



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 PM GMT

PDB ID : 4K17
Title : Crystal Structure of mouse CARMIL residues 1-668
Authors : Zwolak, A.; Dominguez, R.
Deposited on : 2013-04-04
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

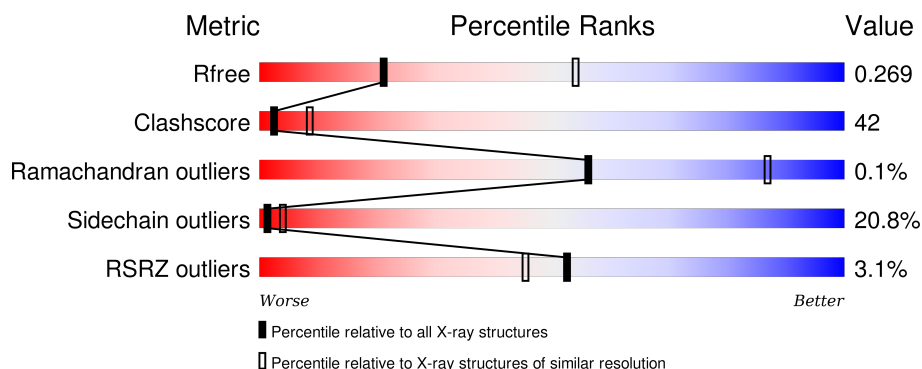
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 ≥ 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	669	<div> <div>2%</div> <div>47% 41% 10% ..</div> </div>
1	B	669	<div> <div>2%</div> <div>48% 39% 11% ..</div> </div>
1	C	669	<div> <div>%</div> <div>42% 46% 10% ..</div> </div>
1	D	669	<div> <div>7%</div> <div>42% 42% 14% ..</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
2	OHB	B	701	-	-	-	X
3	CL	B	702	-	-	X	-
4	ABU	C	701	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20371 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.

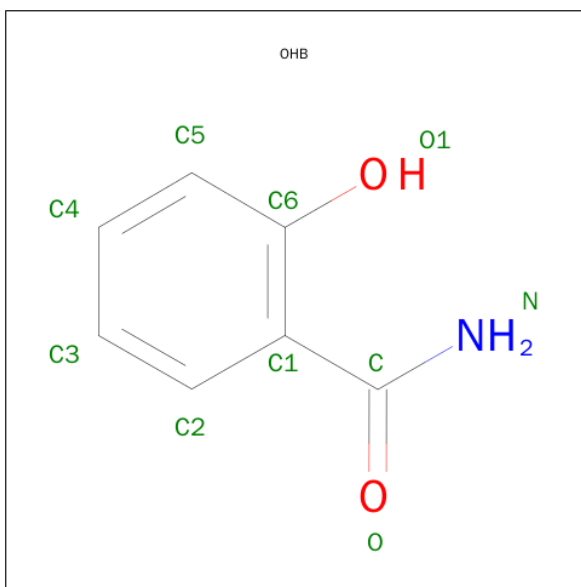
- Molecule 1 is a protein called Leucine-rich repeat-containing protein 16A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	Se	0	2	0
			5112	3220	888	969	17	18			
1	B	660	Total	C	N	O	S	Se	0	0	0
			5102	3211	884	973	16	18			
1	C	656	Total	C	N	O	S	Se	0	0	0
			5073	3196	880	963	16	18			
1	D	655	Total	C	N	O	S	Se	0	0	0
			5066	3191	879	962	16	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q6EDY6
B	0	SER	-	EXPRESSION TAG	UNP Q6EDY6
C	0	SER	-	EXPRESSION TAG	UNP Q6EDY6
D	0	SER	-	EXPRESSION TAG	UNP Q6EDY6

- Molecule 2 is SALICYLAMIDE (three-letter code: OHB) (formula: C₇H₇NO₂).

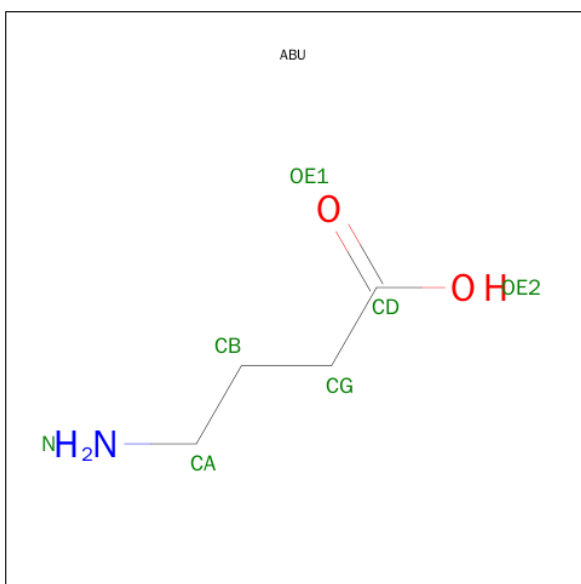


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: C₄H₉NO₂).

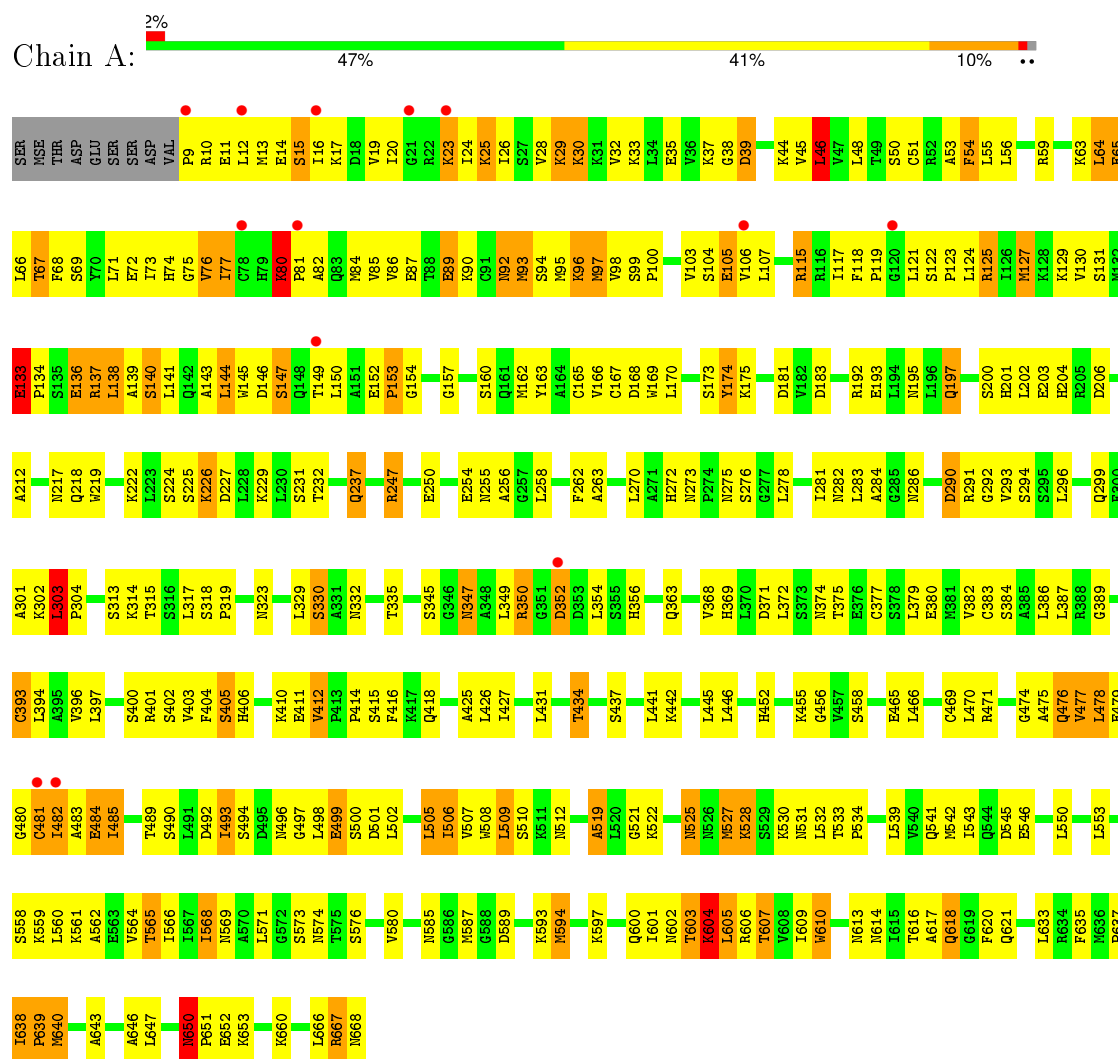


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			7	4	1	2		

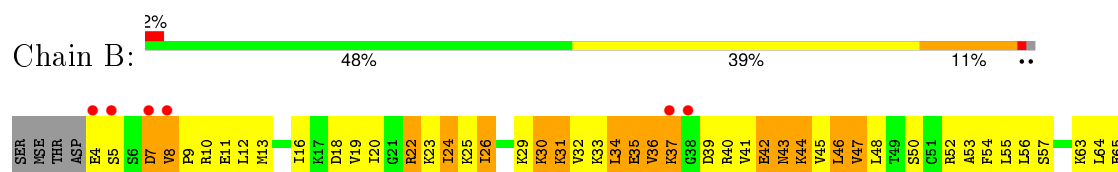
3 Residue-property plots

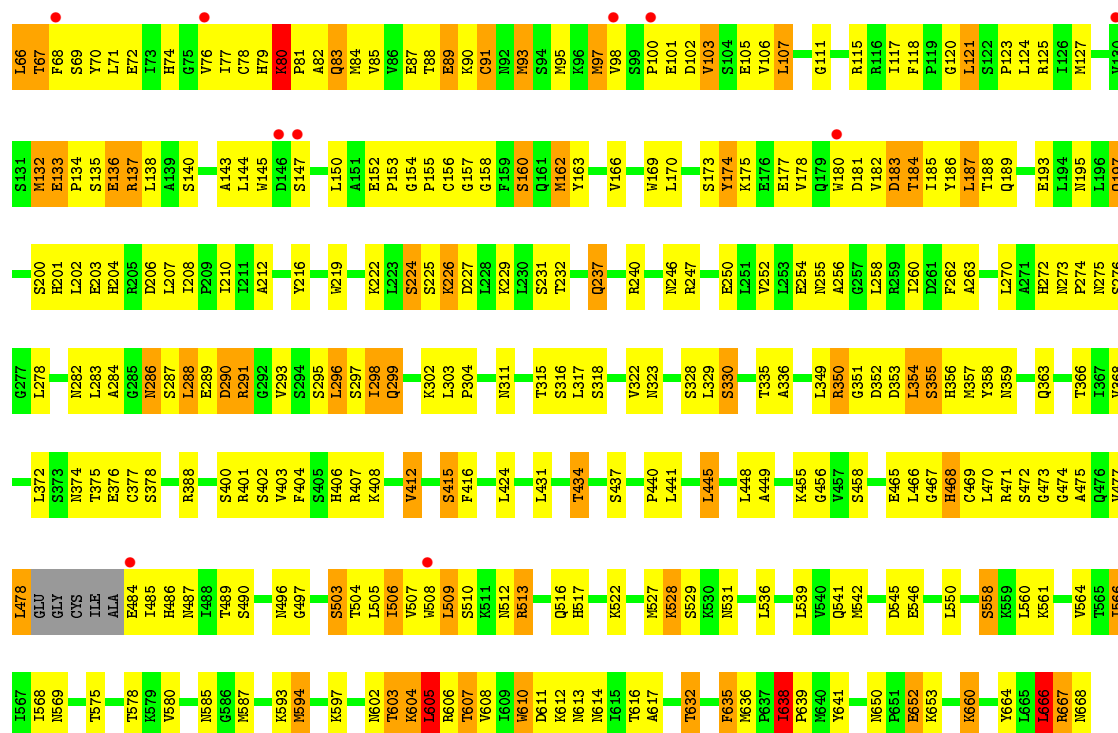
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

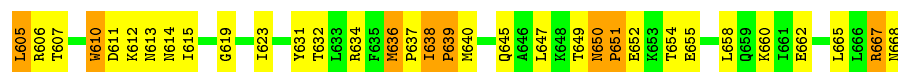
- Molecule 1: Leucine-rich repeat-containing protein 16A



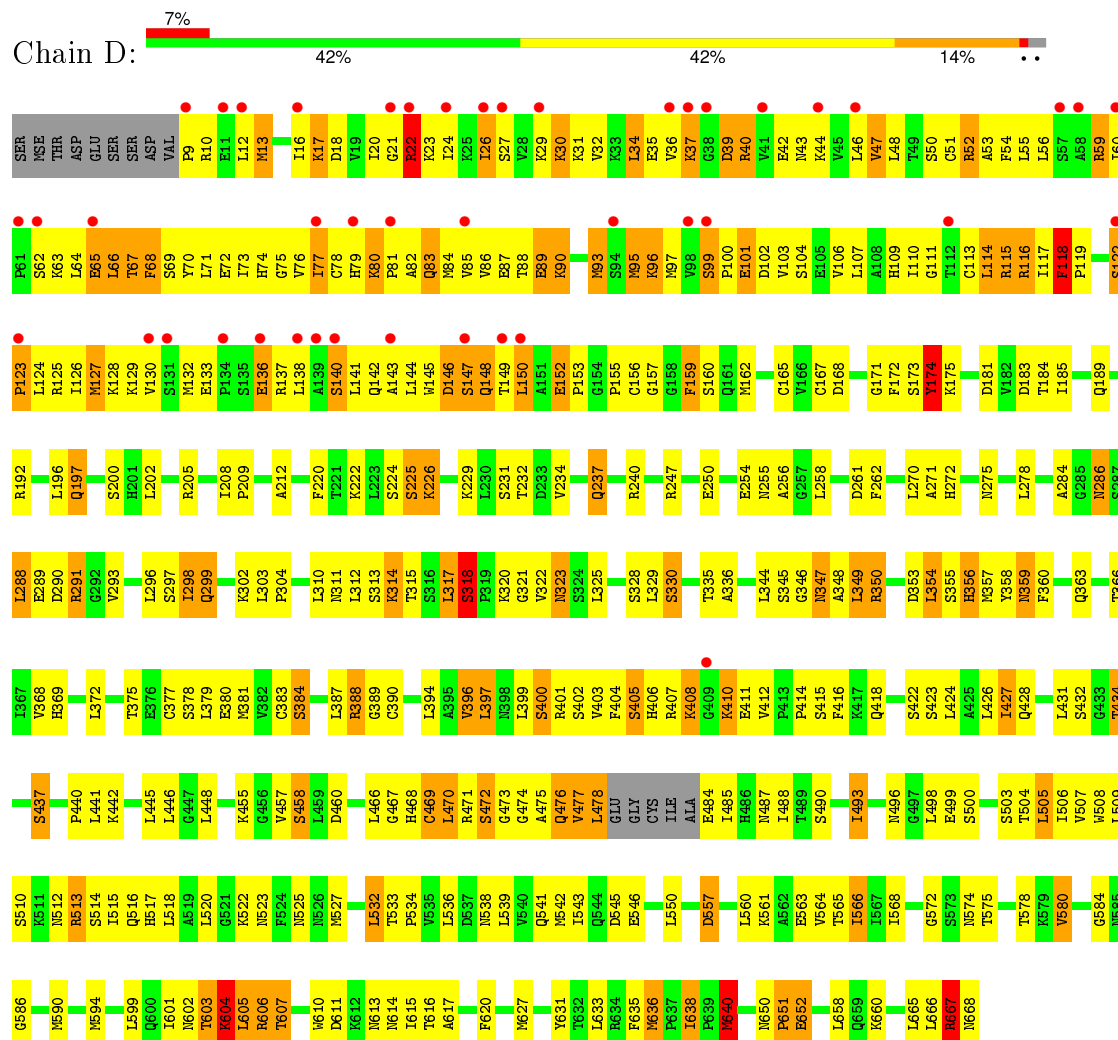
- Molecule 1: Leucine-rich repeat-containing protein 16A







• Molecule 1: Leucine-rich repeat-containing protein 16A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.17Å 67.99Å 212.15Å 92.73° 96.95° 110.15°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.4 (49.76-2.90) 66.5 (49.76-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.259 0.219 , 0.269	Depositor DCC
R_{free} test set	1913 reflections (3.47%)	DCC
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 45379 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20371	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ABU, OHB, CL

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	1.09	5/5179 (0.1%)	0.99	15/6967 (0.2%)
1	B	1.03	5/5160 (0.1%)	0.98	15/6941 (0.2%)
1	C	0.99	5/5131 (0.1%)	0.96	12/6902 (0.2%)
1	D	0.87	5/5124 (0.1%)	1.08	26/6891 (0.4%)
All	All	1.00	20/20594 (0.1%)	1.01	68/27701 (0.2%)

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	3
1	C	0	3
All	All	0	6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	666	LEU	CG-CD1	-6.07	1.29	1.51
1	D	174	TYR	CE2-CZ	-5.92	1.30	1.38
1	A	519	ALA	CA-CB	-5.77	1.40	1.52
1	B	605	LEU	CG-CD1	-5.72	1.30	1.51
1	A	237	GLN	CD-NE2	-5.55	1.19	1.32
1	C	580	VAL	CB-CG2	-5.51	1.41	1.52
1	C	61	PRO	N-CD	5.40	1.55	1.47
1	C	165	CYS	CB-SG	-5.40	1.73	1.81
1	B	641	TYR	CE1-CZ	-5.32	1.31	1.38
1	B	153	PRO	N-CD	5.31	1.55	1.47
1	A	639	PRO	N-CD	5.29	1.55	1.47
1	D	167	CYS	CB-SG	-5.29	1.73	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	123	PRO	N-CD	5.24	1.55	1.47
1	D	119	PRO	N-CD	5.09	1.54	1.47
1	D	651	PRO	N-CD	5.08	1.54	1.47
1	A	153	PRO	N-CD	5.08	1.54	1.47
1	B	605	LEU	CG-CD2	-5.05	1.33	1.51
1	A	281	ILE	CA-CB	-5.05	1.43	1.54
1	C	174	TYR	CE1-CZ	-5.03	1.32	1.38
1	C	164	ALA	CA-CB	-5.03	1.41	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	ARG	NE-CZ-NH2	-23.32	108.64	120.30
1	D	192	ARG	NE-CZ-NH1	-18.59	111.01	120.30
1	D	192	ARG	NE-CZ-NH2	18.24	129.42	120.30
1	D	22	ARG	NE-CZ-NH1	16.50	128.55	120.30
1	D	17	LYS	CD-CE-NZ	8.39	131.00	111.70
1	A	527	MSE	N-CA-CB	-8.29	95.68	110.60
1	D	192	ARG	CD-NE-CZ	7.83	134.56	123.60
1	D	640	MSE	CB-CG-SE	-7.42	90.43	112.70
1	A	455	LYS	CD-CE-NZ	7.38	128.67	111.70
1	D	23	LYS	CD-CE-NZ	6.76	127.24	111.70
1	B	351	GLY	N-CA-C	-6.74	96.25	113.10
1	D	640	MSE	CB-CA-C	-6.66	97.07	110.40
1	C	638	ILE	C-N-CD	6.25	141.53	128.40
1	D	240	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	22	ARG	CD-NE-CZ	6.19	132.27	123.60
1	D	640	MSE	CA-CB-CG	-6.19	102.78	113.30
1	C	650	ASN	C-N-CD	6.17	141.35	128.40
1	A	133	GLU	C-N-CD	6.16	141.34	128.40
1	B	650	ASN	C-N-CD	6.08	141.17	128.40
1	A	154	GLY	C-N-CD	6.06	141.12	128.40
1	B	80	LYS	C-N-CD	6.05	141.11	128.40
1	B	240	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	8	VAL	C-N-CD	6.04	141.08	128.40
1	A	650	ASN	C-N-CD	6.01	141.03	128.40
1	C	154	GLY	C-N-CD	5.99	140.98	128.40
1	B	154	GLY	C-N-CD	5.97	140.93	128.40
1	A	604	LYS	N-CA-C	5.95	127.06	111.00
1	B	636	MSE	C-N-CD	5.93	140.86	128.40
1	D	318	SER	C-N-CD	5.92	140.84	128.40
1	A	303	LEU	C-N-CD	5.91	140.82	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	ILE	C-N-CD	5.91	140.82	128.40
1	D	636	MSE	C-N-CD	5.89	140.76	128.40
1	C	636	MSE	C-N-CD	5.87	140.73	128.40
1	D	314	LYS	CD-CE-NZ	5.87	125.20	111.70
1	B	133	GLU	C-N-CD	5.86	140.71	128.40
1	A	80	LYS	C-N-CD	5.82	140.62	128.40
1	C	117	ILE	CB-CA-C	-5.80	100.00	111.60
1	C	133	GLU	C-N-CD	5.80	140.58	128.40
1	A	46	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	389	GLY	N-CA-C	5.77	127.54	113.10
1	D	557	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	118	PHE	C-N-CD	5.74	140.45	128.40
1	D	122	SER	C-N-CD	5.74	140.46	128.40
1	B	152	GLU	C-N-CD	5.74	140.45	128.40
1	B	132	MSE	N-CA-C	-5.73	95.53	111.00
1	C	240	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	118	PHE	C-N-CD	5.71	140.39	128.40
1	C	533	THR	C-N-CD	5.70	140.36	128.40
1	B	8	VAL	C-N-CD	5.68	140.32	128.40
1	D	118	PHE	C-N-CD	5.63	140.23	128.40
1	D	650	ASN	C-N-CD	5.62	140.20	128.40
1	B	473	GLY	N-CA-C	-5.54	99.26	113.10
1	A	638	ILE	C-N-CD	5.53	140.01	128.40
1	C	605	LEU	CA-CB-CG	5.51	127.97	115.30
1	D	317	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	D	389	GLY	N-CA-C	5.37	126.53	113.10
1	D	611	ASP	CB-CG-OD1	5.33	123.09	118.30
1	D	17	LYS	CG-CD-CE	5.31	127.84	111.90
1	D	60	ILE	C-N-CD	5.31	139.55	128.40
1	D	604	LYS	CA-CB-CG	5.23	124.91	113.40
1	B	296	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	666	LEU	CD1-CG-CD2	-5.11	95.17	110.50
1	A	455	LYS	CG-CD-CE	5.08	127.13	111.90
1	C	38	GLY	N-CA-C	-5.07	100.42	113.10
1	B	605	LEU	CB-CG-CD1	5.07	119.62	111.00
1	D	667	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	605	LEU	CA-CB-CG	5.02	126.85	115.30
1	A	393	CYS	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	LYS	Peptide
1	A	481	CYS	Peptide
1	A	525	ASN	Peptide
1	C	410	LYS	Peptide
1	C	604	LYS	Mainchain
1	C	651	PRO	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	5112	0	5253	411	1
1	B	5102	0	5239	368	1
1	C	5073	0	5217	458	3
1	D	5066	0	5213	515	3
2	B	10	0	7	2	0
3	B	1	0	0	3	1
4	C	7	0	5	0	0
All	All	20371	0	20934	1733	5

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 42.

