



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2016 – 07:54 PM EDT

PDB ID : 5HXB
Title : Cereblon in complex with DDB1, CC-885, and GSPT1
Authors : Chamberlain, P.P.; Matyskiela, M.; Pagarigan, B.
Deposited on : 2016-01-30
Resolution : 3.60 Å(reported)

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

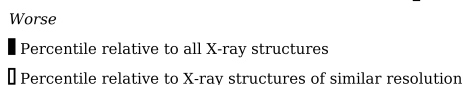
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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-20027790

i

X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

Mol	Chain	Length	Quality of chain	
1	A	199	<div> <div></div> <div>2%</div> <div>36%</div> <div>42%</div> <div>18%</div> <div>• •</div> </div>	
1	X	199	<div> <div></div> <div>2%</div> <div>31%</div> <div>42%</div> <div>20%</div> <div>6%</div> <div>•</div> </div>	
2	B	1140	<div> <div></div> <div>•</div> <div>52%</div> <div>35%</div> <div>6%</div> <div>6%</div> </div>	
2	Y	1140	<div> <div></div> <div>•</div> <div>53%</div> <div>35%</div> <div>7%</div> <div>5%</div> </div>	
3	C	406	<div> <div></div> <div>•</div> <div>52%</div> <div>32%</div> <div>6%</div> <div>•</div> <div>9%</div> </div>	
3	Z	406	<div> <div></div> <div>52%</div> <div>34%</div> <div>7%</div> <div>•</div> <div>6%</div> </div>	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	C	501	-	-	X	-
5	85C	Z	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25089 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 Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	195	Total	C	N	O	S	0	0	0
			1481	941	254	275	11			
1	A	196	Total	C	N	O	S	0	0	0
			1441	919	245	267	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	436	GLY	-	expression tag	UNP P15170
X	437	SER	-	expression tag	UNP P15170
A	436	GLY	-	expression tag	UNP P15170
A	437	SER	-	expression tag	UNP P15170

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	1080	Total	C	N	O	S	0	0	0
			8178	5215	1369	1550	44			
2	B	1075	Total	C	N	O	S	0	0	0
			8096	5164	1351	1536	45			

- Molecule 3 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	380	Total	C	N	O	S	0	0	0
			2960	1891	502	544	23			
3	C	370	Total	C	N	O	S	0	0	0
			2869	1835	485	526	23			

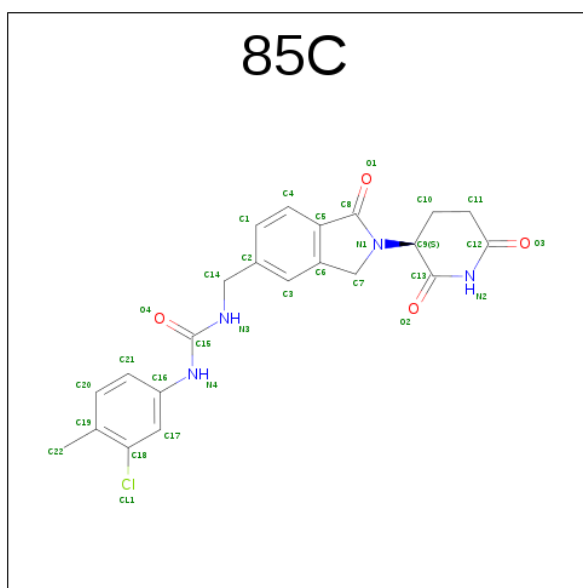
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	37	GLY	-	expression tag	UNP Q96SW2
Z	38	SER	-	expression tag	UNP Q96SW2
Z	39	MET	-	expression tag	UNP Q96SW2
C	37	GLY	-	expression tag	UNP Q96SW2
C	38	SER	-	expression tag	UNP Q96SW2
C	39	MET	-	expression tag	UNP Q96SW2

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is 1-(3-chloro-4-methylphenyl)-3-({2-[(3S)-2,6-dioxopiperidin-3-yl]-1-oxo-2,3-dihydro-1H-isindol-5-yl}methyl)urea (three-letter code: 85C) (formula: C₂₂H₂₁ClN₄O₄).

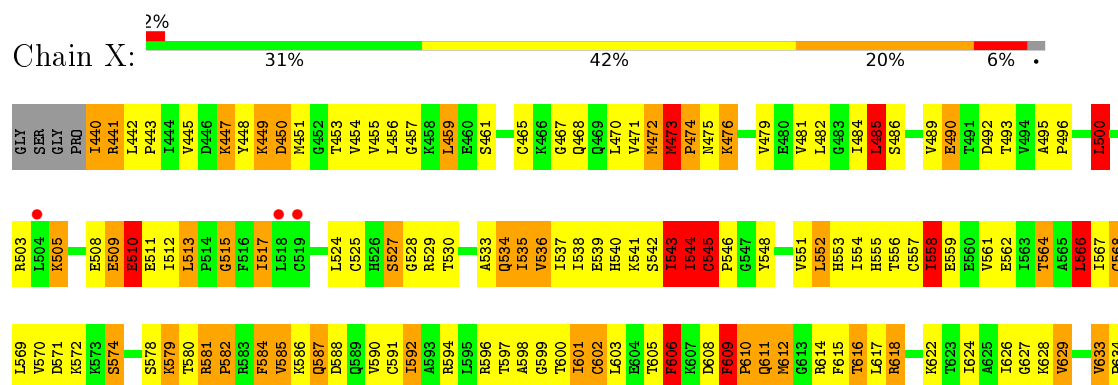


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Z	1	Total C Cl N O 31 22 1 4 4	0	0
5	C	1	Total C Cl N O 31 22 1 4 4	0	0

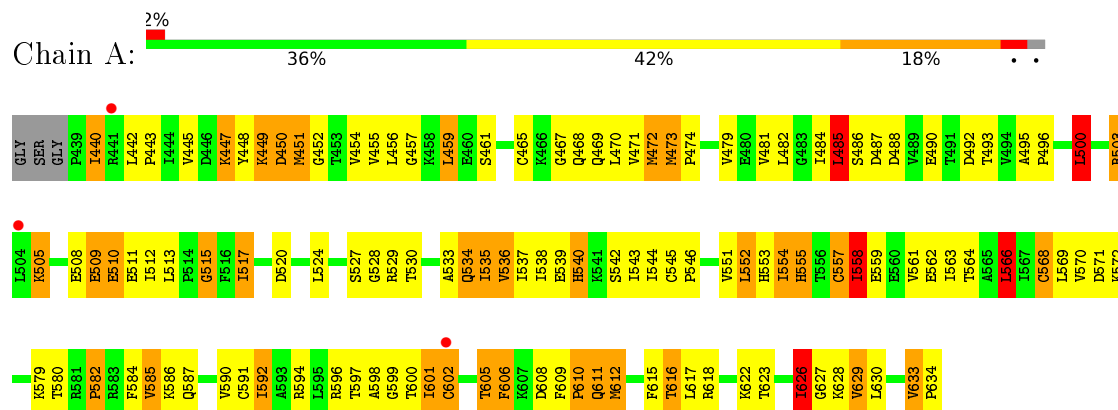
3 Residue-property plots

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

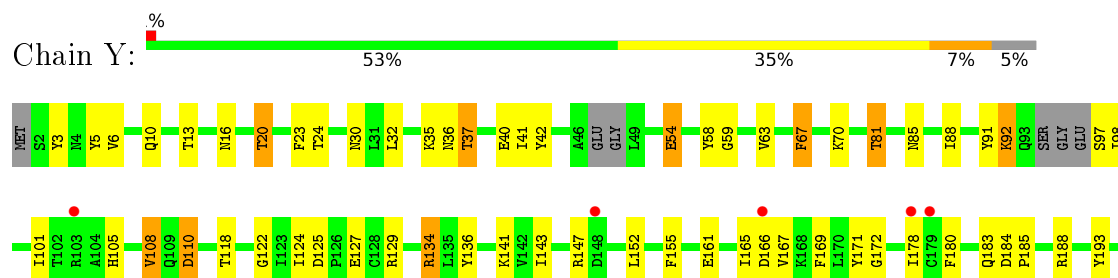
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



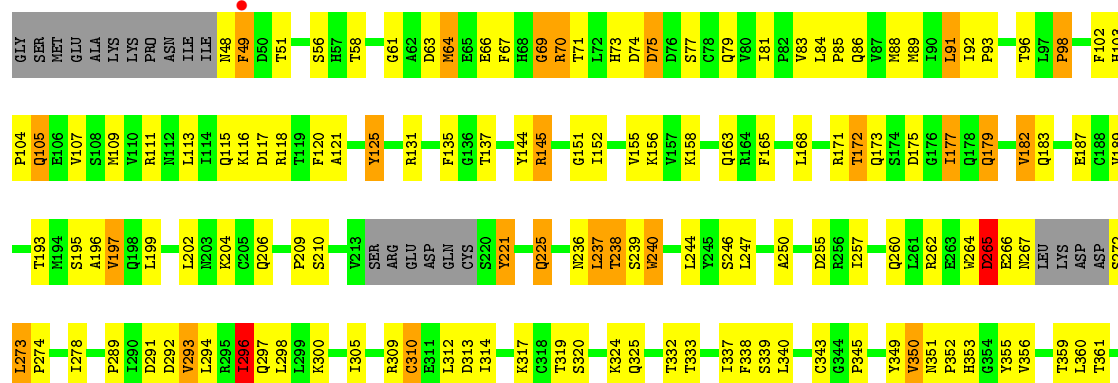
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

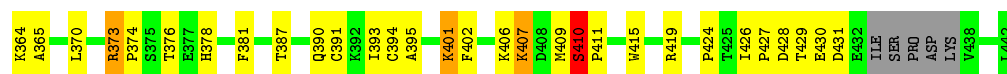


- Molecule 2: DNA damage-binding protein 1

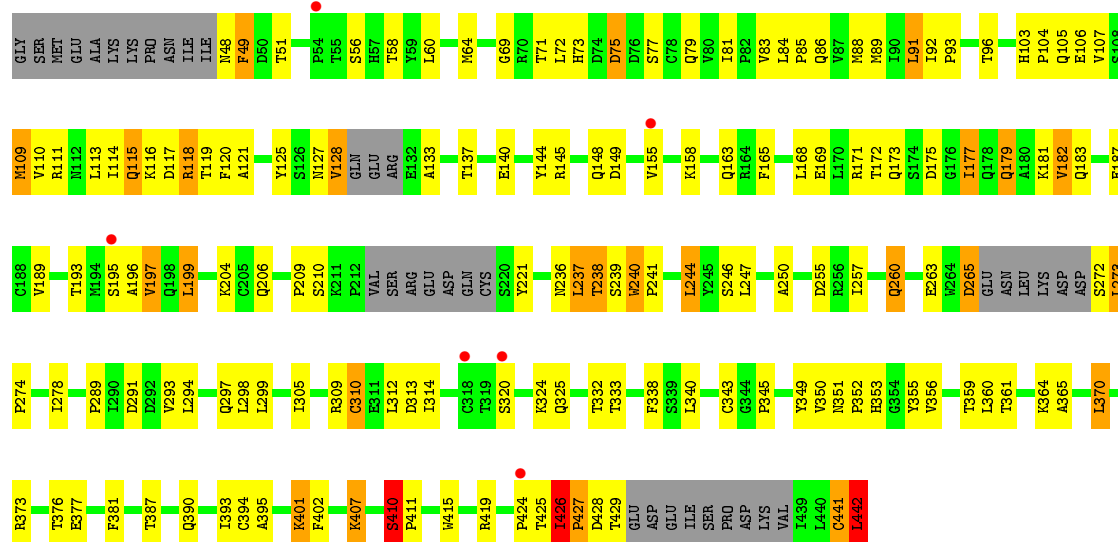








• Molecule 3: Protein cereblon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.75Å 111.52Å 175.06Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.80 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-3.60) 94.5 (49.80-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.272	Depositor DCC
R_{free} test set	3289 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 85.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25089	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 85C

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	0.85	0/1463	0.89	1/1987 (0.1%)
1	X	0.93	0/1502	1.02	10/2032 (0.5%)
2	B	0.85	4/8235 (0.0%)	0.87	6/11187 (0.1%)
2	Y	0.86	6/8319 (0.1%)	0.88	11/11295 (0.1%)
3	C	0.81	0/2937	0.90	5/4003 (0.1%)
3	Z	0.84	0/3030	0.90	5/4125 (0.1%)
All	All	0.85	10/25486 (0.0%)	0.89	38/34629 (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	13
1	X	0	16
2	B	0	17
2	Y	0	19
3	C	0	5
3	Z	0	5
All	All	0	75

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	489	GLU	CG-CD	7.70	1.63	1.51
2	B	489	GLU	CG-CD	7.30	1.62	1.51
2	Y	853	TYR	CB-CG	-6.86	1.41	1.51
2	B	1134	GLU	CG-CD	6.54	1.61	1.51
2	Y	1134	GLU	CG-CD	6.18	1.61	1.51
2	B	668	PHE	CB-CG	-5.88	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	136	TYR	CB-CG	5.79	1.60	1.51
2	Y	411	TRP	CB-CG	-5.47	1.40	1.50
2	Y	136	TYR	CB-CG	5.30	1.59	1.51
2	Y	453	ASP	CB-CG	5.20	1.62	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	426	ILE	C-N-CD	-7.50	104.10	120.60
3	C	442	LEU	CA-CB-CG	7.35	132.21	115.30
2	B	357	GLY	C-N-CD	-7.31	104.52	120.60
2	Y	357	GLY	C-N-CD	-7.28	104.59	120.60
2	Y	597	GLU	N-CA-C	-7.00	92.09	111.00
1	X	536	VAL	CG1-CB-CG2	6.99	122.08	110.90
1	X	510	GLU	N-CA-C	-6.94	92.26	111.00
1	X	485	LEU	CA-CB-CG	6.67	130.65	115.30
3	C	199	LEU	CB-CG-CD1	6.60	122.23	111.00
2	Y	434	ARG	NE-CZ-NH2	-6.52	117.04	120.30
3	Z	265	ASP	N-CA-C	6.49	128.51	111.00
2	B	623	LEU	N-CA-C	-6.19	94.29	111.00
3	Z	296	ILE	CB-CA-C	-6.12	99.35	111.60
2	Y	394	ILE	N-CA-C	-5.97	94.88	111.00
2	Y	606	LEU	CA-CB-CG	-5.92	101.68	115.30
1	A	485	LEU	N-CA-C	-5.92	95.03	111.00
1	X	606	PHE	N-CA-C	-5.88	95.12	111.00
1	X	609	PHE	C-N-CD	5.84	140.66	128.40
3	Z	410	SER	C-N-CD	-5.73	107.99	120.60
1	X	585	VAL	CA-CB-CG2	5.67	119.41	110.90
2	B	98	ILE	CB-CA-C	-5.61	100.39	111.60
2	Y	98	ILE	CB-CA-C	-5.56	100.47	111.60
2	Y	434	ARG	NE-CZ-NH1	5.55	123.08	120.30
3	Z	296	ILE	CG1-CB-CG2	5.48	123.46	111.40
3	C	410	SER	C-N-CD	-5.46	108.60	120.60
2	Y	1013	VAL	N-CA-C	-5.36	96.52	111.00
1	X	585	VAL	CG1-CB-CG2	5.34	119.44	110.90
3	Z	343	CYS	CA-CB-SG	-5.27	104.51	114.00
1	X	536	VAL	CA-CB-CG2	5.27	118.80	110.90
2	B	928	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	C	343	CYS	CA-CB-SG	-5.21	104.62	114.00
2	Y	414	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	B	394	ILE	N-CA-C	-5.18	97.01	111.00
2	B	626	ARG	N-CA-C	-5.18	97.02	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	543	ILE	CB-CA-C	-5.08	101.44	111.60
2	Y	977	CYS	CA-CB-SG	5.03	123.06	114.00
2	Y	1032	THR	N-CA-CB	-5.03	100.75	110.30
1	X	473	MET	C-N-CD	-5.02	109.56	120.60

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	LYS	Peptide
1	A	451	MET	Peptide
1	A	472	MET	Peptide
1	A	500	LEU	Peptide
1	A	509	GLU	Peptide
1	A	515	GLY	Peptide
1	A	534	GLN	Peptide
1	A	555	HIS	Peptide
1	A	564	THR	Peptide
1	A	566	LEU	Peptide
1	A	601	ILE	Peptide
1	A	626	ILE	Peptide
1	A	633	VAL	Peptide
2	B	1015	GLN	Peptide
2	B	1116	ASP	Peptide
2	B	209	GLN	Peptide
2	B	224	GLU	Peptide
2	B	332	GLN	Peptide
2	B	345	SER	Peptide
2	B	357	GLY	Peptide
2	B	465	HIS	Sidechain
2	B	476	VAL	Peptide
2	B	482	GLU	Peptide
2	B	571	LEU	Peptide
2	B	660	TYR	Mainchain,Peptide
2	B	664	HIS	Peptide
2	B	805	HIS	Sidechain
2	B	853	TYR	Sidechain
2	B	965	PHE	Sidechain
3	C	103	HIS	Sidechain
3	C	181	LYS	Peptide
3	C	410	SER	Peptide
3	C	426	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	441	CYS	Peptide
1	X	472	MET	Peptide
1	X	473	MET	Peptide
1	X	500	LEU	Peptide
1	X	509	GLU	Peptide
1	X	515	GLY	Peptide
1	X	534	GLN	Peptide
1	X	543	ILE	Mainchain
1	X	544	ILE	Peptide
1	X	545	CYS	Peptide
1	X	564	THR	Peptide
1	X	566	LEU	Peptide
1	X	574	SER	Peptide
1	X	587	GLN	Peptide
1	X	601	ILE	Peptide
1	X	603	LEU	Peptide
1	X	633	VAL	Peptide
2	Y	1014	MET	Peptide
2	Y	224	GLU	Peptide
2	Y	332	GLN	Peptide
2	Y	337	ASN	Mainchain
2	Y	338	VAL	Peptide
2	Y	342	GLU	Peptide
2	Y	345	SER	Peptide
2	Y	357	GLY	Peptide
2	Y	392	ASN	Peptide
2	Y	482	GLU	Peptide
2	Y	571	LEU	Peptide
2	Y	660	TYR	Mainchain,Peptide
2	Y	664	HIS	Peptide
2	Y	706	GLU	Peptide
2	Y	805	HIS	Sidechain
2	Y	891	TYR	Sidechain
2	Y	950	ASN	Peptide
2	Y	965	PHE	Sidechain
3	Z	125	TYR	Peptide
3	Z	151	GLY	Peptide
3	Z	410	SER	Peptide
3	Z	430	GLU	Peptide
3	Z	69	GLY	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	1441	0	1439	151	2
1	X	1481	0	1519	209	0
2	B	8096	0	7807	344	0
2	Y	8178	0	7930	342	0
3	C	2869	0	2758	126	0
3	Z	2960	0	2851	138	2
4	C	1	0	0	2	0
4	Z	1	0	0	0	0
5	C	31	0	0	4	0
5	Z	31	0	0	10	0
All	All	25089	0	24304	1265	2

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 26.

