Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 08:14 PM EDT

PDB ID	:	2B5L
Title	:	Crystal Structure of DDB1 In Complex with Simian Virus 5 V Protein
Authors	:	Li, T.; Chen, X.; Garbutt, K.C.; Zhou, P.; Zheng, N.
Deposited on	:	2005-09-28
Resolution	:	2.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

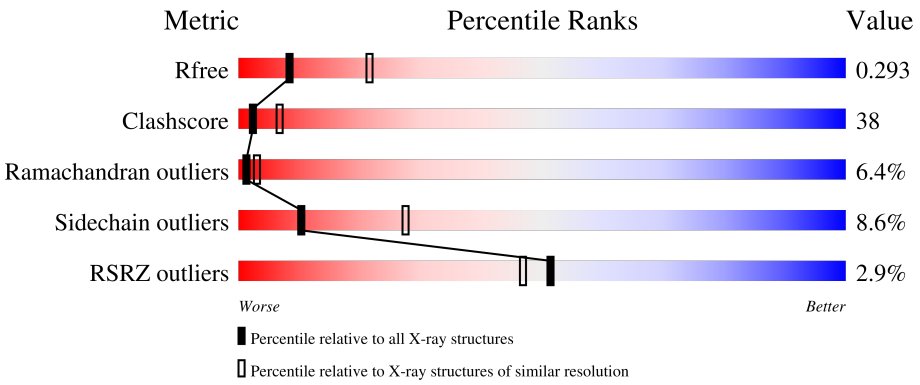
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	1140	%, 54%, 37%, 7% ••
1	B	1140	3%, 41%, 48%, 10% ••
2	C	222	5%, 30%, 37%, 9% •, 22%
2	D	222	9%, 25%, 37%, 13% •, 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20399 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 damage-specific DNA binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1132	8860	5610	1493	1708	49	0	0	0
1	B	1134	8876	5619	1495	1713	49	0	0	0

- Molecule 2 is a protein called Nonstructural protein V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	174	1324	826	229	261	8	0	0	0
2	D	175	1335	834	233	260	8	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

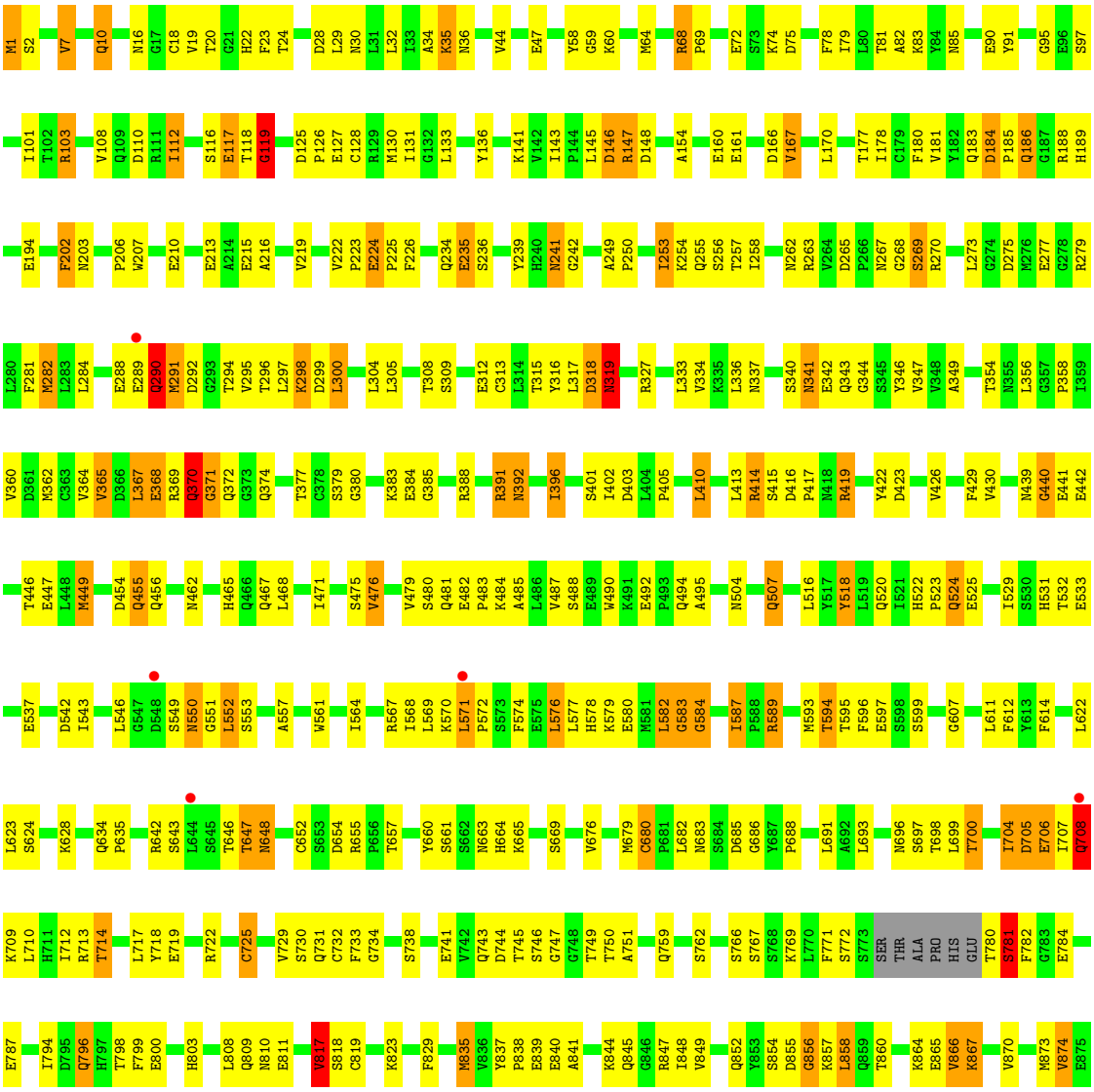
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	C	2	2	2	0	0
3	D	2	2	2	0	0