All (1733) 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:C:478:LEU:HG	1:C:508:TRP:CZ2	1.28	1.59
1:B:350:ARG:HG3	1:B:406:HIS:CE1	1.35	1.57
1:D:258:LEU:HD23	1:D:262:PHE:CE2	1.44	1.53
1:B:54:PHE:CD1	1:B:67:THR:HG21	1.46	1.49
1:A:474:GLY:HA2	1:A:477:VAL:CG1	1.43	1.46
1:B:350:ARG:CG	1:B:406:HIS:CE1	1.97	1.46
1:C:478:LEU:CG	1:C:508:TRP:CZ2	1.97	1.45
1:C:350:ARG:HD3	1:C:406:HIS:CE1	1.53	1.41
1:B:484:GLU:HG2	1:B:508:TRP:NE1	1.23	1.40
1:C:350:ARG:HD3	1:C:406:HIS:ND1	1.41	1.35
1:A:319:PRO:HB2	1:A:352:ASP:CB	1.56	1.35

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PRO:CG	1:A:352:ASP:HB2	1.56	1.33
1:C:478:LEU:HG	1:C:508:TRP:CH2	1.62	1.33
1:C:65:GLU:O	1:C:66:LEU:HD23	1.21	1.31
1:D:499:GLU:C	1:D:527:MSE:CE	2.01	1.28
1:B:54:PHE:CD1	1:B:67:THR:CG2	2.15	1.28
1:A:319:PRO:CB	1:A:352:ASP:HB3	1.64	1.28
1:A:374:ASN:OD1	1:A:401:ARG:HD2	1.34	1.27
1:D:258:LEU:CD2	1:D:262:PHE:CE2	2.19	1.26
1:C:55:LEU:HD11	1:C:95:MSE:CE	1.66	1.25
1:D:145:TRP:HA	1:D:148:GLN:OE1	1.37	1.24
1:A:319:PRO:CB	1:A:352:ASP:CB	2.14	1.24
1:B:484:GLU:HG2	1:B:508:TRP:CD1	1.70	1.24
1:C:484:GLU:OE2	1:C:511:LYS:HB3	1.38	1.23
1:C:44:LYS:NZ	1:C:65:GLU:CD	1.92	1.22
1:A:9:PRO:CB	1:A:12:LEU:HD21	1.68	1.22
1:A:402:SER:O	1:A:434:THR:CG2	1.86	1.22
1:A:474:GLY:CA	1:A:477:VAL:HG12	1.69	1.22
1:C:477:VAL:O	1:C:508:TRP:CZ3	1.90	1.21
1:D:258:LEU:HD23	1:D:262:PHE:CD2	1.75	1.21
1:C:374:ASN:OD1	1:C:401:ARG:HG3	1.36	1.21
1:C:448:LEU:O	1:C:487:ASN:ND2	1.70	1.21
1:C:478:LEU:CB	1:C:508:TRP:CZ2	2.19	1.20
1:C:504:THR:O	1:C:507:VAL:HG22	1.41	1.20
1:C:350:ARG:CD	1:C:406:HIS:CE1	2.22	1.19
1:B:484:GLU:OE2	1:B:508:TRP:O	1.57	1.19
1:C:484:GLU:OE2	1:C:511:LYS:CB	1.88	1.19
1:B:484:GLU:CG	1:B:508:TRP:NE1	2.07	1.18
1:B:36:VAL:HG21	1:B:42:GLU:CG	1.72	1.17
1:A:9:PRO:HB2	1:A:12:LEU:HD21	1.17	1.17
1:A:349:LEU:HG	1:A:375:THR:OG1	1.44	1.16
1:D:136:GLU:O	1:D:140:SER:OG	1.63	1.16
1:A:484:GLU:HG3	1:A:508:TRP:NE1	1.59	1.16
1:C:478:LEU:CG	1:C:508:TRP:HZ2	1.46	1.14
1:D:349:LEU:CD1	1:D:357:MSE:HE1	1.76	1.13
1:D:499:GLU:HA	1:D:527:MSE:HE3	1.28	1.13
1:D:118:PHE:CD2	1:D:126:ILE:CD1	2.32	1.12
1:B:24:ILE:HD12	1:B:25:LYS:H	1.14	1.12
1:A:402:SER:O	1:A:434:THR:HG23	1.43	1.12
1:D:349:LEU:HB3	1:D:354:LEU:HD21	1.33	1.11
1:A:484:GLU:CG	1:A:508:TRP:HE1	1.62	1.11
1:A:485:ILE:HG22	1:A:512:ASN:HD22	1.12	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ILE:O	1:A:496:ASN:ND2	1.83	1.10
1:A:374:ASN:OD1	1:A:401:ARG:CD	1.99	1.09
1:D:144:LEU:O	1:D:148:GLN:OE1	1.71	1.09
1:A:484:GLU:HG3	1:A:508:TRP:HE1	0.95	1.09
1:C:474:GLY:HA2	1:C:475:ALA:CB	1.82	1.09
1:D:474:GLY:HA2	1:D:475:ALA:HB3	1.29	1.09
1:C:349:LEU:HG	1:C:375:THR:OG1	1.50	1.09
1:C:36:VAL:HG12	1:C:37:LYS:HD2	1.32	1.08
1:B:323:ASN:ND2	1:B:356:HIS:ND1	2.01	1.08
1:A:652:GLU:HG2	1:A:653:LYS:H	1.17	1.08
1:D:118:PHE:HD2	1:D:126:ILE:CD1	1.67	1.08
1:D:499:GLU:C	1:D:527:MSE:HE1	1.75	1.07
1:A:485:ILE:CG2	1:A:512:ASN:ND2	2.18	1.07
1:C:44:LYS:NZ	1:C:65:GLU:OE1	1.85	1.06
1:B:36:VAL:HG21	1:B:42:GLU:HG3	1.07	1.06
1:B:354:LEU:HB3	1:B:358:TYR:CE2	1.90	1.06
1:B:54:PHE:HD1	1:B:67:THR:CG2	1.58	1.06
1:C:68:PHE:CD2	1:C:93:MSE:CE	2.39	1.06
1:D:411:GLU:OE2	1:D:412:VAL:N	1.88	1.06
1:A:498:LEU:HD12	1:A:502:LEU:HD13	1.32	1.06
1:A:485:ILE:HG22	1:A:512:ASN:ND2	1.69	1.06
1:B:448:LEU:O	1:B:487:ASN:ND2	1.89	1.06
1:D:322:VAL:HG11	1:D:357:MSE:HE3	1.37	1.06
1:D:145:TRP:CA	1:D:148:GLN:OE1	2.04	1.05
1:B:182:VAL:O	1:B:186:TYR:HB2	1.55	1.05
1:D:349:LEU:HD11	1:D:357:MSE:HE1	1.34	1.05
1:A:638:ILE:HD12	1:B:638:ILE:HG12	1.34	1.05
1:B:374:ASN:OD1	1:B:401:ARG:HD3	1.55	1.05
1:D:513:ARG:HH21	1:D:513:ARG:HG3	1.22	1.05
1:B:350:ARG:HG2	1:B:406:HIS:CE1	1.87	1.05
1:C:44:LYS:NZ	1:C:65:GLU:OE2	1.89	1.04
1:C:610:TRP:CE2	1:C:636:MSE:HE2	1.91	1.04
1:C:562:ALA:O	1:C:565:THR:OG1	1.76	1.04
1:C:474:GLY:HA3	1:C:476:GLN:H	1.21	1.04
1:C:68:PHE:CD2	1:C:93:MSE:HE2	1.93	1.04
1:B:74:HIS:CE1	1:B:89:GLU:HB2	1.93	1.04
1:C:474:GLY:CA	1:C:475:ALA:HB3	1.87	1.03
1:B:349:LEU:HG	1:B:375:THR:OG1	1.57	1.03
1:C:478:LEU:HB2	1:C:508:TRP:CZ2	1.90	1.02
1:C:113:CYS:O	1:C:117:ILE:HD12	1.59	1.02
1:B:177:GLU:N	1:B:177:GLU:OE1	1.91	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:CG1	1:C:37:LYS:HD2	1.89	1.02
1:C:44:LYS:HZ2	1:C:65:GLU:CD	1.52	1.02
1:B:402:SER:O	1:B:434:THR:HB	1.58	1.01
1:C:36:VAL:HG12	1:C:37:LYS:H	1.20	1.01
1:C:350:ARG:HG2	1:C:406:HIS:HE1	1.26	1.01
1:D:499:GLU:CA	1:D:527:MSE:HE3	1.89	1.01
1:C:402:SER:O	1:C:434:THR:HB	1.60	1.01
1:B:78:CYS:HB2	1:B:132:MSE:HA	1.43	1.01
1:A:303:LEU:HD23	1:A:304:PRO:HD2	1.39	1.00
1:B:484:GLU:CG	1:B:508:TRP:CD1	2.41	1.00
1:C:478:LEU:CB	1:C:508:TRP:HZ2	1.67	0.99
1:B:88:THR:HG23	1:B:91:CYS:H	1.23	0.99
1:C:399:LEU:O	1:C:402:SER:OG	1.81	0.99
1:C:350:ARG:CG	1:C:406:HIS:HE1	1.76	0.99
1:B:80:LYS:CE	1:B:81:PRO:HD2	1.92	0.99
1:C:474:GLY:HA2	1:C:475:ALA:HB3	1.02	0.99
1:A:24:ILE:HD12	1:A:25:LYS:H	1.24	0.98
1:C:477:VAL:O	1:C:508:TRP:HZ3	1.03	0.98
1:D:37:LYS:HA	1:D:39:ASP:H	1.25	0.98
1:C:114:LEU:O	1:C:117:ILE:O	1.81	0.98
1:D:291:ARG:HB3	1:D:291:ARG:HH21	1.29	0.98
1:D:118:PHE:CD2	1:D:126:ILE:HD13	1.98	0.97
1:C:474:GLY:CA	1:C:476:GLN:H	1.77	0.97
1:C:478:LEU:CG	1:C:508:TRP:CH2	2.23	0.97
1:D:322:VAL:CG1	1:D:357:MSE:HE3	1.94	0.97
1:A:652:GLU:HG2	1:A:653:LYS:N	1.71	0.97
1:B:484:GLU:CD	1:B:508:TRP:O	2.02	0.97
1:A:369:HIS:CD2	1:A:396:VAL:HG21	2.00	0.96
1:A:319:PRO:CB	1:A:352:ASP:HB2	1.87	0.96
1:D:26:ILE:HD12	1:D:47:VAL:CG2	1.94	0.96
1:A:319:PRO:CG	1:A:352:ASP:CB	2.41	0.96
1:D:78:CYS:SG	1:D:103:VAL:HG11	2.04	0.96
1:C:353:ASP:OD1	1:C:355:SER:OG	1.83	0.96
1:C:431:LEU:O	1:C:434:THR:HG23	1.66	0.96
1:D:638:ILE:HD12	1:D:638:ILE:H	1.28	0.96
1:A:319:PRO:HG2	1:A:352:ASP:HB2	0.99	0.96
1:B:66:LEU:HD12	1:B:93:MSE:HE1	1.46	0.95
1:B:456:GLY:HA2	1:B:489:THR:HG23	1.48	0.95
1:B:36:VAL:CG2	1:B:42:GLU:HG3	1.95	0.95
1:C:68:PHE:CE2	1:C:93:MSE:HE2	2.01	0.95
1:C:55:LEU:HD21	1:C:95:MSE:HE2	1.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASP:O	1:A:294:SER:N	1.99	0.95
1:D:13:MSE:HE1	1:D:26:ILE:HD11	1.46	0.95
1:B:66:LEU:CD1	1:B:93:MSE:HE1	1.97	0.95
1:A:474:GLY:CA	1:A:477:VAL:CG1	2.36	0.95
1:A:293:VAL:HG21	1:A:317:LEU:HD11	1.46	0.94
1:A:9:PRO:CB	1:A:12:LEU:CD2	2.46	0.94
1:D:507:VAL:O	1:D:510:SER:OG	1.85	0.94
1:D:258:LEU:HD23	1:D:262:PHE:HE2	1.32	0.94
1:B:611:ASP:OD1	1:B:612:LYS:N	2.00	0.94
1:C:350:ARG:CD	1:C:406:HIS:ND1	2.30	0.94
1:D:467:GLY:CA	1:D:498:LEU:HD23	1.98	0.94
1:C:543:ILE:CG2	1:C:574:ASN:ND2	2.31	0.93
1:D:18:ASP:OD1	1:D:22:ARG:NH2	2.02	0.93
1:A:9:PRO:HB2	1:A:12:LEU:CD2	1.98	0.93
1:D:344:LEU:O	1:D:347:ASN:ND2	2.00	0.93
2:B:701:OHB:O	3:B:702:CL:CL	2.24	0.93
1:B:88:THR:HG23	1:B:91:CYS:N	1.84	0.93
1:B:54:PHE:CE1	1:B:67:THR:HG21	2.04	0.92
1:C:68:PHE:CE2	1:C:93:MSE:CE	2.52	0.92
1:D:512:ASN:OD1	1:D:515:ILE:HG13	1.68	0.92
1:B:80:LYS:HE3	1:B:81:PRO:HD2	1.48	0.92
1:C:381:MSE:HA	1:C:381:MSE:HE3	1.51	0.92
1:B:178:VAL:O	1:B:182:VAL:HG23	1.68	0.92
1:C:610:TRP:NE1	1:C:636:MSE:HE2	1.84	0.91
1:A:319:PRO:HG2	1:A:352:ASP:CB	1.96	0.91
1:C:256:ALA:HB3	1:C:258:LEU:HD13	1.51	0.91
1:B:180:TRP:O	1:B:184:THR:OG1	1.88	0.91
1:B:185:ILE:O	1:B:189:GLN:HG3	1.71	0.91
1:C:55:LEU:HD11	1:C:95:MSE:HE3	1.53	0.90
1:C:350:ARG:HG2	1:C:406:HIS:CE1	2.05	0.90
1:D:13:MSE:CE	1:D:26:ILE:HD11	2.01	0.90
1:C:68:PHE:HD2	1:C:93:MSE:HE1	1.33	0.90
1:D:322:VAL:HG11	1:D:357:MSE:CE	2.01	0.90
1:C:506:ILE:HG23	1:C:542:MSE:CE	2.03	0.89
1:B:484:GLU:OE2	1:B:508:TRP:CD1	2.26	0.89
1:D:34:LEU:CD2	1:D:42:GLU:HB2	2.02	0.89
1:C:350:ARG:CG	1:C:406:HIS:CE1	2.54	0.89
1:C:509:LEU:CD2	1:C:518:LEU:HD22	2.03	0.89
1:C:528:LYS:O	1:C:531:ASN:ND2	2.04	0.89
1:C:484:GLU:OE1	1:C:484:GLU:N	2.06	0.89
1:D:64:LEU:HD23	1:D:65:GLU:N	1.88	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ALA:O	1:B:486:HIS:HE1	1.56	0.89
1:D:499:GLU:O	1:D:527:MSE:HE1	1.71	0.89
1:B:7:ASP:O	1:B:31:LYS:HG3	1.72	0.89
1:C:134:PRO:HD2	1:C:137:ARG:HH21	1.37	0.88
1:D:431:LEU:O	1:D:434:THR:HG23	1.73	0.88
1:C:55:LEU:HD11	1:C:95:MSE:HE1	1.54	0.88
1:C:8:VAL:HG12	1:C:9:PRO:CD	2.04	0.88
1:D:423:SER:OG	1:D:426:LEU:HD13	1.73	0.88
1:C:117:ILE:HB	1:C:118:PHE:CD2	2.09	0.88
1:A:605:LEU:O	1:A:633:LEU:HD12	1.74	0.88
1:C:115:ARG:HB3	1:C:115:ARG:HH21	1.36	0.88
1:A:319:PRO:HB2	1:A:352:ASP:HB3	0.87	0.87
1:C:115:ARG:HH21	1:C:115:ARG:CB	1.88	0.87
1:A:349:LEU:HG	1:A:375:THR:HG1	1.39	0.87
1:D:350:ARG:HD3	1:D:350:ARG:H	1.37	0.87
1:A:402:SER:O	1:A:434:THR:HG22	1.75	0.86
1:B:350:ARG:HG2	1:B:406:HIS:NE2	1.90	0.86
1:B:24:ILE:HD12	1:B:25:LYS:N	1.88	0.86
1:D:543:ILE:HG22	1:D:574:ASN:ND2	1.90	0.86
1:A:374:ASN:HD21	1:A:401:ARG:HH21	1.20	0.86
1:C:531:ASN:O	1:C:534:PRO:HD2	1.76	0.86
1:C:193:GLU:HG3	1:C:222:LYS:HD3	1.54	0.86
1:D:143:ALA:O	1:D:147:SER:OG	1.93	0.86
1:D:32:VAL:HG23	1:D:96:LYS:O	1.76	0.86
1:A:24:ILE:HD12	1:A:25:LYS:N	1.91	0.85
1:A:138:LEU:HD23	1:A:139:ALA:N	1.91	0.85
1:C:68:PHE:CD2	1:C:93:MSE:HE1	2.08	0.85
1:C:543:ILE:CG2	1:C:574:ASN:HD22	1.90	0.85
1:C:12:LEU:HD12	1:C:12:LEU:O	1.77	0.85
1:C:113:CYS:O	1:C:117:ILE:CD1	2.24	0.85
1:A:372:LEU:O	1:A:375:THR:CG2	2.25	0.85
1:A:258:LEU:HD23	1:A:262:PHE:CE2	2.12	0.85
1:A:562:ALA:O	1:A:565:THR:OG1	1.95	0.85
1:B:484:GLU:HG2	1:B:508:TRP:HE1	1.04	0.84
1:C:484:GLU:OE1	1:C:508:TRP:CD1	2.30	0.84
1:C:504:THR:O	1:C:507:VAL:CG2	2.24	0.84
1:D:26:ILE:HD12	1:D:47:VAL:HG21	1.58	0.84
1:D:499:GLU:C	1:D:527:MSE:HE3	1.93	0.84
1:D:467:GLY:HA2	1:D:498:LEU:CD2	2.08	0.84
1:A:258:LEU:HD23	1:A:262:PHE:CD2	2.13	0.84
1:C:555:LEU:O	1:C:558:SER:OG	1.94	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:MSE:O	1:B:166:VAL:HG23	1.78	0.84
1:D:46:LEU:HD13	1:D:95:MSE:HE1	1.60	0.84
1:B:431:LEU:O	1:B:434:THR:HG23	1.78	0.83
1:D:118:PHE:CD2	1:D:126:ILE:HD11	2.10	0.83
1:D:496:ASN:O	1:D:523:ASN:OD1	1.94	0.83
1:A:121:LEU:HD22	1:A:125:ARG:NH1	1.92	0.83
1:A:117:ILE:CD1	1:A:165:CYS:SG	2.66	0.83
1:A:474:GLY:HA2	1:A:477:VAL:HG11	1.54	0.83
1:A:474:GLY:HA2	1:A:477:VAL:HG12	0.84	0.83
1:A:9:PRO:HB3	1:A:12:LEU:HD21	1.56	0.83
1:B:74:HIS:ND1	1:B:89:GLU:HB2	1.93	0.83
1:C:8:VAL:HG12	1:C:9:PRO:HD2	1.59	0.83
1:A:256:ALA:HB3	1:A:258:LEU:HD13	1.61	0.83
1:B:484:GLU:CD	1:B:508:TRP:CD1	2.51	0.83
1:D:117:ILE:HD13	1:D:165:CYS:SG	2.18	0.83
1:C:26:ILE:HG23	1:C:47:VAL:CG1	2.08	0.83
1:D:610:TRP:CZ3	1:D:615:ILE:HD12	2.14	0.82
1:C:374:ASN:OD1	1:C:401:ARG:CG	2.23	0.82
1:C:65:GLU:O	1:C:66:LEU:CD2	2.17	0.82
1:A:44:LYS:NZ	1:A:65:GLU:OE2	2.12	0.82
1:A:372:LEU:O	1:A:375:THR:HG22	1.78	0.82
1:D:325:LEU:HD12	1:D:325:LEU:O	1.79	0.82
1:D:404:PHE:CE1	1:D:440:PRO:HB3	2.14	0.82
1:A:68:PHE:CD1	1:A:93:MSE:CE	2.62	0.82
1:A:374:ASN:HD21	1:A:401:ARG:NH2	1.76	0.81
1:C:353:ASP:OD1	1:C:355:SER:N	2.12	0.81
1:D:610:TRP:CZ3	1:D:615:ILE:CD1	2.62	0.81
1:D:318:SER:O	1:D:322:VAL:HG23	1.79	0.81
1:D:504:THR:O	1:D:507:VAL:HG22	1.81	0.81
1:C:407:ARG:HH21	1:C:407:ARG:HG3	1.43	0.81
1:C:65:GLU:C	1:C:66:LEU:HD23	1.99	0.81
1:C:373:SER:HB3	1:C:398:ASN:OD1	1.80	0.81
1:D:467:GLY:HA3	1:D:498:LEU:HD23	1.63	0.81
1:C:505:LEU:O	1:C:509:LEU:HD12	1.81	0.81
1:D:318:SER:OG	1:D:320:LYS:N	2.14	0.81
1:D:117:ILE:CD1	1:D:165:CYS:SG	2.68	0.81
1:D:467:GLY:CA	1:D:498:LEU:CD2	2.58	0.81
1:A:485:ILE:HG23	1:A:512:ASN:ND2	1.94	0.81
1:B:65:GLU:O	1:B:66:LEU:HD23	1.79	0.80
1:D:474:GLY:HA2	1:D:475:ALA:CB	2.11	0.80
1:C:474:GLY:O	1:C:477:VAL:HG12	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PHE:CD2	1:D:209:PRO:HD3	2.16	0.80
1:A:485:ILE:HG23	1:A:512:ASN:HD21	1.44	0.80
1:D:34:LEU:HD22	1:D:42:GLU:HB2	1.62	0.80
1:B:124:LEU:O	1:B:127:MSE:O	2.00	0.80
1:A:484:GLU:CG	1:A:508:TRP:NE1	2.30	0.80
1:B:456:GLY:HA2	1:B:489:THR:CG2	2.11	0.80
1:D:37:LYS:HA	1:D:39:ASP:N	1.96	0.80
1:C:258:LEU:HD23	1:C:262:PHE:CE2	2.17	0.80
1:D:349:LEU:HD13	1:D:357:MSE:HE1	1.63	0.80
1:B:256:ALA:HB3	1:B:258:LEU:HD13	1.62	0.80
1:B:54:PHE:HD1	1:B:67:THR:HG21	0.97	0.79
1:D:499:GLU:CA	1:D:527:MSE:CE	2.55	0.79
1:D:44:LYS:NZ	1:D:65:GLU:OE2	2.13	0.79
1:D:500:SER:N	1:D:527:MSE:CE	2.45	0.79
1:B:258:LEU:HD23	1:B:262:PHE:CE2	2.18	0.79
1:D:142:GLN:O	1:D:146:ASP:OD1	2.00	0.79
1:D:99:SER:HB2	1:D:101:GLU:HG3	1.63	0.78
1:D:500:SER:N	1:D:527:MSE:HE2	1.98	0.78
1:D:36:VAL:HG12	1:D:37:LYS:O	1.83	0.78
1:D:117:ILE:HG22	1:D:118:PHE:CD1	2.18	0.78
1:A:283:LEU:O	1:A:286:ASN:ND2	2.16	0.78
1:A:638:ILE:HD13	1:A:640:MSE:HE1	1.64	0.78
1:B:283:LEU:O	1:B:286:ASN:ND2	2.15	0.78
1:C:51:CYS:HB3	1:C:165:CYS:SG	2.24	0.78
1:A:16:ILE:O	1:A:19:VAL:HG12	1.83	0.78
1:C:509:LEU:CD2	1:C:518:LEU:CD2	2.62	0.78
1:D:116:ARG:HH21	1:D:116:ARG:HB2	1.49	0.77
1:C:418:GLN:O	1:C:422:SER:OG	2.02	0.77
1:D:468:HIS:O	1:D:472:SER:HB3	1.84	0.77
1:A:638:ILE:HD13	1:A:640:MSE:CE	2.13	0.77
1:D:256:ALA:HB3	1:D:258:LEU:HD13	1.64	0.77
1:B:7:ASP:O	1:B:31:LYS:CG	2.31	0.77
1:A:13:MSE:SE	1:A:29:LYS:HD2	2.34	0.77
1:A:484:GLU:HG3	1:A:508:TRP:CE2	2.19	0.77
1:A:638:ILE:CD1	1:B:638:ILE:HG12	2.14	0.77
1:D:610:TRP:CE2	1:D:636:MSE:HE2	2.19	0.77
1:B:350:ARG:CG	1:B:406:HIS:NE2	2.47	0.77
1:A:374:ASN:ND2	1:A:401:ARG:HH21	1.81	0.77
1:D:26:ILE:HD12	1:D:47:VAL:HG23	1.67	0.77
1:D:478:LEU:HB3	1:D:508:TRP:NE1	1.98	0.77
1:B:258:LEU:HD23	1:B:262:PHE:CD2	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LEU:HD22	1:B:666:LEU:CD1	2.15	0.77
1:B:115:ARG:NH2	1:B:150:LEU:HD11	1.99	0.77
1:C:476:GLN:N	1:C:476:GLN:HE21	1.82	0.76
1:B:65:GLU:C	1:B:66:LEU:HD23	2.04	0.76
1:A:160:SER:OG	1:A:183:ASP:OD1	2.02	0.76
1:B:183:ASP:O	1:B:187:LEU:HB3	1.86	0.76
1:C:372:LEU:O	1:C:375:THR:CG2	2.34	0.76
1:B:354:LEU:CB	1:B:358:TYR:CE2	2.66	0.76
1:C:77:ILE:HB	1:C:85:VAL:HG22	1.67	0.76
1:C:407:ARG:NH2	1:C:407:ARG:HG3	2.00	0.76
1:B:350:ARG:HG3	1:B:406:HIS:HE1	0.93	0.76
1:D:288:LEU:HD12	1:D:288:LEU:O	1.86	0.76
1:B:372:LEU:O	1:B:375:THR:CG2	2.33	0.76
1:C:379:LEU:HD13	1:C:402:SER:CB	2.16	0.76
1:B:353:ASP:OD1	1:B:355:SER:OG	2.02	0.76
1:A:23:LYS:HE3	1:A:23:LYS:HA	1.68	0.76
1:C:543:ILE:HG23	1:C:574:ASN:ND2	2.00	0.75
1:A:143:ALA:O	1:A:147:SER:N	2.19	0.75
1:C:350:ARG:CD	1:C:406:HIS:HE1	1.90	0.75
1:C:474:GLY:HA3	1:C:476:GLN:HG2	1.67	0.75
1:A:498:LEU:CD1	1:A:502:LEU:HD13	2.15	0.75
1:B:136:GLU:OE2	1:B:136:GLU:N	2.20	0.75
1:C:411:GLU:OE2	1:C:411:GLU:HA	1.87	0.75
1:D:114:LEU:HD23	1:D:123:PRO:HB3	1.69	0.75
1:C:610:TRP:CE2	1:C:636:MSE:CE	2.70	0.75
1:C:485:ILE:HG22	1:C:487:ASN:HB2	1.68	0.74
1:B:32:VAL:HG21	1:B:95:MSE:HB3	1.70	0.74
1:D:372:LEU:O	1:D:375:THR:CG2	2.36	0.74
1:B:513:ARG:HH11	1:B:513:ARG:CB	2.00	0.74
1:D:258:LEU:HD21	1:D:262:PHE:CE2	2.22	0.74
1:B:54:PHE:HA	1:B:67:THR:HG22	1.67	0.74
1:A:73:ILE:HG21	1:A:127:MSE:HE2	1.68	0.74
1:C:456:GLY:HA2	1:C:489:THR:HG23	1.68	0.74
1:B:484:GLU:OE2	1:B:508:TRP:C	2.26	0.74
1:C:475:ALA:C	1:C:476:GLN:HE21	1.90	0.74
1:B:484:GLU:OE1	1:B:508:TRP:O	2.04	0.74
1:D:54:PHE:CD1	1:D:67:THR:HG23	2.22	0.74
1:C:640:MSE:SE	1:D:640:MSE:HG3	2.38	0.74
1:A:13:MSE:HG3	1:A:17:LYS:CE	2.18	0.74
1:A:121:LEU:CD2	1:A:125:ARG:NH1	2.49	0.74
1:C:420:PHE:CZ	1:C:444:LEU:HD13	2.23	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD12	1:B:93:MSE:CE	2.18	0.74
1:D:82:ALA:HB1	1:D:97:MSE:O	1.85	0.74
1:B:449:ALA:O	1:B:486:HIS:CE1	2.40	0.74
1:B:604:LYS:O	1:B:604:LYS:HG3	1.88	0.74
1:D:63:LYS:HG3	1:D:63:LYS:O	1.88	0.74
1:C:26:ILE:HG23	1:C:47:VAL:HG12	1.69	0.73
1:D:564:VAL:HG13	1:D:568:ILE:HD12	1.69	0.73
1:A:104:SER:OG	1:A:137:ARG:NH1	2.20	0.73
1:C:133:GLU:OE1	1:C:133:GLU:HA	1.87	0.73
1:D:13:MSE:HE1	1:D:26:ILE:CD1	2.19	0.73
1:C:509:LEU:HD22	1:C:518:LEU:CD2	2.18	0.73
1:B:115:ARG:HG3	1:B:123:PRO:HG3	1.69	0.73
1:B:134:PRO:HD2	1:B:137:ARG:HH21	1.53	0.73
1:A:76:VAL:HG23	1:A:130:VAL:HG12	1.71	0.73
1:D:349:LEU:HD23	1:D:349:LEU:N	2.04	0.73
1:A:498:LEU:HD12	1:A:502:LEU:CD1	2.15	0.73
1:B:115:ARG:CZ	1:B:150:LEU:HD11	2.17	0.73
1:D:323:ASN:ND2	1:D:356:HIS:HB2	2.03	0.73
1:D:315:THR:OG1	1:D:317:LEU:CD1	2.36	0.73
1:D:68:PHE:CE2	1:D:86:VAL:HG11	2.24	0.73
1:C:604:LYS:HG3	1:C:604:LYS:O	1.89	0.73
1:B:638:ILE:HD12	1:B:638:ILE:N	2.03	0.73
1:A:68:PHE:CD1	1:A:93:MSE:HE2	2.24	0.73
1:B:293:VAL:HG21	1:B:317:LEU:HD11	1.71	0.73
1:A:369:HIS:CD2	1:A:396:VAL:CG2	2.72	0.73
1:D:485:ILE:O	1:D:512:ASN:ND2	2.21	0.73
1:D:114:LEU:O	1:D:117:ILE:O	2.06	0.72
1:A:638:ILE:CG2	1:A:640:MSE:HE3	2.19	0.72
1:B:134:PRO:HB2	1:B:137:ARG:HB2	1.71	0.72
1:B:80:LYS:HG2	1:B:81:PRO:CD	2.19	0.72
1:B:132:MSE:SE	1:B:138:LEU:HD13	2.39	0.72
1:D:349:LEU:HG	1:D:375:THR:OG1	1.89	0.72
1:D:474:GLY:HA3	1:D:476:GLN:CG	2.20	0.72
1:C:509:LEU:HD23	1:C:518:LEU:HD22	1.71	0.72
1:D:604:LYS:HG3	1:D:604:LYS:O	1.89	0.72
1:C:498:LEU:HD13	1:C:505:LEU:HD12	1.71	0.72
1:B:115:ARG:HG3	1:B:123:PRO:CG	2.19	0.72
1:B:64:LEU:HD11	1:B:66:LEU:O	1.90	0.72
1:B:66:LEU:CD1	1:B:93:MSE:CE	2.68	0.72
1:D:478:LEU:HB3	1:D:508:TRP:HE1	1.52	0.72
1:A:13:MSE:HG3	1:A:17:LYS:HE2	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LEU:HD23	1:D:335:THR:HG21	1.71	0.72
1:D:118:PHE:CE2	1:D:126:ILE:HD13	2.24	0.71
1:C:503:SER:O	1:C:506:ILE:HB	1.90	0.71
1:C:505:LEU:O	1:C:509:LEU:CD1	2.38	0.71
1:D:77:ILE:O	1:D:85:VAL:HG12	1.90	0.71
1:B:177:GLU:O	1:B:181:ASP:HB2	1.90	0.71
1:C:498:LEU:HD11	1:C:505:LEU:HD13	1.72	0.71
1:D:64:LEU:HD23	1:D:65:GLU:H	1.53	0.71
1:B:484:GLU:CG	1:B:508:TRP:HE1	1.86	0.71
1:C:395:ALA:O	1:C:427:ILE:HG22	1.90	0.71
1:A:124:LEU:HD22	1:A:130:VAL:HG21	1.72	0.71
1:D:54:PHE:CD1	1:D:67:THR:CG2	2.74	0.71
1:C:77:ILE:HB	1:C:85:VAL:CG2	2.20	0.71
1:D:580:VAL:CG1	1:D:605:LEU:HD21	2.21	0.71
1:D:507:VAL:HG23	1:D:508:TRP:N	2.05	0.71
1:C:352:ASP:OD1	1:C:352:ASP:N	2.20	0.71
1:B:32:VAL:CG2	1:B:95:MSE:HB3	2.21	0.71
1:C:543:ILE:HG23	1:C:574:ASN:HD21	1.56	0.71
1:C:506:ILE:HG23	1:C:542:MSE:HE1	1.72	0.71
1:C:478:LEU:HB2	1:C:508:TRP:HZ2	1.39	0.70
1:D:34:LEU:HD21	1:D:42:GLU:OE2	1.91	0.70
1:A:479:GLU:HA	1:A:481:CYS:SG	2.31	0.70
1:C:543:ILE:HG22	1:C:574:ASN:ND2	2.04	0.70
1:A:73:ILE:HD13	1:A:127:MSE:CE	2.21	0.70
1:C:117:ILE:HB	1:C:118:PHE:HD2	1.55	0.70
1:A:480:GLY:N	1:A:481:CYS:HA	2.06	0.70
1:D:349:LEU:CB	1:D:354:LEU:HD21	2.16	0.70
1:B:54:PHE:CD1	1:B:67:THR:HG22	2.24	0.70
1:B:80:LYS:CD	1:B:81:PRO:HD2	2.22	0.70
1:A:134:PRO:O	1:A:137:ARG:HG3	1.92	0.70
1:D:99:SER:HB3	1:D:100:PRO:HD2	1.73	0.70
1:B:652:GLU:HG2	1:B:653:LYS:N	2.05	0.70
1:D:291:ARG:NH2	1:D:291:ARG:HB3	2.05	0.70
1:C:502:LEU:O	1:C:502:LEU:HD12	1.91	0.70
1:C:610:TRP:CZ3	1:C:615:ILE:HD13	2.26	0.70
1:C:256:ALA:HB3	1:C:258:LEU:CD1	2.19	0.70
1:A:76:VAL:HG13	1:A:86:VAL:HG22	1.74	0.70
1:A:323:ASN:OD1	1:A:354:LEU:HA	1.91	0.70
1:C:543:ILE:HG22	1:C:574:ASN:HD22	1.54	0.70
1:D:616:THR:HG22	1:D:617:ALA:N	2.07	0.70
1:D:499:GLU:C	1:D:527:MSE:HE2	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLN:HE21	1:A:618:GLN:C	1.95	0.69
1:C:484:GLU:OE2	1:C:511:LYS:CG	2.39	0.69
1:B:36:VAL:HG21	1:B:42:GLU:HG2	1.71	0.69
1:D:513:ARG:NH2	1:D:513:ARG:HG3	1.94	0.69
1:D:77:ILE:HD12	1:D:85:VAL:HG11	1.73	0.69
1:C:55:LEU:CD1	1:C:95:MSE:CE	2.59	0.69
1:C:530:LYS:O	1:C:534:PRO:HD3	1.91	0.69
1:B:4:GLU:HG2	1:B:5:SER:N	2.07	0.69