All (1265) 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:X:606:PHE:CD2	1:X:628:LYS:HG2	1.44	1.49
1:A:606:PHE:CE2	1:A:628:LYS:HG2	1.50	1.47
1:A:606:PHE:CD2	1:A:628:LYS:HG2	1.48	1.45
1:X:606:PHE:CE2	1:X:628:LYS:HG2	1.64	1.30
3:Z:352:PRO:HG3	3:Z:378:HIS:ND1	1.44	1.29
1:X:606:PHE:CD2	1:X:628:LYS:CG	2.15	1.28
1:X:628:LYS:HG3	5:Z:502:85C:CL1	1.73	1.25
1:A:606:PHE:CD2	1:A:628:LYS:CG	2.19	1.23
1:X:606:PHE:HD2	1:X:628:LYS:CG	1.49	1.20
1:X:540:HIS:CE1	1:X:542:SER:H	1.66	1.13
1:A:606:PHE:HD2	1:A:628:LYS:CB	1.62	1.11
1:X:554:ILE:HG22	1:X:555:HIS:HD2	1.13	1.11
2:Y:35:LYS:HE3	2:Y:40:GLU:OE1	1.50	1.11
1:X:453:THR:O	1:X:503:ARG:HG3	1.52	1.08
3:Z:352:PRO:CG	3:Z:378:HIS:ND1	2.17	1.07
1:A:606:PHE:CE2	1:A:628:LYS:CG	2.37	1.05
1:X:441:ARG:HG2	1:X:612:MET:SD	1.98	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:PHE:HD2	1:A:628:LYS:CG	1.61	1.02
1:A:606:PHE:HD2	1:A:628:LYS:HB3	1.27	0.99
1:X:449:LYS:NZ	1:X:510:GLU:OE2	1.96	0.99
1:A:540:HIS:CD2	1:A:544:ILE:HG22	1.98	0.98
3:C:199:LEU:HD21	3:C:237:LEU:HD11	1.42	0.98
1:X:554:ILE:HG22	1:X:555:HIS:CD2	1.99	0.96
3:Z:265:ASP:OD1	3:Z:266:GLU:N	1.97	0.96
2:Y:595:THR:OG1	2:Y:600:HIS:CE1	2.19	0.95
1:X:606:PHE:HD2	1:X:628:LYS:CB	1.78	0.95
2:Y:595:THR:OG1	2:Y:600:HIS:ND1	1.98	0.95
1:X:628:LYS:CG	5:Z:502:85C:CL1	2.53	0.93
2:Y:741:GLU:OE1	2:Y:749:THR:HG23	1.68	0.92
1:X:606:PHE:CE2	1:X:628:LYS:CG	2.47	0.92
1:A:485:LEU:HA	1:A:490:GLU:CB	2.01	0.91
1:A:606:PHE:HE2	1:A:628:LYS:HG2	1.28	0.91
2:B:808:LEU:H	2:B:808:LEU:HD12	1.34	0.91
1:X:552:LEU:HD11	1:X:554:ILE:CG1	2.01	0.91
3:C:125:TYR:CE1	3:C:133:ALA:HB2	2.06	0.90
2:Y:660:TYR:O	2:Y:667:VAL:N	2.04	0.90
3:Z:173:GLN:CB	3:Z:179:GLN:NE2	2.35	0.90
1:A:540:HIS:CD2	1:A:544:ILE:CG2	2.55	0.90
1:X:467:GLY:HA2	1:X:481:VAL:O	1.72	0.89
3:Z:401:LYS:HG3	3:Z:415:TRP:CE2	2.08	0.89
2:B:660:TYR:O	2:B:667:VAL:N	2.06	0.88
3:C:115:GLN:HE21	3:C:115:GLN:HA	1.38	0.88
1:A:467:GLY:HA2	1:A:481:VAL:O	1.72	0.88
3:C:394:CYS:HG	4:C:501:ZN:ZN	0.56	0.88
2:Y:988:GLU:HA	2:Y:988:GLU:OE1	1.73	0.88
1:A:606:PHE:CD2	1:A:628:LYS:CB	2.55	0.87
2:Y:908:ASN:OD1	2:Y:908:ASN:N	2.08	0.87
1:A:606:PHE:CD2	1:A:628:LYS:HB3	2.09	0.87
1:X:540:HIS:CE1	1:X:542:SER:N	2.43	0.86
3:Z:352:PRO:CD	3:Z:378:HIS:ND1	2.37	0.86
1:X:486:SER:O	1:X:489:VAL:O	1.93	0.86
2:B:988:GLU:OE1	2:B:988:GLU:HA	1.76	0.85
1:X:605:THR:OG1	1:X:608:ASP:HB2	1.75	0.85
1:X:451:MET:CB	1:X:503:ARG:HD3	2.06	0.85
3:C:125:TYR:HE1	3:C:133:ALA:HB2	1.41	0.84
2:Y:629:VAL:HG11	2:Y:668:PHE:CE2	2.12	0.84
1:A:558:ILE:HG22	1:A:558:ILE:O	1.76	0.84
1:X:540:HIS:ND1	1:X:542:SER:N	2.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:997:LEU:HB3	2:Y:1076:PHE:HD2	1.42	0.83
1:A:605:THR:HG22	1:A:630:LEU:O	1.77	0.83
3:C:425:THR:HG22	3:C:426:ILE:H	1.44	0.82
1:A:538:ILE:HD11	1:A:623:THR:HG22	1.60	0.82
1:X:515:GLY:HA2	1:X:556:THR:OG1	1.80	0.82
1:A:515:GLY:HA3	1:A:557:CYS:HB2	1.61	0.82
3:Z:352:PRO:N	3:Z:378:HIS:HE1	1.79	0.81
1:X:510:GLU:O	1:X:511:GLU:HB3	1.81	0.80
3:C:394:CYS:SG	4:C:501:ZN:ZN	1.69	0.80
2:Y:327:ARG:HD3	3:Z:199:LEU:HD22	1.63	0.80
3:Z:352:PRO:N	3:Z:378:HIS:CE1	2.48	0.80
2:Y:204:LYS:HA	2:Y:204:LYS:HE2	1.63	0.80
3:Z:199:LEU:HD21	3:Z:237:LEU:HD11	1.62	0.80
2:B:279:ARG:HG3	2:B:279:ARG:NH1	1.95	0.80
3:C:401:LYS:HG3	3:C:415:TRP:CE2	2.18	0.79
1:X:489:VAL:HG22	1:X:490:GLU:O	1.82	0.79
3:Z:70:ARG:HD2	3:Z:70:ARG:H	1.47	0.79
2:Y:451:PHE:CE2	2:Y:470:GLN:HB2	2.18	0.79
1:X:558:ILE:O	1:X:558:ILE:HG22	1.81	0.78
2:B:889:ARG:HD3	2:B:901:THR:HG23	1.66	0.78
1:X:533:ALA:HB1	1:X:628:LYS:O	1.83	0.78
1:A:512:ILE:C	1:A:513:LEU:HD12	2.04	0.78
3:Z:401:LYS:HG3	3:Z:415:TRP:NE1	1.98	0.78
2:Y:118:THR:HG21	2:Y:165:ILE:O	1.84	0.78
2:B:900:ARG:HG3	2:B:900:ARG:O	1.80	0.77
1:X:548:TYR:OH	1:X:624:ILE:CD1	2.32	0.77
2:B:546:LEU:O	2:B:549:SER:N	2.17	0.77
3:C:426:ILE:HG12	3:C:427:PRO:HA	1.65	0.77
1:X:606:PHE:HD2	1:X:628:LYS:HB3	1.47	0.77
2:B:118:THR:HG21	2:B:165:ILE:O	1.85	0.77
1:X:540:HIS:HE1	1:X:542:SER:OG	1.68	0.77
1:X:605:THR:HA	1:X:629:VAL:HG22	1.65	0.77
2:Y:889:ARG:HD3	2:Y:901:THR:HG23	1.66	0.77
3:Z:165:PHE:CD1	3:Z:182:VAL:CG2	2.67	0.76
3:C:127:ASN:ND2	3:C:128:VAL:H	1.83	0.76
1:A:557:CYS:SG	1:A:558:ILE:N	2.57	0.76
3:C:48:ASN:HA	3:C:410:SER:HB3	1.66	0.76
2:Y:753:ARG:HB2	2:Y:754:PRO:HD2	1.65	0.76
3:Z:273:LEU:HB2	3:Z:274:PRO:CD	2.15	0.76
2:Y:118:THR:O	2:Y:118:THR:HG22	1.84	0.76
3:C:273:LEU:HB2	3:C:274:PRO:CD	2.16	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:485:LEU:HD11	1:X:503:ARG:NH2	2.00	0.76
1:A:552:LEU:HD11	1:A:554:ILE:HG12	1.66	0.76
3:Z:125:TYR:HE2	3:Z:131:ARG:HA	1.49	0.76
1:A:543:ILE:HG22	1:A:586:LYS:HG2	1.68	0.75
2:Y:997:LEU:HB3	2:Y:1076:PHE:CD2	2.22	0.75
2:Y:35:LYS:CE	2:Y:40:GLU:OE1	2.33	0.75
2:Y:928:ARG:O	2:Y:928:ARG:HD2	1.86	0.75
1:X:441:ARG:CZ	1:X:525:CYS:SG	2.74	0.75
1:A:633:VAL:HG12	1:A:634:PRO:CD	2.16	0.75
2:B:118:THR:HG22	2:B:118:THR:O	1.86	0.75
2:Y:927:MET:O	2:Y:928:ARG:HB3	1.85	0.75
2:Y:900:ARG:O	2:Y:900:ARG:HG3	1.84	0.75
1:X:474:PRO:O	1:X:476:LYS:HE2	1.87	0.74
3:Z:48:ASN:HA	3:Z:410:SER:HB3	1.69	0.74
2:B:883:SER:HB2	2:B:911:ALA:HB3	1.68	0.74
3:C:313:ASP:OD2	3:C:441:CYS:O	2.06	0.74
1:X:554:ILE:CG2	1:X:555:HIS:HD2	1.98	0.74
2:B:304:LEU:O	2:B:304:LEU:HG	1.86	0.74
2:B:753:ARG:HB2	2:B:754:PRO:HD2	1.68	0.74
2:B:972:PHE:CZ	3:C:196:ALA:O	2.40	0.74
1:A:540:HIS:NE2	1:A:544:ILE:HG22	2.01	0.74
3:C:175:ASP:OD1	3:C:177:ILE:HB	1.88	0.74
2:Y:279:ARG:HG3	2:Y:279:ARG:NH1	2.00	0.73
2:B:327:ARG:HD3	3:C:199:LEU:HD22	1.68	0.73
2:B:997:LEU:HB3	2:B:1076:PHE:HD2	1.53	0.73
2:Y:987:GLU:OE1	2:Y:989:ARG:NH2	2.21	0.73
2:Y:928:ARG:NH2	2:Y:994:GLU:OE2	2.21	0.73
2:Y:59:GLY:HA2	2:Y:1073:TRP:CZ3	2.23	0.73
3:Z:352:PRO:HD3	3:Z:378:HIS:ND1	2.03	0.73
1:X:633:VAL:HG12	1:X:634:PRO:HD2	1.70	0.73
2:Y:304:LEU:O	2:Y:304:LEU:HG	1.87	0.73
3:Z:165:PHE:CD1	3:Z:182:VAL:HG22	2.22	0.73
1:X:548:TYR:OH	1:X:624:ILE:HD13	1.88	0.73
1:X:606:PHE:CE2	1:X:628:LYS:HD2	2.24	0.73
3:Z:352:PRO:CD	3:Z:378:HIS:CE1	2.72	0.73
1:A:508:GLU:HG3	1:A:511:GLU:HB3	1.70	0.73
1:A:533:ALA:HB1	1:A:628:LYS:O	1.88	0.73
1:A:535:ILE:HG22	1:A:535:ILE:O	1.89	0.72
2:B:279:ARG:HG3	2:B:279:ARG:HH11	1.54	0.72
3:Z:69:GLY:O	3:Z:118:ARG:NH2	2.21	0.72
2:B:928:ARG:HD2	2:B:928:ARG:O	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:TYR:CE2	2:B:1045:GLU:HG3	2.25	0.72
2:Y:660:TYR:HB2	2:Y:661:SER:HB3	1.70	0.72
2:B:808:LEU:CD1	2:B:847:ARG:HH21	2.03	0.72
1:A:447:LYS:H	1:A:447:LYS:HD3	1.55	0.72
2:Y:279:ARG:HG3	2:Y:279:ARG:HH11	1.53	0.72
2:Y:35:LYS:HE3	2:Y:40:GLU:CD	2.10	0.72
2:B:596:PHE:HD2	2:B:601:TYR:HD2	1.38	0.71
2:Y:118:THR:HB	2:Y:134:ARG:NH2	2.05	0.71
1:X:606:PHE:CD2	1:X:628:LYS:CD	2.73	0.71
2:B:928:ARG:NH2	2:B:994:GLU:OE2	2.23	0.71
3:Z:144:TYR:HE1	3:Z:155:VAL:HG13	1.55	0.71
1:A:450:ASP:O	1:A:452:GLY:N	2.24	0.71
3:C:114:ILE:HG13	3:C:144:TYR:CE2	2.25	0.71
2:B:927:MET:O	2:B:928:ARG:HB3	1.89	0.71
2:B:59:GLY:HA2	2:B:1073:TRP:CZ3	2.26	0.71
2:B:660:TYR:HB2	2:B:661:SER:HB3	1.72	0.71
1:X:606:PHE:CD2	1:X:628:LYS:HB3	2.25	0.71
2:Y:3:TYR:CE2	2:Y:1045:GLU:HG3	2.26	0.71
1:X:453:THR:O	1:X:454:VAL:HG22	1.91	0.71
2:Y:118:THR:HB	2:Y:134:ARG:HH22	1.56	0.71
2:B:661:SER:OG	2:B:663:ASN:ND2	2.23	0.70
2:B:629:VAL:HG11	2:B:668:PHE:CE2	2.26	0.70
2:B:808:LEU:N	2:B:808:LEU:HD12	2.06	0.70
1:X:449:LYS:HZ1	1:X:510:GLU:CD	1.93	0.70
2:B:808:LEU:HD11	2:B:847:ARG:NH2	2.06	0.70
2:Y:471:ILE:HG23	2:Y:476:VAL:HG22	1.73	0.70
1:X:535:ILE:O	1:X:535:ILE:HG22	1.90	0.70
1:X:618:ARG:HG3	1:X:622:LYS:O	1.91	0.70
1:X:537:ILE:HG22	1:X:587:GLN:HA	1.74	0.70
2:B:997:LEU:HB3	2:B:1076:PHE:CD2	2.27	0.70
1:X:447:LYS:H	1:X:447:LYS:HD3	1.56	0.70
2:Y:377:THR:HG1	2:Y:379:SER:HG	1.36	0.70
2:B:471:ILE:HG23	2:B:476:VAL:HG22	1.73	0.70
1:X:515:GLY:CA	1:X:556:THR:OG1	2.39	0.70
1:A:445:VAL:HG23	1:A:457:GLY:HA2	1.74	0.70
2:Y:906:TYR:N	2:Y:906:TYR:CD1	2.58	0.70
1:A:605:THR:CG2	1:A:630:LEU:O	2.40	0.69
5:C:502:85C:C20	1:A:628:LYS:HD3	2.22	0.69
2:Y:714:THR:HG22	2:Y:716:PRO:HD3	1.73	0.69
2:Y:716:PRO:HB3	2:Y:718:TYR:CE1	2.27	0.69
2:B:118:THR:HB	2:B:134:ARG:HH22	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:THR:HB	2:B:134:ARG:NH2	2.07	0.69
1:A:484:ILE:O	1:A:490:GLU:CB	2.41	0.69
3:C:427:PRO:O	3:C:428:ASP:HB2	1.93	0.69
3:Z:351:ASN:C	3:Z:378:HIS:HE1	1.96	0.69
1:X:453:THR:HG22	1:X:454:VAL:N	2.08	0.69
2:Y:629:VAL:HG11	2:Y:668:PHE:HE2	1.56	0.69
3:Z:273:LEU:HB2	3:Z:274:PRO:HD2	1.75	0.69
2:B:987:GLU:OE1	2:B:989:ARG:NH2	2.26	0.68
1:X:610:PRO:HD2	1:X:611:GLN:H	1.58	0.68
1:A:535:ILE:O	1:A:535:ILE:CG2	2.41	0.68
3:C:75:ASP:OD1	3:C:75:ASP:N	2.26	0.68
1:X:512:ILE:C	1:X:513:LEU:HD12	2.14	0.68
1:X:535:ILE:CG2	1:X:535:ILE:O	2.42	0.68
3:C:127:ASN:HD22	3:C:128:VAL:H	1.39	0.68
2:B:5:TYR:CE2	2:B:1136:LEU:HD22	2.28	0.68
3:C:273:LEU:HB2	3:C:274:PRO:HD2	1.74	0.68
2:B:914:LEU:HD21	2:B:921:ILE:HG23	1.75	0.68
2:B:715:VAL:O	2:B:715:VAL:HG12	1.92	0.68
2:Y:914:LEU:HD21	2:Y:921:ILE:HG23	1.76	0.68
1:A:534:GLN:O	1:A:627:GLY:HA2	1.94	0.68
1:X:606:PHE:CE2	1:X:628:LYS:CD	2.77	0.68
2:Y:563:ASP:OD1	2:Y:565:SER:HB3	1.93	0.68
3:Z:173:GLN:CB	3:Z:179:GLN:HE21	2.04	0.68
3:C:144:TYR:HE1	3:C:155:VAL:HG13	1.60	0.67
3:C:353:HIS:NE2	5:C:502:85C:O4	2.25	0.67
3:Z:262:ARG:O	3:Z:265:ASP:HA	1.93	0.67
3:Z:264:TRP:CD1	3:Z:337:ILE:HG22	2.30	0.67
2:B:20:THR:HG23	2:B:315:THR:HG21	1.77	0.67
2:B:714:THR:HG22	2:B:716:PRO:HD3	1.75	0.67
2:B:716:PRO:HB3	2:B:718:TYR:CE1	2.30	0.67
2:Y:715:VAL:HG12	2:Y:715:VAL:O	1.93	0.67
1:A:605:THR:OG1	1:A:608:ASP:HB2	1.95	0.67
2:B:414:ARG:N	2:B:462:ASN:HD21	1.92	0.67
1:A:558:ILE:O	1:A:558:ILE:CG2	2.42	0.66
2:B:914:LEU:HD21	2:B:921:ILE:CG2	2.25	0.66
2:Y:537:GLU:HG3	2:Y:561:TRP:CG	2.31	0.66
1:A:510:GLU:HG2	1:A:510:GLU:O	1.96	0.66
2:B:913:TYR:CE1	3:C:240:TRP:HH2	2.13	0.66
3:Z:70:ARG:H	3:Z:70:ARG:CD	2.08	0.66
1:A:606:PHE:O	1:A:606:PHE:HD1	1.79	0.66
2:B:377:THR:HG1	2:B:379:SER:HG	1.41	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:606:PHE:CD2	1:X:628:LYS:CB	2.66	0.66
2:Y:404:LEU:HD22	2:Y:407:ILE:HD11	1.77	0.66
2:B:166:ASP:OD2	3:C:204:LYS:HD3	1.95	0.66
2:B:744:ASP:CB	2:B:749:THR:N	2.59	0.66
1:X:552:LEU:HD11	1:X:554:ILE:HG12	1.77	0.66
3:Z:266:GLU:HA	3:Z:266:GLU:OE1	1.96	0.66
1:X:552:LEU:HD11	1:X:554:ILE:HG13	1.78	0.65
2:B:541:LEU:HD23	2:B:558:ILE:CD1	2.26	0.65
1:X:606:PHE:HA	1:X:609:PHE:O	1.96	0.65
3:Z:264:TRP:NE1	3:Z:337:ILE:HG22	2.11	0.65
3:Z:75:ASP:N	3:Z:75:ASP:OD1	2.29	0.65
1:X:445:VAL:HG23	1:X:457:GLY:HA2	1.77	0.65
2:Y:20:THR:HG23	2:Y:315:THR:HG21	1.76	0.65
1:A:537:ILE:HG22	1:A:587:GLN:HA	1.79	0.65
1:A:633:VAL:HG12	1:A:634:PRO:HD2	1.78	0.65
3:C:165:PHE:CD1	3:C:182:VAL:CG2	2.80	0.65
2:Y:569:LEU:HD13	2:Y:576:LEU:CB	2.27	0.65
1:A:552:LEU:HD11	1:A:554:ILE:CG1	2.27	0.65
2:Y:913:TYR:CE1	3:Z:240:TRP:HH2	2.15	0.65
2:B:928:ARG:HB3	2:B:952:ASN:O	1.97	0.64
2:Y:275:ASP:OD2	2:Y:279:ARG:HB2	1.96	0.64
1:A:566:LEU:CD2	1:A:585:VAL:HG12	2.28	0.64
3:C:117:ASP:O	3:C:119:THR:N	2.31	0.64
1:X:615:PHE:HE1	1:X:617:LEU:CD1	2.10	0.64
1:A:606:PHE:CE2	1:A:628:LYS:CD	2.80	0.64
2:Y:914:LEU:HD21	2:Y:921:ILE:CG2	2.28	0.64
3:Z:63:ASP:O	3:Z:145:ARG:NH2	2.31	0.64
2:B:394:ILE:HD11	2:B:669:SER:CB	2.28	0.64
2:B:404:LEU:HD22	2:B:407:ILE:HD11	1.78	0.64
2:Y:805:HIS:CD2	2:Y:806:GLN:N	2.66	0.64
2:B:451:PHE:CE2	2:B:470:GLN:HB2	2.32	0.64
3:Z:310:CYS:O	3:Z:314:ILE:HD12	1.98	0.64
1:A:545:CYS:HB3	1:A:546:PRO:HD2	1.79	0.63
2:Y:394:ILE:HD12	2:Y:658:VAL:HB	1.80	0.63
2:Y:913:TYR:CE1	3:Z:240:TRP:CH2	2.87	0.63
2:B:511:ALA:HB1	2:B:538:VAL:HG11	1.80	0.63
2:Y:541:LEU:HD23	2:Y:558:ILE:CD1	2.27	0.63
2:B:394:ILE:HD12	2:B:658:VAL:HB	1.80	0.63
3:C:401:LYS:HG3	3:C:415:TRP:NE1	2.12	0.63
2:B:913:TYR:CE1	3:C:240:TRP:CH2	2.86	0.63
1:X:633:VAL:HG12	1:X:634:PRO:CD	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:HIS:ND1	1:A:572:LYS:HD3	2.14	0.63
1:X:601:ILE:HG22	1:X:602:CYS:N	2.12	0.63
2:B:903:CYS:SG	2:B:904:ASN:N	2.72	0.63
1:X:441:ARG:HB2	1:X:461:SER:HB3	1.81	0.63
1:X:558:ILE:CG2	1:X:558:ILE:O	2.46	0.63
2:Y:413:LEU:HB3	2:Y:424:THR:HB	1.80	0.63
1:A:486:SER:H	1:A:490:GLU:HA	1.63	0.63
3:Z:135:PHE:CE1	3:Z:300:LYS:HD3	2.33	0.63
3:C:165:PHE:CD1	3:C:182:VAL:HG22	2.34	0.63
3:C:310:CYS:O	3:C:314:ILE:HD12	1.99	0.63
3:C:425:THR:CG2	3:C:426:ILE:H	2.12	0.63
2:Y:558:ILE:HG22	2:Y:559:GLY:N	2.13	0.63
3:C:49:PHE:CE1	3:C:340:LEU:HD22	2.33	0.62
2:Y:928:ARG:HB3	2:Y:952:ASN:O	1.99	0.62
2:B:482:GLU:HA	2:B:482:GLU:OE2	1.99	0.62
1:X:628:LYS:HD3	5:Z:502:85C:C17	2.29	0.62
2:Y:361:ASP:OD1	2:Y:362:MET:N	2.32	0.62
2:Y:634:GLN:CB	2:Y:654:ASP:OD1	2.46	0.62
2:B:596:PHE:HD2	2:B:601:TYR:CD2	2.17	0.62
1:A:606:PHE:CE2	1:A:628:LYS:HD2	2.34	0.62
1:X:537:ILE:CG2	1:X:587:GLN:HA	2.30	0.62
1:X:515:GLY:HA3	1:X:557:CYS:HB2	1.81	0.62
1:X:606:PHE:HE2	1:X:628:LYS:HG2	1.57	0.62
2:Y:802:LEU:N	2:Y:802:LEU:HD23	2.13	0.62
3:Z:144:TYR:CE1	3:Z:155:VAL:HG13	2.35	0.62
2:Y:403:ASP:O	2:B:768:SER:OG	2.09	0.61
2:B:361:ASP:OD1	2:B:362:MET:N	2.32	0.61
3:Z:352:PRO:CG	3:Z:378:HIS:CE1	2.84	0.61
1:A:510:GLU:CG	1:A:510:GLU:O	2.47	0.61
3:Z:264:TRP:NE1	3:Z:337:ILE:CG2	2.64	0.61
1:X:441:ARG:CB	1:X:461:SER:HB3	2.30	0.61
3:C:115:GLN:NE2	3:C:115:GLN:HA	2.14	0.61
1:X:610:PRO:CD	1:X:611:GLN:H	2.13	0.61
2:Y:642:ARG:NH2	2:Y:645:SER:O	2.34	0.61
2:B:558:ILE:HG22	2:B:559:GLY:N	2.16	0.61
2:Y:511:ALA:HB1	2:Y:538:VAL:HG11	1.82	0.61
2:B:275:ASP:OD2	2:B:279:ARG:HB2	2.01	0.61
2:Y:691:LEU:HD23	2:Y:693:LEU:HD11	1.83	0.61
3:Z:49:PHE:CE1	3:Z:340:LEU:HD22	2.35	0.61
2:Y:13:THR:OG1	2:Y:355:ASN:OD1	2.19	0.60
2:Y:394:ILE:HD11	2:Y:669:SER:CB	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ILE:HG22	1:A:602:CYS:N	2.16	0.60
2:B:537:GLU:HG3	2:B:561:TRP:CG	2.36	0.60
1:X:451:MET:CB	1:X:503:ARG:CD	2.78	0.60
1:A:543:ILE:HD12	1:A:545:CYS:SG	2.41	0.60
2:Y:466:GLN:OE1	2:Y:466:GLN:HA	2.01	0.60
2:B:413:LEU:HB3	2:B:424:THR:HB	1.82	0.60
1:X:597:THR:HG21	1:X:601:ILE:HG13	1.83	0.60
1:A:508:GLU:O	1:A:509:GLU:OE2	2.20	0.60
2:B:466:GLN:OE1	2:B:466:GLN:HA	2.01	0.60
2:Y:903:CYS:SG	2:Y:904:ASN:N	2.74	0.60