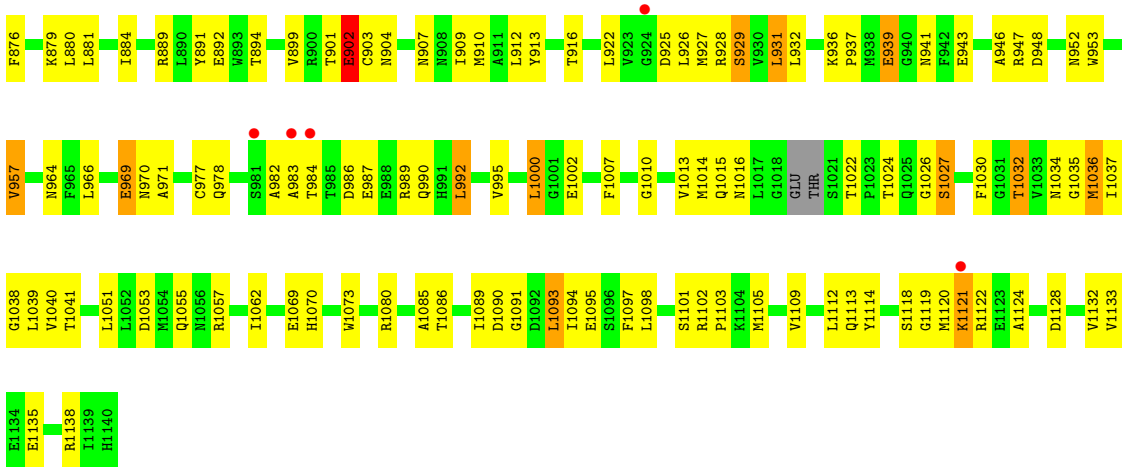
3 Residue-property plots (i)

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

- Molecule 1: damage-specific DNA binding protein 1

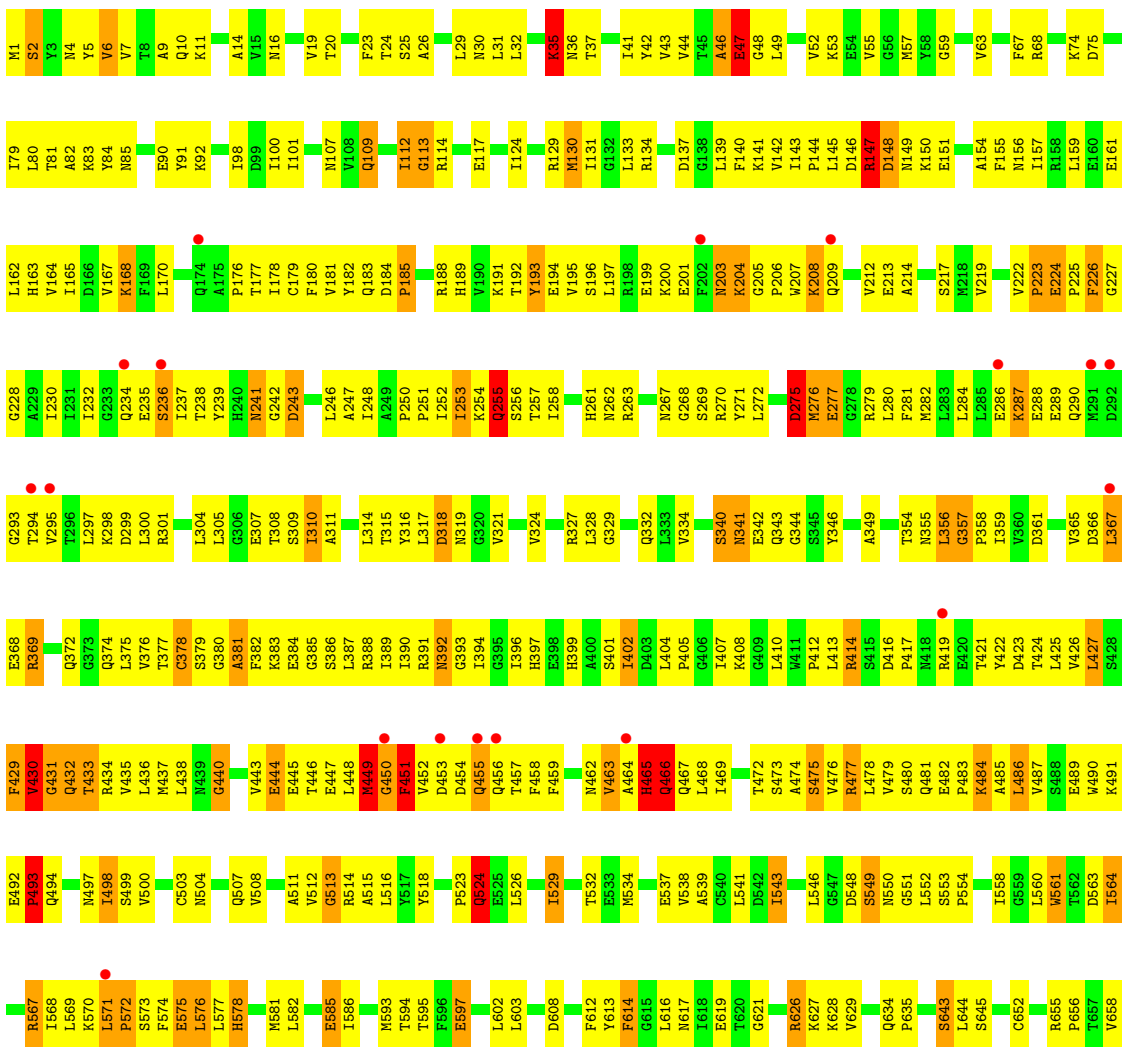
Chain A:

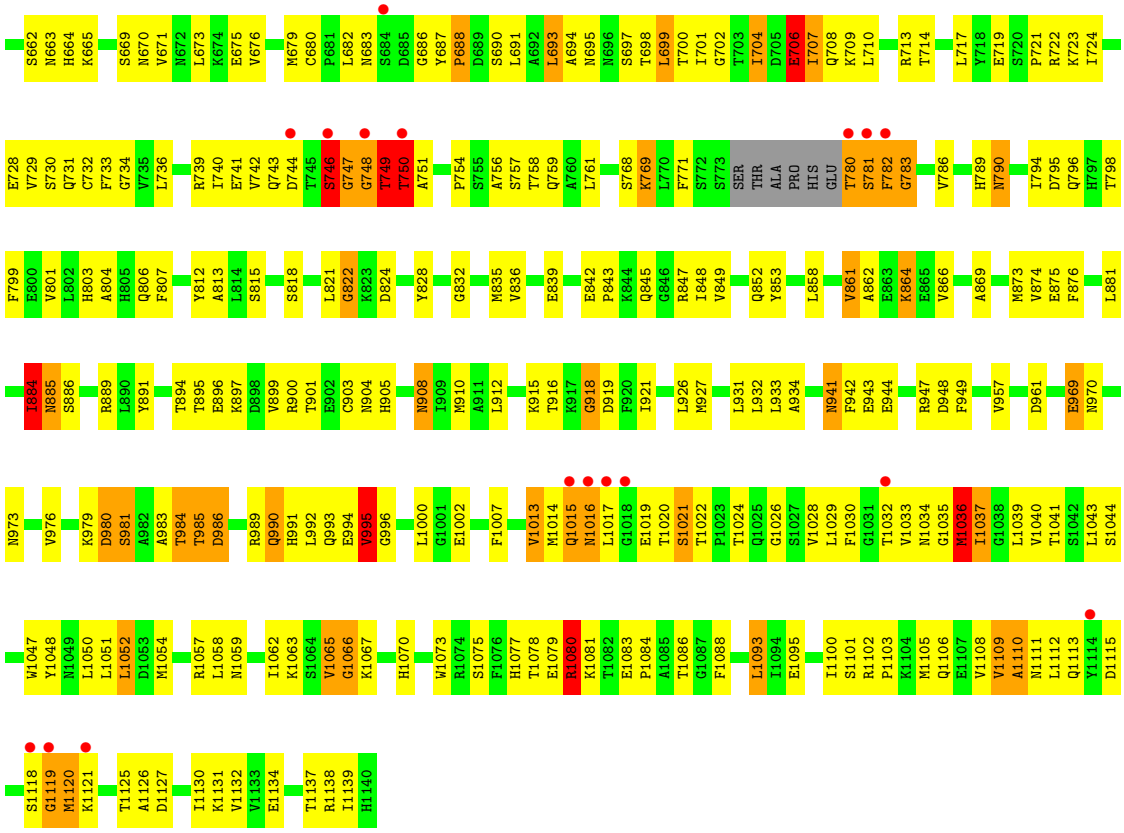




• Molecule 1: damage-specific DNA binding protein 1

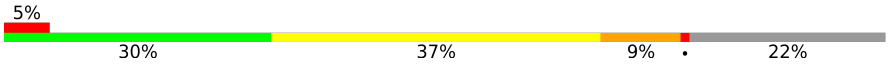
Chain B: 3% 41% 48% 10%

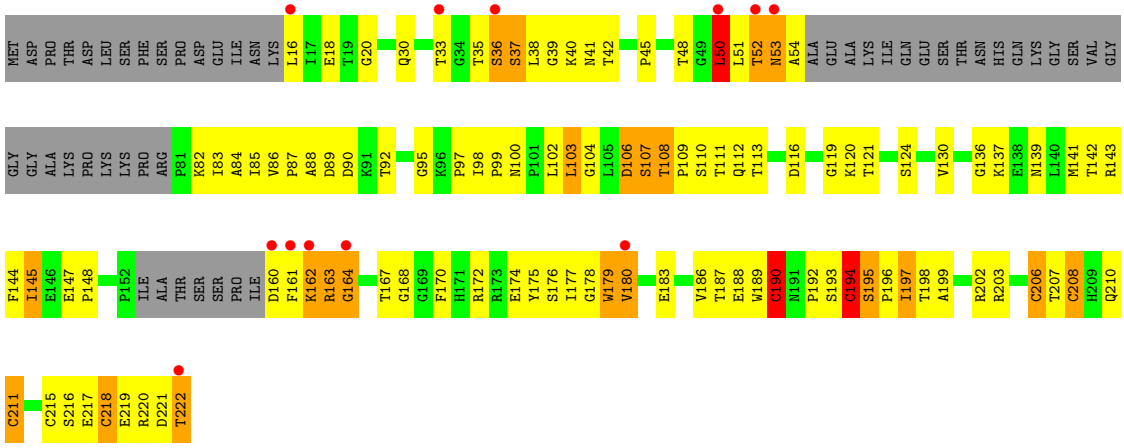




- Molecule 2: Nonstructural protein V

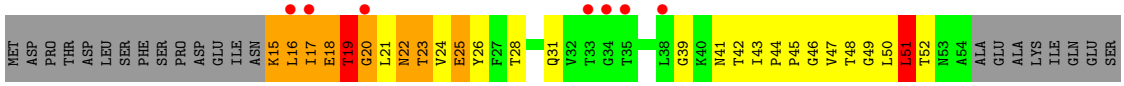
Chain C:

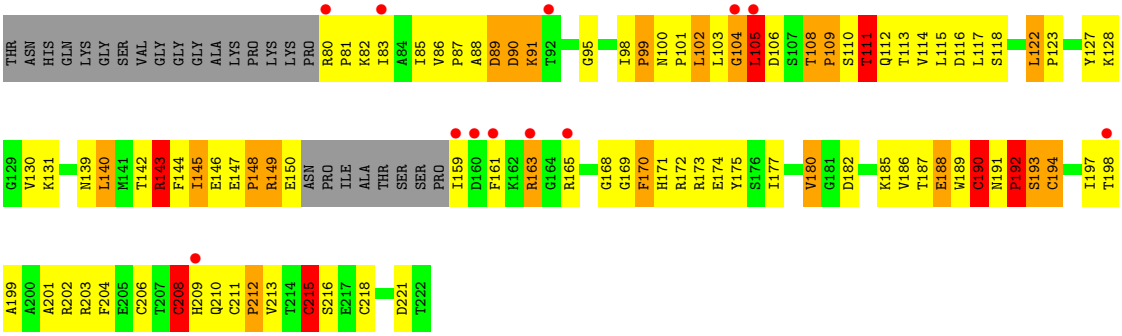




- Molecule 2: Nonstructural protein V

Chain D:




THR ASN HIS GLN LYS GLY SER VAL GLY GLY GLY ALA LYS PRO LYS LYS PRO R80 P81 K82 I83 A84 I85 V86 P87 A88 D89 D90 K91 T92 G95 I98 P99 N100 P101 L102 L103 G104 L105 D106 S107 T108 P109 S110 T111 Q112 T113 V114 L115 D116 L117 S118 L122 P123 Y127 K128
G129 V130 K131 N139 L140 M141 T142 R143 F144 I145 E146 E147 P148 R149 E150 ASN PRO ILE ALA THR SER SER PRO I159 D160 F161 K162 R163 G164 R165 G168 G169 F170 H171 R172 R173 E174 Y175 S176 I177 V180 G181 D182 K185 V186 T187 E188 W189 C190 N191 P192 S193 C194 I197 T198
A199 A200 A201 R202 R203 F204 E205 C206 T207 C208 H209 Q210 C211 P212 V213 T214 C215 S216 E217 C218 D221 T222

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.76Å 240.79Å 117.18Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	47.80 – 2.85 47.77 – 2.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.80-2.85) 86.6 (47.77-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.299 0.226 , 0.293	Depositor DCC
R_{free} test set	3805 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20399	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.45	1/9022 (0.0%)	0.77	7/12219 (0.1%)
1	B	0.45	3/9039 (0.0%)	0.91	41/12244 (0.3%)
2	C	0.56	0/1351	0.95	9/1832 (0.5%)
2	D	0.71	2/1361 (0.1%)	1.24	19/1843 (1.0%)
All	All	0.48	6/20773 (0.0%)	0.88	76/28138 (0.3%)

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	B	1	1
2	D	0	1
All	All	1	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	189	TRP	C-N	-15.06	0.99	1.34
2	D	190	CYS	C-N	11.09	1.59	1.34
1	B	748	GLY	N-CA	-7.48	1.34	1.46
1	B	431	GLY	N-CA	-6.93	1.35	1.46
1	A	725	CYS	CB-SG	-5.43	1.73	1.81
1	B	455	GLN	N-CA	-5.34	1.35	1.46