1:D:258:LEU:CD2	1:D:262:PHE:CD2	2.61	0.69
1:B:80:LYS:HG2	1:B:81:PRO:HD3	1.74	0.69
1:A:568:ILE:O	1:A:571:LEU:HB2	1.93	0.69
1:C:603:THR:OG1	1:C:603:THR:O	2.10	0.69
1:A:9:PRO:O	1:A:12:LEU:HG	1.92	0.69
1:B:323:ASN:ND2	1:B:356:HIS:CG	2.61	0.69
1:D:377:CYS:O	1:D:403:VAL:HG22	1.92	0.69
1:C:610:TRP:NE1	1:C:636:MSE:CE	2.56	0.69
1:A:77:ILE:O	1:A:85:VAL:HG12	1.92	0.69
1:B:156:CYS:HA	1:B:219:TRP:CD1	2.28	0.69
1:B:36:VAL:HB	1:B:41:VAL:HA	1.74	0.69
1:C:379:LEU:HD13	1:C:402:SER:HB3	1.74	0.69
1:A:470:LEU:CD2	1:A:477:VAL:HG11	2.23	0.69
1:D:53:ALA:HB3	1:D:68:PHE:CE1	2.28	0.69
1:D:30:LYS:HE3	1:D:102:ASP:OD1	1.93	0.69
1:D:506:ILE:HG21	1:D:538:ASN:HB3	1.74	0.69
1:A:414:PRO:O	1:A:418:GLN:HB2	1.93	0.68
1:B:8:VAL:HA	1:B:31:LYS:HD2	1.75	0.68
1:B:135:SER:HB3	1:B:136:GLU:OE2	1.93	0.68
1:C:290:ASP:OD2	1:C:321:GLY:N	2.26	0.68
1:D:43:ASN:O	1:D:44:LYS:CE	2.41	0.68
1:A:117:ILE:HD13	1:A:165:CYS:SG	2.33	0.68
1:A:618:GLN:NE2	1:A:618:GLN:O	2.15	0.68
1:A:12:LEU:C	1:A:12:LEU:HD12	2.14	0.68
1:A:638:ILE:HG21	1:A:640:MSE:HE3	1.75	0.68
1:D:507:VAL:HG23	1:D:508:TRP:H	1.58	0.68
1:A:73:ILE:CD1	1:A:127:MSE:HE3	2.23	0.68
1:B:78:CYS:HB2	1:B:132:MSE:CA	2.21	0.68
1:D:651:PRO:HG2	1:D:652:GLU:N	2.09	0.68
1:C:98:VAL:HG22	1:C:102:ASP:OD2	1.94	0.68
1:B:54:PHE:HA	1:B:67:THR:CG2	2.23	0.68
1:D:638:ILE:HD12	1:D:638:ILE:N	2.04	0.68
1:D:144:LEU:C	1:D:148:GLN:OE1	2.31	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HB	1:B:40:ARG:O	1.93	0.68
1:A:73:ILE:HG21	1:A:127:MSE:CE	2.24	0.68
1:A:374:ASN:OD1	1:A:401:ARG:HD3	1.89	0.67
1:C:256:ALA:CB	1:C:258:LEU:HD13	2.24	0.67
1:B:513:ARG:HH11	1:B:513:ARG:CG	2.07	0.67
1:D:34:LEU:HD21	1:D:36:VAL:HG21	1.75	0.67
1:C:36:VAL:HG12	1:C:37:LYS:CD	2.18	0.67
1:D:543:ILE:CG2	1:D:574:ASN:ND2	2.57	0.67
1:A:95:MSE:HB2	1:A:97:MSE:CE	2.25	0.67
1:A:452:HIS:CD2	1:A:452:HIS:H	2.11	0.67
1:C:478:LEU:CD2	1:C:508:TRP:CH2	2.77	0.67
1:B:56:LEU:HD23	1:B:64:LEU:HB2	1.76	0.67
1:C:563:GLU:O	1:C:566:ILE:HG23	1.94	0.67
1:D:46:LEU:CD1	1:D:95:MSE:HE1	2.25	0.67
1:C:578:THR:HG22	1:C:604:LYS:HD2	1.75	0.67
1:D:80:LYS:HD2	1:D:81:PRO:HD2	1.77	0.67
1:D:610:TRP:CE3	1:D:615:ILE:HD12	2.29	0.67
1:A:80:LYS:HD2	1:A:81:PRO:N	2.10	0.67
1:A:141:LEU:HD23	1:A:144:LEU:HD23	1.77	0.67
1:A:143:ALA:HA	1:A:146:ASP:HB2	1.77	0.67
1:B:143:ALA:O	1:B:147:SER:HB3	1.95	0.67
1:C:217:ASN:OD1	1:C:219:TRP:N	2.19	0.67
1:C:185:ILE:HA	1:D:601:ILE:HD11	1.76	0.67
1:D:349:LEU:CD1	1:D:357:MSE:CE	2.64	0.67
1:B:52:ARG:HD3	1:B:67:THR:HB	1.76	0.66
1:C:378:SER:O	1:C:382:VAL:HG23	1.95	0.66
1:C:478:LEU:HD23	1:C:508:TRP:HH2	1.58	0.66
1:D:46:LEU:HD13	1:D:95:MSE:CE	2.24	0.66
1:A:98:VAL:HG23	1:A:99:SER:N	2.09	0.66
1:B:372:LEU:O	1:B:375:THR:HG22	1.94	0.66
1:C:134:PRO:CD	1:C:137:ARG:HH21	2.07	0.66
1:B:18:ASP:OD1	1:B:22:ARG:NH2	2.29	0.66
1:B:478:LEU:HB3	1:B:508:TRP:CZ3	2.31	0.66
1:C:372:LEU:O	1:C:375:THR:HG22	1.94	0.66
1:A:597:LYS:HE3	1:B:201:HIS:CE1	2.31	0.66
1:B:212:ALA:HB2	1:B:237:GLN:CG	2.25	0.66
1:C:527:MSE:CE	1:C:532:LEU:HG	2.25	0.66
1:D:100:PRO:CD	1:D:101:GLU:H	2.08	0.66
1:C:636:MSE:HB3	1:C:665:LEU:HD11	1.78	0.66
1:D:46:LEU:HD22	1:D:95:MSE:CE	2.25	0.66
1:B:485:ILE:HG22	1:B:512:ASN:ND2	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MSE:CE	1:A:26:ILE:CD1	2.73	0.66
1:D:474:GLY:CA	1:D:475:ALA:HB3	2.16	0.66
1:D:99:SER:CB	1:D:100:PRO:HD2	2.26	0.66
1:B:7:ASP:OD1	1:B:7:ASP:N	2.28	0.66
1:C:115:ARG:NH2	1:C:150:LEU:HD21	2.09	0.66
1:C:484:GLU:OE2	1:C:511:LYS:HB2	1.89	0.66
1:D:318:SER:HG	1:D:320:LYS:HG3	1.61	0.66
1:A:35:GLU:HB2	1:A:94:SER:HB3	1.78	0.66
1:D:160:SER:OG	1:D:183:ASP:OD1	2.13	0.66
1:D:427:ILE:HD13	1:D:427:ILE:O	1.94	0.66
1:A:13:MSE:CE	1:A:26:ILE:HD12	2.25	0.65
1:A:97:MSE:SE	1:A:103:VAL:HG12	2.46	0.65
1:B:355:SER:O	1:B:359:ASN:HB2	1.97	0.65
1:C:478:LEU:CD2	1:C:508:TRP:HH2	2.09	0.65
1:C:478:LEU:CD1	1:C:508:TRP:HZ2	2.09	0.65
1:B:478:LEU:HB3	1:B:508:TRP:CE3	2.32	0.65
1:D:117:ILE:HG22	1:D:118:PHE:CE1	2.31	0.65
1:C:193:GLU:CG	1:C:222:LYS:HD3	2.27	0.65
1:D:563:GLU:O	1:D:564:VAL:C	2.30	0.65
1:C:256:ALA:CB	1:C:258:LEU:CD1	2.74	0.65
1:C:315:THR:OG1	1:C:317:LEU:HD13	1.95	0.65
1:D:478:LEU:CB	1:D:508:TRP:HE1	2.10	0.65
1:A:89:GLU:OE2	1:A:89:GLU:HA	1.96	0.65
1:C:503:SER:HA	1:C:506:ILE:HG13	1.77	0.65
1:D:172:PHE:CE2	1:D:209:PRO:HD3	2.32	0.65
1:A:119:PRO:HG2	1:A:153:PRO:HB3	1.79	0.65
1:D:499:GLU:HA	1:D:527:MSE:CE	2.16	0.65
1:D:117:ILE:HD11	1:D:165:CYS:SG	2.37	0.65
1:D:474:GLY:HA3	1:D:476:GLN:HG2	1.79	0.65
1:D:448:LEU:O	1:D:487:ASN:ND2	2.30	0.65
1:D:34:LEU:O	1:D:36:VAL:HG23	1.97	0.65
1:A:138:LEU:HD23	1:A:138:LEU:C	2.16	0.65
1:D:84:MSE:SE	1:D:107:LEU:CD1	2.95	0.65
1:C:474:GLY:CA	1:C:476:GLN:N	2.57	0.65
1:A:138:LEU:HD23	1:A:139:ALA:CA	2.27	0.64
1:B:52:ARG:HG3	1:B:68:PHE:O	1.97	0.64
1:C:160:SER:OG	1:C:183:ASP:OD1	2.13	0.64
1:C:349:LEU:HG	1:C:375:THR:HG1	1.62	0.64
1:D:610:TRP:CE3	1:D:615:ILE:CD1	2.81	0.64
1:D:437:SER:O	1:D:440:PRO:HD2	1.98	0.64
1:A:394:LEU:HD21	1:A:397:LEU:HD13	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASP:N	1:D:146:ASP:OD1	2.31	0.64
1:B:256:ALA:HB3	1:B:258:LEU:CD1	2.27	0.64
1:D:113:CYS:O	1:D:116:ARG:HB3	1.98	0.64
1:D:76:VAL:O	1:D:130:VAL:HA	1.98	0.64
1:D:40:ARG:CG	1:D:40:ARG:HH21	2.10	0.64
1:A:23:LYS:HD2	1:A:23:LYS:N	2.12	0.64
1:D:78:CYS:SG	1:D:103:VAL:CG1	2.83	0.64
1:D:110:ILE:HG21	1:D:127:MSE:HE1	1.80	0.64
1:D:37:LYS:CA	1:D:39:ASP:H	2.06	0.64
1:A:593:LYS:HE2	1:B:200:SER:OG	1.98	0.64
1:D:408:LYS:HE3	1:D:408:LYS:HA	1.79	0.64
1:B:8:VAL:HG22	1:B:31:LYS:HG2	1.80	0.64
1:C:381:MSE:HA	1:C:381:MSE:CE	2.27	0.64
1:C:193:GLU:HG3	1:C:222:LYS:CD	2.28	0.64
1:A:258:LEU:CD2	1:A:262:PHE:CE2	2.81	0.64
1:B:32:VAL:CG2	1:B:95:MSE:HG2	2.28	0.63
1:C:484:GLU:N	1:C:508:TRP:HE1	1.96	0.63
1:D:115:ARG:HG3	1:D:115:ARG:HH11	1.62	0.63
1:D:53:ALA:O	1:D:67:THR:HG22	1.99	0.63
1:A:84:MSE:HE1	1:A:106:VAL:HG11	1.80	0.63
1:C:290:ASP:O	1:C:294:SER:OG	2.16	0.63
1:C:602:ASN:ND2	1:C:605:LEU:HD23	2.13	0.63
1:C:449:ALA:HA	1:C:485:ILE:HG23	1.80	0.63
1:D:36:VAL:O	1:D:39:ASP:N	2.32	0.63
1:A:601:ILE:HD11	1:B:184:THR:O	1.97	0.63
1:C:404:PHE:CE1	1:C:440:PRO:HB3	2.32	0.63
1:D:70:TYR:CD1	1:D:110:ILE:HG23	2.32	0.63
1:A:117:ILE:HD11	1:A:165:CYS:SG	2.37	0.63
1:A:543:ILE:CG2	1:A:574:ASN:ND2	2.61	0.63
1:C:611:ASP:OD1	1:C:612:LYS:N	2.31	0.63
1:A:638:ILE:CD1	1:A:640:MSE:HE1	2.27	0.63
1:A:290:ASP:HA	1:A:293:VAL:HB	1.81	0.63
1:A:143:ALA:O	1:A:146:ASP:HB2	1.98	0.63
1:B:288:LEU:O	1:B:289:GLU:HB2	1.97	0.63
1:C:55:LEU:CD2	1:C:95:MSE:HE2	2.27	0.63
1:C:134:PRO:HD2	1:C:137:ARG:HD3	1.81	0.63
1:B:115:ARG:HG3	1:B:123:PRO:CD	2.29	0.63
1:C:441:LEU:HD11	1:C:445:LEU:HD11	1.81	0.63
1:B:580:VAL:HG12	1:B:608:VAL:HG22	1.81	0.63
1:B:8:VAL:HG21	1:B:45:VAL:HG13	1.81	0.62
1:C:12:LEU:HD12	1:C:12:LEU:C	2.19	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:HG3	1:B:123:PRO:HD3	1.80	0.62
1:D:48:LEU:HD11	1:D:106:VAL:HG13	1.80	0.62
1:D:144:LEU:C	1:D:144:LEU:HD13	2.20	0.62
1:B:80:LYS:HB3	1:B:83:GLN:HB3	1.82	0.62
1:C:470:LEU:HD11	1:C:505:LEU:HD11	1.81	0.62
1:B:474:GLY:O	1:B:475:ALA:HB3	2.00	0.62
1:C:36:VAL:HG12	1:C:37:LYS:N	2.01	0.62
1:D:43:ASN:O	1:D:44:LYS:HE2	1.97	0.62
1:B:513:ARG:HH11	1:B:513:ARG:CA	2.12	0.62
1:A:301:ALA:O	1:A:332:ASN:HB2	1.99	0.62
1:C:474:GLY:HA3	1:C:476:GLN:N	2.05	0.62
1:B:484:GLU:OE2	1:B:508:TRP:CA	2.48	0.62
1:A:617:ALA:O	1:A:621:GLN:HG3	2.00	0.62
1:C:532:LEU:CD2	1:C:536:LEU:HG	2.29	0.62
1:D:379:LEU:HD13	1:D:402:SER:OG	2.00	0.62
1:C:484:GLU:CD	1:C:511:LYS:HB3	2.16	0.62
1:C:509:LEU:HD22	1:C:518:LEU:HD22	1.77	0.62
1:A:68:PHE:CD1	1:A:93:MSE:HE1	2.34	0.62
1:D:378:SER:HB2	1:D:406:HIS:CD2	2.35	0.61
1:B:638:ILE:HD12	1:B:638:ILE:H	1.65	0.61
1:B:349:LEU:HG	1:B:375:THR:HG1	1.63	0.61
1:D:43:ASN:O	1:D:44:LYS:CD	2.48	0.61
1:A:133:GLU:HA	1:A:133:GLU:OE1	1.98	0.61
1:B:496:ASN:O	1:B:497:GLY:C	2.37	0.61
1:D:256:ALA:HB3	1:D:258:LEU:CD1	2.30	0.61
1:D:26:ILE:CD1	1:D:47:VAL:HG21	2.29	0.61
1:D:470:LEU:O	1:D:473:GLY:O	2.18	0.61
1:A:349:LEU:CG	1:A:375:THR:OG1	2.35	0.61
1:D:348:ALA:C	1:D:349:LEU:HD23	2.20	0.61
1:A:589:ASP:OD1	1:A:616:THR:OG1	2.18	0.61
1:D:313:SER:HA	1:D:345:SER:O	2.01	0.61
1:C:477:VAL:HG13	1:C:477:VAL:O	2.00	0.61
1:B:477:VAL:HG23	1:B:478:LEU:HG	1.81	0.61
1:D:477:VAL:O	1:D:478:LEU:HD23	2.00	0.61
1:B:157:GLY:O	1:B:162:MSE:HE3	2.00	0.61
1:B:115:ARG:NH1	1:B:150:LEU:HD11	2.16	0.61
1:A:482:ILE:HG23	1:A:483:ALA:N	2.15	0.61
1:D:372:LEU:O	1:D:375:THR:HB	2.01	0.61
1:D:39:ASP:N	1:D:39:ASP:OD1	2.29	0.61
1:C:387:LEU:O	1:C:391:LEU:HD21	2.01	0.61
1:B:298:ILE:HG22	1:B:299:GLN:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:PHE:CD1	1:C:67:THR:HG23	2.35	0.61
1:C:498:LEU:CD1	1:C:505:LEU:CD1	2.79	0.61
1:A:479:GLU:C	1:A:481:CYS:HB2	2.21	0.61
1:D:318:SER:OG	1:D:320:LYS:HG3	2.01	0.61
1:A:76:VAL:HG12	1:A:85:VAL:O	2.01	0.61
1:C:80:LYS:HG2	1:C:81:PRO:HD2	1.82	0.61
1:D:322:VAL:HG12	1:D:357:MSE:HE3	1.83	0.61
1:D:34:LEU:HD23	1:D:34:LEU:O	2.00	0.61
1:D:82:ALA:O	1:D:97:MSE:N	2.25	0.61
1:A:478:LEU:HD13	1:A:508:TRP:CB	2.31	0.60
1:D:54:PHE:CE1	1:D:67:THR:HG21	2.36	0.60
1:A:602:ASN:ND2	1:A:605:LEU:HD23	2.16	0.60
1:D:284:ALA:HB1	1:D:313:SER:HB3	1.84	0.60
1:D:474:GLY:HA3	1:D:476:GLN:HG3	1.83	0.60
1:B:349:LEU:CG	1:B:375:THR:OG1	2.44	0.60
1:D:97:MSE:HE2	1:D:103:VAL:HA	1.83	0.60
1:B:36:VAL:CG2	1:B:42:GLU:CG	2.65	0.60
1:A:65:GLU:O	1:A:66:LEU:HD23	2.02	0.60
1:A:666:LEU:HD22	1:B:666:LEU:HD11	1.83	0.60
1:D:355:SER:O	1:D:359:ASN:N	2.30	0.60
1:C:509:LEU:HD22	1:C:518:LEU:HD21	1.84	0.60
1:D:325:LEU:HD11	1:D:329:LEU:HD11	1.84	0.60
1:C:185:ILE:O	1:C:189:GLN:HG3	2.01	0.60
1:C:650:ASN:O	1:C:652:GLU:HB3	2.00	0.60
1:B:182:VAL:O	1:B:186:TYR:CB	2.43	0.60
1:A:431:LEU:O	1:A:434:THR:OG1	2.18	0.60
1:C:115:ARG:CG	1:C:115:ARG:HH21	2.14	0.60
1:D:586:GLY:HA2	1:D:614:ASN:HD22	1.65	0.60
1:A:263:ALA:CB	1:A:292:GLY:HA3	2.32	0.60
1:D:115:ARG:CG	1:D:115:ARG:HH11	2.14	0.60
1:D:638:ILE:CD1	1:D:638:ILE:H	1.99	0.60
1:A:254:GLU:O	1:A:255:ASN:C	2.38	0.60
1:A:303:LEU:HD23	1:A:304:PRO:CD	2.23	0.59
1:C:122:SER:O	1:C:125:ARG:N	2.35	0.59
1:A:506:ILE:HG23	1:A:542:MSE:HE3	1.83	0.59
1:C:169:TRP:CZ3	1:C:170:LEU:HD21	2.36	0.59
1:B:66:LEU:HD13	1:B:93:MSE:HE1	1.81	0.59
1:C:350:ARG:HG3	1:C:376:GLU:HG2	1.83	0.59
1:A:483:ALA:O	1:A:484:GLU:HB3	2.02	0.59
1:A:256:ALA:HB3	1:A:258:LEU:CD1	2.29	0.59
1:D:314:LYS:HG3	1:D:346:GLY:HA3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MSE:HE1	1:B:106:VAL:HB	1.84	0.59
1:A:56:LEU:HD23	1:A:63:LYS:O	2.01	0.59
1:C:117:ILE:CG2	1:C:118:PHE:CE2	2.85	0.59
1:B:136:GLU:CD	1:B:136:GLU:H	2.04	0.59
1:C:651:PRO:N	1:C:652:GLU:HB2	2.16	0.59
1:A:9:PRO:HB3	1:A:12:LEU:CD2	2.26	0.59
1:D:117:ILE:HG22	1:D:118:PHE:CG	2.38	0.59
1:B:374:ASN:OD1	1:B:401:ARG:CD	2.43	0.59
1:D:142:GLN:OE1	1:D:146:ASP:OD1	2.20	0.59
1:A:506:ILE:HG23	1:A:542:MSE:CE	2.32	0.59
1:A:162:MSE:O	1:A:166:VAL:HG23	2.02	0.59
1:B:44:LYS:HB3	1:B:56:LEU:O	2.02	0.59
1:C:414:PRO:O	1:C:418:GLN:HB2	2.02	0.59
1:A:652:GLU:CG	1:A:653:LYS:H	2.05	0.59
1:B:354:LEU:HD23	1:B:358:TYR:OH	2.03	0.59
1:D:16:ILE:HG23	1:D:56:LEU:HD13	1.83	0.59
1:D:34:LEU:HD21	1:D:36:VAL:CG2	2.33	0.59
1:A:32:VAL:HG21	1:A:95:MSE:HB3	1.85	0.59
1:A:574:ASN:OD1	1:A:576:SER:N	2.31	0.59
1:D:620:PHE:CD1	1:D:658:LEU:HD21	2.38	0.59
1:A:528:LYS:O	1:A:531:ASN:HB2	2.02	0.59
1:D:422:SER:O	1:D:424:LEU:CD1	2.51	0.59
1:C:36:VAL:HG21	1:C:42:GLU:HG3	1.85	0.59
1:D:616:THR:CG2	1:D:617:ALA:N	2.66	0.59
1:B:76:VAL:HG11	1:B:107:LEU:HD21	1.85	0.59
1:B:56:LEU:CD2	1:B:64:LEU:HB2	2.33	0.59
1:D:372:LEU:O	1:D:375:THR:HG22	2.01	0.59
1:A:121:LEU:HD22	1:A:125:ARG:HH11	1.66	0.59
1:A:28:VAL:HB	1:A:48:LEU:HB2	1.85	0.59
1:D:64:LEU:CD2	1:D:65:GLU:N	2.64	0.58
1:B:174:TYR:CD1	1:B:174:TYR:C	2.76	0.58
1:B:558:SER:HB2	1:B:560:LEU:HG	1.84	0.58
1:D:144:LEU:O	1:D:148:GLN:CD	2.40	0.58
1:B:564:VAL:HG22	1:B:564:VAL:O	2.03	0.58
1:D:117:ILE:CG2	1:D:118:PHE:CE1	2.86	0.58
1:C:536:LEU:O	1:C:540:VAL:HG23	2.02	0.58
1:C:498:LEU:CD1	1:C:505:LEU:HD13	2.33	0.58
1:B:54:PHE:CA	1:B:67:THR:HG22	2.34	0.58
1:A:470:LEU:CD2	1:A:477:VAL:CG1	2.81	0.58
1:A:403:VAL:HG23	1:A:403:VAL:O	2.04	0.58
1:C:509:LEU:H	1:C:509:LEU:HD12	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:LEU:O	1:C:391:LEU:HD11	2.03	0.58
1:C:53:ALA:O	1:C:67:THR:HG22	2.02	0.58
1:C:647:LEU:HD23	1:C:654:THR:HB	1.83	0.58
1:A:13:MSE:O	1:A:16:ILE:HB	2.02	0.58
1:A:610:TRP:O	1:A:613:ASN:ND2	2.28	0.58
1:A:667:ARG:HG3	1:A:668:ASN:N	2.19	0.58
1:D:504:THR:O	1:D:507:VAL:CG2	2.51	0.58
1:D:397:LEU:HD11	1:D:399:LEU:HD11	1.84	0.58
1:D:208:ILE:HG23	1:D:237:GLN:HE21	1.68	0.58
1:D:563:GLU:O	1:D:566:ILE:HG23	2.04	0.58
1:A:543:ILE:HG22	1:A:574:ASN:ND2	2.19	0.58
1:C:16:ILE:HA	1:C:19:VAL:HG12	1.86	0.58
1:B:53:ALA:O	1:B:67:THR:HG22	2.04	0.58
1:C:117:ILE:CB	1:C:118:PHE:CD2	2.85	0.58
1:A:222:LYS:HG3	1:A:250:GLU:HB2	1.84	0.58
1:D:336:ALA:O	1:D:366:THR:HG22	2.03	0.58
1:C:476:GLN:CA	1:C:476:GLN:HE21	2.16	0.58
1:D:115:ARG:NH2	1:D:150:LEU:HD22	2.18	0.58
1:B:322:VAL:HG21	1:B:349:LEU:HD21	1.86	0.58
1:B:80:LYS:HD3	1:B:82:ALA:H	1.68	0.58
1:D:80:LYS:HD2	1:D:81:PRO:CD	2.34	0.58
1:D:477:VAL:C	1:D:478:LEU:HG	2.23	0.58
1:D:610:TRP:HZ3	1:D:615:ILE:CD1	2.17	0.58
1:B:270:LEU:HD21	1:B:278:LEU:HD12	1.85	0.58
1:A:23:LYS:HE3	1:A:23:LYS:CA	2.34	0.57
1:A:603:THR:OG1	1:A:603:THR:O	2.21	0.57
1:D:174:TYR:HD1	1:D:174:TYR:C	2.08	0.57
1:D:56:LEU:HD23	1:D:64:LEU:HA	1.85	0.57
1:B:258:LEU:CD2	1:B:262:PHE:CE2	2.86	0.57
1:D:97:MSE:HG3	1:D:103:VAL:HG22	1.87	0.57
1:D:110:ILE:CG2	1:D:127:MSE:HE1	2.34	0.57
1:D:110:ILE:HG21	1:D:127:MSE:CE	2.34	0.57
1:D:174:TYR:C	1:D:174:TYR:CD1	2.76	0.57
1:C:493:ILE:O	1:C:496:ASN:ND2	2.34	0.57
1:C:69:SER:N	1:C:72:GLU:OE1	2.34	0.57
1:B:503:SER:O	1:B:504:THR:C	2.42	0.57
1:C:510:SER:O	1:C:513:ARG:NH1	2.37	0.57
1:B:132:MSE:SE	1:B:138:LEU:CD1	3.02	0.57
1:D:37:LYS:H	1:D:37:LYS:CD	2.18	0.57
1:A:212:ALA:HB2	1:A:237:GLN:CG	2.35	0.57
1:C:407:ARG:CG	1:C:407:ARG:HH21	2.15	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:SER:OG	1:A:100:PRO:HD2	2.05	0.57
1:A:19:VAL:HG13	1:A:20:ILE:HG23	1.86	0.57
1:D:290:ASP:OD2	1:D:321:GLY:N	2.38	0.57
1:A:650:ASN:HB3	1:A:652:GLU:OE2	2.05	0.57
1:A:638:ILE:HG23	1:A:640:MSE:CE	2.35	0.57
1:D:70:TYR:CE1	1:D:110:ILE:HG12	2.39	0.57
1:D:212:ALA:HB2	1:D:237:GLN:CG	2.35	0.57
1:A:589:ASP:OD2	1:A:616:THR:OG1	2.22	0.57
1:D:499:GLU:OE2	1:D:499:GLU:HA	2.04	0.57
1:A:290:ASP:OD1	1:A:317:LEU:HA	2.04	0.57
1:A:380:GLU:CD	1:A:405:SER:OG	2.43	0.57
1:D:114:LEU:HB3	1:D:123:PRO:HG3	1.87	0.57
1:C:26:ILE:CG2	1:C:47:VAL:CG1	2.81	0.57
1:C:486:HIS:HA	1:C:514:SER:HB3	1.87	0.57
1:A:13:MSE:HG3	1:A:17:LYS:HE3	1.86	0.57
1:C:524:PHE:N	1:C:524:PHE:CD1	2.73	0.57
1:D:196:LEU:HB2	1:D:225:SER:HB2	1.87	0.57
1:B:485:ILE:HG22	1:B:512:ASN:HD22	1.70	0.57
1:C:610:TRP:CD1	1:C:636:MSE:HE3	2.40	0.57
1:D:66:LEU:HD13	1:D:93:MSE:HE2	1.87	0.57
1:B:315:THR:OG1	1:B:317:LEU:HD13	2.05	0.57
1:A:604:LYS:O	1:A:604:LYS:HG3	2.05	0.57
1:C:381:MSE:HE3	1:C:381:MSE:CA	2.27	0.56
1:C:420:PHE:CZ	1:C:444:LEU:CD1	2.87	0.56
1:C:587:MSE:HG2	1:C:613:ASN:CG	2.25	0.56
1:C:613:ASN:O	1:C:614:ASN:HB2	2.03	0.56
1:B:468:HIS:O	1:B:472:SER:HB3	2.05	0.56
1:A:471:ARG:NH2	1:A:471:ARG:HG3	2.19	0.56
1:C:461:LEU:O	1:C:464:CYS:SG	2.62	0.56
1:C:34:LEU:HD23	1:C:36:VAL:HG22	1.87	0.56
1:D:27:SER:HB2	1:D:109:HIS:HE1	1.70	0.56
1:D:466:LEU:O	1:D:469:CYS:HB3	2.06	0.56
1:A:323:ASN:ND2	1:A:356:HIS:HB2	2.20	0.56
1:D:325:LEU:HD12	1:D:325:LEU:C	2.26	0.56
1:D:159:PHE:O	1:D:159:PHE:HD1	1.88	0.56
1:D:516:GLN:C	1:D:517:HIS:CD2	2.78	0.56
1:B:46:LEU:HA	1:B:55:LEU:HD23	1.88	0.56
1:C:68:PHE:HD2	1:C:93:MSE:CE	1.92	0.56
1:A:479:GLU:CA	1:A:481:CYS:SG	2.93	0.56
1:D:506:ILE:HG23	1:D:542:MSE:HE3	1.88	0.56
1:C:545:ASP:OD1	1:C:546:GLU:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:HIS:CG	1:A:396:VAL:CG2	2.89	0.56
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.71	0.56
1:A:13:MSE:HE2	1:A:26:ILE:HD11	1.87	0.56
1:D:375:THR:HG23	1:D:377:CYS:HB3	1.88	0.56
1:A:652:GLU:HG2	1:A:653:LYS:HG3	1.88	0.56
1:C:498:LEU:HD13	1:C:505:LEU:CD1	2.35	0.56
1:B:323:ASN:ND2	1:B:356:HIS:HB2	2.21	0.56
1:B:88:THR:HG23	1:B:91:CYS:CA	2.36	0.56
1:D:563:GLU:O	1:D:565:THR:N	2.39	0.56
1:C:602:ASN:HD21	1:C:605:LEU:HD23	1.70	0.56
1:A:558:SER:HB2	1:A:585:ASN:OD1	2.06	0.56
1:A:46:LEU:HD23	1:A:55:LEU:HD23	1.86	0.56
1:A:13:MSE:HE2	1:A:26:ILE:CD1	2.36	0.56
1:A:369:HIS:HA	1:A:396:VAL:HG22	1.88	0.56
1:B:284:ALA:HB2	1:B:311:ASN:OD1	2.05	0.56
1:C:29:LYS:O	1:C:30:LYS:HD2	2.05	0.56
1:D:512:ASN:OD1	1:D:514:SER:OG	2.24	0.56
1:B:183:ASP:N	1:B:183:ASP:OD1	2.38	0.56
1:A:119:PRO:HG2	1:A:153:PRO:CB	2.36	0.56
1:A:115:ARG:NH2	1:A:145:TRP:O	2.39	0.55
1:C:586:GLY:N	1:C:613:ASN:OD1	2.38	0.55
1:B:32:VAL:HG22	1:B:95:MSE:HG2	1.88	0.55
1:B:32:VAL:HG21	1:B:95:MSE:CG	2.37	0.55
1:D:390:CYS:HB3	1:D:394:LEU:HB2	1.87	0.55
1:A:587:MSE:HG2	1:A:613:ASN:OD1	2.06	0.55
1:C:323:ASN:ND2	1:C:356:HIS:ND1	2.54	0.55
1:A:601:ILE:HD11	1:B:184:THR:C	2.27	0.55
1:D:159:PHE:HD2	1:D:220:PHE:CE2	2.24	0.55
1:B:77:ILE:HG23	1:B:79:HIS:CE1	2.40	0.55
1:C:36:VAL:CG1	1:C:37:LYS:H	2.05	0.55
1:A:471:ARG:CG	1:A:471:ARG:HH21	2.18	0.55
1:C:270:LEU:HD21	1:C:278:LEU:HD12	1.88	0.55
1:C:368:VAL:O	1:C:368:VAL:HG12	2.04	0.55
1:A:284:ALA:HB1	1:A:313:SER:HB3	1.88	0.55
1:B:375:THR:HG23	1:B:377:CYS:H	1.71	0.55
1:D:100:PRO:HD2	1:D:101:GLU:H	1.71	0.55
1:B:84:MSE:HE3	1:B:103:VAL:HB	1.87	0.55
1:B:117:ILE:HG22	1:B:118:PHE:CD2	2.42	0.55
1:D:16:ILE:HG23	1:D:56:LEU:CD1	2.36	0.55
1:C:84:MSE:HE1	1:C:106:VAL:HG11	1.88	0.55
1:C:561:LYS:O	1:C:562:ALA:HB3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:TYR:HD1	1:B:175:LYS:N	2.05	0.55
1:C:197:GLN:OE1	1:C:226:LYS:N	2.32	0.55
1:C:174:TYR:HD1	1:C:175:LYS:N	2.05	0.55
1:D:651:PRO:HG2	1:D:652:GLU:H	1.71	0.55
1:B:561:LYS:O	1:B:564:VAL:HG12	2.06	0.55
1:C:55:LEU:HD11	1:C:95:MSE:HE2	1.79	0.55
1:C:502:LEU:O	1:C:506:ILE:HG12	2.07	0.55
1:A:32:VAL:HG23	1:A:96:LYS:O	2.05	0.55
1:C:422:SER:O	1:C:424:LEU:CD1	2.55	0.55
1:C:474:GLY:C	1:C:476:GLN:H	2.10	0.55
1:D:408:LYS:CE	1:D:408:LYS:CA	2.85	0.55
1:A:218:GLN:HA	1:A:247:ARG:HG3	1.89	0.55
1:A:494:SER:HB2	1:A:521:GLY:O	2.07	0.55
1:A:456:GLY:HA2	1:A:489:THR:HG23	1.89	0.55
1:D:290:ASP:OD2	1:D:318:SER:HB3	2.08	0.54
1:B:88:THR:CG2	1:B:91:CYS:CB	2.86	0.54
1:D:99:SER:CB	1:D:101:GLU:HG3	2.36	0.54
1:D:84:MSE:SE	1:D:107:LEU:HD11	2.57	0.54
1:D:372:LEU:O	1:D:375:THR:CB	2.55	0.54
1:D:34:LEU:CD2	1:D:36:VAL:CG2	2.85	0.54
1:C:531:ASN:H	1:C:531:ASN:ND2	2.05	0.54
1:B:513:ARG:HH11	1:B:513:ARG:HA	1.71	0.54
1:C:14:GLU:OE1	1:C:14:GLU:HA	2.06	0.54
1:C:372:LEU:O	1:C:375:THR:HB	2.08	0.54
1:C:8:VAL:HG11	1:C:13:MSE:HE3	1.88	0.54
1:B:134:PRO:CD	1:B:137:ARG:HH21	2.19	0.54
1:D:118:PHE:HD2	1:D:126:ILE:HD12	1.66	0.54
1:C:610:TRP:CE3	1:C:615:ILE:CD1	2.90	0.54
1:A:174:TYR:CD1	1:A:174:TYR:C	2.81	0.54
1:C:287:SER:OG	1:C:287:SER:O	2.26	0.54
1:D:603:THR:OG1	1:D:603:THR:O	2.26	0.54
1:B:80:LYS:CG	1:B:81:PRO:CD	2.86	0.54