2:Y:910:MET:HG2	2:Y:912:LEU:HD21	1.84	0.60
1:A:540:HIS:N	1:A:587:GLN:OE1	2.32	0.60
2:B:884:ILE:HD12	2:B:884:ILE:N	2.17	0.59
2:Y:59:GLY:CA	2:Y:1073:TRP:CZ3	2.84	0.59
2:B:222:VAL:HG12	2:B:223:PRO:HD2	1.83	0.59
2:B:691:LEU:HD23	2:B:693:LEU:HD11	1.83	0.59
1:X:540:HIS:CD2	1:X:544:ILE:HG22	2.37	0.59
1:A:543:ILE:CD1	1:A:545:CYS:SG	2.91	0.59
2:B:802:LEU:HD23	2:B:802:LEU:N	2.16	0.59
2:Y:661:SER:OG	2:Y:663:ASN:ND2	2.35	0.59
2:Y:883:SER:HB2	2:Y:911:ALA:HB3	1.82	0.59
2:B:1008:CYS:SG	2:B:1008:CYS:O	2.61	0.59
2:B:1097:PHE:CE2	2:B:1129:LEU:HB3	2.37	0.59
2:B:245:TYR:CD1	2:B:245:TYR:C	2.76	0.59
2:B:913:TYR:OH	3:C:240:TRP:HZ3	1.85	0.59
2:B:914:LEU:CD2	2:B:921:ILE:HG23	2.32	0.59
2:Y:913:TYR:OH	3:Z:240:TRP:HZ3	1.86	0.59
3:Z:173:GLN:CB	3:Z:179:GLN:HE22	2.15	0.59
2:B:735:VAL:HB	2:B:792:LEU:HB2	1.84	0.59
2:B:868:GLY:HA3	2:B:885:ASN:ND2	2.17	0.59
1:X:534:GLN:O	1:X:627:GLY:HA2	2.02	0.59
2:B:167:VAL:HG23	2:B:180:PHE:HB3	1.84	0.59
1:A:471:VAL:HG12	1:A:472:MET:N	2.18	0.59
2:B:13:THR:OG1	2:B:355:ASN:OD1	2.20	0.59
3:C:265:ASP:C	3:C:265:ASP:OD1	2.40	0.59
2:Y:414:ARG:N	2:Y:462:ASN:HD21	2.00	0.59
1:X:628:LYS:HD3	5:Z:502:85C:CL1	2.40	0.59
1:A:468:GLN:O	1:A:470:LEU:HG	2.03	0.59
1:X:517:ILE:HD11	1:X:602:CYS:HB2	1.85	0.59
2:Y:36:ASN:ND2	2:Y:37:THR:HG23	2.18	0.59
2:Y:972:PHE:CZ	3:Z:196:ALA:O	2.56	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:427:PRO:O	3:C:428:ASP:CB	2.49	0.58
2:Y:1032:THR:HG22	2:Y:1034:ASN:N	2.17	0.58
2:B:1097:PHE:CZ	2:B:1129:LEU:HB3	2.39	0.58
2:B:23:PHE:H	2:B:30:ASN:ND2	2.01	0.58
2:B:465:HIS:O	2:B:467:GLN:HG3	2.03	0.58
1:X:449:LYS:HZ2	1:X:510:GLU:HB3	1.67	0.58
2:Y:884:ILE:HD12	2:Y:884:ILE:N	2.18	0.58
3:Z:264:TRP:CD1	3:Z:337:ILE:O	2.56	0.58
1:A:539:GLU:O	1:A:540:HIS:HB2	2.03	0.58
2:B:1050:LEU:HD12	2:B:1050:LEU:O	2.03	0.58
2:B:695:ASN:OD1	2:B:696:ASN:N	2.36	0.58
1:X:510:GLU:O	1:X:511:GLU:CB	2.50	0.58
2:Y:23:PHE:H	2:Y:30:ASN:ND2	2.00	0.58
3:Z:352:PRO:HG3	3:Z:378:HIS:CE1	2.32	0.58
3:C:425:THR:HG22	3:C:426:ILE:N	2.16	0.58
1:X:500:LEU:CD1	1:X:500:LEU:N	2.66	0.58
3:C:104:PRO:HA	3:C:107:VAL:HB	1.86	0.58
2:B:972:PHE:CE1	3:C:196:ALA:O	2.56	0.58
2:Y:832:GLY:N	2:Y:873:MET:HE1	2.18	0.58
1:X:557:CYS:SG	1:X:558:ILE:N	2.77	0.58
2:Y:245:TYR:C	2:Y:245:TYR:CD1	2.77	0.57
2:Y:628:LYS:HG2	2:Y:629:VAL:N	2.18	0.57
2:Y:167:VAL:HG23	2:Y:180:PHE:HB3	1.86	0.57
2:Y:537:GLU:O	2:Y:561:TRP:HB2	2.04	0.57
3:Z:144:TYR:CD1	3:Z:145:ARG:N	2.72	0.57
3:Z:61:GLY:HA3	3:Z:145:ARG:NH1	2.19	0.57
2:Y:868:GLY:HA3	2:Y:885:ASN:ND2	2.19	0.57
1:A:448:TYR:CE1	1:A:454:VAL:HB	2.40	0.57
1:A:606:PHE:HE2	1:A:628:LYS:CG	1.99	0.57
1:X:515:GLY:N	1:X:556:THR:OG1	2.37	0.57
2:B:32:LEU:HD11	2:B:41:ILE:HG12	1.86	0.57
1:X:453:THR:O	1:X:454:VAL:CG2	2.52	0.57
2:Y:1050:LEU:HD12	2:Y:1050:LEU:O	2.04	0.57
1:X:597:THR:HG21	1:X:601:ILE:CG1	2.35	0.57
2:Y:1032:THR:HG22	2:Y:1034:ASN:H	1.68	0.57
2:Y:222:VAL:HG12	2:Y:223:PRO:HD2	1.84	0.57
2:Y:695:ASN:OD1	2:Y:696:ASN:N	2.37	0.57
1:A:537:ILE:CG2	1:A:587:GLN:HA	2.35	0.57
2:Y:998:PHE:HB2	2:Y:1088:PHE:CD2	2.40	0.57
3:Z:175:ASP:OD1	3:Z:177:ILE:HB	2.04	0.57
1:A:487:ASP:CG	1:A:488:ASP:H	2.08	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:CYS:HB3	1:A:592:ILE:HD11	1.87	0.57
2:B:1058:LEU:HD22	2:B:1062:ILE:HD11	1.86	0.57
2:B:642:ARG:NH2	2:B:645:SER:O	2.38	0.57
2:Y:394:ILE:CD1	2:Y:658:VAL:HB	2.35	0.57
2:B:414:ARG:H	2:B:462:ASN:HD21	1.51	0.57
3:Z:293:VAL:O	3:Z:296:ILE:HG13	2.04	0.57
3:Z:265:ASP:CG	3:Z:266:GLU:HG2	2.25	0.57
2:Y:914:LEU:CD2	2:Y:921:ILE:HG23	2.35	0.56
3:Z:115:GLN:NE2	3:Z:115:GLN:HA	2.19	0.56
3:Z:70:ARG:HD2	3:Z:70:ARG:N	2.19	0.56
2:B:465:HIS:CG	2:B:523:PRO:HD3	2.40	0.56
2:B:573:SER:O	2:B:574:PHE:HB2	2.05	0.56
1:X:559:GLU:OE2	1:X:599:GLY:CA	2.53	0.56
2:Y:735:VAL:HB	2:Y:792:LEU:HB2	1.87	0.56
1:A:440:ILE:HA	1:A:461:SER:O	2.06	0.56
2:B:59:GLY:CA	2:B:1073:TRP:CZ3	2.87	0.56
1:X:605:THR:OG1	1:X:608:ASP:CB	2.49	0.56
2:Y:1058:LEU:HD22	2:Y:1062:ILE:HD11	1.86	0.56
2:Y:560:LEU:N	2:Y:560:LEU:HD23	2.21	0.56
2:Y:646:THR:OG1	2:Y:647:THR:N	2.37	0.56
2:Y:395:GLY:N	2:Y:705:ASP:OD1	2.39	0.56
2:B:971:ALA:HB3	2:B:1077:HIS:O	2.06	0.56
1:A:543:ILE:HG22	1:A:586:LYS:CG	2.34	0.56
2:B:1032:THR:HG22	2:B:1034:ASN:H	1.71	0.56
2:B:16:ASN:HD21	2:B:36:ASN:HA	1.70	0.56
1:X:508:GLU:O	1:X:509:GLU:OE2	2.23	0.56
2:B:578:HIS:O	2:B:579:LYS:HB2	2.05	0.56
2:B:913:TYR:HH	3:C:240:TRP:HZ3	1.53	0.56
1:X:471:VAL:HG12	1:X:472:MET:N	2.21	0.56
2:Y:1097:PHE:CE2	2:Y:1129:LEU:HB3	2.40	0.56
2:Y:515:ALA:HB1	2:Y:532:THR:O	2.05	0.56
1:X:515:GLY:HA2	1:X:556:THR:HG1	1.70	0.56
1:X:566:LEU:HD21	1:X:584:PHE:HA	1.88	0.56
2:B:408:LYS:HA	2:B:678:TYR:CE2	2.41	0.56
1:X:552:LEU:HB2	1:X:561:VAL:HG11	1.88	0.56
2:Y:465:HIS:O	2:Y:467:GLN:HG3	2.06	0.56
1:A:517:ILE:HD11	1:A:602:CYS:HB2	1.87	0.56
2:B:634:GLN:CB	2:B:654:ASP:OD1	2.53	0.56
2:B:646:THR:OG1	2:B:647:THR:N	2.39	0.56
1:A:495:ALA:HB1	1:A:496:PRO:CD	2.37	0.55
2:Y:108:VAL:HG23	2:Y:108:VAL:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LYS:HE2	1:A:590:VAL:HG23	1.89	0.55
3:C:56:SER:O	3:C:158:LYS:NZ	2.38	0.55
2:B:515:ALA:HB1	2:B:532:THR:O	2.06	0.55
2:B:394:ILE:CD1	2:B:658:VAL:HB	2.36	0.55
2:B:967:GLY:HA3	2:B:975:PHE:CE2	2.41	0.55
1:X:459:LEU:HD13	1:X:496:PRO:HA	1.87	0.55
2:Y:445:GLU:OE2	2:B:770:LEU:C	2.44	0.55
3:Z:85:PRO:O	3:Z:86:GLN:CB	2.54	0.55
1:A:615:PHE:HE1	1:A:617:LEU:CD1	2.20	0.55
2:B:108:VAL:HG23	2:B:108:VAL:O	2.06	0.55
2:B:448:LEU:HD23	2:B:451:PHE:CD1	2.42	0.55
2:B:765:VAL:HG23	2:B:806:GLN:HB3	1.89	0.55
3:C:349:TYR:HD2	3:C:359:THR:HG22	1.72	0.55
2:Y:928:ARG:CB	2:Y:952:ASN:O	2.54	0.55
2:B:1032:THR:HG22	2:B:1034:ASN:N	2.20	0.55
1:X:566:LEU:CD2	1:X:585:VAL:HG12	2.37	0.55
2:Y:404:LEU:HD23	2:Y:404:LEU:C	2.27	0.55
2:Y:618:ILE:HD12	2:Y:618:ILE:N	2.21	0.55
2:Y:928:ARG:O	2:Y:928:ARG:CD	2.54	0.55
3:Z:85:PRO:O	3:Z:86:GLN:HB2	2.06	0.55
1:A:606:PHE:CE1	1:A:610:PRO:HB3	2.42	0.55
2:B:608:ASP:O	2:B:633:THR:HA	2.07	0.55
2:B:1003:PHE:CD2	3:C:197:VAL:HG23	2.42	0.55
1:X:540:HIS:CE1	1:X:542:SER:C	2.79	0.55
1:X:572:LYS:HE2	1:X:590:VAL:HG23	1.88	0.55
2:Y:32:LEU:HD11	2:Y:41:ILE:HG12	1.88	0.55
2:Y:869:ALA:O	2:Y:884:ILE:HA	2.06	0.55
3:Z:351:ASN:HB2	3:Z:352:PRO:CD	2.37	0.55
2:B:920:PHE:HE2	2:B:962:ASP:HB3	1.72	0.55
1:X:568:CYS:HB3	1:X:592:ILE:HD11	1.89	0.55
1:X:537:ILE:HG12	1:X:585:VAL:HG21	1.88	0.55
1:X:553:HIS:HB2	1:X:616:THR:HG23	1.88	0.55
2:Y:1097:PHE:CZ	2:Y:1129:LEU:HB3	2.42	0.55
2:Y:944:GLU:OE1	2:Y:947:ARG:NH2	2.37	0.55
3:Z:172:THR:O	3:Z:173:GLN:C	2.44	0.55
1:A:597:THR:HG21	1:A:601:ILE:HG13	1.87	0.55
2:Y:608:ASP:O	2:Y:633:THR:HA	2.07	0.55
1:A:529:ARG:HD2	1:A:599:GLY:O	2.07	0.55
2:B:513:GLY:O	2:B:538:VAL:HG12	2.07	0.55
3:C:426:ILE:HD13	3:C:426:ILE:H	1.72	0.55
2:Y:118:THR:O	2:Y:118:THR:CG2	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:817:VAL:HG13	2:Y:830:ILE:HB	1.89	0.55
1:A:472:MET:O	1:A:473:MET:CB	2.55	0.55
1:A:552:LEU:HB2	1:A:561:VAL:HG11	1.89	0.55
3:C:351:ASN:HB2	3:C:352:PRO:CD	2.37	0.55
1:X:559:GLU:OE2	1:X:599:GLY:N	2.40	0.55
1:A:569:LEU:H	1:A:582:PRO:HG3	1.72	0.54
1:X:615:PHE:HE1	1:X:617:LEU:HD13	1.71	0.54
2:B:63:VAL:HG11	2:B:122:GLY:HA3	1.89	0.54
2:B:628:LYS:HG2	2:B:629:VAL:N	2.20	0.54
1:X:440:ILE:HA	1:X:461:SER:O	2.08	0.54
1:X:443:PRO:HA	1:X:517:ILE:HG22	1.88	0.54
2:Y:765:VAL:HG23	2:Y:806:GLN:HB3	1.90	0.54
2:B:652:CYS:HB3	2:B:676:VAL:O	2.07	0.54
2:Y:513:GLY:O	2:Y:538:VAL:HG12	2.07	0.54
2:Y:754:PRO:HB2	2:Y:759:GLN:NE2	2.22	0.54
1:A:527:SER:HB2	1:A:602:CYS:HA	1.89	0.54
2:B:808:LEU:CD1	2:B:847:ARG:NH2	2.66	0.54
3:C:69:GLY:HA2	3:C:118:ARG:NH2	2.21	0.54
1:A:597:THR:HG21	1:A:601:ILE:CG1	2.38	0.54
1:X:476:LYS:HE3	1:X:476:LYS:N	2.22	0.54
2:Y:913:TYR:CZ	3:Z:240:TRP:CH2	2.95	0.54
3:Z:352:PRO:CA	3:Z:378:HIS:CE1	2.91	0.54
2:B:537:GLU:O	2:B:561:TRP:HB2	2.08	0.54
2:B:928:ARG:O	2:B:928:ARG:CG	2.56	0.54
1:X:601:ILE:CG2	1:X:602:CYS:N	2.70	0.54
2:Y:427:LEU:N	2:Y:427:LEU:HD12	2.23	0.54
3:Z:352:PRO:HG3	3:Z:378:HIS:CG	2.36	0.54
1:A:540:HIS:ND1	1:A:542:SER:O	2.41	0.54
1:A:615:PHE:HE1	1:A:617:LEU:HD13	1.72	0.54
2:B:1030:PHE:CZ	2:B:1038:GLY:HA3	2.43	0.54
2:B:389:ILE:N	2:B:389:ILE:HD12	2.23	0.54
2:B:427:LEU:N	2:B:427:LEU:HD12	2.22	0.54
2:B:817:VAL:HG13	2:B:830:ILE:HB	1.90	0.54
1:A:559:GLU:OE2	1:A:599:GLY:CA	2.55	0.54
5:C:502:85C:C21	1:A:628:LYS:HD3	2.37	0.54
3:Z:104:PRO:HA	3:Z:107:VAL:HB	1.90	0.54
2:B:1076:PHE:CD1	2:B:1076:PHE:C	2.81	0.54
3:C:85:PRO:O	3:C:86:GLN:CB	2.56	0.54
2:Y:63:VAL:HG11	2:Y:122:GLY:HA3	1.89	0.54
1:A:566:LEU:HD23	1:A:585:VAL:HG12	1.89	0.54
3:C:353:HIS:CG	1:A:572:LYS:HD3	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:928:ARG:CB	2:B:952:ASN:O	2.55	0.53
1:X:448:TYR:O	1:X:449:LYS:C	2.47	0.53
2:Y:1058:LEU:O	2:Y:1062:ILE:HD12	2.08	0.53
2:Y:541:LEU:HD23	2:Y:558:ILE:HD13	1.89	0.53
1:X:628:LYS:CD	5:Z:502:85C:CL1	2.92	0.53
1:A:443:PRO:HA	1:A:517:ILE:HG22	1.90	0.53
2:B:541:LEU:HD23	2:B:558:ILE:HD13	1.89	0.53
2:B:928:ARG:CD	2:B:928:ARG:O	2.55	0.53
3:Z:56:SER:O	3:Z:158:LYS:NZ	2.42	0.53
2:B:908:ASN:OD1	2:B:908:ASN:N	2.41	0.53
3:C:85:PRO:O	3:C:86:GLN:HB2	2.08	0.53
1:X:453:THR:CG2	1:X:454:VAL:N	2.71	0.53
1:X:574:SER:O	5:Z:502:85C:C8	2.56	0.53
3:Z:264:TRP:HD1	3:Z:337:ILE:O	1.91	0.53
2:B:1102:ARG:N	2:B:1103:PRO:HD2	2.23	0.53
2:B:118:THR:CG2	2:B:118:THR:O	2.56	0.53
2:B:414:ARG:HB2	2:B:462:ASN:ND2	2.23	0.53
2:B:538:VAL:HG23	2:B:558:ILE:HG23	1.88	0.53
2:Y:1076:PHE:CD1	2:Y:1076:PHE:C	2.82	0.53
1:A:538:ILE:HD11	1:A:623:THR:CG2	2.36	0.53
2:B:433:THR:O	2:B:434:ARG:CD	2.57	0.53
1:X:552:LEU:CD1	1:X:554:ILE:HG13	2.37	0.53
2:B:660:TYR:O	2:B:667:VAL:HB	2.09	0.53
1:X:448:TYR:O	1:X:448:TYR:CG	2.61	0.53
1:A:510:GLU:OE1	1:A:510:GLU:C	2.47	0.53
1:A:615:PHE:C	1:A:615:PHE:CD1	2.82	0.53
2:B:807:PHE:CZ	2:B:831:VAL:HG11	2.44	0.53
2:B:808:LEU:H	2:B:808:LEU:CD1	2.16	0.53
2:B:869:ALA:O	2:B:884:ILE:HA	2.08	0.53
1:X:552:LEU:CD1	1:X:554:ILE:CG1	2.83	0.53
2:Y:317:LEU:HB2	2:Y:321:VAL:HG12	1.91	0.53
2:Y:538:VAL:HG23	2:Y:558:ILE:HG23	1.90	0.53
2:B:584:GLY:O	2:B:586:ILE:N	2.42	0.53
1:X:495:ALA:HB1	1:X:496:PRO:CD	2.39	0.53
1:X:511:GLU:HA	1:X:511:GLU:OE1	2.09	0.53
1:X:544:ILE:O	1:X:544:ILE:HG12	2.08	0.53
2:Y:910:MET:HG2	2:Y:912:LEU:CD2	2.38	0.53
1:X:495:ALA:HB1	1:X:496:PRO:HD2	1.91	0.53
2:Y:736:LEU:HD13	2:Y:813:ALA:HB1	1.90	0.53
2:Y:971:ALA:HB3	2:Y:1077:HIS:O	2.08	0.53
2:Y:596:PHE:O	2:Y:597:GLU:C	2.46	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ALA:HB1	1:A:496:PRO:HD2	1.91	0.52
2:B:995:VAL:HG23	2:B:995:VAL:O	2.09	0.52
1:X:473:MET:C	1:X:475:ASN:H	2.11	0.52
1:X:513:LEU:N	1:X:513:LEU:CD1	2.72	0.52
2:Y:389:ILE:N	2:Y:389:ILE:HD12	2.24	0.52
2:Y:663:ASN:HB2	2:Y:1134:GLU:OE2	2.09	0.52
1:X:605:THR:C	1:X:606:PHE:O	2.38	0.52
1:A:515:GLY:HA3	1:A:557:CYS:CB	2.37	0.52
1:A:597:THR:O	1:A:599:GLY:N	2.41	0.52
2:Y:20:THR:HG23	2:Y:315:THR:CG2	2.40	0.52
1:A:513:LEU:N	1:A:513:LEU:CD1	2.73	0.52
2:B:317:LEU:HB2	2:B:321:VAL:HG12	1.92	0.52
2:B:88:ILE:HD12	2:B:152:LEU:HD21	1.92	0.52
3:C:117:ASP:C	3:C:119:THR:H	2.13	0.52
1:X:448:TYR:CE1	1:X:454:VAL:HB	2.44	0.52
2:Y:88:ILE:HD12	2:Y:152:LEU:HD21	1.90	0.52
3:Z:83:VAL:HG22	3:Z:121:ALA:HB3	1.91	0.52
1:A:485:LEU:N	1:A:485:LEU:CD1	2.73	0.52
2:B:560:LEU:HD23	2:B:560:LEU:N	2.24	0.52
1:X:450:ASP:OD1	1:X:451:MET:N	2.43	0.52
1:X:537:ILE:HG21	1:X:586:LYS:O	2.09	0.52
2:Y:805:HIS:HD2	2:Y:806:GLN:C	2.13	0.52
3:Z:91:LEU:HD22	3:Z:92:ILE:H	1.75	0.52
2:B:972:PHE:HZ	3:C:196:ALA:O	1.91	0.52
2:Y:912:LEU:HB3	3:Z:240:TRP:CZ2	2.45	0.52
2:Y:618:ILE:CD1	2:Y:618:ILE:H	2.23	0.52
2:Y:618:ILE:HD12	2:Y:618:ILE:H	1.74	0.52
2:Y:995:VAL:HG23	2:Y:995:VAL:O	2.09	0.52
3:Z:237:LEU:HD23	3:Z:237:LEU:N	2.24	0.52
3:Z:135:PHE:CZ	3:Z:300:LYS:HD3	2.44	0.52
2:B:812:TYR:CZ	3:C:241:PRO:HB3	2.45	0.52
2:B:868:GLY:HA3	2:B:885:ASN:HD21	1.75	0.52
3:C:173:GLN:CB	3:C:179:GLN:NE2	2.73	0.52
1:A:606:PHE:HA	1:A:609:PHE:O	2.10	0.52
3:C:407:LYS:N	3:C:407:LYS:HD2	2.25	0.52
3:C:79:GLN:HA	3:C:79:GLN:HE21	1.75	0.52
2:Y:928:ARG:O	2:Y:928:ARG:CG	2.58	0.52
3:Z:407:LYS:N	3:Z:407:LYS:HD2	2.24	0.52
1:A:555:HIS:HB3	1:A:557:CYS:H	1.75	0.51
1:A:566:LEU:HD21	1:A:584:PHE:HA	1.91	0.51
1:X:443:PRO:HB3	1:X:556:THR:HG23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:36:ASN:ND2	2:Y:37:THR:CG2	2.73	0.51
2:Y:408:LYS:HA	2:Y:678:TYR:CE2	2.45	0.51
2:B:535:GLU:CB	2:B:536:HIS:CE1	2.93	0.51
1:X:537:ILE:HG12	1:X:585:VAL:CG2	2.39	0.51
2:Y:660:TYR:O	2:Y:667:VAL:HB	2.10	0.51
3:Z:265:ASP:OD1	3:Z:266:GLU:HG2	2.09	0.51
1:A:568:CYS:O	1:A:592:ILE:CG1	2.58	0.51
2:B:1072:PHE:CD1	2:B:1072:PHE:C	2.83	0.51
2:B:998:PHE:HB2	2:B:1088:PHE:CD2	2.45	0.51
3:C:310:CYS:HA	3:C:442:LEU:HA	1.90	0.51
1:X:468:GLN:O	1:X:470:LEU:HG	2.09	0.51
3:Z:364:LYS:O	3:Z:365:ALA:HB2	2.10	0.51
1:A:513:LEU:N	1:A:513:LEU:HD12	2.24	0.51
2:B:736:LEU:HD13	2:B:813:ALA:HB1	1.91	0.51
1:X:610:PRO:CD	1:X:611:GLN:N	2.73	0.51
2:Y:996:GLY:O	2:Y:997:LEU:HD23	2.11	0.51
3:C:237:LEU:N	3:C:237:LEU:HD23	2.24	0.51
3:C:238:THR:OG1	3:C:239:SER:N	2.40	0.51
1:X:474:PRO:O	1:X:476:LYS:CE	2.56	0.51
2:B:429:PHE:N	2:B:429:PHE:CD1	2.77	0.51
2:Y:652:CYS:HB3	2:Y:676:VAL:O	2.11	0.51
1:A:553:HIS:HB2	1:A:616:THR:HG23	1.93	0.51
1:X:473:MET:CE	1:X:476:LYS:HD3	2.40	0.51
1:X:552:LEU:HD11	1:X:554:ILE:CD1	2.40	0.51
2:Y:486:LEU:HG	2:Y:486:LEU:O	2.10	0.51
3:Z:250:ALA:HB2	3:Z:305:ILE:HD13	1.93	0.51
1:A:610:PRO:O	1:A:612:MET:N	2.44	0.51
2:B:484:LYS:O	2:B:485:ALA:HB2	2.11	0.51
3:C:83:VAL:HG22	3:C:121:ALA:HB3	1.92	0.51
3:C:91:LEU:HD22	3:C:92:ILE:H	1.75	0.51
2:Y:166:ASP:OD2	3:Z:204:LYS:HD3	2.11	0.51
1:X:597:THR:O	1:X:599:GLY:N	2.44	0.51
3:Z:349:TYR:HD2	3:Z:359:THR:HG22	1.76	0.51
2:B:944:GLU:OE1	2:B:947:ARG:NH2	2.41	0.50
1:X:540:HIS:CE1	1:X:542:SER:CA	2.94	0.50
2:Y:10:GLN:HB3	2:Y:1037:ILE:HB	1.93	0.50
2:Y:273:LEU:HB2	2:Y:281:PHE:HB2	1.93	0.50
2:Y:868:GLY:HA3	2:Y:885:ASN:HD21	1.77	0.50
3:Z:338:PHE:CE2	3:Z:340:LEU:HG	2.45	0.50
2:B:517:TYR:CD1	2:B:517:TYR:N	2.80	0.50