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	749	THR	N-CA-C	-19.59	58.10	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	35	LYS	CB-CA-C	18.15	146.70	110.40
2	D	15	LYS	N-CA-C	-16.98	65.16	111.00
1	B	431	GLY	N-CA-C	-16.54	71.75	113.10
1	B	749	THR	N-CA-CB	14.29	137.44	110.30
1	B	884	ILE	CB-CA-C	13.67	138.94	111.60
1	B	2	SER	N-CA-CB	-13.37	90.44	110.50
1	B	942	PHE	CB-CA-C	-12.45	85.50	110.40
1	B	451	PHE	CB-CG-CD1	-12.41	112.11	120.80
1	B	980	ASP	N-CA-C	-12.21	78.02	111.00
1	B	981	SER	N-CA-CB	-11.22	93.67	110.50
2	D	16	LEU	CB-CA-C	-10.79	89.69	110.20
1	A	202	PHE	CB-CA-C	-10.52	89.36	110.40
1	B	748	GLY	N-CA-C	10.49	139.33	113.10
1	B	980	ASP	CB-CA-C	-10.47	89.46	110.40
2	D	143	ARG	CB-CA-C	-10.28	89.84	110.40
2	D	16	LEU	N-CA-CB	-10.27	89.87	110.40
2	D	170	PHE	CB-CG-CD2	-10.05	113.77	120.80
1	B	185	PRO	CA-N-CD	-9.86	97.70	111.50
2	D	192	PRO	CA-N-CD	-9.54	98.15	111.50
2	D	170	PHE	CB-CG-CD1	9.38	127.36	120.80
1	B	885	ASN	N-CA-CB	-9.33	93.81	110.60
1	B	451	PHE	CB-CG-CD2	9.16	127.21	120.80
1	B	451	PHE	CB-CA-C	-8.92	92.56	110.40
1	A	290	GLN	CB-CA-C	8.86	128.12	110.40
2	D	19	THR	C-N-CA	-8.73	103.96	122.30
1	B	36	ASN	N-CA-CB	-8.54	95.24	110.60
1	B	1	MET	CB-CA-C	8.33	127.06	110.40
2	D	15	LYS	CB-CA-C	8.24	126.87	110.40
1	B	561	TRP	CB-CA-C	-7.59	95.23	110.40
2	D	189	TRP	C-N-CA	7.55	140.58	121.70
2	C	194	CYS	CA-CB-SG	7.51	127.52	114.00
2	D	111	THR	N-CA-C	-7.46	90.86	111.00
1	A	35	LYS	CB-CA-C	7.23	124.85	110.40
2	D	208	CYS	CA-CB-SG	7.18	126.93	114.00
1	B	429	PHE	N-CA-C	-7.17	91.63	111.00
2	D	20	GLY	N-CA-C	7.14	130.95	113.10
2	D	190	CYS	CA-C-N	-7.13	101.51	117.20
1	B	455	GLN	N-CA-C	-7.12	91.77	111.00
2	C	53	ASN	CA-C-N	-7.03	101.73	117.20
2	C	37	SER	N-CA-C	-6.99	92.14	111.00
1	B	430	VAL	C-N-CA	-6.88	107.85	122.30
2	C	37	SER	N-CA-CB	6.77	120.66	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	17	ILE	N-CA-CB	-6.65	95.51	110.80
2	C	52	THR	C-N-CA	-6.62	105.15	121.70
1	B	561	TRP	N-CA-C	6.60	128.82	111.00
1	A	902	GLU	CA-CB-CG	6.56	127.83	113.40
1	B	185	PRO	N-CA-C	6.47	128.92	112.10
1	B	455	GLN	CB-CA-C	6.21	122.82	110.40
2	C	36	SER	N-CA-C	-6.14	94.42	111.00
1	B	750	THR	CB-CA-C	-6.12	95.06	111.60
1	B	35	LYS	N-CA-C	-6.12	94.47	111.00
2	C	190	CYS	O-C-N	6.11	132.47	122.70
1	B	885	ASN	N-CA-C	-6.03	94.72	111.00
2	C	53	ASN	CB-CA-C	5.97	122.35	110.40
1	B	747	GLY	CA-C-N	-5.86	104.48	116.20
1	B	193	TYR	N-CA-C	-5.84	95.23	111.00
1	B	431	GLY	C-N-CA	5.82	136.25	121.70
2	D	215	CYS	CA-CB-SG	5.75	124.36	114.00
1	B	36	ASN	N-CA-C	-5.75	95.49	111.00
1	B	465	HIS	CB-CA-C	-5.61	99.17	110.40
1	A	902	GLU	N-CA-CB	5.56	120.61	110.60
2	D	102	LEU	N-CA-CB	-5.47	99.46	110.40
1	B	431	GLY	CA-C-N	-5.42	105.28	117.20
1	B	780	THR	CA-C-N	-5.40	105.33	117.20
2	D	189	TRP	O-C-N	-5.36	114.12	122.70
2	D	17	ILE	N-CA-C	-5.34	96.57	111.00
1	B	449	MET	C-N-CA	5.31	133.45	122.30
1	B	366	ASP	CA-C-N	-5.30	105.54	117.20
1	A	902	GLU	N-CA-C	-5.26	96.79	111.00
1	B	378	CYS	N-CA-C	-5.18	97.02	111.00
1	B	117	GLU	N-CA-C	5.16	124.94	111.00
1	A	119	GLY	N-CA-C	5.16	125.99	113.10
1	B	746	SER	CB-CA-C	-5.15	100.31	110.10
2	C	36	SER	CB-CA-C	5.11	119.81	110.10
1	B	463	VAL	C-N-CA	5.08	134.41	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	430	VAL	Peptide
2	D	190	CYS	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8860	0	8828	466	0
1	B	8876	0	8842	793	0
2	C	1324	0	1306	128	0
2	D	1335	0	1323	177	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	20399	0	20299	1549	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1549) 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:B:367:LEU:HD21	1:B:374:GLN:CG	1.51	1.38
1:B:367:LEU:HD21	1:B:374:GLN:CB	1.50	1.37
1:B:367:LEU:CD2	1:B:374:GLN:HB2	1.53	1.37
1:B:742:VAL:CG2	1:B:750:THR:HG21	1.57	1.35
1:B:367:LEU:CD2	1:B:374:GLN:CG	2.06	1.34
2:D:169:GLY:O	2:D:212:PRO:CD	1.75	1.33