1:D:43:ASN:O	1:D:44:LYS:HD3	2.08	0.54
1:A:394:LEU:O	1:A:425:ALA:HB3	2.06	0.54
1:D:408:LYS:HE3	1:D:408:LYS:CA	2.37	0.54
1:A:471:ARG:NH1	1:A:497:GLY:O	2.41	0.54
1:B:9:PRO:HG2	1:B:12:LEU:HB3	1.90	0.54
1:C:484:GLU:OE1	1:C:508:TRP:HD1	1.89	0.54
1:A:478:LEU:HD13	1:A:508:TRP:HB2	1.90	0.54
1:A:600:GLN:OE1	1:B:185:ILE:HD13	2.07	0.54
1:A:104:SER:HG	1:A:137:ARG:HH11	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LYS:N	1:D:345:SER:O	2.41	0.54
1:B:404:PHE:CE1	1:B:440:PRO:HB3	2.43	0.54
1:C:212:ALA:HB2	1:C:237:GLN:CG	2.38	0.54
1:B:477:VAL:HG23	1:B:478:LEU:N	2.22	0.54
1:A:290:ASP:OD1	1:A:290:ASP:N	2.40	0.54
1:D:315:THR:OG1	1:D:317:LEU:HD12	2.07	0.54
1:B:415:SER:OG	3:B:702:CL:CL	2.60	0.54
1:C:381:MSE:CA	1:C:381:MSE:CE	2.85	0.54
1:A:98:VAL:CG2	1:A:99:SER:N	2.71	0.54
1:B:174:TYR:HD1	1:B:174:TYR:C	2.10	0.54
1:A:200:SER:OG	1:B:593:LYS:HE2	2.08	0.54
1:D:172:PHE:HE2	1:D:208:ILE:HB	1.72	0.54
1:D:222:LYS:HG3	1:D:250:GLU:HB2	1.90	0.54
1:D:289:GLU:O	1:D:293:VAL:HG23	2.06	0.54
1:B:24:ILE:CD1	1:B:25:LYS:N	2.68	0.54
1:C:54:PHE:CD1	1:C:67:THR:CG2	2.91	0.54
1:C:141:LEU:O	1:C:144:LEU:N	2.41	0.54
1:C:639:PRO:O	1:C:639:PRO:HG2	2.07	0.54
1:C:386:LEU:HD23	1:C:390:CYS:SG	2.47	0.54
1:A:485:ILE:CG2	1:A:512:ASN:HD22	1.90	0.53
1:C:329:LEU:HD23	1:C:335:THR:HG21	1.91	0.53
1:B:607:THR:HB	1:B:635:PHE:HD2	1.73	0.53
1:A:319:PRO:HD2	1:A:352:ASP:OD2	2.07	0.53
1:D:442:LYS:HG3	1:D:477:VAL:HG13	1.91	0.53
1:D:578:THR:HG22	1:D:604:LYS:HD2	1.90	0.53
1:C:162:MSE:HE1	1:C:217:ASN:HA	1.91	0.53
1:B:484:GLU:OE2	1:B:508:TRP:HA	2.08	0.53
1:B:80:LYS:CD	1:B:81:PRO:CD	2.85	0.53
1:A:601:ILE:CD1	1:B:184:THR:O	2.57	0.53
1:D:46:LEU:HD22	1:D:95:MSE:HE1	1.91	0.53
1:D:610:TRP:HZ3	1:D:615:ILE:HD13	1.74	0.53
1:C:162:MSE:O	1:C:166:VAL:HG23	2.09	0.53
1:B:506:ILE:CD1	1:B:539:LEU:HD13	2.38	0.53
1:A:638:ILE:CG2	1:A:640:MSE:CE	2.85	0.53
1:D:80:LYS:HE2	1:D:82:ALA:HB3	1.90	0.53
1:D:408:LYS:CE	1:D:408:LYS:HA	2.38	0.53
1:D:261:ASP:OD1	1:D:262:PHE:N	2.42	0.53
1:B:32:VAL:HG21	1:B:95:MSE:CB	2.36	0.53
1:A:474:GLY:O	1:A:475:ALA:HB3	2.07	0.53
1:A:474:GLY:C	1:A:477:VAL:HG12	2.29	0.53
1:A:76:VAL:HG13	1:A:86:VAL:CG2	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ALA:O	1:B:366:THR:HG22	2.09	0.53
1:B:197:GLN:OE1	1:B:226:LYS:N	2.36	0.53
1:B:484:GLU:OE2	1:B:508:TRP:CG	2.62	0.53
1:D:99:SER:CB	1:D:100:PRO:CD	2.87	0.53
1:D:516:GLN:HB2	1:D:517:HIS:CD2	2.44	0.53
1:B:16:ILE:O	1:B:19:VAL:HG12	2.09	0.53
1:C:498:LEU:HD11	1:C:505:LEU:CD1	2.39	0.53
1:B:117:ILE:CG2	1:B:118:PHE:CD2	2.92	0.53
1:A:607:THR:HB	1:A:635:PHE:HB2	1.90	0.53
1:C:107:LEU:O	1:C:108:ALA:C	2.42	0.53
1:C:466:LEU:HA	1:C:469:CYS:HB3	1.91	0.53
1:C:195:ASN:OD1	1:C:197:GLN:HG2	2.08	0.53
1:D:74:HIS:N	1:D:87:GLU:O	2.42	0.53
1:C:71:LEU:N	1:C:71:LEU:HD12	2.23	0.53
1:B:74:HIS:CE1	1:B:89:GLU:CB	2.81	0.53
1:D:68:PHE:CE2	1:D:86:VAL:CG1	2.91	0.53
1:A:543:ILE:HG22	1:A:574:ASN:HD22	1.74	0.53
1:B:77:ILE:O	1:B:85:VAL:HG12	2.09	0.53
1:B:297:SER:HB2	1:B:328:SER:HB2	1.90	0.53
1:D:256:ALA:N	1:D:286:ASN:OD1	2.42	0.53
1:D:172:PHE:CE2	1:D:208:ILE:HB	2.44	0.53
1:D:145:TRP:C	1:D:148:GLN:OE1	2.47	0.52
1:C:610:TRP:CD1	1:C:636:MSE:CE	2.92	0.52
1:D:51:CYS:C	1:D:70:TYR:CE2	2.82	0.52
1:B:46:LEU:HG	1:B:55:LEU:HD21	1.90	0.52
1:C:116:ARG:HG3	1:C:116:ARG:NH1	2.24	0.52
1:C:456:GLY:HA2	1:C:489:THR:CG2	2.38	0.52
1:D:408:LYS:O	1:D:408:LYS:HE2	2.08	0.52
1:D:72:GLU:OE2	1:D:90:LYS:HE3	2.09	0.52
1:A:382:VAL:O	1:A:386:LEU:HG	2.08	0.52
1:A:169:TRP:CZ3	1:A:170:LEU:HD21	2.44	0.52
1:D:111:GLY:O	1:D:115:ARG:N	2.36	0.52
1:A:73:ILE:HD12	1:A:127:MSE:HE3	1.90	0.52
1:D:298:ILE:HG22	1:D:299:GLN:HE21	1.75	0.52
1:A:368:VAL:O	1:A:368:VAL:HG12	2.09	0.52
1:A:602:ASN:HD21	1:A:605:LEU:CD2	2.23	0.52
1:C:411:GLU:O	1:C:413:PRO:HD3	2.10	0.52
1:B:604:LYS:CG	1:B:604:LYS:O	2.57	0.52
1:D:71:LEU:HD12	1:D:71:LEU:N	2.24	0.52
1:D:349:LEU:HD13	1:D:357:MSE:CE	2.33	0.52
1:B:71:LEU:HD21	1:B:118:PHE:CZ	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:HIS:HA	1:D:133:GLU:HB2	1.91	0.52
1:A:647:LEU:HD23	1:A:651:PRO:HA	1.92	0.52
1:C:478:LEU:CD1	1:C:508:TRP:CZ2	2.87	0.52
1:A:480:GLY:N	1:A:481:CYS:CA	2.72	0.52
1:A:485:ILE:O	1:A:512:ASN:ND2	2.42	0.52
1:A:640:MSE:HE2	1:A:640:MSE:HA	1.92	0.52
1:C:610:TRP:CH2	1:C:623:ILE:HG13	2.45	0.52
1:C:117:ILE:HG21	1:C:118:PHE:CE2	2.45	0.52
1:C:558:SER:HB2	1:C:585:ASN:OD1	2.09	0.52
1:B:513:ARG:CG	1:B:513:ARG:NH1	2.72	0.52
1:C:16:ILE:O	1:C:19:VAL:HG12	2.10	0.52
1:A:558:SER:O	1:A:559:LYS:HB2	2.10	0.52
1:D:72:GLU:HG2	1:D:89:GLU:CG	2.40	0.52
1:C:155:PRO:HB3	1:C:187:LEU:HD13	1.91	0.52
1:D:152:GLU:HG2	1:D:153:PRO:CD	2.40	0.52
1:C:556:ALA:HA	1:C:583:SER:O	2.09	0.52
1:D:52:ARG:N	1:D:70:TYR:CE2	2.78	0.52
1:D:424:LEU:CD1	1:D:424:LEU:N	2.72	0.52
1:B:195:ASN:OD1	1:B:197:GLN:HG2	2.10	0.52
1:B:16:ILE:HG23	1:B:56:LEU:HD13	1.90	0.52
1:D:13:MSE:CE	1:D:26:ILE:CD1	2.82	0.52
1:B:158:GLY:O	1:B:162:MSE:CG	2.58	0.52
1:B:158:GLY:O	1:B:162:MSE:HG3	2.09	0.52
1:C:655:GLU:HA	1:D:640:MSE:HE1	1.91	0.52
1:D:85:VAL:O	1:D:85:VAL:HG13	2.09	0.52
1:A:380:GLU:OE2	1:A:405:SER:OG	2.28	0.52
1:D:384:SER:HA	1:D:415:SER:HB3	1.92	0.52
1:A:330:SER:HB3	1:A:363:GLN:OE1	2.09	0.52
1:B:36:VAL:CG1	1:B:37:LYS:N	2.73	0.52
1:D:474:GLY:CA	1:D:475:ALA:CB	2.85	0.52
1:C:98:VAL:CG2	1:C:102:ASP:OD2	2.58	0.52
1:C:441:LEU:HD22	1:C:466:LEU:HD22	1.92	0.52
1:D:150:LEU:N	1:D:150:LEU:HD23	2.24	0.52
1:C:115:ARG:NH1	1:C:145:TRP:O	2.42	0.52
1:D:208:ILE:CG2	1:D:237:GLN:HE21	2.23	0.52
1:D:100:PRO:CG	1:D:101:GLU:N	2.73	0.52
1:D:397:LEU:HD11	1:D:399:LEU:CD1	2.40	0.52
1:A:174:TYR:C	1:A:174:TYR:HD1	2.13	0.52
1:C:645:GLN:HA	1:C:645:GLN:OE1	2.10	0.52
1:A:323:ASN:OD1	1:A:354:LEU:CA	2.58	0.51
1:B:36:VAL:HG13	1:B:37:LYS:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:ILE:HG22	1:D:574:ASN:HD22	1.71	0.51
1:D:54:PHE:CD1	1:D:67:THR:HG21	2.45	0.51
1:D:30:LYS:CE	1:D:102:ASP:OD1	2.57	0.51
1:C:169:TRP:CE3	1:C:170:LEU:HD21	2.45	0.51
1:B:16:ILE:HD11	1:B:45:VAL:HG21	1.92	0.51
1:C:513:ARG:HH21	1:C:547:ASP:HB3	1.76	0.51
1:C:662:GLU:OE1	1:D:638:ILE:HD11	2.09	0.51
1:C:503:SER:HA	1:C:506:ILE:CG1	2.40	0.51
1:C:8:VAL:HG11	1:C:13:MSE:CE	2.39	0.51
1:B:212:ALA:HB2	1:B:237:GLN:HG2	1.93	0.51
1:B:34:LEU:HD12	1:B:35:GLU:O	2.10	0.51
1:D:616:THR:CG2	1:D:617:ALA:H	2.22	0.51
1:A:54:PHE:CD2	1:A:67:THR:CG2	2.93	0.51
1:A:13:MSE:HE2	1:A:29:LYS:HD3	1.93	0.51
1:D:355:SER:O	1:D:359:ASN:HB2	2.11	0.51
1:D:115:ARG:CG	1:D:115:ARG:NH1	2.73	0.51
1:A:270:LEU:HD21	1:A:278:LEU:HD12	1.93	0.51
1:C:476:GLN:CA	1:C:476:GLN:NE2	2.73	0.51
1:A:352:ASP:O	1:A:354:LEU:HG	2.10	0.51
1:D:375:THR:CG2	1:D:377:CYS:HB3	2.41	0.51
1:D:80:LYS:HD2	1:D:81:PRO:N	2.26	0.51
1:B:184:THR:O	1:B:188:THR:OG1	2.16	0.51
1:A:138:LEU:HD23	1:A:139:ALA:HA	1.92	0.51
1:C:293:VAL:HG21	1:C:317:LEU:HD11	1.91	0.51
1:C:174:TYR:C	1:C:174:TYR:CD1	2.84	0.51
1:A:470:LEU:HD23	1:A:477:VAL:HG11	1.93	0.51
1:A:478:LEU:HD13	1:A:508:TRP:CG	2.46	0.51
1:A:484:GLU:HG3	1:A:508:TRP:CZ2	2.45	0.51
1:A:638:ILE:HG23	1:A:640:MSE:HE3	1.89	0.51
1:D:40:ARG:NH2	1:D:40:ARG:CG	2.72	0.51
1:C:512:ASN:OD1	1:C:514:SER:N	2.43	0.51
1:B:32:VAL:HG21	1:B:95:MSE:HG2	1.91	0.51
1:B:484:GLU:OE1	1:B:512:ASN:HB2	2.10	0.51
1:D:115:ARG:CZ	1:D:115:ARG:CB	2.89	0.51
1:D:507:VAL:CG2	1:D:508:TRP:N	2.73	0.51
1:C:144:LEU:O	1:C:147:SER:OG	2.28	0.51
1:D:72:GLU:CD	1:D:90:LYS:HE3	2.31	0.51
1:C:203:GLU:O	1:C:206:ASP:HB2	2.11	0.51
1:D:667:ARG:HG3	1:D:668:ASN:N	2.24	0.51
1:C:310:LEU:HD11	1:C:312:LEU:HD11	1.93	0.51
1:D:64:LEU:HD21	1:D:66:LEU:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:HD22	1:C:422:SER:HB2	1.92	0.51
1:D:475:ALA:C	1:D:476:GLN:HG2	2.31	0.51
1:C:636:MSE:HB3	1:C:665:LEU:CD1	2.41	0.51
1:D:99:SER:HB3	1:D:100:PRO:CD	2.40	0.51
1:D:383:CYS:O	1:D:384:SER:C	2.47	0.51
1:D:197:GLN:OE1	1:D:226:LYS:N	2.42	0.51
1:B:478:LEU:HB2	1:B:508:TRP:CD2	2.46	0.50
1:A:484:GLU:CD	1:A:508:TRP:HE1	2.11	0.50
1:B:375:THR:HG23	1:B:377:CYS:N	2.27	0.50
1:A:23:LYS:CD	1:A:23:LYS:N	2.73	0.50
1:B:652:GLU:HG2	1:B:653:LYS:H	1.74	0.50
1:D:506:ILE:CD1	1:D:539:LEU:HD13	2.41	0.50
1:C:68:PHE:HE1	1:C:73:ILE:HD11	1.75	0.50
1:A:589:ASP:CG	1:A:616:THR:OG1	2.50	0.50
1:B:366:THR:O	1:B:366:THR:OG1	2.26	0.50
1:B:93:MSE:HG3	1:B:95:MSE:HE2	1.93	0.50
1:C:531:ASN:C	1:C:534:PRO:HD2	2.32	0.50
1:B:222:LYS:HG3	1:B:250:GLU:HB2	1.93	0.50
1:A:478:LEU:O	1:A:480:GLY:N	2.41	0.50
1:C:258:LEU:HD23	1:C:262:PHE:CD2	2.45	0.50
1:C:478:LEU:HD23	1:C:508:TRP:CH2	2.42	0.50
1:D:355:SER:HA	1:D:358:TYR:CD2	2.46	0.50
1:D:355:SER:HA	1:D:358:TYR:HD2	1.76	0.50
1:B:78:CYS:CB	1:B:132:MSE:HA	2.28	0.50
1:D:68:PHE:N	1:D:68:PHE:CD1	2.80	0.50
1:A:143:ALA:O	1:A:146:ASP:N	2.45	0.50
1:C:115:ARG:HB3	1:C:115:ARG:NH2	2.17	0.50
1:D:350:ARG:HD3	1:D:350:ARG:N	2.07	0.50
1:C:80:LYS:HD3	1:C:80:LYS:C	2.32	0.50
1:B:561:LYS:HA	1:B:585:ASN:O	2.11	0.50
1:C:498:LEU:CD1	1:C:505:LEU:HD12	2.41	0.50
1:D:208:ILE:N	1:D:209:PRO:HD2	2.26	0.50
1:B:506:ILE:HG23	1:B:542:MSE:CE	2.42	0.50
1:A:192:ARG:NH1	1:A:219:TRP:CZ3	2.80	0.50
1:C:667:ARG:HG3	1:C:668:ASN:N	2.25	0.50
1:D:115:ARG:HB2	1:D:115:ARG:NH1	2.27	0.50
1:A:23:LYS:N	1:A:24:ILE:O	2.45	0.50
1:A:53:ALA:HB3	1:A:68:PHE:CE1	2.47	0.50
1:D:174:TYR:HD1	1:D:175:LYS:N	2.10	0.50
1:A:92:ASN:N	1:A:92:ASN:OD1	2.44	0.50
1:B:7:ASP:O	1:B:31:LYS:CD	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:VAL:HG23	1:B:508:TRP:N	2.27	0.50
1:C:86:VAL:HB	1:C:93:MSE:HG3	1.94	0.50
1:A:638:ILE:HD13	1:A:640:MSE:HE3	1.91	0.50
1:C:117:ILE:CG2	1:C:118:PHE:CD2	2.95	0.50
1:D:55:LEU:O	1:D:64:LEU:HD23	2.12	0.50
1:A:602:ASN:HD21	1:A:605:LEU:HD23	1.76	0.49
1:D:613:ASN:O	1:D:614:ASN:HB2	2.12	0.49
1:D:631:TYR:O	1:D:668:ASN:CG	2.50	0.49
1:C:372:LEU:O	1:C:375:THR:CB	2.60	0.49
1:C:503:SER:O	1:C:506:ILE:CB	2.59	0.49
1:C:611:ASP:O	1:C:612:LYS:HB2	2.11	0.49
1:B:569:ASN:OD1	1:B:594:MSE:HG3	2.12	0.49
1:B:52:ARG:CG	1:B:53:ALA:N	2.75	0.49
1:B:484:GLU:CB	1:B:508:TRP:NE1	2.73	0.49
1:C:386:LEU:CD2	1:C:390:CYS:SG	3.00	0.49
1:A:493:ILE:C	1:A:496:ASN:ND2	2.58	0.49
1:C:379:LEU:CD1	1:C:402:SER:CB	2.88	0.49
1:A:73:ILE:HD13	1:A:127:MSE:HE1	1.94	0.49
1:A:506:ILE:CD1	1:A:539:LEU:HD13	2.43	0.49
1:A:212:ALA:HB2	1:A:237:GLN:HG2	1.94	0.49
1:B:610:TRP:N	1:B:610:TRP:CD1	2.80	0.49
1:C:536:LEU:CB	1:C:566:ILE:HD11	2.42	0.49
1:D:54:PHE:HD1	1:D:64:LEU:HD11	1.78	0.49
1:A:602:ASN:ND2	1:A:605:LEU:CD2	2.76	0.49
1:C:387:LEU:O	1:C:387:LEU:HD12	2.13	0.49
1:D:323:ASN:ND2	1:D:356:HIS:CB	2.75	0.49
1:B:667:ARG:HG3	1:B:668:ASN:N	2.27	0.49
1:D:394:LEU:O	1:D:426:LEU:HD12	2.12	0.49
1:B:134:PRO:HD2	1:B:137:ARG:HD3	1.94	0.49
1:C:647:LEU:O	1:C:651:PRO:HB3	2.12	0.49
1:A:506:ILE:HD13	1:A:539:LEU:HD13	1.95	0.49
1:B:416:PHE:HE2	1:B:440:PRO:O	1.96	0.49
1:D:72:GLU:HG2	1:D:89:GLU:HG3	1.93	0.49
1:D:231:SER:OG	1:D:234:VAL:HG23	2.12	0.49
1:A:197:GLN:OE1	1:A:226:LYS:N	2.39	0.49
1:B:69:SER:O	1:B:72:GLU:N	2.46	0.49
1:C:282:ASN:OD1	1:C:282:ASN:C	2.51	0.49
1:D:412:VAL:HG23	1:D:412:VAL:O	2.12	0.49
1:D:636:MSE:HB3	1:D:665:LEU:HD11	1.92	0.49
1:C:604:LYS:CG	1:C:604:LYS:O	2.60	0.49
1:C:69:SER:O	1:C:72:GLU:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PHE:HD1	1:D:159:PHE:C	2.16	0.49
1:C:174:TYR:C	1:C:174:TYR:HD1	2.15	0.49
1:B:160:SER:O	1:B:163:TYR:HB3	2.11	0.49
1:A:12:LEU:O	1:A:16:ILE:HG13	2.11	0.49
1:C:379:LEU:HD13	1:C:402:SER:HB2	1.92	0.49
1:A:618:GLN:NE2	1:A:618:GLN:CA	2.76	0.49
1:C:474:GLY:C	1:C:476:GLN:N	2.66	0.49
1:D:97:MSE:HG3	1:D:103:VAL:CG2	2.43	0.49
1:C:16:ILE:HG12	1:C:56:LEU:HD13	1.94	0.49
1:C:260:ILE:O	1:C:263:ALA:HB3	2.12	0.49
1:D:145:TRP:N	1:D:148:GLN:OE1	2.46	0.49
1:A:484:GLU:CG	1:A:508:TRP:CE2	2.89	0.49
1:C:348:ALA:C	1:C:349:LEU:HD23	2.33	0.49
1:A:640:MSE:HA	1:A:640:MSE:CE	2.40	0.49
1:C:431:LEU:O	1:C:434:THR:CG2	2.50	0.49
1:D:80:LYS:HG3	1:D:83:GLN:H	1.77	0.49
1:D:68:PHE:CZ	1:D:86:VAL:HG11	2.47	0.49
1:D:303:LEU:HD23	1:D:304:PRO:HD2	1.95	0.49
1:D:297:SER:HB2	1:D:328:SER:HB2	1.95	0.49
1:B:290:ASP:N	1:B:290:ASP:OD1	2.43	0.49
1:D:26:ILE:CD1	1:D:47:VAL:CG2	2.80	0.48
1:C:397:LEU:HD11	1:C:399:LEU:HD11	1.95	0.48
1:D:310:LEU:HD11	1:D:312:LEU:CD1	2.43	0.48
1:A:68:PHE:HD1	1:A:93:MSE:HE1	1.78	0.48
1:C:647:LEU:CD2	1:C:654:THR:HB	2.43	0.48
1:A:174:TYR:HD1	1:A:175:LYS:N	2.11	0.48
1:C:224:SER:HB2	1:C:252:VAL:HB	1.95	0.48
1:D:354:LEU:O	1:D:357:MSE:HB3	2.13	0.48
1:D:507:VAL:CG2	1:D:508:TRP:H	2.23	0.48
1:B:124:LEU:HD13	1:B:145:TRP:HZ3	1.78	0.48
1:B:115:ARG:HH22	1:B:150:LEU:HD11	1.75	0.48
1:B:506:ILE:HG23	1:B:542:MSE:HE3	1.94	0.48
1:B:474:GLY:HA2	1:B:477:VAL:HG13	1.95	0.48
1:A:14:GLU:O	1:A:16:ILE:N	2.46	0.48
1:C:610:TRP:CZ3	1:C:623:ILE:HG13	2.48	0.48
1:D:64:LEU:CD2	1:D:66:LEU:N	2.76	0.48
1:A:80:LYS:HD2	1:A:80:LYS:C	2.33	0.48
1:D:185:ILE:O	1:D:189:GLN:HG3	2.13	0.48
1:A:12:LEU:HD12	1:A:13:MSE:N	2.28	0.48
1:D:330:SER:HB3	1:D:363:GLN:OE1	2.14	0.48
1:B:97:MSE:CG	1:B:103:VAL:HG12	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:HIS:CE1	1:B:597:LYS:HE3	2.49	0.48
1:D:159:PHE:CD1	1:D:159:PHE:C	2.86	0.48
1:D:516:GLN:HB2	1:D:517:HIS:HD2	1.79	0.48
1:B:12:LEU:O	1:B:12:LEU:HD12	2.13	0.48
1:A:441:LEU:HD22	1:A:466:LEU:HD22	1.96	0.48
1:C:638:ILE:O	1:C:638:ILE:HG23	2.13	0.48
1:D:322:VAL:HG21	1:D:349:LEU:HD22	1.95	0.48
1:D:586:GLY:HA2	1:D:614:ASN:ND2	2.28	0.48
1:B:254:GLU:O	1:B:255:ASN:C	2.51	0.48
1:D:478:LEU:HA	1:D:508:TRP:CZ2	2.49	0.48
1:D:478:LEU:CB	1:D:508:TRP:NE1	2.73	0.48
1:D:310:LEU:HD11	1:D:312:LEU:HD11	1.96	0.48
1:D:73:ILE:CD1	1:D:127:MSE:HE2	2.43	0.48
1:D:602:ASN:HD21	1:D:605:LEU:HD12	1.79	0.48
1:C:602:ASN:HD21	1:C:605:LEU:CD2	2.26	0.48
1:D:79:HIS:O	1:D:133:GLU:HB3	2.13	0.48
1:A:56:LEU:HD23	1:A:64:LEU:HA	1.96	0.48
1:B:528:LYS:O	1:B:531:ASN:HB2	2.14	0.48
1:C:449:ALA:CA	1:C:485:ILE:HG23	2.43	0.47
1:D:111:GLY:O	1:D:115:ARG:CG	2.61	0.47
1:C:375:THR:HG23	1:C:377:CYS:HB3	1.95	0.47
1:D:312:LEU:C	1:D:315:THR:HG23	2.34	0.47
1:D:323:ASN:HD21	1:D:356:HIS:HB2	1.74	0.47
1:C:81:PRO:O	1:C:100:PRO:HB3	2.13	0.47
1:A:558:SER:HB3	1:A:560:LEU:HG	1.96	0.47
1:B:118:PHE:CD1	1:B:216:TYR:HB2	2.49	0.47
1:B:26:ILE:O	1:B:26:ILE:HG12	2.14	0.47
1:D:369:HIS:CD2	1:D:396:VAL:HG21	2.49	0.47
1:B:368:VAL:HG12	1:B:368:VAL:O	2.13	0.47
1:C:513:ARG:NH2	1:C:547:ASP:HB3	2.28	0.47
1:C:610:TRP:CZ3	1:C:615:ILE:CD1	2.97	0.47
1:C:212:ALA:HB2	1:C:237:GLN:HE21	1.79	0.47
1:B:474:GLY:O	1:B:475:ALA:CB	2.62	0.47
1:C:68:PHE:HE2	1:C:93:MSE:CE	2.21	0.47
1:A:141:LEU:CD2	1:A:144:LEU:HD23	2.44	0.47
1:A:666:LEU:HD22	1:B:666:LEU:HD13	1.94	0.47
1:B:580:VAL:CG1	1:B:608:VAL:HG22	2.44	0.47
1:B:528:LYS:HE3	1:B:529:SER:H	1.80	0.47
1:D:532:LEU:O	1:D:532:LEU:HD23	2.14	0.47
1:D:100:PRO:CG	1:D:101:GLU:H	2.26	0.47
1:D:506:ILE:HG21	1:D:538:ASN:CB	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:THR:HG22	1:D:617:ALA:H	1.77	0.47
1:A:506:ILE:CG2	1:A:542:MSE:HE3	2.43	0.47
1:B:36:VAL:HG13	1:B:37:LYS:N	2.30	0.47
1:C:353:ASP:OD1	1:C:355:SER:CB	2.62	0.47
1:A:103:VAL:CG2	1:A:104:SER:N	2.78	0.47
1:C:441:LEU:HD11	1:C:445:LEU:CD1	2.44	0.47
1:D:152:GLU:HG2	1:D:153:PRO:HD3	1.97	0.47
1:C:297:SER:HB2	1:C:328:SER:HB2	1.95	0.47
1:C:58:ALA:C	1:C:59:ARG:HG3	2.34	0.47
1:C:484:GLU:N	1:C:508:TRP:NE1	2.63	0.47
1:B:32:VAL:CG2	1:B:95:MSE:CB	2.92	0.47
1:A:9:PRO:C	1:A:12:LEU:HG	2.33	0.47
1:C:157:GLY:O	1:C:162:MSE:HE3	2.14	0.47
1:D:298:ILE:HG22	1:D:299:GLN:N	2.29	0.47
1:D:384:SER:O	1:D:387:LEU:HB3	2.15	0.47
1:D:414:PRO:O	1:D:418:GLN:HB2	2.14	0.47
1:C:61:PRO:HG2	1:C:61:PRO:O	2.14	0.47
1:B:120:GLY:O	1:B:121:LEU:HD23	2.14	0.47
1:A:383:CYS:HG	1:A:416:PHE:HD1	1.56	0.47
1:A:498:LEU:CD1	1:A:502:LEU:CD1	2.84	0.47
1:A:80:LYS:CD	1:A:81:PRO:N	2.78	0.47
1:A:195:ASN:OD1	1:A:197:GLN:HG2	2.14	0.47
1:C:634:ARG:O	1:D:666:LEU:HD11	2.14	0.47
1:B:613:ASN:O	1:B:614:ASN:HB2	2.13	0.47
1:B:401:ARG:N	1:B:434:THR:HG22	2.30	0.47
1:D:442:LYS:HE2	1:D:446:LEU:CD1	2.45	0.47
1:A:93:MSE:HG3	1:A:95:MSE:HE3	1.97	0.47
1:B:513:ARG:NH1	1:B:513:ARG:HA	2.30	0.47
1:A:384:SER:HA	1:A:415:SER:HB3	1.97	0.47
1:D:115:ARG:CB	1:D:115:ARG:NH1	2.78	0.47
1:A:144:LEU:O	1:A:144:LEU:HD12	2.15	0.47
1:B:10:ARG:O	1:B:13:MSE:HB2	2.15	0.47
1:B:57:SER:HB3	1:B:65:GLU:OE2	2.15	0.46
1:A:14:GLU:O	1:A:15:SER:C	2.54	0.46
1:C:261:ASP:OD1	1:C:262:PHE:N	2.48	0.46
1:B:71:LEU:HD11	1:B:118:PHE:HZ	1.80	0.46
1:A:69:SER:HB3	1:A:169:TRP:CD1	2.49	0.46
1:B:660:LYS:O	1:B:664:TYR:CD2	2.67	0.46
1:A:643:ALA:O	1:A:646:ALA:N	2.48	0.46
1:C:128:LYS:CD	1:C:128:LYS:N	2.78	0.46
1:C:128:LYS:HD2	1:C:128:LYS:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:CYS:HB2	1:D:132:MSE:HG2	1.97	0.46
1:D:401:ARG:N	1:D:434:THR:HG22	2.31	0.46
1:A:602:ASN:CG	1:A:605:LEU:HD23	2.35	0.46
1:A:103:VAL:HG23	1:A:104:SER:N	2.28	0.46
1:B:568:ILE:HD11	1:B:587:MSE:SE	2.65	0.46
1:B:330:SER:HB3	1:B:363:GLN:OE1	2.14	0.46
1:B:118:PHE:HD1	1:B:216:TYR:CB	2.27	0.46
1:B:226:LYS:O	1:B:227:ASP:HB2	2.14	0.46
1:D:545:ASP:OD1	1:D:546:GLU:N	2.48	0.46
1:D:258:LEU:CD2	1:D:262:PHE:HE2	1.99	0.46
1:B:354:LEU:HB3	1:B:358:TYR:CD2	2.45	0.46
1:D:44:LYS:NZ	1:D:65:GLU:CD	2.68	0.46
1:D:100:PRO:CD	1:D:101:GLU:N	2.73	0.46
1:A:122:SER:HA	1:A:123:PRO:HD3	1.82	0.46
1:A:427:ILE:O	1:A:427:ILE:HG12	2.14	0.46
1:D:144:LEU:HA	1:D:147:SER:OG	2.15	0.46
1:D:111:GLY:HA2	1:D:114:LEU:HB2	1.97	0.46
1:D:26:ILE:HB	1:D:47:VAL:CG2	2.46	0.46
1:D:325:LEU:CD1	1:D:329:LEU:CD1	2.93	0.46
1:D:100:PRO:HG2	1:D:101:GLU:N	2.30	0.46
1:D:30:LYS:HA	1:D:30:LYS:HD2	1.69	0.46
1:D:254:GLU:HG3	1:D:284:ALA:O	2.15	0.46
1:D:284:ALA:CB	1:D:313:SER:HB3	2.44	0.46
1:C:155:PRO:O	1:C:156:CYS:HB2	2.16	0.46
1:B:610:TRP:HD1	1:B:610:TRP:H	1.63	0.46
1:D:441:LEU:HD11	1:D:445:LEU:HD11	1.97	0.46
1:C:336:ALA:O	1:C:366:THR:HG22	2.15	0.46
1:B:88:THR:CG2	1:B:91:CYS:CA	2.93	0.46
1:C:534:PRO:O	1:C:537:ASP:HB2	2.16	0.46
1:D:599:LEU:HD22	1:D:633:LEU:HD22	1.97	0.46
1:B:117:ILE:HB	1:B:118:PHE:CD2	2.51	0.46
1:C:112:THR:HG23	1:C:148:GLN:OE1	2.15	0.46
1:C:15:SER:O	1:C:18:ASP:HB2	2.16	0.46
1:C:662:GLU:OE1	1:D:638:ILE:CD1	2.64	0.46
1:D:22:ARG:HD3	1:D:22:ARG:HA	1.49	0.46
1:A:138:LEU:O	1:A:141:LEU:HB2	2.16	0.46
1:D:493:ILE:HD11	1:D:520:LEU:CD2	2.44	0.46
1:D:575:THR:O	1:D:604:LYS:HG2	2.16	0.46
1:D:27:SER:CB	1:D:109:HIS:CE1	2.98	0.46
1:B:98:VAL:HG22	1:B:102:ASP:OD2	2.14	0.46
1:D:12:LEU:HD12	1:D:12:LEU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LEU:HA	1:B:210:ILE:HD12	1.98	0.46
2:B:701:OHB:C	3:B:702:CL:CL	3.00	0.46
1:D:437:SER:C	1:D:440:PRO:HD2	2.36	0.46
1:D:516:GLN:CB	1:D:517:HIS:CD2	2.99	0.46
1:D:517:HIS:CD2	1:D:517:HIS:N	2.83	0.46
1:A:441:LEU:HD11	1:A:445:LEU:HD11	1.97	0.46
1:A:561:LYS:O	1:A:564:VAL:HG12	2.15	0.46
1:C:477:VAL:CG2	1:C:478:LEU:HD23	2.46	0.46
1:D:377:CYS:O	1:D:403:VAL:CG2	2.62	0.46
1:D:513:ARG:HH21	1:D:513:ARG:CG	2.07	0.46
1:B:375:THR:HG23	1:B:377:CYS:HB3	1.98	0.46
1:D:312:LEU:O	1:D:315:THR:HG23	2.15	0.46
1:D:379:LEU:HB2	1:D:404:PHE:HA	1.97	0.46
1:D:563:GLU:C	1:D:565:THR:N	2.64	0.46
1:B:52:ARG:HG2	1:B:53:ALA:N	2.30	0.46
1:B:80:LYS:HE3	1:B:81:PRO:CD	2.34	0.46