1:X:513:LEU:N	1:X:513:LEU:HD12	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1030:PHE:CZ	2:Y:1038:GLY:HA3	2.46	0.50
2:Y:920:PHE:HE2	2:Y:962:ASP:HB3	1.77	0.50
1:A:601:ILE:CG2	1:A:602:CYS:N	2.74	0.50
2:B:596:PHE:CD2	2:B:601:TYR:HD2	2.24	0.50
2:B:618:ILE:HD12	2:B:618:ILE:N	2.26	0.50
3:Z:77:SER:O	3:Z:183:GLN:HA	2.12	0.50
2:Y:276:MET:CE	3:Z:202:LEU:HD22	2.41	0.50
3:Z:238:THR:OG1	3:Z:239:SER:N	2.40	0.50
3:C:236:ASN:OD1	3:C:237:LEU:HD23	2.11	0.50
1:X:554:ILE:C	1:X:555:HIS:CD2	2.85	0.50
2:Y:16:ASN:HD21	2:Y:36:ASN:HA	1.76	0.50
2:Y:337:ASN:HB2	2:Y:339:ASP:O	2.11	0.50
1:A:585:VAL:HG11	1:A:591:CYS:SG	2.51	0.50
1:A:606:PHE:HE1	1:A:610:PRO:HB3	1.76	0.50
2:B:649:VAL:HB	2:B:659:ILE:HB	1.94	0.50
2:B:889:ARG:HD3	2:B:901:THR:CG2	2.39	0.50
1:X:559:GLU:OE2	1:X:599:GLY:HA3	2.11	0.50
1:X:533:ALA:HB2	1:X:629:VAL:HA	1.93	0.50
2:Y:1102:ARG:N	2:Y:1103:PRO:HD2	2.25	0.50
2:B:245:TYR:C	2:B:245:TYR:HD1	2.15	0.50
1:X:449:LYS:NZ	1:X:510:GLU:CG	2.75	0.50
1:X:443:PRO:CA	1:X:517:ILE:HG22	2.41	0.50
1:A:448:TYR:CG	1:A:448:TYR:O	2.65	0.50
1:A:459:LEU:HD13	1:A:496:PRO:HA	1.92	0.50
1:X:568:CYS:O	1:X:592:ILE:CG1	2.60	0.50
3:Z:247:LEU:O	3:Z:309:ARG:HD2	2.12	0.50
2:B:10:GLN:HB3	2:B:1037:ILE:HB	1.94	0.50
2:B:805:HIS:CD2	2:B:806:GLN:N	2.80	0.50
2:B:913:TYR:CZ	3:C:240:TRP:CH2	2.99	0.50
3:C:77:SER:O	3:C:183:GLN:HA	2.12	0.50
1:X:527:SER:HB2	1:X:602:CYS:HA	1.92	0.50
1:X:527:SER:OG	1:X:528:GLY:N	2.45	0.50
2:Y:1048:TYR:HD1	2:Y:1089:ILE:HD12	1.77	0.50
2:B:20:THR:HG23	2:B:315:THR:CG2	2.40	0.49
2:Y:1039:LEU:HD23	2:Y:1040:VAL:N	2.27	0.49
2:Y:913:TYR:CZ	3:Z:240:TRP:HH2	2.30	0.49
2:B:582:LEU:HD23	2:B:612:PHE:CG	2.47	0.49
3:C:426:ILE:HG12	3:C:427:PRO:CA	2.38	0.49
1:X:552:LEU:HD12	1:X:552:LEU:C	2.32	0.49
1:X:554:ILE:HG12	1:X:615:PHE:HB2	1.93	0.49
2:Y:393:GLY:O	2:Y:708:GLN:CB	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1003:PHE:CD2	3:Z:197:VAL:HG23	2.48	0.49
1:A:559:GLU:OE2	1:A:599:GLY:HA3	2.11	0.49
2:B:1058:LEU:O	2:B:1062:ILE:HD12	2.13	0.49
3:C:199:LEU:CD2	3:C:237:LEU:HD11	2.30	0.49
2:Y:513:GLY:O	2:Y:537:GLU:HA	2.12	0.49
2:Y:582:LEU:HD23	2:Y:612:PHE:CG	2.48	0.49
2:Y:649:VAL:HB	2:Y:659:ILE:HB	1.95	0.49
2:Y:762:SER:O	2:Y:803:HIS:HA	2.12	0.49
2:Y:81:THR:HG23	2:Y:85:ASN:HB2	1.94	0.49
5:C:502:85C:C4	1:A:572:LYS:O	2.60	0.49
2:B:455:GLN:OE1	2:B:455:GLN:HA	2.12	0.49
1:X:569:LEU:H	1:X:582:PRO:HG3	1.77	0.49
1:X:545:CYS:HB2	1:X:584:PHE:HB3	1.93	0.49
2:Y:1008:CYS:SG	2:Y:1008:CYS:O	2.71	0.49
3:Z:48:ASN:CA	3:Z:410:SER:HB3	2.42	0.49
1:A:559:GLU:OE2	1:A:599:GLY:N	2.45	0.49
2:B:1078:THR:HG1	2:B:1081:LYS:N	2.10	0.49
2:B:555:LEU:HD13	2:B:593:MET:SD	2.52	0.49
1:X:440:ILE:HD11	1:X:470:LEU:HD22	1.94	0.49
2:Y:838:PRO:HB2	3:Z:225:GLN:OE1	2.12	0.49
2:B:127:GLU:HB2	2:B:129:ARG:HG2	1.95	0.49
2:B:275:ASP:HB2	2:B:279:ARG:HB2	1.95	0.49
2:B:404:LEU:HD23	2:B:404:LEU:C	2.33	0.49
2:B:762:SER:O	2:B:803:HIS:HA	2.13	0.49
3:C:247:LEU:O	3:C:309:ARG:HD2	2.13	0.49
2:Y:871:TYR:HE2	2:Y:885:ASN:HA	1.77	0.49
3:Z:64:MET:O	3:Z:66:GLU:OE2	2.30	0.49
2:B:427:LEU:CD1	2:B:427:LEU:N	2.75	0.49
2:B:513:GLY:O	2:B:537:GLU:HA	2.13	0.49
2:B:996:GLY:O	2:B:997:LEU:HD23	2.13	0.49
2:Y:263:ARG:HA	2:Y:271:TYR:CD1	2.48	0.49
2:Y:322:VAL:HG23	2:Y:336:LEU:HD21	1.95	0.49
2:Y:537:GLU:HG3	2:Y:561:TRP:CD1	2.47	0.49
2:Y:596:PHE:O	2:Y:597:GLU:CB	2.61	0.49
3:Z:236:ASN:OD1	3:Z:237:LEU:HD23	2.12	0.49
2:B:40:GLU:HG2	2:B:54:GLU:HG3	1.95	0.49
2:B:390:ILE:CG2	2:B:710:LEU:HD13	2.43	0.49
2:Y:805:HIS:HD2	2:Y:806:GLN:N	2.09	0.49
3:Z:317:LYS:O	3:Z:426:ILE:HD13	2.13	0.48
2:B:1039:LEU:HD23	2:B:1040:VAL:N	2.28	0.48
2:Y:92:LYS:HE2	2:Y:101:ILE:HD13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:HIS:CG	3:C:79:GLN:OE1	2.66	0.48
1:X:581:ARG:HH11	1:X:581:ARG:CG	2.25	0.48
2:Y:427:LEU:CD1	2:Y:427:LEU:N	2.76	0.48
2:Y:817:VAL:CG1	2:Y:830:ILE:HB	2.43	0.48
3:Z:407:LYS:CD	3:Z:407:LYS:N	2.75	0.48
2:B:171:TYR:CG	2:B:223:PRO:HA	2.49	0.48
2:B:663:ASN:HB2	2:B:1134:GLU:OE2	2.14	0.48
2:B:715:VAL:HG21	2:B:799:PHE:CG	2.49	0.48
3:C:364:LYS:O	3:C:365:ALA:HB2	2.13	0.48
2:Y:796:GLN:OE1	2:Y:797:HIS:CE1	2.67	0.48
3:Z:165:PHE:CD1	3:Z:182:VAL:HG21	2.48	0.48
2:B:263:ARG:HA	2:B:271:TYR:CD1	2.48	0.48
2:B:967:GLY:HA3	2:B:975:PHE:CZ	2.48	0.48
3:C:110:VAL:O	3:C:114:ILE:HG12	2.12	0.48
3:C:407:LYS:CD	3:C:407:LYS:N	2.76	0.48
2:Y:484:LYS:O	2:Y:485:ALA:HB2	2.12	0.48
2:Y:517:TYR:N	2:Y:517:TYR:CD1	2.81	0.48
1:A:471:VAL:CG1	1:A:472:MET:N	2.76	0.48
1:A:536:VAL:HG13	1:A:626:ILE:HD12	1.96	0.48
2:B:385:GLY:HA3	2:B:719:GLU:O	2.13	0.48
2:B:874:VAL:HG12	2:B:881:LEU:HB3	1.95	0.48
2:B:950:ASN:HD22	2:B:950:ASN:C	2.17	0.48
2:Y:1055:GLN:HE22	2:Y:1090:ASP:H	1.60	0.48
2:Y:24:THR:HG22	2:Y:91:TYR:CE2	2.49	0.48
2:Y:385:GLY:HA3	2:Y:719:GLU:O	2.14	0.48
2:Y:429:PHE:N	2:Y:429:PHE:CD1	2.81	0.48
2:Y:492:GLU:OE1	2:Y:494:GLN:N	2.37	0.48
2:Y:913:TYR:OH	2:Y:955:SER:C	2.52	0.48
3:Z:401:LYS:CG	3:Z:415:TRP:CE2	2.90	0.48
1:A:443:PRO:CA	1:A:517:ILE:HG22	2.43	0.48
2:B:1051:LEU:HD22	2:B:1094:ILE:HD12	1.96	0.48
2:B:1054:MET:HE2	2:B:1129:LEU:HD12	1.96	0.48
2:B:5:TYR:HE1	2:B:7:VAL:HB	1.79	0.48
2:Y:1051:LEU:HB2	2:Y:1089:ILE:HD13	1.94	0.48
2:Y:183:GLN:HE22	3:Z:209:PRO:HA	1.78	0.48
1:A:500:LEU:CD1	1:A:500:LEU:N	2.76	0.48
1:A:508:GLU:C	1:A:509:GLU:OE2	2.51	0.48
2:B:511:ALA:CB	2:B:538:VAL:HG11	2.43	0.48
2:B:58:TYR:CE1	2:B:1070:HIS:HD2	2.32	0.48
3:C:144:TYR:CE1	3:C:155:VAL:HG13	2.44	0.48
3:C:425:THR:HG23	3:C:426:ILE:HD13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:275:ASP:HB2	2:Y:279:ARG:HB2	1.95	0.48
2:Y:378:CYS:SG	2:Y:721:PRO:HB2	2.54	0.48
2:Y:390:ILE:CG2	2:Y:710:LEU:HD13	2.44	0.48
2:B:624:SER:O	2:B:625:ASP:HB2	2.14	0.48
3:C:250:ALA:HB2	3:C:305:ILE:HD13	1.95	0.48
1:X:500:LEU:N	1:X:500:LEU:HD13	2.29	0.48
1:X:540:HIS:CE1	1:X:543:ILE:N	2.82	0.48
2:Y:537:GLU:HG3	2:Y:561:TRP:CB	2.44	0.48
2:Y:972:PHE:CE1	3:Z:196:ALA:O	2.66	0.48
3:Z:73:HIS:CG	3:Z:79:GLN:OE1	2.67	0.48
1:A:606:PHE:CD2	1:A:628:LYS:CD	2.93	0.48
2:B:537:GLU:HG3	2:B:561:TRP:HB2	1.96	0.48
2:B:871:TYR:HE2	2:B:885:ASN:HA	1.78	0.48
2:B:900:ARG:O	2:B:900:ARG:CG	2.56	0.48
2:Y:414:ARG:H	2:Y:462:ASN:HD21	1.59	0.48
2:Y:40:GLU:HG2	2:Y:54:GLU:HG3	1.96	0.48
2:B:663:ASN:O	2:B:1134:GLU:OE1	2.32	0.47
1:X:453:THR:C	1:X:454:VAL:CG2	2.82	0.47
1:X:581:ARG:HH11	1:X:581:ARG:HG2	1.79	0.47
1:X:568:CYS:O	1:X:592:ILE:HG13	2.14	0.47
2:Y:1072:PHE:CD1	2:Y:1072:PHE:C	2.87	0.47
2:Y:537:GLU:HG3	2:Y:561:TRP:HB2	1.95	0.47
2:Y:558:ILE:CG2	2:Y:559:GLY:N	2.78	0.47
2:Y:5:TYR:HB2	2:Y:1043:LEU:HD11	1.96	0.47
2:Y:931:LEU:HD11	2:Y:947:ARG:NH2	2.29	0.47
3:Z:351:ASN:OD1	3:Z:355:TYR:HB2	2.14	0.47
1:A:482:LEU:HD21	1:A:505:LYS:HB3	1.95	0.47
2:B:5:TYR:HB2	2:B:1043:LEU:HD11	1.96	0.47
3:C:168:LEU:HD11	3:C:183:GLN:HB2	1.96	0.47
1:X:544:ILE:CG1	1:X:544:ILE:O	2.62	0.47
2:Y:188:ARG:NH1	2:Y:216:ALA:O	2.46	0.47
2:Y:663:ASN:O	2:Y:1134:GLU:OE1	2.31	0.47
2:Y:809:GLN:O	2:Y:810:ASN:HB2	2.14	0.47
3:Z:70:ARG:N	3:Z:70:ARG:CD	2.70	0.47
1:A:552:LEU:CD1	1:A:554:ILE:HG12	2.41	0.47
1:A:606:PHE:C	1:A:606:PHE:CD1	2.86	0.47
2:B:81:THR:HG23	2:B:85:ASN:HB2	1.96	0.47
2:Y:889:ARG:HD3	2:Y:901:THR:CG2	2.39	0.47
2:B:618:ILE:H	2:B:618:ILE:HD12	1.80	0.47
2:B:676:VAL:O	2:B:676:VAL:HG12	2.13	0.47
3:C:114:ILE:CD1	3:C:144:TYR:CD2	2.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:PHE:CE2	3:C:340:LEU:HG	2.49	0.47
3:C:349:TYR:HD2	3:C:359:THR:CG2	2.28	0.47
2:Y:127:GLU:HB2	2:Y:129:ARG:HG2	1.96	0.47
2:Y:267:ASN:ND2	2:Y:269:SER:OG	2.47	0.47
2:Y:805:HIS:C	2:Y:805:HIS:CD2	2.86	0.47
2:B:486:LEU:HD11	2:B:488:SER:C	2.35	0.47
2:B:708:GLN:O	2:B:709:LYS:HB3	2.15	0.47
2:B:807:PHE:CE1	2:B:831:VAL:HG11	2.50	0.47
3:C:127:ASN:HD22	3:C:128:VAL:CG1	2.27	0.47
1:X:561:VAL:HG22	1:X:562:GLU:N	2.28	0.47
1:X:474:PRO:HD3	1:X:602:CYS:SG	2.55	0.47
1:X:606:PHE:HE2	1:X:628:LYS:HD2	1.75	0.47
3:Z:120:PHE:N	3:Z:120:PHE:CD1	2.82	0.47
2:B:172:GLY:HA3	2:B:224:GLU:HG3	1.97	0.47
2:B:322:VAL:HG23	2:B:336:LEU:HD21	1.96	0.47
1:X:615:PHE:C	1:X:615:PHE:CD1	2.88	0.47
3:Z:351:ASN:C	3:Z:378:HIS:CE1	2.83	0.47
3:Z:381:PHE:HD2	3:Z:402:PHE:CE2	2.33	0.47
2:B:716:PRO:HB3	2:B:718:TYR:HE1	1.75	0.47
2:B:766:SER:O	2:B:767:SER:HB3	2.14	0.47
3:C:381:PHE:HD2	3:C:402:PHE:CE2	2.33	0.47
1:A:485:LEU:HA	1:A:490:GLU:CA	2.44	0.47
1:A:606:PHE:C	1:A:606:PHE:HD1	2.17	0.47
2:B:1048:TYR:HD1	2:B:1089:ILE:HD12	1.80	0.47
2:B:459:PHE:CD1	2:B:459:PHE:C	2.88	0.47
2:B:970:ASN:O	2:B:973:ASN:ND2	2.47	0.47
1:X:465:CYS:HA	1:X:493:THR:HG22	1.97	0.47
1:A:447:LYS:HD3	1:A:447:LYS:N	2.28	0.47
1:A:465:CYS:HA	1:A:493:THR:HG22	1.96	0.47
1:A:527:SER:OG	1:A:528:GLY:N	2.48	0.47
2:B:792:LEU:O	2:B:793:ILE:HD13	2.15	0.47
2:Y:455:GLN:HA	2:Y:455:GLN:OE1	2.15	0.47
2:B:1051:LEU:HB2	2:B:1089:ILE:HD13	1.96	0.47
2:B:926:LEU:HA	2:B:926:LEU:HD12	1.53	0.47
1:X:540:HIS:ND1	1:X:541:LYS:N	2.63	0.47
2:Y:1054:MET:HE2	2:Y:1129:LEU:HD12	1.97	0.47
2:Y:1055:GLN:NE2	2:Y:1090:ASP:H	2.12	0.47
2:B:535:GLU:C	2:B:536:HIS:CG	2.89	0.47
2:Y:245:TYR:C	2:Y:245:TYR:HD1	2.17	0.47
3:Z:165:PHE:CG	3:Z:182:VAL:HG22	2.50	0.47
1:A:540:HIS:HD2	1:A:544:ILE:CG2	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:GLN:OE1	2:B:434:ARG:NH2	2.45	0.46
2:B:933:LEU:HD22	2:B:944:GLU:HA	1.97	0.46
3:C:310:CYS:HB2	3:C:442:LEU:HB3	1.97	0.46
1:X:628:LYS:N	5:Z:502:85C:CL1	2.85	0.46
2:Y:171:TYR:CG	2:Y:223:PRO:HA	2.50	0.46
2:Y:874:VAL:HG12	2:Y:881:LEU:HB3	1.97	0.46
2:B:596:PHE:HB3	2:B:661:SER:C	2.35	0.46
2:B:817:VAL:CG1	2:B:830:ILE:HB	2.44	0.46
3:C:120:PHE:CD1	3:C:120:PHE:N	2.83	0.46
1:X:572:LYS:HD3	3:Z:353:HIS:ND1	2.29	0.46
2:B:16:ASN:ND2	2:B:36:ASN:H	2.13	0.46
2:B:726:TYR:CD1	2:B:733:PHE:CE1	3.03	0.46
1:X:585:VAL:HG11	1:X:591:CYS:SG	2.56	0.46
3:Z:168:LEU:HD11	3:Z:183:GLN:HB2	1.98	0.46
2:B:390:ILE:HG21	2:B:710:LEU:HD13	1.96	0.46
2:B:426:VAL:C	2:B:427:LEU:HD12	2.35	0.46
2:B:948:ASP:HB2	2:B:992:LEU:HB2	1.97	0.46
2:Y:426:VAL:C	2:Y:427:LEU:HD12	2.35	0.46
2:Y:676:VAL:HG12	2:Y:676:VAL:O	2.14	0.46
3:Z:394:CYS:O	3:Z:395:ALA:HB3	2.16	0.46
3:Z:79:GLN:HA	3:Z:79:GLN:HE21	1.81	0.46
2:B:276:MET:O	2:B:276:MET:HG2	2.15	0.46
2:Y:555:LEU:HD13	2:Y:593:MET:SD	2.55	0.46
3:Z:115:GLN:NE2	3:Z:115:GLN:CA	2.78	0.46
2:B:267:ASN:ND2	2:B:269:SER:OG	2.49	0.46
2:B:652:CYS:HB3	2:B:676:VAL:HG12	1.96	0.46
2:Y:36:ASN:ND2	2:Y:1002:GLU:OE2	2.48	0.46
2:Y:1078:THR:HG1	2:Y:1081:LYS:N	2.13	0.46
2:Y:272:LEU:HD11	2:Y:322:VAL:HG21	1.98	0.46
2:Y:535:GLU:C	2:Y:536:HIS:CG	2.89	0.46
2:Y:596:PHE:HB3	2:Y:661:SER:C	2.35	0.46
1:X:441:ARG:N	1:X:461:SER:HB3	2.30	0.46
1:X:540:HIS:CE1	1:X:542:SER:OG	2.57	0.46
2:Y:279:ARG:CG	2:Y:279:ARG:HH11	2.21	0.46
3:Z:345:PRO:O	3:Z:360:LEU:HD12	2.16	0.46
2:B:930:VAL:HG12	2:B:931:LEU:N	2.31	0.46
3:C:351:ASN:OD1	3:C:355:TYR:HB2	2.16	0.46
2:B:24:THR:HG22	2:B:91:TYR:CE2	2.52	0.45
2:B:328:LEU:HD23	2:B:328:LEU:N	2.32	0.45
2:B:808:LEU:HD11	2:B:847:ARG:CZ	2.46	0.45
2:B:914:LEU:O	2:B:915:LYS:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:913:TYR:CZ	3:C:240:TRP:CZ3	3.04	0.45
3:C:91:LEU:HD22	3:C:92:ILE:N	2.31	0.45
1:X:471:VAL:CG1	1:X:472:MET:N	2.78	0.45
2:Y:715:VAL:HG21	2:Y:799:PHE:CG	2.51	0.45
2:Y:916:THR:OG1	2:Y:917:LYS:N	2.47	0.45
1:A:459:LEU:HB2	1:A:500:LEU:HD22	1.98	0.45
1:A:561:VAL:HG22	1:A:562:GLU:N	2.31	0.45
2:B:913:TYR:OH	2:B:955:SER:C	2.54	0.45
2:Y:511:ALA:HB1	2:Y:538:VAL:CG1	2.46	0.45
1:A:568:CYS:O	1:A:592:ILE:HG13	2.15	0.45
2:B:564:ILE:CD1	2:B:584:GLY:N	2.79	0.45
2:Y:1051:LEU:HD22	2:Y:1094:ILE:HD12	1.99	0.45
2:Y:390:ILE:HG21	2:Y:710:LEU:HD13	1.98	0.45
2:Y:511:ALA:CB	2:Y:538:VAL:HG11	2.45	0.45
2:Y:958:GLU:HA	2:Y:958:GLU:OE1	2.16	0.45
3:Z:91:LEU:HD22	3:Z:92:ILE:N	2.29	0.45
1:A:552:LEU:HD12	1:A:552:LEU:C	2.37	0.45
2:B:537:GLU:HG3	2:B:561:TRP:CB	2.46	0.45
2:B:617:ASN:CB	2:B:620:THR:CB	2.95	0.45
1:X:449:LYS:HZ2	1:X:510:GLU:CB	2.30	0.45
1:X:554:ILE:O	1:X:555:HIS:CD2	2.70	0.45
2:Y:881:LEU:HD12	2:Y:889:ARG:O	2.17	0.45
2:Y:914:LEU:O	2:Y:915:LYS:HG2	2.17	0.45
3:Z:402:PHE:N	3:Z:402:PHE:CD1	2.84	0.45
2:B:1122:ARG:NH1	2:B:1128:ASP:OD2	2.49	0.45
2:B:576:LEU:O	2:B:578:HIS:N	2.49	0.45
2:B:591:ILE:HG13	2:B:603:LEU:O	2.17	0.45
2:B:916:THR:OG1	2:B:917:LYS:N	2.50	0.45
2:B:912:LEU:HD11	3:C:244:LEU:HD21	1.99	0.45
1:X:447:LYS:N	1:X:447:LYS:HD3	2.29	0.45
2:Y:105:HIS:HA	2:Y:152:LEU:HD12	1.98	0.45
1:A:540:HIS:CE1	1:A:542:SER:O	2.70	0.45
1:A:533:ALA:HB2	1:A:629:VAL:HA	1.97	0.45
3:C:351:ASN:CB	3:C:352:PRO:CD	2.95	0.45
3:C:48:ASN:CA	3:C:410:SER:HB3	2.40	0.45
2:Y:161:GLU:OE2	2:Y:193:TYR:OH	2.29	0.45
2:B:119:GLY:O	2:B:134:ARG:NH1	2.50	0.45
2:B:241:ASN:O	2:B:242:GLY:C	2.55	0.45
2:B:618:ILE:H	2:B:618:ILE:CD1	2.28	0.45
1:X:459:LEU:HB2	1:X:500:LEU:HD22	1.97	0.45
1:X:482:LEU:HD21	1:X:505:LYS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:449:LYS:HZ2	1:X:510:GLU:CG	2.30	0.45
1:X:610:PRO:HD2	1:X:611:GLN:HG2	1.98	0.45
2:Y:1039:LEU:HD23	2:Y:1039:LEU:C	2.37	0.45
2:Y:706:GLU:HA	2:Y:707:ILE:HA	1.86	0.45
3:Z:145:ARG:NH2	3:Z:145:ARG:HG3	2.31	0.45
2:B:883:SER:HB2	2:B:911:ALA:CB	2.43	0.45
3:C:114:ILE:HG13	3:C:144:TYR:HE2	1.80	0.45
3:C:394:CYS:O	3:C:395:ALA:HB3	2.16	0.45
1:X:605:THR:HG1	1:X:608:ASP:HB2	1.78	0.45
1:X:610:PRO:CG	1:X:611:GLN:H	2.29	0.45
2:Y:998:PHE:HD2	2:Y:1088:PHE:CB	2.30	0.45
2:Y:268:GLY:O	2:Y:285:LEU:HD12	2.17	0.45
2:B:172:GLY:HA2	2:B:224:GLU:CD	2.37	0.45
2:B:324:VAL:HB	2:B:332:GLN:HB2	1.98	0.45
2:B:486:LEU:O	2:B:486:LEU:HG	2.16	0.45
1:X:581:ARG:NH1	1:X:581:ARG:CG	2.80	0.45
1:X:610:PRO:HD2	1:X:611:GLN:N	2.28	0.45
1:A:508:GLU:OE2	1:A:511:GLU:HG2	2.16	0.45
3:C:117:ASP:C	3:C:119:THR:N	2.70	0.45
1:X:482:LEU:HD21	1:X:505:LYS:CB	2.47	0.45
2:Y:118:THR:CG2	2:Y:165:ILE:O	2.62	0.45
2:Y:172:GLY:HA3	2:Y:224:GLU:HG3	1.99	0.45
2:Y:324:VAL:HB	2:Y:332:GLN:HB2	1.99	0.45
2:Y:414:ARG:HB2	2:Y:462:ASN:ND2	2.31	0.45
2:B:405:PRO:HA	2:B:697:SER:HA	1.99	0.44
2:B:558:ILE:CG2	2:B:559:GLY:N	2.80	0.44
2:Y:913:TYR:CZ	3:Z:240:TRP:CZ3	3.05	0.44
2:B:1125:THR:HG23	2:B:1128:ASP:OD2	2.18	0.44
2:B:273:LEU:HB2	2:B:281:PHE:HB2	1.97	0.44
2:B:459:PHE:CD1	2:B:460:CYS:N	2.85	0.44