1:B:367:LEU:CD2	1:B:374:GLN:CB	2.08	1.31
1:B:367:LEU:CD1	1:B:374:GLN:OE1	1.79	1.31
1:B:432:GLN:OE1	1:B:454:ASP:CB	1.79	1.31
1:B:367:LEU:O	1:B:368:GLU:HG2	1.12	1.29
1:B:367:LEU:HD13	1:B:374:GLN:CD	1.51	1.28
2:D:169:GLY:O	2:D:212:PRO:HD2	1.28	1.27
2:D:190:CYS:SG	2:D:218:CYS:HB3	1.80	1.22
1:B:369:ARG:HB2	1:B:655:ARG:HH12	1.07	1.19
1:A:289:GLU:O	1:A:290:GLN:O	1.55	1.19
1:A:660:TYR:OH	1:A:708:GLN:OE1	1.58	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:THR:O	1:B:750:THR:CG2	1.79	1.19
2:D:170:PHE:O	2:D:193:SER:HB3	1.40	1.19
1:A:16:ASN:ND2	1:A:35:LYS:O	1.74	1.19
2:C:35:THR:HG22	2:C:36:SER:O	1.38	1.18
1:B:742:VAL:CG2	1:B:750:THR:CG2	2.21	1.18
1:B:367:LEU:HD13	1:B:374:GLN:OE1	1.02	1.18
1:B:367:LEU:CD2	1:B:374:GLN:HG3	1.72	1.17
1:B:367:LEU:O	1:B:368:GLU:CG	1.90	1.17
1:B:367:LEU:CD1	1:B:374:GLN:CD	2.12	1.15
1:B:474:ALA:HB3	1:B:477:ARG:HH22	1.08	1.14
1:B:432:GLN:OE1	1:B:454:ASP:HB3	0.97	1.12
1:B:889:ARG:HD3	1:B:904:ASN:HD21	0.98	1.10
1:B:742:VAL:HG23	1:B:750:THR:HG21	1.18	1.08
1:B:367:LEU:HD21	1:B:374:GLN:HG3	1.18	1.08
1:B:456:GLN:NE2	1:B:473:SER:OG	1.86	1.07
1:A:81:THR:HG22	1:A:83:LYS:H	1.19	1.07
1:B:286:GLU:HB2	1:B:299:ASP:H	1.17	1.07
2:C:52:THR:O	2:C:52:THR:HG22	1.52	1.07
1:B:368:GLU:OE1	1:B:391:ARG:NH2	1.88	1.06
1:B:367:LEU:HD11	1:B:374:GLN:HG3	1.37	1.06
2:D:111:THR:O	2:D:188:GLU:OE2	1.74	1.05
1:B:456:GLN:NE2	1:B:473:SER:CB	2.20	1.05
1:B:742:VAL:HG23	1:B:750:THR:CG2	1.83	1.05
1:A:371:GLY:HA3	1:A:1016:ASN:HD21	1.13	1.05
1:A:889:ARG:HD3	1:A:904:ASN:HD21	1.16	1.04
1:B:367:LEU:CD1	1:B:374:GLN:HG3	1.86	1.04
1:B:367:LEU:CD1	1:B:374:GLN:CG	2.35	1.03
1:B:81:THR:HG22	1:B:83:LYS:H	1.22	1.03
1:B:367:LEU:HD22	1:B:374:GLN:HB2	1.40	1.03
1:B:367:LEU:HD11	1:B:374:GLN:CG	1.89	1.03
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.38	1.02
1:B:450:GLY:HA3	1:B:479:VAL:HG11	1.42	1.01
1:B:367:LEU:HD12	1:B:368:GLU:HG2	1.44	1.00
1:B:267:ASN:HD21	1:B:269:SER:HB2	1.26	0.98
1:A:23:PHE:H	1:A:30:ASN:HD22	1.00	0.98
1:B:482:GLU:HB2	1:B:483:PRO:HD3	1.43	0.98
2:C:112:GLN:HE22	2:C:187:THR:HG23	1.28	0.98
2:D:143:ARG:HB3	2:D:143:ARG:CZ	1.89	0.98
2:C:52:THR:HG21	2:C:85:ILE:HG12	1.43	0.97
1:B:178:ILE:HG22	1:B:193:TYR:O	1.65	0.97
1:B:167:VAL:HG12	1:B:180:PHE:HB3	1.47	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLU:HB2	1:B:298:LYS:HB2	1.45	0.97
1:A:706:GLU:O	1:A:707:ILE:HG13	1.63	0.96
1:A:504:ASN:HD21	1:A:507:GLN:HE21	1.02	0.96
1:B:23:PHE:H	1:B:30:ASN:HD22	1.03	0.96
1:B:889:ARG:HD3	1:B:904:ASN:ND2	1.81	0.96
1:B:191:LYS:HG2	1:B:192:THR:H	1.30	0.96
1:A:356:LEU:HD21	1:A:712:ILE:HD13	1.48	0.95
1:B:367:LEU:CG	1:B:374:GLN:HG3	1.97	0.95
1:B:294:THR:HG22	1:B:295:VAL:H	1.30	0.94
1:B:24:THR:H	1:B:30:ASN:HD21	1.12	0.94
1:B:368:GLU:CD	1:B:391:ARG:NH2	2.20	0.93
1:B:368:GLU:OE2	1:B:391:ARG:NH2	2.01	0.93
1:A:889:ARG:HD3	1:A:904:ASN:ND2	1.83	0.93
2:D:171:HIS:NE2	2:D:212:PRO:HG2	1.84	0.93
1:B:478:LEU:HD23	1:B:479:VAL:H	1.31	0.92
2:C:190:CYS:HB2	2:C:218:CYS:SG	2.09	0.92
2:C:208:CYS:SG	2:C:210:GLN:HG2	2.09	0.92
1:B:976:VAL:HG22	1:B:996:GLY:HA3	1.50	0.92
1:B:286:GLU:HG3	1:B:299:ASP:HB3	1.52	0.91
1:B:474:ALA:HB3	1:B:477:ARG:NH2	1.85	0.91
1:B:480:SER:HB3	1:B:485:ALA:H	1.36	0.91
2:C:194:CYS:SG	2:C:208:CYS:N	2.42	0.91
1:B:450:GLY:O	1:B:479:VAL:HG21	1.70	0.91
2:D:108:THR:O	2:D:110:SER:N	2.04	0.91
2:D:80:ARG:HB2	2:D:81:PRO:HD3	1.51	0.90
2:C:52:THR:CG2	2:C:85:ILE:HG23	2.01	0.90
1:B:162:LEU:HD23	1:B:162:LEU:H	1.35	0.90
1:B:1125:THR:HG22	1:B:1127:ASP:H	1.34	0.90
1:B:742:VAL:O	1:B:750:THR:HB	1.71	0.90
1:B:478:LEU:HD23	1:B:479:VAL:N	1.87	0.90
1:B:225:PRO:HG2	1:B:267:ASN:HB2	1.53	0.89
1:B:450:GLY:HA3	1:B:479:VAL:CG1	2.01	0.89
1:A:422:TYR:HD1	1:A:683:ASN:H	1.11	0.89
1:B:1032:THR:HG22	1:B:1034:ASN:H	1.35	0.89
1:B:256:SER:HB2	1:B:276:MET:HB3	1.53	0.89
2:C:109:PRO:HG2	2:C:203:ARG:CZ	2.02	0.89