1:A:315:THR:OG1	1:A:317:LEU:HD13	2.15	0.46
1:D:503:SER:O	1:D:504:THR:C	2.53	0.46
1:B:513:ARG:HH11	1:B:513:ARG:HG2	1.80	0.46
1:D:77:ILE:HB	1:D:85:VAL:CG1	2.44	0.46
1:B:208:ILE:HG23	1:B:237:GLN:HE21	1.81	0.46
1:A:74:HIS:CE1	1:A:89:GLU:HG2	2.51	0.46
1:B:117:ILE:HG22	1:B:118:PHE:N	2.31	0.46
1:C:226:LYS:O	1:C:227:ASP:HB2	2.16	0.46
1:D:369:HIS:CD2	1:D:396:VAL:CG2	2.98	0.46
1:A:329:LEU:HD23	1:A:335:THR:HG21	1.97	0.46
1:B:260:ILE:HD11	1:B:291:ARG:HB3	1.98	0.46
1:D:66:LEU:CD1	1:D:93:MSE:HE2	2.45	0.45
1:C:222:LYS:HG3	1:C:250:GLU:HB2	1.98	0.45
1:A:256:ALA:CB	1:A:258:LEU:CD1	2.93	0.45
1:D:323:ASN:CG	1:D:356:HIS:HB2	2.36	0.45
1:D:604:LYS:CG	1:D:604:LYS:O	2.58	0.45
1:D:605:LEU:O	1:D:633:LEU:HD12	2.16	0.45
1:A:485:ILE:O	1:A:485:ILE:HG23	2.16	0.45
1:B:372:LEU:O	1:B:375:THR:HB	2.16	0.45
1:D:68:PHE:N	1:D:68:PHE:HD1	2.13	0.45
1:D:205:ARG:O	1:D:208:ILE:HG13	2.16	0.45
1:A:528:LYS:HB2	1:A:531:ASN:ND2	2.31	0.45
1:C:193:GLU:HG3	1:C:222:LYS:CG	2.46	0.45
1:A:68:PHE:HE2	1:A:73:ILE:HD11	1.82	0.45
1:D:40:ARG:NH2	1:D:40:ARG:HG2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:LEU:HD13	1:C:457:VAL:HG21	1.99	0.45
1:C:403:VAL:HG23	1:C:403:VAL:O	2.17	0.45
1:B:507:VAL:CG2	1:B:508:TRP:N	2.79	0.45
1:C:610:TRP:CZ2	1:C:636:MSE:HE2	2.46	0.45
1:D:65:GLU:C	1:D:66:LEU:HG	2.37	0.45
1:D:172:PHE:CD2	1:D:209:PRO:CD	2.96	0.45
1:A:618:GLN:HE21	1:A:618:GLN:CA	2.29	0.45
1:A:543:ILE:CG2	1:A:574:ASN:HD22	2.28	0.45
1:A:620:PHE:CE1	1:A:639:PRO:HG3	2.52	0.45
1:D:607:THR:HB	1:D:635:PHE:HB2	1.98	0.45
1:A:484:GLU:CG	1:A:508:TRP:CZ2	2.99	0.45
1:D:477:VAL:C	1:D:478:LEU:CG	2.85	0.45
1:C:258:LEU:HD12	1:C:258:LEU:N	2.32	0.45
1:A:32:VAL:CG2	1:A:95:MSE:HB3	2.45	0.45
1:C:650:ASN:C	1:C:652:GLU:CB	2.85	0.45
1:A:157:GLY:O	1:A:162:MSE:HE3	2.17	0.45
1:C:144:LEU:HA	1:C:147:SER:OG	2.17	0.45
1:C:201:HIS:HB2	1:D:590:MSE:HE1	1.99	0.45
1:B:181:ASP:OD2	1:B:185:ILE:HD12	2.16	0.45
1:C:26:ILE:CG2	1:C:47:VAL:HG13	2.46	0.45
1:A:137:ARG:HE	1:A:137:ARG:HB3	1.63	0.45
1:B:652:GLU:CG	1:B:653:LYS:N	2.79	0.45
1:A:80:LYS:CD	1:A:80:LYS:C	2.85	0.45
1:C:461:LEU:C	1:C:464:CYS:HG	2.19	0.45
1:B:527:MSE:CE	1:B:531:ASN:HB3	2.46	0.45
1:B:329:LEU:HD23	1:B:335:THR:HG21	1.99	0.45
1:B:639:PRO:HG2	1:B:639:PRO:O	2.16	0.45
1:C:375:THR:HG23	1:C:377:CYS:H	1.82	0.45
1:D:54:PHE:HA	1:D:67:THR:HG23	1.99	0.45
1:A:143:ALA:CA	1:A:146:ASP:HB2	2.45	0.45
1:B:315:THR:O	1:B:316:SER:HB2	2.17	0.45
1:D:313:SER:O	1:D:314:LYS:C	2.53	0.45
1:D:71:LEU:HD12	1:D:71:LEU:H	1.81	0.45
1:A:609:ILE:HG13	1:A:637:PRO:HG2	1.99	0.45
1:A:204:HIS:CD2	1:A:231:SER:HB3	2.52	0.45
1:D:410:LYS:HG2	1:D:410:LYS:H	1.56	0.45
1:D:20:ILE:HG13	1:D:21:GLY:N	2.31	0.45
1:A:493:ILE:C	1:A:496:ASN:HD21	2.19	0.45
1:C:117:ILE:HB	1:C:118:PHE:CE2	2.51	0.45
1:D:34:LEU:CD2	1:D:36:VAL:HG23	2.47	0.45
1:D:52:ARG:HG3	1:D:68:PHE:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:MSE:O	1:C:17:LYS:HG2	2.17	0.45
1:C:26:ILE:HG23	1:C:47:VAL:HG13	1.97	0.45
1:A:528:LYS:HD3	1:A:528:LYS:HA	1.61	0.45
1:D:397:LEU:HD11	1:D:399:LEU:CG	2.47	0.45
1:A:313:SER:O	1:A:314:LYS:C	2.54	0.45
1:C:173:SER:O	1:C:174:TYR:C	2.56	0.45
1:A:466:LEU:HA	1:A:469:CYS:HB3	1.99	0.45
1:C:319:PRO:HB3	1:C:354:LEU:HD13	1.98	0.45
1:D:536:LEU:CB	1:D:566:ILE:HD11	2.47	0.45
1:C:54:PHE:CE1	1:C:67:THR:HG21	2.52	0.45
1:A:263:ALA:HB3	1:A:292:GLY:HA3	1.99	0.45
1:B:603:THR:OG1	1:B:603:THR:O	2.34	0.45
1:D:171:GLY:C	1:D:172:PHE:HD1	2.20	0.45
1:B:77:ILE:CG2	1:B:79:HIS:CE1	3.00	0.45
1:C:303:LEU:HD23	1:C:304:PRO:HD2	1.99	0.45
1:A:545:ASP:OD1	1:A:546:GLU:N	2.50	0.45
1:C:288:LEU:HG	1:C:288:LEU:H	1.55	0.45
1:B:408:LYS:HB3	1:B:408:LYS:HE2	1.61	0.45
1:D:111:GLY:O	1:D:115:ARG:HG3	2.17	0.44
1:C:563:GLU:C	1:C:565:THR:H	2.21	0.44
1:B:375:THR:CG2	1:B:377:CYS:HB3	2.46	0.44
1:A:525:ASN:N	1:A:525:ASN:HD22	2.15	0.44
1:B:323:ASN:ND2	1:B:356:HIS:CB	2.81	0.44
1:C:137:ARG:HA	1:C:140:SER:OG	2.17	0.44
1:C:9:PRO:HG2	1:C:12:LEU:HB3	2.00	0.44
1:C:115:ARG:CG	1:C:115:ARG:NH2	2.73	0.44
1:B:115:ARG:NH1	1:B:150:LEU:CD1	2.79	0.44
1:B:219:TRP:CG	1:B:219:TRP:O	2.70	0.44
1:C:286:ASN:O	1:C:315:THR:HA	2.17	0.44
1:C:587:MSE:HG2	1:C:613:ASN:ND2	2.31	0.44
1:B:603:THR:O	1:B:632:THR:HG21	2.17	0.44
1:D:360:PHE:CD1	1:D:360:PHE:O	2.70	0.44
1:A:13:MSE:CE	1:A:26:ILE:HD11	2.44	0.44
1:B:111:GLY:HA3	1:B:145:TRP:CZ2	2.51	0.44
1:C:395:ALA:O	1:C:427:ILE:CG2	2.63	0.44
1:B:48:LEU:HB3	1:B:70:TYR:OH	2.18	0.44
1:C:378:SER:HB2	1:C:406:HIS:CD2	2.52	0.44
1:A:482:ILE:CG2	1:A:483:ALA:N	2.80	0.44
1:A:500:SER:C	1:A:502:LEU:H	2.21	0.44
1:D:34:LEU:CD2	1:D:42:GLU:CB	2.85	0.44
1:B:513:ARG:HG2	1:B:513:ARG:NH1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:LYS:HD3	1:D:408:LYS:O	2.18	0.44
1:A:163:TYR:CE1	1:A:167:CYS:SG	3.10	0.44
1:A:30:LYS:HE2	1:A:105:GLU:OE2	2.18	0.44
1:D:26:ILE:HB	1:D:47:VAL:HG23	2.00	0.44
1:A:80:LYS:HD3	1:A:81:PRO:CD	2.48	0.44
1:A:46:LEU:HD23	1:A:55:LEU:CD2	2.47	0.44
1:A:169:TRP:CE3	1:A:170:LEU:HD21	2.52	0.44
1:C:328:SER:O	1:C:331:ALA:HB3	2.18	0.44
1:A:136:GLU:CD	1:A:136:GLU:H	2.19	0.44
1:C:375:THR:CG2	1:C:377:CYS:HB3	2.48	0.44
1:D:212:ALA:HB2	1:D:237:GLN:HG2	2.00	0.44
1:D:142:GLN:O	1:D:146:ASP:CG	2.56	0.44
1:C:387:LEU:HA	1:C:391:LEU:HD21	1.99	0.44
1:A:387:LEU:HD21	1:A:418:GLN:OE1	2.18	0.44
1:C:310:LEU:HD11	1:C:312:LEU:CD1	2.47	0.44
1:D:380:GLU:OE2	1:D:405:SER:OG	2.35	0.44
1:B:478:LEU:CB	1:B:508:TRP:CD2	3.01	0.44
1:A:509:LEU:O	1:A:512:ASN:HB3	2.18	0.44
1:C:416:PHE:CE1	1:C:420:PHE:HE2	2.35	0.44
1:D:605:LEU:O	1:D:633:LEU:CD1	2.66	0.44
1:A:543:ILE:HG23	1:A:574:ASN:ND2	2.33	0.44
1:C:650:ASN:C	1:C:652:GLU:HB3	2.38	0.44
1:A:456:GLY:HA2	1:A:489:THR:CG2	2.47	0.44
1:B:64:LEU:HD11	1:B:67:THR:HG23	1.99	0.44
1:A:374:ASN:ND2	1:A:401:ARG:NH2	2.50	0.44
1:C:513:ARG:NH2	1:C:547:ASP:CB	2.81	0.44
1:C:610:TRP:HZ3	1:C:615:ILE:HD13	1.80	0.44
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.83	0.44
1:D:73:ILE:HD13	1:D:127:MSE:HE2	1.99	0.44
1:A:77:ILE:HD12	1:A:85:VAL:HG11	1.99	0.44
1:C:189:GLN:O	1:C:190:ASP:C	2.53	0.44
1:C:383:CYS:HA	1:C:386:LEU:HB2	2.00	0.44
1:A:26:ILE:O	1:A:26:ILE:HG13	2.17	0.44
1:A:500:SER:C	1:A:502:LEU:N	2.71	0.44
1:D:80:LYS:HG3	1:D:83:GLN:N	2.33	0.44
1:C:533:THR:N	1:C:534:PRO:CD	2.81	0.44
1:D:64:LEU:C	1:D:64:LEU:CD2	2.86	0.44
1:D:424:LEU:HD12	1:D:424:LEU:N	2.32	0.44
1:A:471:ARG:HH21	1:A:471:ARG:HG3	1.82	0.44
1:A:412:VAL:O	1:A:412:VAL:HG22	2.18	0.44
1:B:354:LEU:HB3	1:B:358:TYR:CZ	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:MSE:HE3	1:D:97:MSE:HB3	1.78	0.43
1:D:602:ASN:ND2	1:D:605:LEU:CD1	2.81	0.43
1:C:474:GLY:CA	1:C:476:GLN:HG2	2.43	0.43
1:A:479:GLU:O	1:A:481:CYS:HB2	2.18	0.43
1:A:93:MSE:HG3	1:A:95:MSE:CE	2.47	0.43
1:A:192:ARG:NH1	1:A:219:TRP:CE3	2.86	0.43
1:B:602:ASN:ND2	1:B:605:LEU:HD22	2.33	0.43
1:D:460:ASP:OD1	1:D:460:ASP:C	2.57	0.43
1:C:536:LEU:HB3	1:C:566:ILE:HD11	1.99	0.43
1:C:563:GLU:C	1:C:565:THR:N	2.72	0.43
1:C:124:LEU:HD21	1:C:145:TRP:CZ3	2.53	0.43
1:C:150:LEU:HD12	1:C:150:LEU:N	2.33	0.43
1:B:666:LEU:HD12	1:B:666:LEU:HA	1.63	0.43
1:D:533:THR:HB	1:D:534:PRO:HD3	1.98	0.43
1:C:485:ILE:CG2	1:C:487:ASN:HB2	2.45	0.43
1:A:479:GLU:C	1:A:481:CYS:CB	2.85	0.43
1:C:543:ILE:CG2	1:C:574:ASN:HD21	2.15	0.43
1:C:258:LEU:CD1	1:C:258:LEU:N	2.81	0.43
1:C:136:GLU:O	1:C:140:SER:OG	2.36	0.43
1:D:40:ARG:HG3	1:D:40:ARG:HH21	1.82	0.43
1:D:69:SER:O	1:D:72:GLU:HB2	2.18	0.43
1:D:271:ALA:HB2	1:D:299:GLN:OE1	2.19	0.43
1:A:533:THR:HB	1:A:534:PRO:HD3	2.01	0.43
1:A:38:GLY:O	1:A:39:ASP:C	2.57	0.43
1:C:259:ARG:HA	1:C:259:ARG:HD3	1.80	0.43
1:A:470:LEU:HD22	1:A:477:VAL:CG1	2.49	0.43
1:D:51:CYS:C	1:D:70:TYR:CD2	2.92	0.43
1:C:8:VAL:CG1	1:C:9:PRO:CD	2.86	0.43
1:D:379:LEU:CD1	1:D:402:SER:OG	2.67	0.43
1:D:77:ILE:HB	1:D:85:VAL:HG11	2.00	0.43
1:A:452:HIS:N	1:A:452:HIS:CD2	2.84	0.43
1:A:226:LYS:O	1:A:227:ASP:HB2	2.17	0.43
1:B:203:GLU:O	1:B:206:ASP:HB2	2.19	0.43
1:C:376:GLU:HG2	1:C:376:GLU:O	2.19	0.43
1:C:498:LEU:HD12	1:C:502:LEU:HD13	2.01	0.43
1:D:40:ARG:HG2	1:D:40:ARG:HH21	1.83	0.43
1:B:297:SER:HB2	1:B:328:SER:CB	2.49	0.43
1:A:442:LYS:HE2	1:A:446:LEU:CD1	2.49	0.43
1:C:254:GLU:O	1:C:255:ASN:C	2.54	0.43
1:A:273:ASN:C	1:A:273:ASN:OD1	2.57	0.43
1:A:14:GLU:C	1:A:16:ILE:N	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ALA:O	1:A:484:GLU:CB	2.66	0.43
1:C:109:HIS:CE1	1:C:113:CYS:SG	3.12	0.43
1:D:16:ILE:CG2	1:D:56:LEU:HD13	2.46	0.43
1:D:325:LEU:HD11	1:D:329:LEU:CD1	2.47	0.43
1:D:404:PHE:CZ	1:D:440:PRO:HB3	2.51	0.43
1:B:539:LEU:HA	1:B:539:LEU:HD12	1.81	0.43
1:B:441:LEU:CD1	1:B:445:LEU:CD1	2.96	0.43
1:D:403:VAL:HG23	1:D:403:VAL:O	2.19	0.43
1:C:375:THR:HG23	1:C:377:CYS:N	2.32	0.43
1:D:93:MSE:HG3	1:D:93:MSE:O	2.19	0.43
1:C:638:ILE:HD11	1:C:658:LEU:HB3	2.01	0.43
1:A:383:CYS:SG	1:A:416:PHE:HD1	2.41	0.43
1:A:505:LEU:HA	1:A:505:LEU:HD13	1.85	0.43
1:D:403:VAL:HG21	1:D:406:HIS:CE1	2.53	0.43
1:D:46:LEU:CD2	1:D:95:MSE:HE1	2.49	0.43
1:B:355:SER:O	1:B:359:ASN:CB	2.65	0.43
1:A:613:ASN:O	1:A:614:ASN:HB2	2.17	0.43
1:C:560:LEU:HG	1:C:560:LEU:H	1.68	0.43
1:B:376:GLU:HG2	1:B:376:GLU:O	2.19	0.43
1:C:631:TYR:CD1	1:C:631:TYR:N	2.87	0.43
1:B:32:VAL:CG2	1:B:95:MSE:CG	2.95	0.43
1:A:638:ILE:HG23	1:A:638:ILE:O	2.18	0.43
1:B:372:LEU:O	1:B:375:THR:CB	2.66	0.43
1:D:514:SER:HG	1:D:515:ILE:N	2.17	0.43
1:C:256:ALA:CB	1:C:258:LEU:HD11	2.48	0.43
1:A:84:MSE:HE2	1:A:97:MSE:HE1	2.00	0.43
1:A:80:LYS:HD2	1:A:82:ALA:H	1.84	0.43
1:C:76:VAL:HG11	1:C:107:LEU:HD11	2.01	0.43
1:A:9:PRO:HB2	1:A:12:LEU:CG	2.47	0.42
1:B:349:LEU:HD13	1:B:357:MSE:SE	2.69	0.42
1:C:117:ILE:C	1:C:118:PHE:CD2	2.92	0.42
1:A:396:VAL:O	1:A:396:VAL:HG23	2.18	0.42
1:B:561:LYS:N	1:B:585:ASN:O	2.52	0.42
1:C:212:ALA:HB2	1:C:237:GLN:HG2	2.01	0.42
1:D:185:ILE:HG22	1:D:189:GLN:HE21	1.84	0.42
1:C:499:GLU:HB3	1:C:500:SER:H	1.67	0.42
1:A:347:ASN:ND2	1:A:347:ASN:N	2.67	0.42
1:A:282:ASN:C	1:A:282:ASN:OD1	2.57	0.42
1:C:17:LYS:O	1:C:21:GLY:N	2.52	0.42
1:D:651:PRO:CG	1:D:652:GLU:N	2.76	0.42
1:C:602:ASN:CG	1:C:605:LEU:HD23	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:LEU:HA	1:A:647:LEU:HD23	1.77	0.42
1:C:297:SER:HB2	1:C:328:SER:CB	2.49	0.42
1:A:203:GLU:O	1:A:206:ASP:HB2	2.19	0.42
1:D:59:ARG:HD2	1:D:59:ARG:H	1.84	0.42
1:A:476:GLN:CD	1:A:476:GLN:N	2.72	0.42
1:C:296:LEU:O	1:C:299:GLN:N	2.50	0.42
1:B:478:LEU:CB	1:B:508:TRP:CE3	3.01	0.42
1:B:88:THR:HG22	1:B:91:CYS:O	2.19	0.42
1:C:256:ALA:O	1:C:258:LEU:HD12	2.18	0.42
1:D:350:ARG:O	1:D:350:ARG:NE	2.52	0.42
1:A:138:LEU:CD2	1:A:139:ALA:N	2.73	0.42
1:B:262:PHE:O	1:B:263:ALA:C	2.57	0.42
1:C:416:PHE:CE1	1:C:420:PHE:CE2	3.07	0.42
1:D:602:ASN:HD21	1:D:605:LEU:CD1	2.31	0.42
1:C:189:GLN:HB2	1:C:191:THR:HG23	2.00	0.42
1:C:602:ASN:ND2	1:C:605:LEU:CD2	2.81	0.42
1:B:117:ILE:CG2	1:B:118:PHE:CE2	3.02	0.42
1:B:193:GLU:CG	1:B:222:LYS:HD3	2.50	0.42
1:A:569:ASN:OD1	1:A:594:MSE:HG3	2.19	0.42
1:A:481:CYS:SG	1:A:481:CYS:O	2.78	0.42
1:D:375:THR:HG23	1:D:377:CYS:N	2.35	0.42
1:A:652:GLU:CG	1:A:653:LYS:HG3	2.48	0.42
1:C:540:VAL:O	1:C:544:GLN:HG2	2.18	0.42
1:B:81:PRO:O	1:B:100:PRO:HB3	2.20	0.42
1:A:124:LEU:HD21	1:A:145:TRP:HZ3	1.83	0.42
1:C:80:LYS:CE	1:C:82:ALA:H	2.33	0.42
1:A:46:LEU:HD23	1:A:54:PHE:O	2.20	0.42
1:D:271:ALA:HA	1:D:299:GLN:OE1	2.19	0.42
1:B:516:GLN:HB2	1:B:517:HIS:CD2	2.54	0.42
1:D:368:VAL:HG12	1:D:368:VAL:O	2.18	0.42
1:D:580:VAL:CG1	1:D:605:LEU:CD2	2.96	0.42
1:A:568:ILE:HD11	1:A:587:MSE:SE	2.70	0.42
1:A:54:PHE:N	1:A:54:PHE:CD1	2.87	0.42
1:D:297:SER:HB2	1:D:328:SER:CB	2.49	0.42
1:B:224:SER:HB2	1:B:252:VAL:HB	2.00	0.42
1:D:270:LEU:HD21	1:D:278:LEU:HD12	2.02	0.42
1:B:536:LEU:CB	1:B:566:ILE:HD11	2.50	0.42
1:C:561:LYS:H	1:C:561:LYS:HG3	1.54	0.42
1:D:64:LEU:HD22	1:D:66:LEU:N	2.35	0.42
1:A:73:ILE:HD13	1:A:127:MSE:HE3	1.87	0.42
1:A:263:ALA:CB	1:A:292:GLY:CA	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLY:CA	1:A:477:VAL:HG11	2.26	0.42
1:C:34:LEU:O	1:C:36:VAL:HG23	2.19	0.42
1:C:507:VAL:HA	1:C:510:SER:OG	2.20	0.42
1:B:88:THR:CG2	1:B:91:CYS:HB3	2.49	0.42
1:D:312:LEU:N	1:D:312:LEU:HD12	2.35	0.42
1:D:315:THR:OG1	1:D:317:LEU:HD11	2.17	0.42
1:D:543:ILE:HG22	1:D:574:ASN:HD21	1.77	0.42
1:D:493:ILE:O	1:D:496:ASN:ND2	2.53	0.42
1:A:604:LYS:O	1:A:604:LYS:CG	2.68	0.42
1:A:620:PHE:HE1	1:A:639:PRO:HG3	1.84	0.42
1:D:322:VAL:CG1	1:D:357:MSE:CE	2.76	0.42
1:D:354:LEU:HB2	1:D:358:TYR:CZ	2.55	0.42
1:B:155:PRO:O	1:B:156:CYS:HB2	2.19	0.42
1:D:606:ARG:HA	1:D:606:ARG:HD3	1.83	0.42
1:B:477:VAL:CG2	1:B:478:LEU:HG	2.49	0.42
1:A:402:SER:H	1:A:434:THR:HG23	1.84	0.42
1:A:375:THR:HG23	1:A:377:CYS:HB3	2.02	0.42
1:D:311:ASN:C	1:D:311:ASN:OD1	2.57	0.42
1:C:256:ALA:HB1	1:C:258:LEU:HD11	2.02	0.42
1:C:529:SER:O	1:C:533:THR:OG1	2.37	0.42
1:D:127:MSE:O	1:D:128:LYS:HB2	2.20	0.42
1:D:518:LEU:HD21	1:D:520:LEU:HD21	2.01	0.42
1:A:568:ILE:CD1	1:A:587:MSE:SE	3.17	0.42
1:A:75:GLY:H	1:A:87:GLU:HG3	1.85	0.42
1:B:282:ASN:C	1:B:282:ASN:OD1	2.59	0.42
1:C:36:VAL:CG1	1:C:37:LYS:N	2.73	0.41
1:A:507:VAL:CG2	1:A:508:TRP:N	2.83	0.41
1:A:638:ILE:HG23	1:A:640:MSE:HE2	2.02	0.41
1:A:84:MSE:HB3	1:A:97:MSE:HE3	2.01	0.41
1:D:572:GLY:O	1:D:601:ILE:HG22	2.20	0.41
1:A:136:GLU:O	1:A:140:SER:OG	2.38	0.41
1:D:380:GLU:CD	1:D:405:SER:OG	2.58	0.41
1:B:30:LYS:HE2	1:B:105:GLU:OE2	2.19	0.41
1:A:374:ASN:CG	1:A:401:ARG:HH21	2.22	0.41
1:B:39:ASP:O	1:B:41:VAL:HG13	2.20	0.41
1:C:368:VAL:O	1:C:368:VAL:CG1	2.67	0.41
1:B:117:ILE:HG21	1:B:118:PHE:CE2	2.54	0.41
1:D:560:LEU:HA	1:D:560:LEU:HD23	1.83	0.41
1:D:122:SER:O	1:D:125:ARG:HB2	2.20	0.41
1:A:71:LEU:HD12	1:A:71:LEU:N	2.34	0.41
1:B:412:VAL:HG22	1:B:412:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLU:C	1:C:36:VAL:HG23	2.40	0.41
1:A:499:GLU:HB3	1:A:500:SER:H	1.59	0.41
1:C:532:LEU:HD22	1:C:536:LEU:CD1	2.50	0.41
1:D:99:SER:O	1:D:102:ASP:N	2.54	0.41
1:C:386:LEU:HD23	1:C:386:LEU:HA	1.71	0.41
1:C:58:ALA:O	1:C:59:ARG:HG3	2.20	0.41
1:B:568:ILE:CD1	1:B:587:MSE:SE	3.18	0.41
1:A:476:GLN:NE2	1:A:476:GLN:C	2.73	0.41
1:A:345:SER:HB3	1:A:371:ASP:OD1	2.19	0.41
1:B:545:ASP:OD1	1:B:546:GLU:N	2.53	0.41
1:B:273:ASN:HA	1:B:274:PRO:HD2	1.92	0.41
1:D:317:LEU:HB2	1:D:347:ASN:HB3	2.02	0.41
1:D:565:THR:HG22	1:D:565:THR:O	2.21	0.41
1:A:77:ILE:O	1:A:85:VAL:CG1	2.63	0.41
1:C:556:ALA:O	1:C:557:ASP:HB2	2.20	0.41
1:A:350:ARG:HG2	1:A:406:HIS:CE1	2.56	0.41
1:C:42:GLU:HB2	1:C:44:LYS:HE2	2.02	0.41
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.76	0.41
1:A:500:SER:O	1:A:502:LEU:N	2.53	0.41
1:C:77:ILE:O	1:C:85:VAL:HG22	2.20	0.41
1:C:169:TRP:CE3	1:C:170:LEU:CD2	3.03	0.41
1:D:27:SER:HB2	1:D:109:HIS:CE1	2.52	0.41
1:B:26:ILE:HB	1:B:47:VAL:HG12	2.01	0.41
1:D:560:LEU:O	1:D:561:LYS:HB2	2.20	0.41
1:D:9:PRO:HG2	1:D:10:ARG:H	1.86	0.41
1:C:509:LEU:HD21	1:C:518:LEU:CD1	2.51	0.41
1:D:30:LYS:HE3	1:D:102:ASP:CG	2.41	0.41
1:D:298:ILE:HG22	1:D:299:GLN:NE2	2.36	0.41
1:C:593:LYS:HE2	1:D:200:SER:OG	2.21	0.41
1:D:75:GLY:HA2	1:D:129:LYS:O	2.21	0.41
1:D:400:SER:HB3	1:D:432:SER:OG	2.21	0.41
1:C:532:LEU:HD23	1:C:536:LEU:HG	2.02	0.41
1:D:37:LYS:H	1:D:37:LYS:HD3	1.85	0.41
1:D:311:ASN:C	1:D:312:LEU:HD12	2.41	0.41
1:D:51:CYS:O	1:D:70:TYR:CD2	2.74	0.41
1:C:150:LEU:HD12	1:C:150:LEU:H	1.85	0.41
1:A:258:LEU:CD2	1:A:262:PHE:CD2	2.95	0.41
1:D:172:PHE:HD2	1:D:209:PRO:HD3	1.79	0.41
1:B:441:LEU:HD22	1:B:466:LEU:HD22	2.01	0.41
1:D:557:ASP:HA	1:D:584:GLY:O	2.21	0.41
1:B:19:VAL:HG13	1:B:20:ILE:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LEU:C	1:C:487:ASN:HD22	2.11	0.41
1:C:470:LEU:CD1	1:C:505:LEU:HD11	2.47	0.41
1:D:68:PHE:CD2	1:D:88:THR:HG21	2.55	0.41
1:C:10:ARG:O	1:C:12:LEU:N	2.54	0.41
1:A:602:ASN:OD1	1:A:605:LEU:HD23	2.20	0.41
1:B:256:ALA:CB	1:B:258:LEU:CD1	2.98	0.41
1:D:539:LEU:HD12	1:D:539:LEU:HA	1.81	0.41
1:B:470:LEU:HD12	1:B:470:LEU:HA	1.80	0.41
1:A:410:LYS:C	1:A:411:GLU:O	2.55	0.41
1:B:65:GLU:H	1:B:65:GLU:HG2	1.63	0.41
1:B:43:ASN:N	1:B:43:ASN:OD1	2.54	0.41
1:A:10:ARG:O	1:A:13:MSE:N	2.38	0.41
1:B:374:ASN:HD21	1:B:401:ARG:NH1	2.19	0.41
1:D:254:GLU:O	1:D:255:ASN:C	2.58	0.41
1:D:387:LEU:HD23	1:D:388:ARG:CZ	2.51	0.41
1:B:193:GLU:CD	1:B:222:LYS:HD3	2.41	0.41
1:A:217:ASN:OD1	1:A:219:TRP:N	2.46	0.41
1:B:587:MSE:HG2	1:B:613:ASN:OD1	2.21	0.41
1:A:492:ASP:HA	1:A:519:ALA:HB3	2.03	0.41
1:C:205:ARG:HB2	1:C:205:ARG:HH11	1.86	0.41
1:A:379:LEU:HB2	1:A:404:PHE:HA	2.02	0.41
1:D:155:PRO:O	1:D:156:CYS:HB2	2.20	0.41
1:D:141:LEU:HA	1:D:141:LEU:HD12	1.77	0.41
1:B:43:ASN:C	1:B:44:LYS:HG2	2.42	0.41
1:C:374:ASN:OD1	1:C:401:ARG:CD	2.69	0.41
1:C:527:MSE:HE1	1:C:532:LEU:HG	2.01	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.80	0.41
1:D:512:ASN:ND2	1:D:514:SER:OG	2.54	0.41
1:C:10:ARG:C	1:C:12:LEU:N	2.73	0.41
1:C:580:VAL:CG1	1:C:605:LEU:HD11	2.51	0.41
1:A:543:ILE:HG21	1:A:543:ILE:HD13	1.88	0.41
1:A:193:GLU:CG	1:A:222:LYS:HD3	2.50	0.41
1:C:524:PHE:CG	1:C:560:LEU:HD21	2.55	0.41
1:C:116:ARG:HH11	1:C:116:ARG:CG	2.34	0.41
1:A:533:THR:N	1:A:534:PRO:CD	2.83	0.41
1:B:169:TRP:CZ3	1:B:170:LEU:HD21	2.56	0.41
1:B:374:ASN:HD21	1:B:401:ARG:HH11	1.69	0.40
1:D:34:LEU:HG	1:D:36:VAL:CG2	2.51	0.40
1:A:32:VAL:CG2	1:A:33:LYS:N	2.84	0.40
1:B:378:SER:HB2	1:B:406:HIS:CD2	2.56	0.40
1:C:615:ILE:HG23	1:C:619:GLY:HA3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LEU:CD1	1:C:445:LEU:CD1	3.00	0.40
1:B:441:LEU:HD11	1:B:445:LEU:CD1	2.51	0.40
1:A:476:GLN:H	1:A:476:GLN:CD	2.24	0.40
1:D:270:LEU:HD21	1:D:278:LEU:CD1	2.51	0.40
1:C:97:MSE:HB3	1:C:97:MSE:HE3	2.01	0.40
1:A:507:VAL:HG23	1:A:508:TRP:N	2.35	0.40
1:D:359:ASN:O	1:D:363:GLN:HG3	2.21	0.40
1:D:485:ILE:HD13	1:D:488:ILE:HD12	2.04	0.40
1:C:509:LEU:CD2	1:C:518:LEU:HD21	2.44	0.40
1:A:138:LEU:C	1:A:138:LEU:CD2	2.85	0.40
1:D:208:ILE:N	1:D:209:PRO:CD	2.84	0.40
1:A:263:ALA:HB1	1:A:292:GLY:CA	2.51	0.40
1:C:313:SER:O	1:C:314:LYS:C	2.60	0.40
1:B:616:THR:O	1:B:617:ALA:C	2.59	0.40
1:D:157:GLY:O	1:D:162:MSE:HE3	2.20	0.40
1:D:457:VAL:HG12	1:D:458:SER:N	2.37	0.40
1:B:204:HIS:CD2	1:B:231:SER:HB3	2.57	0.40
1:B:509:LEU:O	1:B:512:ASN:HB3	2.21	0.40
1:A:484:GLU:HA	1:A:485:ILE:HA	1.68	0.40
1:A:638:ILE:CD1	1:A:640:MSE:CE	2.88	0.40
1:B:74:HIS:HE1	1:B:89:GLU:HB2	1.71	0.40
1:B:258:LEU:CD2	1:B:262:PHE:CD2	2.99	0.40
1:A:130:VAL:O	1:A:130:VAL:HG23	2.22	0.40
1:D:627:MSE:HE1	1:D:633:LEU:HB3	2.02	0.40
1:D:397:LEU:HD11	1:D:399:LEU:HG	2.03	0.40
1:D:383:CYS:HG	1:D:416:PHE:HE1	1.67	0.40
1:B:587:MSE:HG2	1:B:613:ASN:CG	2.42	0.40
1:C:204:HIS:CE1	1:C:234:VAL:HG21	2.57	0.40
1:B:467:GLY:O	1:B:471:ARG:HG3	2.22	0.40
1:C:121:LEU:HA	1:C:121:LEU:HD23	1.80	0.40
1:B:303:LEU:HD23	1:B:304:PRO:HD2	2.03	0.40
1:C:477:VAL:HA	1:C:478:LEU:HA	1.73	0.40
1:B:638:ILE:H	1:B:638:ILE:CD1	2.27	0.40
1:B:401:ARG:H	1:B:434:THR:HG22	1.87	0.40
1:C:379:LEU:CD1	1:C:402:SER:HB3	2.47	0.40
1:B:78:CYS:HB2	1:B:132:MSE:CB	2.51	0.40
1:B:578:THR:HG22	1:B:604:LYS:HD2	2.02	0.40
1:A:543:ILE:HD11	1:A:553:LEU:HD22	2.03	0.40
1:C:16:ILE:O	1:C:19:VAL:CG1	2.70	0.40
1:A:150:LEU:HA	1:A:150:LEU:HD23	1.86	0.40
1:D:505:LEU:HD13	1:D:505:LEU:HA	1.81	0.40