2:B:378:CYS:SG	2:B:721:PRO:HB2	2.57	0.44
2:B:881:LEU:HD12	2:B:889:ARG:O	2.17	0.44
1:X:443:PRO:CB	1:X:556:THR:HG23	2.48	0.44
1:X:606:PHE:HB2	1:X:628:LYS:HB3	1.99	0.44
2:Y:410:LEU:HA	2:Y:410:LEU:HD12	1.80	0.44
2:Y:571:LEU:O	2:Y:573:SER:N	2.44	0.44
2:Y:584:GLY:O	2:Y:586:ILE:N	2.50	0.44
2:Y:808:LEU:HB2	2:Y:811:GLU:HB2	1.99	0.44
2:Y:821:LEU:HD11	2:Y:830:ILE:HD11	1.99	0.44
3:Z:104:PRO:HD2	3:Z:105:GLN:OE1	2.18	0.44
3:Z:351:ASN:CB	3:Z:352:PRO:CD	2.94	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:391:CYS:HB3	3:Z:394:CYS:SG	2.57	0.44
1:A:485:LEU:N	1:A:485:LEU:HD12	2.33	0.44
1:A:503:ARG:HB2	1:A:503:ARG:CZ	2.46	0.44
3:C:351:ASN:ND2	1:A:572:LYS:O	2.50	0.44
2:B:571:LEU:O	2:B:573:SER:N	2.45	0.44
1:X:553:HIS:CE1	1:X:558:ILE:HG12	2.52	0.44
1:X:606:PHE:O	1:X:608:ASP:N	2.48	0.44
2:Y:183:GLN:HB2	2:Y:188:ARG:HG2	1.99	0.44
2:Y:792:LEU:O	2:Y:793:ILE:HD13	2.18	0.44
2:Y:873:MET:HE2	2:Y:873:MET:HB2	1.89	0.44
2:B:183:GLN:NE2	3:C:209:PRO:HA	2.32	0.44
3:C:93:PRO:HD3	3:C:137:THR:HG21	2.00	0.44
1:X:552:LEU:HD11	1:X:554:ILE:HD11	1.98	0.44
2:Y:569:LEU:N	2:Y:569:LEU:HD22	2.33	0.44
1:X:536:VAL:HG11	5:Z:502:85C:C20	2.47	0.44
2:B:931:LEU:HD23	2:B:933:LEU:HD21	1.99	0.44
1:X:537:ILE:CG1	1:X:585:VAL:HG22	2.48	0.44
2:Y:184:ASP:HB2	2:Y:185:PRO:HD2	2.00	0.44
2:Y:930:VAL:HG12	2:Y:931:LEU:N	2.32	0.44
1:A:530:THR:HG23	1:A:596:ARG:HG2	2.00	0.44
2:B:110:ASP:N	2:B:110:ASP:OD1	2.50	0.44
2:B:832:GLY:N	2:B:873:MET:HE2	2.32	0.44
2:B:873:MET:HE3	2:B:873:MET:HB2	1.87	0.44
2:Y:998:PHE:HD2	2:Y:1088:PHE:HB2	1.82	0.44
2:Y:241:ASN:O	2:Y:242:GLY:C	2.55	0.44
3:Z:187:GLU:HG2	3:Z:278:ILE:HG12	1.98	0.44
2:B:118:THR:CG2	2:B:165:ILE:O	2.63	0.44
2:Y:110:ASP:N	2:Y:110:ASP:OD1	2.50	0.44
2:Y:67:PHE:CG	2:Y:124:ILE:HD13	2.53	0.44
2:Y:172:GLY:HA2	2:Y:224:GLU:CD	2.38	0.44
2:Y:889:ARG:HG2	2:Y:891:TYR:CE2	2.53	0.44
2:Y:937:PRO:HD2	2:Y:938:MET:CE	2.47	0.44
2:B:217:SER:HB2	3:C:204:LYS:HB3	1.98	0.44
2:B:511:ALA:HB1	2:B:538:VAL:CG1	2.45	0.44
2:B:478:LEU:HD22	2:B:526:LEU:HG	1.99	0.44
2:B:578:HIS:O	2:B:579:LYS:CB	2.66	0.44
2:Y:1122:ARG:NH1	2:Y:1128:ASP:OD2	2.50	0.44
2:Y:1125:THR:HG23	2:Y:1128:ASP:OD2	2.18	0.44
2:Y:405:PRO:HA	2:Y:697:SER:HA	1.99	0.44
2:Y:933:LEU:HD22	2:Y:944:GLU:HA	1.99	0.44
3:Z:338:PHE:HE2	3:Z:340:LEU:HG	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:443:PRO:HA	1:X:517:ILE:CG2	2.47	0.44
1:X:538:ILE:HG13	1:X:539:GLU:N	2.33	0.44
1:X:545:CYS:SG	1:X:546:PRO:HD2	2.58	0.44
2:Y:591:ILE:HG13	2:Y:603:LEU:O	2.18	0.44
2:Y:932:LEU:HA	2:Y:932:LEU:HD12	1.79	0.44
2:B:718:TYR:CD1	2:B:718:TYR:N	2.85	0.43
2:B:821:LEU:HD11	2:B:830:ILE:HD11	2.00	0.43
3:C:173:GLN:CB	3:C:179:GLN:HE21	2.31	0.43
3:C:425:THR:CG2	3:C:426:ILE:HD13	2.47	0.43
1:X:449:LYS:NZ	1:X:510:GLU:CD	2.65	0.43
3:Z:292:ASP:O	3:Z:296:ILE:HG12	2.18	0.43
2:B:796:GLN:OE1	2:B:797:HIS:CE1	2.71	0.43
2:B:847:ARG:NH1	2:B:849:VAL:HG22	2.33	0.43
2:Y:1030:PHE:CE2	2:Y:1040:VAL:HG23	2.53	0.43
2:Y:723:LYS:O	2:Y:735:VAL:HA	2.18	0.43
2:Y:900:ARG:CG	2:Y:900:ARG:O	2.59	0.43
1:X:545:CYS:HB2	1:X:584:PHE:CB	2.48	0.43
1:X:553:HIS:ND1	1:X:558:ILE:HD11	2.33	0.43
2:Y:110:ASP:OD1	2:Y:141:LYS:NZ	2.51	0.43
2:Y:328:LEU:HD23	2:Y:328:LEU:N	2.32	0.43
3:Z:105:GLN:CD	3:Z:105:GLN:H	2.22	0.43
1:A:605:THR:HA	1:A:629:VAL:HG22	2.00	0.43
2:B:58:TYR:HE1	2:B:1070:HIS:HD2	1.65	0.43
2:B:110:ASP:OD1	2:B:141:LYS:NZ	2.51	0.43
2:B:268:GLY:O	2:B:285:LEU:HD12	2.18	0.43
2:B:805:HIS:HD2	2:B:806:GLN:C	2.20	0.43
2:B:998:PHE:CZ	2:B:1074:ARG:HD2	2.53	0.43
2:Y:329:GLY:O	2:Y:355:ASN:ND2	2.50	0.43
2:Y:448:LEU:HD23	2:Y:451:PHE:CD1	2.53	0.43
2:Y:478:LEU:HD22	2:Y:526:LEU:HG	2.00	0.43
2:Y:564:ILE:O	2:Y:582:LEU:HD12	2.19	0.43
2:B:869:ALA:HB3	2:B:871:TYR:CZ	2.53	0.43
2:Y:40:GLU:HB3	2:Y:42:TYR:CE1	2.54	0.43
2:Y:616:LEU:HD12	2:Y:616:LEU:HA	1.92	0.43
2:Y:652:CYS:HB3	2:Y:676:VAL:HG12	2.01	0.43
2:Y:718:TYR:N	2:Y:718:TYR:CD1	2.86	0.43
3:Z:340:LEU:HD23	3:Z:340:LEU:HA	1.79	0.43
1:A:482:LEU:HD21	1:A:505:LYS:CB	2.48	0.43
2:B:359:ILE:HB	2:B:1032:THR:H	1.84	0.43
2:B:1030:PHE:CE2	2:B:1040:VAL:HG23	2.54	0.43
2:B:958:GLU:OE1	2:B:958:GLU:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:250:ALA:HB2	3:Z:305:ILE:CD1	2.48	0.43
2:B:492:GLU:OE1	2:B:494:GLN:N	2.39	0.43
1:X:441:ARG:NE	1:X:525:CYS:SG	2.92	0.43
2:Y:457:THR:HG23	2:Y:470:GLN:HG3	2.00	0.43
2:Y:631:LEU:HD12	2:Y:636:THR:HG21	2.01	0.43
2:B:571:LEU:HB3	2:B:572:PRO:CD	2.49	0.43
2:B:723:LYS:O	2:B:735:VAL:HA	2.18	0.43
3:C:260:GLN:O	3:C:263:GLU:HG2	2.18	0.43
2:Y:204:LYS:CA	2:Y:204:LYS:HE2	2.42	0.43
2:Y:573:SER:O	2:Y:574:PHE:CB	2.66	0.43
1:X:540:HIS:C	1:X:540:HIS:ND1	2.72	0.43
2:B:809:GLN:O	2:B:810:ASN:HB2	2.19	0.43
3:C:199:LEU:HD21	3:C:237:LEU:CD1	2.31	0.43
1:X:508:GLU:C	1:X:509:GLU:OE2	2.57	0.43
1:X:572:LYS:O	5:Z:502:85C:C4	2.66	0.43
2:Y:487:VAL:CG2	2:Y:524:GLN:HA	2.49	0.43
2:Y:883:SER:OG	2:Y:883:SER:O	2.37	0.43
1:A:554:ILE:O	1:A:557:CYS:O	2.37	0.42
2:B:1032:THR:CG2	2:B:1033:VAL:N	2.81	0.42
2:B:16:ASN:OD1	2:B:16:ASN:N	2.51	0.42
2:B:410:LEU:HD12	2:B:410:LEU:HA	1.78	0.42
2:B:487:VAL:CG2	2:B:524:GLN:HA	2.48	0.42
2:B:538:VAL:HG23	2:B:558:ILE:CG2	2.49	0.42
3:C:49:PHE:CD1	3:C:49:PHE:C	2.92	0.42
1:X:572:LYS:O	3:Z:351:ASN:ND2	2.51	0.42
2:Y:1121:LYS:O	2:Y:1122:ARG:HB3	2.19	0.42
1:A:563:ILE:CG1	1:A:563:ILE:O	2.67	0.42
2:B:161:GLU:OE2	2:B:193:TYR:OH	2.31	0.42
2:B:932:LEU:HB3	2:B:945:ILE:HB	2.00	0.42
2:B:960:LEU:HA	2:B:960:LEU:HD23	1.80	0.42
3:C:313:ASP:C	3:C:313:ASP:OD1	2.58	0.42
1:X:628:LYS:HD3	5:Z:502:85C:C18	2.49	0.42
2:Y:1061:VAL:HG21	2:Y:1108:VAL:CG2	2.49	0.42
2:Y:58:TYR:CE1	2:Y:1070:HIS:HD2	2.37	0.42
3:Z:289:PRO:O	3:Z:424:PRO:HG3	2.19	0.42
3:Z:113:LEU:HA	3:Z:113:LEU:HD12	1.82	0.42
3:Z:345:PRO:O	3:Z:360:LEU:HA	2.18	0.42
1:A:486:SER:O	1:A:487:ASP:HB3	2.20	0.42
1:A:440:ILE:HG13	1:A:520:ASP:H	1.84	0.42
1:A:553:HIS:CE1	1:A:558:ILE:HG12	2.54	0.42
2:B:281:PHE:HD1	2:B:304:LEU:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:537:GLU:HG3	2:B:561:TRP:CD1	2.53	0.42
2:B:5:TYR:CE1	2:B:7:VAL:HB	2.54	0.42
2:B:913:TYR:CZ	3:C:240:TRP:HH2	2.36	0.42
3:C:426:ILE:N	3:C:426:ILE:HD13	2.34	0.42
1:X:537:ILE:HG13	1:X:585:VAL:HG22	2.00	0.42
2:Y:6:VAL:HG22	2:Y:1040:VAL:HG22	2.01	0.42
2:Y:805:HIS:CD2	2:Y:806:GLN:C	2.92	0.42
2:Y:998:PHE:CD2	2:Y:1088:PHE:HB3	2.54	0.42
3:Z:67:PHE:CD2	3:Z:118:ARG:HD3	2.54	0.42
2:B:937:PRO:HD2	2:B:938:MET:CE	2.49	0.42
3:C:113:LEU:HA	3:C:113:LEU:HD12	1.82	0.42
3:C:119:THR:HG22	3:C:140:GLU:HA	2.01	0.42
2:Y:492:GLU:HB3	2:Y:496:LYS:H	1.84	0.42
3:Z:221:TYR:O	3:Z:225:GLN:NE2	2.51	0.42
1:A:474:PRO:HD3	1:A:602:CYS:SG	2.60	0.42
2:B:40:GLU:CG	2:B:54:GLU:HG3	2.49	0.42
3:C:187:GLU:HG2	3:C:278:ILE:HG12	2.01	0.42
1:X:447:LYS:HG2	1:X:447:LYS:O	2.20	0.42
2:Y:535:GLU:CB	2:Y:536:HIS:CE1	3.03	0.42
2:Y:537:GLU:O	2:Y:561:TRP:CD1	2.73	0.42
2:Y:541:LEU:HD23	2:Y:558:ILE:HD12	2.00	0.42
1:A:442:LEU:HB2	1:A:459:LEU:HD23	2.01	0.42
1:A:610:PRO:HD2	1:A:611:GLN:NE2	2.35	0.42
2:B:955:SER:OG	2:B:1004:VAL:O	2.23	0.42
2:B:912:LEU:HD23	2:B:912:LEU:HA	1.72	0.42
2:B:932:LEU:HA	2:B:932:LEU:HD12	1.77	0.42
2:Y:1032:THR:CG2	2:Y:1033:VAL:N	2.82	0.42
2:Y:913:TYR:OH	3:Z:240:TRP:CZ3	2.70	0.42
3:Z:319:THR:OG1	3:Z:427:PRO:HG3	2.19	0.42
2:B:821:LEU:HB3	2:B:893:TRP:CB	2.49	0.42
1:X:554:ILE:CG2	1:X:555:HIS:CD2	2.85	0.42
3:Z:93:PRO:HD3	3:Z:137:THR:HG21	2.02	0.42
2:B:283:LEU:HD12	2:B:302:VAL:HG22	2.02	0.42
3:C:349:TYR:CD2	3:C:359:THR:CG2	3.03	0.42
2:Y:1056:ASN:N	2:Y:1056:ASN:HD22	2.18	0.42
2:Y:5:TYR:CE2	2:Y:1136:LEU:HD22	2.55	0.42
3:Z:117:ASP:O	3:Z:118:ARG:HB2	2.20	0.42
3:Z:81:ILE:HB	3:Z:121:ALA:HB2	2.01	0.42
2:B:1070:HIS:CE1	2:B:1093:LEU:CD2	3.02	0.42
2:B:1051:LEU:CD2	2:B:1094:ILE:HD12	2.49	0.42
2:B:358:PRO:O	2:B:379:SER:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:GLU:HB3	2:B:496:LYS:H	1.85	0.42
2:B:541:LEU:HD23	2:B:558:ILE:HD12	1.99	0.42
2:B:543:ILE:O	2:B:543:ILE:HG23	2.20	0.42
1:X:475:ASN:C	1:X:476:LYS:HE3	2.40	0.42
1:X:610:PRO:CG	1:X:611:GLN:N	2.82	0.42
2:Y:998:PHE:CZ	2:Y:1074:ARG:HD2	2.55	0.42
2:Y:40:GLU:CG	2:Y:54:GLU:HG3	2.49	0.42
2:Y:571:LEU:HB3	2:Y:572:PRO:CD	2.50	0.42
3:Z:145:ARG:HH21	3:Z:145:ARG:HG3	1.85	0.42
2:B:155:PHE:C	2:B:155:PHE:CD1	2.94	0.41
1:X:442:LEU:HB2	1:X:459:LEU:HD23	2.01	0.41
2:Y:404:LEU:HD22	2:Y:407:ILE:CD1	2.47	0.41
2:Y:455:GLN:HE21	2:Y:474:ALA:HB2	1.85	0.41
2:Y:486:LEU:HD11	2:Y:488:SER:C	2.40	0.41
2:Y:716:PRO:HB3	2:Y:718:TYR:HE1	1.80	0.41
1:A:511:GLU:OE1	1:A:511:GLU:HA	2.19	0.41
1:A:538:ILE:HG13	1:A:539:GLU:N	2.34	0.41
2:B:169:PHE:CD1	2:B:178:ILE:HG22	2.55	0.41
2:B:588:PRO:HA	2:B:606:LEU:HD23	2.01	0.41
3:C:85:PRO:HD2	3:C:106:GLU:HG2	2.02	0.41
2:B:234:GLN:OE1	2:B:257:THR:HG23	2.21	0.41
2:B:661:SER:H	2:B:666:LEU:HA	1.85	0.41
2:B:925:ASP:OD1	2:B:925:ASP:C	2.58	0.41
3:C:93:PRO:HD3	3:C:137:THR:CG2	2.51	0.41
1:X:540:HIS:HE1	1:X:542:SER:CA	2.32	0.41
1:X:530:THR:HG23	1:X:596:ARG:HG2	2.00	0.41
2:Y:663:ASN:C	2:Y:663:ASN:HD22	2.23	0.41
2:Y:930:VAL:CG1	2:Y:931:LEU:N	2.83	0.41
2:Y:965:PHE:N	2:Y:965:PHE:CD2	2.88	0.41
2:B:1121:LYS:O	2:B:1122:ARG:HB3	2.19	0.41
2:B:575:GLU:O	2:B:576:LEU:C	2.59	0.41
2:B:631:LEU:HD12	2:B:636:THR:HG21	2.02	0.41
2:B:893:TRP:CZ2	2:B:897:LYS:HG3	2.56	0.41
3:C:81:ILE:HB	3:C:121:ALA:HB2	2.01	0.41
1:X:551:VAL:HG12	1:X:552:LEU:N	2.35	0.41
2:Y:485:ALA:O	2:Y:487:VAL:HG13	2.20	0.41
2:Y:641:PHE:CE1	2:Y:648:ASN:HB2	2.56	0.41
3:Z:266:GLU:O	3:Z:267:ASN:C	2.54	0.41
1:X:572:LYS:HD3	3:Z:353:HIS:CG	2.55	0.41
3:Z:406:LYS:HE2	3:Z:409:MET:CE	2.51	0.41
2:B:928:ARG:HB2	2:B:954:MET:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:MET:HE2	3:C:109:MET:CA	2.49	0.41
3:C:250:ALA:HB2	3:C:305:ILE:CD1	2.50	0.41
1:X:447:LYS:HD2	1:X:512:ILE:O	2.20	0.41
2:Y:359:ILE:HB	2:Y:1032:THR:H	1.85	0.41
2:Y:459:PHE:CD1	2:Y:459:PHE:C	2.93	0.41
2:Y:543:ILE:HG23	2:Y:543:ILE:O	2.21	0.41
3:Z:137:THR:HA	3:Z:163:GLN:O	2.21	0.41
2:B:272:LEU:HD11	2:B:322:VAL:HG21	2.02	0.41
2:B:451:PHE:HA	2:B:470:GLN:NE2	2.36	0.41
2:B:558:ILE:HG22	2:B:560:LEU:HD23	2.01	0.41
2:B:569:LEU:HD22	2:B:569:LEU:N	2.35	0.41
1:X:584:PHE:CD1	1:X:584:PHE:C	2.93	0.41
2:Y:23:PHE:H	2:Y:30:ASN:HD22	1.68	0.41
2:Y:358:PRO:O	2:Y:379:SER:HA	2.21	0.41
2:Y:538:VAL:HG23	2:Y:558:ILE:CG2	2.51	0.41
2:B:1055:GLN:HE22	2:B:1090:ASP:H	1.69	0.41
3:C:165:PHE:CG	3:C:182:VAL:HG22	2.55	0.41
1:X:564:THR:HG21	1:X:596:ARG:HG3	2.03	0.41
2:Y:744:ASP:CB	2:Y:749:THR:N	2.83	0.41
2:Y:770:LEU:HD23	2:B:445:GLU:HG3	2.03	0.41
2:Y:931:LEU:HD23	2:Y:933:LEU:HD21	2.01	0.41
2:B:1072:PHE:CD1	2:B:1072:PHE:O	2.74	0.41
2:B:183:GLN:HE22	3:C:209:PRO:HA	1.84	0.41
3:C:257:ILE:CG1	3:C:312:LEU:HG	2.51	0.41
3:C:425:THR:CG2	3:C:426:ILE:N	2.81	0.41
1:X:481:VAL:HG11	1:X:484:ILE:HD11	2.03	0.41
1:X:540:HIS:HE1	1:X:542:SER:N	2.12	0.41
1:X:567:ILE:HA	1:X:581:ARG:HH12	1.85	0.41
2:Y:467:GLN:HE22	2:Y:524:GLN:H	1.67	0.41
2:Y:811:GLU:OE1	2:Y:847:ARG:NH2	2.47	0.41
2:Y:906:TYR:HD1	2:Y:906:TYR:H	1.64	0.41
3:Z:313:ASP:C	3:Z:313:ASP:OD1	2.59	0.41
1:A:568:CYS:O	1:A:592:ILE:HG12	2.20	0.41
2:B:378:CYS:SG	2:B:724:ILE:HB	2.60	0.41
2:B:930:VAL:CG1	2:B:931:LEU:N	2.83	0.41
2:B:932:LEU:C	2:B:933:LEU:HD23	2.41	0.41
1:X:578:SER:OG	1:X:579:LYS:N	2.53	0.41
2:Y:1134:GLU:HA	2:Y:1137:THR:OG1	2.21	0.41
2:Y:411:TRP:O	2:Y:425:LEU:HD12	2.21	0.41
2:Y:658:VAL:HG23	2:Y:671:VAL:HG22	2.03	0.41
3:Z:102:PHE:N	3:Z:102:PHE:CD1	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1007:PHE:CD1	2:B:1030:PHE:HB3	2.56	0.41
2:B:216:ALA:HA	2:B:233:GLY:HA2	2.03	0.41
3:C:72:LEU:HD23	3:C:163:GLN:HE21	1.86	0.41
2:B:1003:PHE:CG	3:C:197:VAL:HG23	2.56	0.41
3:C:370:LEU:HD21	3:C:401:LYS:HD3	2.02	0.41
2:Y:497:ASN:O	2:Y:512:VAL:HG13	2.21	0.41
2:Y:722:ARG:C	2:Y:723:LYS:HG2	2.41	0.41
2:Y:821:LEU:HB3	2:Y:893:TRP:CB	2.51	0.41
2:Y:960:LEU:HA	2:Y:960:LEU:HD23	1.76	0.41
2:B:184:ASP:HB2	2:B:185:PRO:HD2	2.02	0.41
2:B:479:VAL:HG12	2:B:480:SER:O	2.21	0.41
2:B:658:VAL:HG23	2:B:671:VAL:HG22	2.03	0.41
3:C:289:PRO:O	3:C:424:PRO:HG3	2.21	0.41
3:Z:257:ILE:CG1	3:Z:312:LEU:HG	2.51	0.41
3:Z:98:PRO:HB2	3:Z:350:VAL:HG22	2.02	0.41
1:A:487:ASP:CG	1:A:488:ASP:N	2.73	0.40
1:A:512:ILE:O	1:A:513:LEU:HD12	2.19	0.40
2:B:40:GLU:HB3	2:B:42:TYR:CE1	2.56	0.40
2:B:624:SER:O	2:B:625:ASP:CB	2.69	0.40
3:C:426:ILE:HG13	3:C:429:THR:HB	2.03	0.40
3:C:60:LEU:HB3	3:C:64:MET:CE	2.51	0.40
1:X:503:ARG:HB2	1:X:503:ARG:CZ	2.51	0.40
3:Z:373:ARG:HB3	3:Z:374:PRO:CD	2.50	0.40
3:Z:49:PHE:C	3:Z:49:PHE:CD1	2.94	0.40
1:A:447:LYS:HG2	1:A:447:LYS:O	2.20	0.40
1:A:469:GLN:O	1:A:470:LEU:HD23	2.22	0.40
1:A:551:VAL:HG12	1:A:552:LEU:N	2.36	0.40
2:Y:1044:SER:OG	2:Y:1047:TRP:HD1	2.04	0.40
2:Y:588:PRO:HA	2:Y:606:LEU:HD23	2.03	0.40
2:Y:922:LEU:HD13	2:Y:965:PHE:CD1	2.56	0.40
2:Y:1003:PHE:CG	3:Z:197:VAL:HG23	2.57	0.40
1:A:443:PRO:HA	1:A:517:ILE:CG2	2.49	0.40
2:B:457:THR:HG23	2:B:470:GLN:HG3	2.04	0.40
2:B:616:LEU:HA	2:B:616:LEU:HD12	1.91	0.40
2:Y:155:PHE:C	2:Y:155:PHE:CD1	2.94	0.40
2:Y:452:VAL:HG12	2:Y:470:GLN:NE2	2.37	0.40
2:Y:791:LEU:HD12	2:Y:792:LEU:N	2.36	0.40
2:B:1072:PHE:HD1	2:B:1072:PHE:C	2.24	0.40
2:B:322:VAL:CG2	2:B:336:LEU:HD21	2.51	0.40
2:B:928:ARG:HG3	2:B:928:ARG:O	2.20	0.40
3:C:345:PRO:O	3:C:360:LEU:HA	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:410:LEU:C	2:Y:411:TRP:CD2	2.95	0.40
2:Y:594:THR:OG1	2:Y:595:THR:N	2.55	0.40
2:B:1115:ASP:CG	2:B:1115:ASP:O	2.60	0.40
2:B:172:GLY:CA	2:B:224:GLU:CD	2.90	0.40
2:B:430:VAL:HA	2:B:456:GLN:NE2	2.36	0.40
2:B:502:SER:HB3	2:B:541:LEU:HB2	2.04	0.40
2:B:872:SER:OG	2:B:914:LEU:HB2	2.22	0.40
2:B:931:LEU:HD11	2:B:947:ARG:NH2	2.36	0.40
3:C:338:PHE:HE2	3:C:340:LEU:HG	1.87	0.40
3:C:351:ASN:HB2	3:C:352:PRO:HD2	2.03	0.40
1:X:606:PHE:HE2	1:X:628:LYS:CG	2.17	0.40
2:Y:1048:TYR:HD1	2:Y:1089:ILE:CD1	2.33	0.40
2:Y:169:PHE:CD1	2:Y:178:ILE:HG22	2.57	0.40
2:Y:171:TYR:CD2	2:Y:223:PRO:HA	2.56	0.40
2:Y:215:GLU:HB3	2:Y:234:GLN:HG2	2.04	0.40
2:Y:322:VAL:CG2	2:Y:336:LEU:HD21	2.51	0.40
2:Y:378:CYS:SG	2:Y:724:ILE:HB	2.61	0.40
2:Y:59:GLY:HA2	2:Y:1073:TRP:CE3	2.54	0.40