2:D:190:CYS:SG	2:D:218:CYS:CB	2.47	0.89
1:A:889:ARG:HH11	1:A:904:ASN:ND2	1.69	0.88
1:B:594:THR:HG22	1:B:595:THR:H	1.36	0.88
2:C:52:THR:HG21	2:C:85:ILE:HG23	1.54	0.88
1:B:453:ASP:OD2	1:B:472:THR:HG21	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:THR:H	1:B:30:ASN:ND2	1.70	0.88
1:A:253:ILE:HD12	1:A:258:ILE:HD11	1.55	0.87
1:B:456:GLN:CD	1:B:473:SER:HB3	1.94	0.87
2:D:169:GLY:O	2:D:212:PRO:HD3	1.71	0.87
1:B:570:LYS:HG3	1:B:572:PRO:HD2	1.56	0.87
2:C:52:THR:O	2:C:54:ALA:N	2.07	0.87
1:B:178:ILE:CG2	1:B:193:TYR:O	2.22	0.87
1:B:232:ILE:HG21	1:B:258:ILE:HD12	1.56	0.87
1:B:746:SER:OG	1:B:746:SER:O	1.78	0.87
2:C:52:THR:HG21	2:C:85:ILE:CG1	2.05	0.87
1:A:699:LEU:HD13	1:A:700:THR:N	1.90	0.86
1:A:396:ILE:HD13	1:A:396:ILE:H	1.38	0.86
1:B:507:GLN:HE22	1:B:553:SER:H	1.22	0.86
1:B:430:VAL:HG13	1:B:456:GLN:HB3	1.55	0.86
1:A:660:TYR:HH	1:A:708:GLN:CD	1.79	0.85
1:B:790:ASN:HB3	1:B:806:GLN:HA	1.59	0.85
1:B:404:LEU:O	1:B:407:ILE:HD11	1.75	0.85
2:C:194:CYS:SG	2:C:207:THR:N	2.49	0.85
2:D:171:HIS:HB2	2:D:215:CYS:CB	2.06	0.85
1:B:367:LEU:HD22	1:B:374:GLN:CG	2.07	0.85
1:B:436:LEU:HD12	1:B:445:GLU:HB3	1.59	0.85
1:B:869:ALA:O	1:B:884:ILE:O	1.94	0.85
1:B:433:THR:HG21	1:B:457:THR:OG1	1.76	0.85
1:B:329:GLY:HA3	1:B:384:GLU:HG2	1.59	0.84
1:B:369:ARG:HB2	1:B:655:ARG:NH1	1.92	0.84
1:B:994:GLU:O	1:B:995:VAL:HG22	1.78	0.84
1:A:743:GLN:HA	1:A:749:THR:HG22	1.59	0.84
1:B:432:GLN:CD	1:B:454:ASP:HB3	1.98	0.84
1:A:23:PHE:H	1:A:30:ASN:ND2	1.74	0.83
1:A:553:SER:O	1:A:571:LEU:HD12	1.79	0.83
1:B:742:VAL:HG21	1:B:750:THR:HG21	1.60	0.83
2:C:51:LEU:HD22	2:C:142:THR:H	1.43	0.83
1:B:742:VAL:HG22	1:B:750:THR:CG2	2.09	0.83
1:A:24:THR:H	1:A:30:ASN:HD21	1.25	0.83
1:A:417:PRO:HG3	1:A:481:GLN:HB3	1.61	0.82
1:B:731:GLN:HA	1:B:796:GLN:NE2	1.94	0.82
1:B:451:PHE:C	1:B:451:PHE:CD2	2.52	0.82
1:B:756:ALA:HB1	1:B:801:VAL:HG21	1.61	0.82
1:A:873:MET:HE2	1:A:880:LEU:HD11	1.61	0.82
1:A:186:GLN:H	1:A:186:GLN:HE21	1.28	0.82
1:B:255:GLN:H	1:B:255:GLN:HE21	1.28	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:HB3	1:B:1037:ILE:HB	1.61	0.82
2:C:168:GLY:HA2	2:C:193:SER:HB2	1.61	0.82
1:A:780:THR:O	1:A:781:SER:O	1.96	0.81
1:A:1032:THR:HG23	1:A:1034:ASN:H	1.44	0.81
1:B:981:SER:HA	1:B:989:ARG:HG3	1.63	0.81
1:B:367:LEU:C	1:B:368:GLU:HG2	2.01	0.81
1:B:367:LEU:O	1:B:367:LEU:HD12	1.80	0.81
1:B:437:MET:HB3	1:B:444:GLU:O	1.80	0.81
2:D:114:VAL:HG22	2:D:185:LYS:HD3	1.62	0.81
1:B:750:THR:O	1:B:750:THR:HG22	1.01	0.81
1:B:803:HIS:HD2	1:B:804:ALA:H	1.29	0.81
2:C:190:CYS:CB	2:C:218:CYS:SG	2.69	0.81
1:B:290:GLN:HE21	1:B:293:GLY:HA3	1.43	0.80
2:D:88:ALA:HA	2:D:199:ALA:HB3	1.61	0.80
1:A:81:THR:HG22	1:A:83:LYS:N	1.96	0.80
1:B:25:SER:O	1:B:74:LYS:HB3	1.82	0.80
1:B:297:LEU:HD21	1:B:300:LEU:HD11	1.63	0.80
1:A:705:ASP:OD2	1:A:709:LYS:HE2	1.82	0.80
1:B:476:VAL:HG13	1:B:490:TRP:HB3	1.64	0.80
2:C:112:GLN:NE2	2:C:187:THR:HG23	1.96	0.80
1:B:1101:SER:OG	1:B:1103:PRO:HD2	1.80	0.80
2:D:192:PRO:O	2:D:194:CYS:N	2.15	0.80
1:B:275:ASP:HB2	1:B:279:ARG:H	1.45	0.79
1:B:466:GLN:O	1:B:481:GLN:HB2	1.82	0.79
1:B:1105:MET:HE3	1:B:1126:ALA:HB1	1.65	0.79
1:B:139:LEU:HB3	1:B:156:ASN:HD22	1.45	0.79
2:D:116:ASP:O	2:D:182:ASP:HB3	1.83	0.78
1:A:454:ASP:O	1:A:455:GLN:HG2	1.83	0.78
1:A:889:ARG:HH11	1:A:904:ASN:HD21	1.27	0.78
1:A:416:ASP:HB3	1:A:419:ARG:HG3	1.66	0.78
1:B:894:THR:HG22	1:B:896:GLU:H	1.49	0.78
1:A:112:ILE:HD13	1:A:112:ILE:H	1.46	0.78
1:B:419:ARG:HH11	1:B:423:ASP:HB3	1.48	0.78
1:B:47:GLU:HG2	1:B:48:GLY:H	1.48	0.78
1:A:186:GLN:H	1:A:186:GLN:NE2	1.81	0.78
1:A:24:THR:H	1:A:30:ASN:ND2	1.81	0.77
1:B:432:GLN:OE1	1:B:454:ASP:CA	2.32	0.77
1:A:429:PHE:O	1:A:456:GLN:HG3	1.84	0.77
1:A:706:GLU:O	1:A:707:ILE:CG1	2.31	0.77
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.66	0.77
1:A:440:GLY:O	1:A:686:GLY:HA3	1.82	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:THR:O	2:C:52:THR:CG2	2.24	0.77