All (5) 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)
1:C:392:GLN:O	1:C:649:THR:OG1[1_655]	1.32	0.88
1:C:289:GLU:OE1	1:D:513:ARG:CG[1_545]	1.55	0.65
1:C:289:GLU:OE2	1:D:513:ARG:NH2[1_545]	1.64	0.56
1:A:415:SER:OG	3:B:702:CL:CL[1_465]	1.74	0.46
1:B:35:GLU:OE2	1:D:476:GLN:NE2[1_545]	1.90	0.30

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	660/669 (99%)	628 (95%)	31 (5%)	1 (0%)	52	84
1	B	656/669 (98%)	635 (97%)	21 (3%)	0	100	100
1	C	652/669 (98%)	631 (97%)	20 (3%)	1 (0%)	52	84
1	D	651/669 (97%)	628 (96%)	23 (4%)	0	100	100
All	All	2619/2676 (98%)	2522 (96%)	95 (4%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	C	11	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	585/573 (102%)	472 (81%)	113 (19%)	2	5
1	B	585/573 (102%)	464 (79%)	121 (21%)	1	4
1	C	581/573 (101%)	460 (79%)	121 (21%)	1	4
1	D	580/573 (101%)	450 (78%)	130 (22%)	1	3
All	All	2331/2292 (102%)	1846 (79%)	485 (21%)	1	4