All (2) 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)
3:Z:103:HIS:CD2	1:A:542:SER:OG[2_546]	2.05	0.15
3:Z:116:LYS:CB	1:A:448:TYR:CB[1_544]	2.18	0.02

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	194/199 (98%)	155 (80%)	30 (16%)	9 (5%)	3 31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	193/199 (97%)	152 (79%)	33 (17%)	8 (4%)	3	34
2	B	1039/1140 (91%)	955 (92%)	76 (7%)	8 (1%)	24	69
2	Y	1046/1140 (92%)	959 (92%)	78 (8%)	9 (1%)	21	67
3	C	360/406 (89%)	322 (89%)	32 (9%)	6 (2%)	11	55
3	Z	372/406 (92%)	332 (89%)	37 (10%)	3 (1%)	24	69
All	All	3204/3490 (92%)	2875 (90%)	286 (9%)	43 (1%)	15	60

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	474	PRO
1	X	610	PRO
2	Y	224	GLU
2	Y	358	PRO
2	Y	483	PRO
2	Y	572	PRO
3	Z	411	PRO
2	B	224	GLU
2	B	358	PRO
2	B	483	PRO
2	B	572	PRO
3	C	116	LYS
3	C	118	ARG
3	C	411	PRO
3	C	427	PRO
1	A	473	MET
1	A	610	PRO
1	X	473	MET
2	Y	225	PRO
2	Y	513	GLY
2	B	225	PRO
2	B	513	GLY
3	Z	195	SER
3	Z	265	ASP
3	C	195	SER
1	A	450	ASP
1	X	582	PRO
1	X	598	ALA
2	Y	371	GLY
2	B	579	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	MET
1	A	540	HIS
1	A	582	PRO
2	Y	543	ILE
2	Y	1015	GLN
1	A	598	ALA
1	X	584	PHE
3	C	377	GLU
1	A	558	ILE
2	B	543	ILE
1	X	558	ILE
1	X	479	VAL
1	A	479	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	153/175 (87%)	113 (74%)	40 (26%)	0	5
1	X	165/175 (94%)	117 (71%)	48 (29%)	0	4
2	B	855/999 (86%)	699 (82%)	156 (18%)	2	14
2	Y	868/999 (87%)	709 (82%)	159 (18%)	2	14
3	C	306/368 (83%)	240 (78%)	66 (22%)	1	9
3	Z	316/368 (86%)	247 (78%)	69 (22%)	1	9
All	All	2663/3084 (86%)	2125 (80%)	538 (20%)	1	11

All (538) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	440	ILE
1	X	441	ARG
1	X	447	LYS
1	X	449	LYS
1	X	450	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	455	VAL
1	X	456	LEU
1	X	459	LEU
1	X	473	MET
1	X	476	LYS
1	X	485	LEU
1	X	490	GLU
1	X	492	ASP
1	X	500	LEU
1	X	505	LYS
1	X	510	GLU
1	X	513	LEU
1	X	517	ILE
1	X	524	LEU
1	X	527	SER
1	X	529	ARG
1	X	535	ILE
1	X	543	ILE
1	X	544	ILE
1	X	545	CYS
1	X	552	LEU
1	X	558	ILE
1	X	566	LEU
1	X	568	CYS
1	X	570	VAL
1	X	571	ASP
1	X	579	LYS
1	X	580	THR
1	X	581	ARG
1	X	588	ASP
1	X	592	ILE
1	X	594	ARG
1	X	600	THR
1	X	602	CYS
1	X	606	PHE
1	X	609	PHE
1	X	611	GLN
1	X	612	MET
1	X	614	ARG
1	X	616	THR
1	X	618	ARG
1	X	626	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	629	VAL
2	Y	20	THR
2	Y	37	THR
2	Y	54	GLU
2	Y	67	PHE
2	Y	70	LYS
2	Y	81	THR
2	Y	92	LYS
2	Y	97	SER
2	Y	108	VAL
2	Y	110	ASP
2	Y	125	ASP
2	Y	134	ARG
2	Y	143	ILE
2	Y	147	ARG
2	Y	197	LEU
2	Y	200	LYS
2	Y	201	GLU
2	Y	204	LYS
2	Y	208	LYS
2	Y	213	GLU
2	Y	226	PHE
2	Y	232	ILE
2	Y	235	GLU
2	Y	245	TYR
2	Y	253	ILE
2	Y	262	ASN
2	Y	269	SER
2	Y	277	GLU
2	Y	299	ASP
2	Y	304	LEU
2	Y	305	LEU
2	Y	309	SER
2	Y	310	ILE
2	Y	318	ASP
2	Y	321	VAL
2	Y	335	LYS
2	Y	336	LEU
2	Y	354	THR
2	Y	360	VAL
2	Y	377	THR
2	Y	396	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	407	ILE
2	Y	410	LEU
2	Y	414	ARG
2	Y	420	GLU
2	Y	421	THR
2	Y	427	LEU
2	Y	428	SER
2	Y	429	PHE
2	Y	432	GLN
2	Y	437	MET
2	Y	454	ASP
2	Y	463	VAL
2	Y	466	GLN
2	Y	468	LEU
2	Y	473	SER
2	Y	477	ARG
2	Y	488	SER
2	Y	492	GLU
2	Y	505	SER
2	Y	510	VAL
2	Y	514	ARG
2	Y	517	TYR
2	Y	519	LEU
2	Y	524	GLN
2	Y	526	LEU
2	Y	532	THR
2	Y	533	GLU
2	Y	534	MET
2	Y	555	LEU
2	Y	560	LEU
2	Y	561	TRP
2	Y	562	THR
2	Y	571	LEU
2	Y	582	LEU
2	Y	586	ILE
2	Y	595	THR
2	Y	602	LEU
2	Y	611	LEU
2	Y	618	ILE
2	Y	624	SER
2	Y	625	ASP
2	Y	630	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	636	THR
2	Y	647	THR
2	Y	653	SER
2	Y	657	THR
2	Y	660	TYR
2	Y	663	ASN
2	Y	672	ASN
2	Y	673	LEU
2	Y	676	VAL
2	Y	697	SER
2	Y	698	THR
2	Y	699	LEU
2	Y	700	THR
2	Y	705	ASP
2	Y	709	LYS
2	Y	729	VAL
2	Y	742	VAL
2	Y	749	THR
2	Y	750	THR
2	Y	752	LEU
2	Y	753	ARG
2	Y	755	SER
2	Y	763	SER
2	Y	764	SER
2	Y	766	SER
2	Y	767	SER
2	Y	786	VAL
2	Y	796	GLN
2	Y	818	SER
2	Y	823	LYS
2	Y	839	GLU
2	Y	840	GLU
2	Y	842	GLU
2	Y	844	LYS
2	Y	845	GLN
2	Y	854	SER
2	Y	860	THR
2	Y	864	LYS
2	Y	874	VAL
2	Y	886	SER
2	Y	889	ARG
2	Y	895	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	898	GLU
2	Y	900	ARG
2	Y	903	CYS
2	Y	904	ASN
2	Y	906	TYR
2	Y	908	ASN
2	Y	914	LEU
2	Y	916	THR
2	Y	919	ASP
2	Y	927	MET
2	Y	933	LEU
2	Y	947	ARG
2	Y	950	ASN
2	Y	957	VAL
2	Y	962	ASP
2	Y	987	GLU
2	Y	990	GLN
2	Y	1006	VAL
2	Y	1008	CYS
2	Y	1011	SER
2	Y	1012	LEU
2	Y	1052	LEU
2	Y	1064	SER
2	Y	1071	SER
2	Y	1072	PHE
2	Y	1096	SER
2	Y	1100	ILE
2	Y	1106	GLN
2	Y	1115	ASP
2	Y	1116	ASP
2	Y	1122	ARG
2	Y	1125	THR
2	Y	1131	LYS
2	Y	1137	THR
3	Z	49	PHE
3	Z	51	THR
3	Z	58	THR
3	Z	64	MET
3	Z	70	ARG
3	Z	71	THR
3	Z	74	ASP
3	Z	75	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Z	84	LEU
3	Z	88	MET
3	Z	89	MET
3	Z	91	LEU
3	Z	96	THR
3	Z	98	PRO
3	Z	105	GLN
3	Z	109	MET
3	Z	111	ARG
3	Z	145	ARG
3	Z	152	ILE
3	Z	156	LYS
3	Z	171	ARG
3	Z	172	THR
3	Z	177	ILE
3	Z	179	GLN
3	Z	182	VAL
3	Z	189	VAL
3	Z	193	THR
3	Z	197	VAL
3	Z	206	GLN
3	Z	210	SER
3	Z	221	TYR
3	Z	225	GLN
3	Z	237	LEU
3	Z	238	THR
3	Z	240	TRP
3	Z	244	LEU
3	Z	246	SER
3	Z	255	ASP
3	Z	260	GLN
3	Z	272	SER
3	Z	273	LEU
3	Z	291	ASP
3	Z	293	VAL
3	Z	294	LEU
3	Z	296	ILE
3	Z	297	GLN
3	Z	298	LEU
3	Z	310	CYS
3	Z	320	SER
3	Z	324	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Z	325	GLN
3	Z	332	THR
3	Z	333	THR
3	Z	339	SER
3	Z	350	VAL
3	Z	356	VAL
3	Z	361	THR
3	Z	370	LEU
3	Z	373	ARG
3	Z	376	THR
3	Z	387	THR
3	Z	390	GLN
3	Z	393	ILE
3	Z	401	LYS
3	Z	407	LYS
3	Z	419	ARG
3	Z	428	ASP
3	Z	429	THR
3	Z	431	ASP
2	B	20	THR
2	B	37	THR
2	B	54	GLU
2	B	67	PHE
2	B	70	LYS
2	B	81	THR
2	B	97	SER
2	B	108	VAL
2	B	110	ASP
2	B	125	ASP
2	B	134	ARG
2	B	143	ILE
2	B	197	LEU
2	B	200	LYS
2	B	201	GLU
2	B	226	PHE
2	B	232	ILE
2	B	245	TYR
2	B	253	ILE
2	B	262	ASN
2	B	269	SER
2	B	299	ASP
2	B	304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	305	LEU
2	B	309	SER
2	B	310	ILE
2	B	318	ASP
2	B	321	VAL
2	B	335	LYS
2	B	336	LEU
2	B	354	THR
2	B	360	VAL
2	B	377	THR
2	B	396	ILE
2	B	407	ILE
2	B	410	LEU
2	B	414	ARG
2	B	420	GLU
2	B	421	THR
2	B	427	LEU
2	B	428	SER
2	B	429	PHE
2	B	432	GLN
2	B	437	MET
2	B	454	ASP
2	B	463	VAL
2	B	466	GLN
2	B	468	LEU
2	B	477	ARG
2	B	482	GLU
2	B	488	SER
2	B	492	GLU
2	B	505	SER
2	B	510	VAL
2	B	514	ARG
2	B	517	TYR
2	B	519	LEU
2	B	524	GLN
2	B	526	LEU
2	B	527	ARG
2	B	532	THR
2	B	533	GLU
2	B	534	MET
2	B	555	LEU
2	B	560	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	561	TRP
2	B	562	THR
2	B	571	LEU
2	B	579	LYS
2	B	582	LEU
2	B	586	ILE
2	B	595	THR
2	B	598	SER
2	B	602	LEU
2	B	611	LEU
2	B	618	ILE
2	B	630	THR
2	B	636	THR
2	B	647	THR
2	B	653	SER
2	B	657	THR
2	B	660	TYR
2	B	663	ASN
2	B	672	ASN
2	B	673	LEU
2	B	676	VAL
2	B	697	SER
2	B	698	THR
2	B	700	THR
2	B	709	LYS
2	B	713	ARG
2	B	722	ARG
2	B	729	VAL
2	B	732	CYS
2	B	742	VAL
2	B	750	THR
2	B	752	LEU
2	B	753	ARG
2	B	755	SER
2	B	763	SER
2	B	764	SER
2	B	768	SER
2	B	786	VAL
2	B	796	GLN
2	B	808	LEU
2	B	814	LEU
2	B	818	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	823	LYS
2	B	839	GLU
2	B	840	GLU
2	B	842	GLU
2	B	844	LYS
2	B	845	GLN
2	B	854	SER
2	B	860	THR
2	B	864	LYS
2	B	874	VAL
2	B	886	SER
2	B	889	ARG
2	B	895	THR
2	B	898	GLU
2	B	900	ARG
2	B	903	CYS
2	B	904	ASN
2	B	907	ASN
2	B	908	ASN
2	B	909	ILE
2	B	914	LEU
2	B	916	THR
2	B	919	ASP
2	B	927	MET
2	B	933	LEU
2	B	947	ARG
2	B	950	ASN
2	B	957	VAL
2	B	962	ASP
2	B	987	GLU
2	B	990	GLN
2	B	1006	VAL
2	B	1008	CYS
2	B	1011	SER
2	B	1012	LEU
2	B	1013	VAL
2	B	1052	LEU
2	B	1064	SER
2	B	1071	SER
2	B	1072	PHE
2	B	1096	SER
2	B	1100	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1106	GLN
2	B	1115	ASP
2	B	1116	ASP
2	B	1122	ARG
2	B	1125	THR
2	B	1131	LYS
2	B	1137	THR
3	C	49	PHE
3	C	51	THR
3	C	58	THR
3	C	71	THR
3	C	75	ASP
3	C	84	LEU
3	C	88	MET
3	C	89	MET
3	C	91	LEU
3	C	96	THR
3	C	105	GLN
3	C	109	MET
3	C	111	ARG
3	C	115	GLN
3	C	128	VAL
3	C	145	ARG
3	C	148	GLN
3	C	149	ASP
3	C	169	GLU
3	C	171	ARG
3	C	172	THR
3	C	177	ILE
3	C	179	GLN
3	C	182	VAL
3	C	189	VAL
3	C	193	THR
3	C	197	VAL
3	C	206	GLN
3	C	210	SER
3	C	221	TYR
3	C	237	LEU
3	C	238	THR
3	C	240	TRP
3	C	244	LEU
3	C	246	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	255	ASP
3	C	260	GLN
3	C	265	ASP
3	C	272	SER
3	C	273	LEU
3	C	291	ASP
3	C	293	VAL
3	C	294	LEU
3	C	297	GLN
3	C	298	LEU
3	C	299	LEU
3	C	310	CYS
3	C	320	SER
3	C	324	LYS
3	C	325	GLN
3	C	332	THR
3	C	333	THR
3	C	350	VAL
3	C	356	VAL
3	C	361	THR
3	C	370	LEU
3	C	373	ARG
3	C	376	THR
3	C	387	THR
3	C	390	GLN
3	C	393	ILE
3	C	401	LYS
3	C	407	LYS
3	C	419	ARG
3	C	426	ILE
3	C	442	LEU
1	A	440	ILE
1	A	447	LYS
1	A	449	LYS
1	A	455	VAL
1	A	456	LEU
1	A	459	LEU
1	A	485	LEU
1	A	492	ASP
1	A	500	LEU
1	A	503	ARG
1	A	505	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	510	GLU
1	A	517	ILE
1	A	524	LEU
1	A	535	ILE
1	A	536	VAL
1	A	552	LEU
1	A	554	ILE
1	A	557	CYS
1	A	558	ILE
1	A	566	LEU
1	A	568	CYS
1	A	570	VAL
1	A	571	ASP
1	A	579	LYS
1	A	580	THR
1	A	585	VAL
1	A	592	ILE
1	A	594	ARG
1	A	600	THR
1	A	602	CYS
1	A	605	THR
1	A	606	PHE
1	A	611	GLN
1	A	612	MET
1	A	616	THR
1	A	618	ARG
1	A	622	LYS
1	A	626	ILE
1	A	629	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	540	HIS
1	X	555	HIS
2	Y	30	ASN
2	Y	36	ASN
2	Y	156	ASN
2	Y	255	GLN
2	Y	267	ASN
2	Y	432	GLN
2	Y	439	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	456	GLN
2	Y	462	ASN
2	Y	467	GLN
2	Y	470	GLN
2	Y	663	ASN
2	Y	672	ASN
2	Y	796	GLN
2	Y	803	HIS
2	Y	805	HIS
2	Y	852	GLN
2	Y	885	ASN
2	Y	950	ASN
2	Y	990	GLN
2	Y	999	HIS
2	Y	1034	ASN
2	Y	1055	GLN
2	Y	1056	ASN
2	Y	1070	HIS
3	Z	86	GLN
3	Z	95	GLN
3	Z	112	ASN
3	Z	115	GLN
3	Z	163	GLN
3	Z	179	GLN
3	Z	198	GLN
3	Z	260	GLN
2	B	16	ASN
2	B	30	ASN
2	B	36	ASN
2	B	156	ASN
2	B	183	GLN
2	B	255	GLN
2	B	267	ASN
2	B	397	HIS
2	B	439	ASN
2	B	456	GLN
2	B	462	ASN
2	B	467	GLN
2	B	470	GLN
2	B	520	GLN
2	B	536	HIS
2	B	663	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	672	ASN
2	B	796	GLN
2	B	803	HIS
2	B	805	HIS
2	B	852	GLN
2	B	885	ASN
2	B	950	ASN
2	B	990	GLN
2	B	999	HIS
2	B	1034	ASN
2	B	1055	GLN
2	B	1056	ASN
2	B	1070	HIS
3	C	86	GLN
3	C	95	GLN
3	C	112	ASN
3	C	115	GLN
3	C	127	ASN
3	C	163	GLN
3	C	179	GLN
3	C	198	GLN
3	C	260	GLN
1	A	611	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	85C	C	502	-	34,34,34	1.53	4 (11%)	46,49,49	2.53	13 (28%)
5	85C	Z	502	-	34,34,34	1.51	4 (11%)	46,49,49	2.51	11 (23%)