All (485) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	25	LYS
1	A	29	LYS
1	A	30	LYS
1	A	37	LYS
1	A	39	ASP
1	A	45	VAL
1	A	46	LEU
1	A	50	SER
1	A	51	CYS
1	A	54	PHE
1	A	59	ARG
1	A	64	LEU
1	A	65	GLU
1	A	67	THR
1	A	72	GLU
1	A	76	VAL
1	A	77	ILE
1	A	80	LYS
1	A	89	GLU
1	A	90	LYS
1	A	92	ASN
1	A	93	MSE
1	A	96	LYS
1	A	97	MSE
1	A	105	GLU
1	A	107	LEU
1	A	115	ARG
1	A	125	ARG
1	A	127	MSE
1	A	129	LYS
1	A	131	SER
1	A	133	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	136	GLU
1	A	137	ARG
1	A	138	LEU
1	A	140	SER
1	A	144	LEU
1	A	147	SER
1	A	149	THR
1	A	152	GLU
1	A	168	ASP
1	A	173	SER
1	A	174	TYR
1	A	181	ASP
1	A	197	GLN
1	A	202	LEU
1	A	224	SER
1	A	225	SER
1	A	226	LYS
1	A	229	LYS
1	A	232	THR
1	A	247	ARG
1	A	272	HIS
1	A	275	ASN
1	A	276	SER
1	A	290	ASP
1	A	291	ARG
1	A	296	LEU
1	A	299	GLN
1	A	302	LYS
1	A	303	LEU
1	A	318	SER
1	A	330	SER
1	A	347	ASN
1	A	350	ARG
1	A	352	ASP
1	A	393	CYS
1	A	400	SER
1	A	405	SER
1	A	412	VAL
1	A	426	LEU
1	A	434	THR
1	A	437	SER
1	A	458	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	465	GLU
1	A	476	GLN
1	A	477	VAL
1	A	478	LEU
1	A	482	ILE
1	A	484	GLU
1	A	485	ILE
1	A	490	SER
1	A	493	ILE
1	A	499	GLU
1	A	501	ASP
1	A	505	LEU
1	A	506	ILE
1	A	509	LEU
1	A	510	SER
1	A	522	LYS
1	A	527	MSE
1	A	528	LYS
1	A	530	LYS
1	A	532	LEU
1	A	541	GLN
1	A	550	LEU
1	A	565	THR
1	A	566	ILE
1	A	568	ILE
1	A	573	SER
1	A	580	VAL
1	A	594	MSE
1	A	603	THR
1	A	604	LYS
1	A	606	ARG
1	A	607	THR
1	A	610	TRP
1	A	618	GLN
1	A	640	MSE
1	A	650	ASN
1	A	660	LYS
1	A	667	ARG
1	B	7	ASP
1	B	11	GLU
1	B	22	ARG
1	B	23	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	24	ILE
1	B	26	ILE
1	B	29	LYS
1	B	30	LYS
1	B	31	LYS
1	B	33	LYS
1	B	34	LEU
1	B	35	GLU
1	B	36	VAL
1	B	37	LYS
1	B	42	GLU
1	B	43	ASN
1	B	44	LYS
1	B	46	LEU
1	B	47	VAL
1	B	50	SER
1	B	63	LYS
1	B	66	LEU
1	B	67	THR
1	B	80	LYS
1	B	83	GLN
1	B	87	GLU
1	B	89	GLU
1	B	90	LYS
1	B	91	CYS
1	B	93	MSE
1	B	97	MSE
1	B	101	GLU
1	B	103	VAL
1	B	107	LEU
1	B	121	LEU
1	B	125	ARG
1	B	133	GLU
1	B	136	GLU
1	B	137	ARG
1	B	140	SER
1	B	144	LEU
1	B	160	SER
1	B	162	MSE
1	B	173	SER
1	B	174	TYR
1	B	183	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	THR
1	B	187	LEU
1	B	197	GLN
1	B	202	LEU
1	B	224	SER
1	B	225	SER
1	B	226	LYS
1	B	229	LYS
1	B	232	THR
1	B	237	GLN
1	B	246	ASN
1	B	247	ARG
1	B	272	HIS
1	B	275	ASN
1	B	276	SER
1	B	286	ASN
1	B	287	SER
1	B	288	LEU
1	B	290	ASP
1	B	291	ARG
1	B	295	SER
1	B	296	LEU
1	B	298	ILE
1	B	299	GLN
1	B	302	LYS
1	B	318	SER
1	B	330	SER
1	B	350	ARG
1	B	352	ASP
1	B	354	LEU
1	B	355	SER
1	B	388	ARG
1	B	400	SER
1	B	403	VAL
1	B	407	ARG
1	B	412	VAL
1	B	415	SER
1	B	424	LEU
1	B	434	THR
1	B	437	SER
1	B	445	LEU
1	B	455	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	458	SER
1	B	465	GLU
1	B	468	HIS
1	B	469	CYS
1	B	478	LEU
1	B	490	SER
1	B	503	SER
1	B	505	LEU
1	B	506	ILE
1	B	509	LEU
1	B	510	SER
1	B	513	ARG
1	B	522	LYS
1	B	528	LYS
1	B	541	GLN
1	B	550	LEU
1	B	558	SER
1	B	566	ILE
1	B	575	THR
1	B	594	MSE
1	B	603	THR
1	B	604	LYS
1	B	605	LEU
1	B	606	ARG
1	B	607	THR
1	B	610	TRP
1	B	632	THR
1	B	635	PHE
1	B	638	ILE
1	B	652	GLU
1	B	660	LYS
1	B	666	LEU
1	B	667	ARG
1	C	10	ARG
1	C	12	LEU
1	C	17	LYS
1	C	22	ARG
1	C	25	LYS
1	C	29	LYS
1	C	31	LYS
1	C	32	VAL
1	C	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	37	LYS
1	C	39	ASP
1	C	46	LEU
1	C	50	SER
1	C	51	CYS
1	C	52	ARG
1	C	55	LEU
1	C	56	LEU
1	C	61	PRO
1	C	64	LEU
1	C	67	THR
1	C	78	CYS
1	C	79	HIS
1	C	80	LYS
1	C	83	GLN
1	C	90	LYS
1	C	93	MSE
1	C	94	SER
1	C	97	MSE
1	C	115	ARG
1	C	129	LYS
1	C	131	SER
1	C	133	GLU
1	C	136	GLU
1	C	140	SER
1	C	144	LEU
1	C	147	SER
1	C	150	LEU
1	C	152	GLU
1	C	168	ASP
1	C	173	SER
1	C	174	TYR
1	C	181	ASP
1	C	184	THR
1	C	188	THR
1	C	194	LEU
1	C	197	GLN
1	C	202	LEU
1	C	205	ARG
1	C	224	SER
1	C	226	LYS
1	C	229	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	232	THR
1	C	247	ARG
1	C	272	HIS
1	C	275	ASN
1	C	276	SER
1	C	287	SER
1	C	288	LEU
1	C	294	SER
1	C	296	LEU
1	C	298	ILE
1	C	302	LYS
1	C	313	SER
1	C	318	SER
1	C	330	SER
1	C	352	ASP
1	C	354	LEU
1	C	381	MSE
1	C	384	SER
1	C	388	ARG
1	C	393	CYS
1	C	396	VAL
1	C	407	ARG
1	C	408	LYS
1	C	411	GLU
1	C	412	VAL
1	C	418	GLN
1	C	421	SER
1	C	422	SER
1	C	426	LEU
1	C	434	THR
1	C	437	SER
1	C	451	ASN
1	C	455	LYS
1	C	458	SER
1	C	465	GLU
1	C	476	GLN
1	C	484	GLU
1	C	486	HIS
1	C	490	SER
1	C	499	GLU
1	C	500	SER
1	C	501	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	503	SER
1	C	505	LEU
1	C	508	TRP
1	C	511	LYS
1	C	513	ARG
1	C	522	LYS
1	C	525	ASN
1	C	527	MSE
1	C	531	ASN
1	C	533	THR
1	C	541	GLN
1	C	550	LEU
1	C	559	LYS
1	C	560	LEU
1	C	561	LYS
1	C	566	ILE
1	C	580	VAL
1	C	594	MSE
1	C	603	THR
1	C	604	LYS
1	C	606	ARG
1	C	607	THR
1	C	610	TRP
1	C	632	THR
1	C	637	PRO
1	C	639	PRO
1	C	660	LYS
1	C	667	ARG
1	D	13	MSE
1	D	17	LYS
1	D	22	ARG
1	D	24	ILE
1	D	26	ILE
1	D	29	LYS
1	D	30	LYS
1	D	31	LYS
1	D	34	LEU
1	D	35	GLU
1	D	37	LYS
1	D	39	ASP
1	D	40	ARG
1	D	47	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	50	SER
1	D	52	ARG
1	D	59	ARG
1	D	62	SER
1	D	65	GLU
1	D	66	LEU
1	D	67	THR
1	D	68	PHE
1	D	77	ILE
1	D	80	LYS
1	D	83	GLN
1	D	89	GLU
1	D	90	LYS
1	D	93	MSE
1	D	95	MSE
1	D	96	LYS
1	D	99	SER
1	D	101	GLU
1	D	104	SER
1	D	114	LEU
1	D	115	ARG
1	D	116	ARG
1	D	118	PHE
1	D	124	LEU
1	D	127	MSE
1	D	136	GLU
1	D	137	ARG
1	D	138	LEU
1	D	140	SER
1	D	146	ASP
1	D	147	SER
1	D	148	GLN
1	D	149	THR
1	D	150	LEU
1	D	152	GLU
1	D	159	PHE
1	D	168	ASP
1	D	173	SER
1	D	174	TYR
1	D	181	ASP
1	D	184	THR
1	D	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	202	LEU
1	D	224	SER
1	D	225	SER
1	D	226	LYS
1	D	229	LYS
1	D	232	THR
1	D	237	GLN
1	D	247	ARG
1	D	272	HIS
1	D	275	ASN
1	D	286	ASN
1	D	288	LEU
1	D	291	ARG
1	D	296	LEU
1	D	298	ILE
1	D	299	GLN
1	D	302	LYS
1	D	318	SER
1	D	323	ASN
1	D	330	SER
1	D	347	ASN
1	D	349	LEU
1	D	350	ARG
1	D	353	ASP
1	D	354	LEU
1	D	356	HIS
1	D	359	ASN
1	D	381	MSE
1	D	384	SER
1	D	388	ARG
1	D	396	VAL
1	D	397	LEU
1	D	400	SER
1	D	405	SER
1	D	407	ARG
1	D	408	LYS
1	D	410	LYS
1	D	427	ILE
1	D	428	GLN
1	D	434	THR
1	D	437	SER
1	D	455	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	458	SER
1	D	469	CYS
1	D	470	LEU
1	D	471	ARG
1	D	472	SER
1	D	476	GLN
1	D	477	VAL
1	D	478	LEU
1	D	484	GLU
1	D	490	SER
1	D	493	ILE
1	D	505	LEU
1	D	509	LEU
1	D	513	ARG
1	D	522	LYS
1	D	525	ASN
1	D	532	LEU
1	D	541	GLN
1	D	550	LEU
1	D	566	ILE
1	D	580	VAL
1	D	594	MSE
1	D	603	THR
1	D	604	LYS
1	D	605	LEU
1	D	606	ARG
1	D	607	THR
1	D	638	ILE
1	D	640	MSE
1	D	652	GLU
1	D	660	LYS
1	D	667	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	369	HIS
1	A	452	HIS
1	A	463	ASN
1	A	476	GLN
1	A	512	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	525	ASN
1	A	618	GLN
1	A	650	ASN
1	B	79	HIS
1	B	83	GLN
1	B	148	GLN
1	B	201	HIS
1	B	323	ASN
1	B	486	HIS
1	B	525	ASN
1	B	645	GLN
1	C	109	HIS
1	C	189	GLN
1	C	246	ASN
1	C	323	ASN
1	C	369	HIS
1	C	406	HIS
1	C	476	GLN
1	D	109	HIS
1	D	189	GLN
1	D	237	GLN
1	D	323	ASN
1	D	369	HIS
1	D	406	HIS
1	D	512	ASN
1	D	517	HIS
1	D	614	ASN