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
5	85C	C	502	-	-	0/13/38/38	0/4/4/4
5	85C	Z	502	-	-	0/13/38/38	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	85C	C5-C8	-5.75	1.39	1.48
5	Z	502	85C	C5-C8	-5.32	1.40	1.48
5	Z	502	85C	C16-N4	-4.58	1.33	1.41
5	C	502	85C	C16-N4	-4.26	1.33	1.41
5	C	502	85C	C8-N1	-2.99	1.32	1.36
5	Z	502	85C	C8-N1	-2.70	1.33	1.36
5	C	502	85C	C15-N4	-2.29	1.33	1.37
5	Z	502	85C	C15-N4	-2.11	1.33	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	85C	C7-N1-C8	-9.77	109.76	113.03
5	Z	502	85C	C7-N1-C8	-8.76	110.09	113.03
5	C	502	85C	C7-C6-C5	-4.16	107.03	109.71
5	Z	502	85C	C7-C6-C5	-3.38	107.53	109.71
5	Z	502	85C	C16-N4-C15	-3.33	120.07	126.65
5	C	502	85C	C16-N4-C15	-3.18	120.36	126.65
5	Z	502	85C	C12-N2-C13	-2.99	121.03	126.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	85C	C12-N2-C13	-2.95	121.11	126.28
5	C	502	85C	C17-C18-C19	-2.84	119.61	122.72
5	C	502	85C	O1-C8-C5	-2.83	123.14	128.70
5	C	502	85C	C10-C11-C12	-2.31	110.01	114.34
5	C	502	85C	O1-C8-N1	-2.28	123.57	125.17
5	Z	502	85C	C17-C18-C19	-2.25	120.26	122.72
5	Z	502	85C	O1-C8-C5	-2.22	124.33	128.70
5	Z	502	85C	C2-C14-N3	-2.17	108.25	112.98
5	C	502	85C	C10-C9-N1	-2.01	109.07	112.23
5	C	502	85C	C11-C12-N2	2.85	119.63	116.62
5	Z	502	85C	C20-C19-C18	3.04	120.03	116.22
5	Z	502	85C	C11-C12-N2	3.27	120.08	116.62
5	C	502	85C	C20-C19-C18	3.34	120.41	116.22
5	C	502	85C	C9-C13-N2	4.41	121.46	116.50
5	Z	502	85C	C9-C13-N2	4.94	122.06	116.50
5	C	502	85C	C5-C8-N1	8.05	110.93	106.48
5	Z	502	85C	C5-C8-N1	9.30	111.63	106.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	85C	4	0
5	Z	502	85C	10	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	196/199 (98%)	-0.08	3 (1%) 76 64	56, 112, 160, 183	0
1	X	195/199 (97%)	-0.09	3 (1%) 76 64	66, 109, 160, 185	0
2	B	1075/1140 (94%)	-0.15	11 (1%) 84 73	60, 114, 185, 240	5 (0%)
2	Y	1080/1140 (94%)	-0.18	9 (0%) 87 78	54, 113, 174, 221	5 (0%)
3	C	370/406 (91%)	-0.22	6 (1%) 74 61	63, 111, 165, 225	0
3	Z	380/406 (93%)	-0.25	1 (0%) 94 90	64, 109, 169, 213	0
All	All	3296/3490 (94%)	-0.17	33 (1%) 84 73	54, 112, 174, 240	10 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	566	ALA	5.2
2	B	103	ARG	3.9
2	Y	179	CYS	3.8
2	B	16	ASN	3.3
2	B	88	ILE	3.3
2	Y	566	ALA	3.3
2	Y	148	ASP	3.1
1	A	504	LEU	2.8
2	B	72	GLU	2.8
1	A	602	CYS	2.8
2	B	980	ASP	2.8
1	X	504	LEU	2.6
2	Y	306	GLY	2.6
3	C	424	PRO	2.5
2	Y	943	GLU	2.4
2	B	104	ALA	2.4
2	B	221	ALA	2.4
3	C	54	PRO	2.4
2	Y	178	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	441	ARG	2.4
3	C	320	SER	2.4
3	C	318	CYS	2.3
2	B	102	THR	2.3
1	X	519	CYS	2.2
3	C	155	VAL	2.2
1	X	518	LEU	2.2
3	Z	49	PHE	2.1
2	Y	166	ASP	2.1
2	Y	315	THR	2.1
3	C	195	SER	2.0
2	Y	103	ARG	2.0
2	B	214	ALA	2.0
2	B	632	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	85C	C	502	31/31	0.93	0.30	0.56	61,90,177,227	0
5	85C	Z	502	31/31	0.94	0.29	0.56	70,95,210,235	0
4	ZN	C	501	1/1	0.98	0.14	-0.23	187,187,187,187	0
4	ZN	Z	501	1/1	0.98	0.14	-0.62	191,191,191,191	0

6.5 Other polymers

There are no such residues in this entry.