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 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	OHB	B	701	-	10,10,10	1.74	1 (10%)	12,13,13	1.28	1 (8%)
4	ABU	C	701	-	3,6,6	0.37	0	3,6,6	1.95	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OHB	B	701	-	-	0/4/4/4	0/1/1/1
4	ABU	C	701	-	-	0/2/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	OHB	C-N	5.07	1.43	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	ABU	CA-CB-CG	2.14	120.29	113.24
4	C	701	ABU	CB-CG-CD	2.27	124.81	112.58
2	B	701	OHB	O-C-C1	2.55	123.46	120.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	OHB	2	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	642/669 (95%)	-0.28	13 (2%) 68 64	8, 38, 107, 159	0
1	B	642/669 (95%)	-0.20	16 (2%) 61 55	8, 41, 113, 176	0
1	C	638/669 (95%)	-0.35	6 (0%) 85 84	13, 43, 89, 142	0
1	D	637/669 (95%)	0.14	44 (6%) 20 14	20, 52, 120, 175	0
All	All	2559/2676 (95%)	-0.18	79 (3%) 52 45	8, 45, 109, 176	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	VAL	6.1
1	D	140	SER	5.2
1	D	61	PRO	5.0
1	D	131	SER	4.8
1	D	37	LYS	4.7
1	A	9	PRO	4.3
1	A	352	ASP	4.2
1	D	136	GLU	4.2
1	D	143	ALA	4.1
1	D	150	LEU	4.1
1	A	12	LEU	4.0
1	D	22	ARG	3.9
1	C	485	ILE	3.9
1	D	11	GLU	3.8
1	A	481	CYS	3.8
1	B	7	ASP	3.8
1	B	38	GLY	3.6
1	C	476	GLN	3.6
1	B	100	PRO	3.4
1	B	484	GLU	3.4
1	D	24	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	81	PRO	3.3
1	D	60	ILE	3.2
1	B	76	VAL	3.1
1	D	36	VAL	3.1
1	B	130	VAL	3.1
1	B	37	LYS	3.0
1	D	85	VAL	3.0
1	D	21	GLY	3.0
1	B	4	GLU	3.0
1	B	5	SER	2.9
1	A	23	LYS	2.9
1	D	16	ILE	2.9
1	D	27	SER	2.9
1	D	9	PRO	2.9
1	A	16	ILE	2.9
1	D	139	ALA	2.8
1	D	65	GLU	2.7
1	D	138	LEU	2.7
1	C	500	SER	2.6
1	B	147	SER	2.6
1	B	146	ASP	2.5
1	D	123	PRO	2.5
1	A	21	GLY	2.5
1	B	508	TRP	2.5
1	D	57	SER	2.5
1	D	38	GLY	2.4
1	C	475	ALA	2.3
1	D	409	GLY	2.3
1	D	29	LYS	2.3
1	D	58	ALA	2.3
1	D	41	VAL	2.3
1	B	98	VAL	2.3
1	D	62	SER	2.2
1	D	94	SER	2.2
1	A	120	GLY	2.2
1	D	46	LEU	2.2
1	C	484	GLU	2.2
1	A	106	VAL	2.2
1	D	134	PRO	2.2
1	B	180	TRP	2.2
1	A	78	CYS	2.1
1	A	149	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	12	LEU	2.1
1	D	122	SER	2.1
1	D	147	SER	2.1
1	D	44	LYS	2.1
1	D	79	HIS	2.1
1	D	130	VAL	2.1
1	D	112	THR	2.1
1	D	149	THR	2.1
1	D	99	SER	2.1
1	D	26	ILE	2.1
1	D	98	VAL	2.1
1	A	482	ILE	2.0
1	C	509	LEU	2.0
1	D	77	ILE	2.0
1	B	68	PHE	2.0
1	A	81	PRO	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
4	ABU	C	701	7/7	0.89	0.30	7.88	31,54,83,85	0
2	OHB	B	701	10/10	0.95	0.21	3.03	10,42,92,98	0
3	CL	B	702	1/1	0.98	0.14	-1.56	2,2,2,2	0

6.5 Other polymers

There are no such residues in this entry.