2:C:52:THR:HG21	2:C:85:ILE:CG2	2.15	0.77
1:A:68:ARG:HD3	1:A:75:ASP:OD2	1.84	0.77
1:A:504:ASN:HD21	1:A:507:GLN:NE2	1.81	0.77
1:A:262:ASN:ND2	1:A:316:TYR:H	1.81	0.77
1:A:504:ASN:ND2	1:A:507:GLN:HE21	1.81	0.77
2:C:50:LEU:HD21	2:C:197:ILE:HG13	1.65	0.77
1:A:867:LYS:HE2	1:A:889:ARG:HH22	1.48	0.77
1:B:81:THR:HB	1:B:85:ASN:H	1.50	0.77
2:C:208:CYS:SG	2:C:211:CYS:N	2.58	0.77
1:A:909:ILE:HG12	1:A:928:ARG:HD2	1.67	0.76
1:B:255:GLN:H	1:B:255:GLN:NE2	1.82	0.76
2:D:15:LYS:HD2	2:D:41:ASN:ND2	1.99	0.76
1:A:589:ARG:HG3	1:A:635:PRO:HB2	1.67	0.76
1:B:23:PHE:N	1:B:30:ASN:HD22	1.82	0.76
1:B:450:GLY:CA	1:B:479:VAL:CG1	2.64	0.76
2:D:15:LYS:HD2	2:D:41:ASN:HD22	1.48	0.76
1:A:901:THR:HG22	1:A:902:GLU:O	1.85	0.76
1:B:367:LEU:HD22	1:B:374:GLN:CB	1.98	0.76
1:A:234:GLN:HE22	1:A:257:THR:HA	1.51	0.76
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.67	0.76
2:D:170:PHE:O	2:D:193:SER:CB	2.30	0.76
1:A:415:SER:HB3	1:A:423:ASP:OD1	1.86	0.76
1:B:466:GLN:H	1:B:466:GLN:HE21	1.34	0.76
1:B:492:GLU:HG3	1:B:512:VAL:HG11	1.68	0.76
1:B:286:GLU:HB2	1:B:299:ASP:N	1.96	0.76
1:A:910:MET:CE	1:A:912:LEU:HD21	2.16	0.76
1:B:396:ILE:HD11	1:B:673:LEU:HD11	1.66	0.75
1:B:478:LEU:HB2	1:B:526:LEU:HD21	1.68	0.75
2:D:122:LEU:HD12	2:D:122:LEU:H	1.50	0.75
1:A:371:GLY:HA3	1:A:1016:ASN:ND2	1.95	0.75
1:B:742:VAL:HG22	1:B:750:THR:HG22	1.66	0.75
1:B:405:PRO:HA	1:B:697:SER:HA	1.68	0.75
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.15	0.75
2:D:98:ILE:HB	2:D:201:ALA:HB1	1.68	0.75
1:B:191:LYS:HG2	1:B:192:THR:N	2.02	0.75
1:B:594:THR:HG22	1:B:595:THR:N	2.02	0.75
1:B:803:HIS:CD2	1:B:804:ALA:H	2.05	0.74
2:D:50:LEU:O	2:D:52:THR:HG23	1.86	0.74
1:B:235:GLU:H	1:B:253:ILE:HG22	1.52	0.74
1:A:146:ASP:C	1:A:148:ASP:H	1.89	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LEU:HD12	1:B:368:GLU:CG	2.17	0.74
1:A:342:GLU:HG2	1:A:343:GLN:HG3	1.68	0.74
1:A:798:THR:OG1	1:A:800:GLU:HG2	1.88	0.74
1:B:159:LEU:HD23	1:B:161:GLU:H	1.52	0.74
1:B:864:LYS:HE2	1:B:891:TYR:HE2	1.52	0.74
1:B:663:ASN:HB2	1:B:1134:GLU:HG3	1.69	0.74
1:A:931:LEU:HD23	1:A:932:LEU:N	2.03	0.74
1:A:1032:THR:HG22	1:A:1036:MET:H	1.53	0.74
1:B:1070:HIS:CE1	1:B:1093:LEU:HD12	2.23	0.73
2:D:208:CYS:O	2:D:210:GLN:N	2.21	0.73
1:A:750:THR:HG22	1:A:751:ALA:H	1.52	0.73
1:A:903:CYS:SG	1:A:941:ASN:HA	2.28	0.73
1:A:282:MET:HG2	1:A:305:LEU:HD11	1.69	0.73
1:A:642:ARG:HG2	1:A:647:THR:HB	1.69	0.73
1:B:368:GLU:OE2	1:B:391:ARG:CZ	2.36	0.73
1:A:855:ASP:O	1:A:857:LYS:N	2.21	0.73
1:B:314:LEU:O	1:B:314:LEU:HD12	1.88	0.73
1:A:803:HIS:CD2	1:A:858:LEU:HB2	2.24	0.73
1:B:267:ASN:ND2	1:B:269:SER:HB2	2.03	0.73
2:D:108:THR:HB	2:D:109:PRO:HD3	1.71	0.73
1:B:367:LEU:CD2	1:B:374:GLN:CD	2.56	0.73
1:B:407:ILE:HD12	1:B:407:ILE:H	1.52	0.73
2:D:102:LEU:HD11	2:D:180:VAL:HG22	1.70	0.73
1:A:936:LYS:HE2	1:A:943:GLU:OE2	1.89	0.72
1:B:707:ILE:CG2	1:B:709:LYS:HE3	2.20	0.72
1:B:450:GLY:CA	1:B:479:VAL:HG13	2.19	0.72
1:B:368:GLU:OE2	1:B:374:GLN:OE1	2.07	0.72
2:D:170:PHE:C	2:D:193:SER:HB3	2.09	0.72
2:C:109:PRO:HG2	2:C:203:ARG:NH2	2.03	0.72
1:B:597:GLU:HG2	1:B:664:HIS:CE1	2.24	0.72
2:C:52:THR:HG21	2:C:85:ILE:CB	2.19	0.72
1:B:129:ARG:NH1	1:B:176:PRO:HD3	2.04	0.72
2:D:19:THR:HG22	2:D:20:GLY:H	1.55	0.71
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.25	0.71
1:A:564:ILE:HG22	1:A:582:LEU:HD12	1.72	0.71
1:B:141:LYS:HD2	1:B:156:ASN:OD1	1.90	0.71
1:B:147:ARG:HE	1:B:147:ARG:HA	1.56	0.71
1:B:451:PHE:CD2	1:B:451:PHE:O	2.43	0.71
1:B:504:ASN:HD21	1:B:507:GLN:HB2	1.55	0.71
2:C:30:GLN:HE21	2:C:36:SER:HA	1.54	0.71
1:B:634:GLN:HB3	1:B:635:PRO:HD2	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD13	1:B:300:LEU:HD13	1.71	0.71
1:A:867:LYS:CE	1:A:889:ARG:HH22	2.04	0.71
1:B:367:LEU:HD22	1:B:374:GLN:CD	2.10	0.71
1:B:23:PHE:H	1:B:30:ASN:ND2	1.83	0.71
1:B:456:GLN:HE22	1:B:473:SER:CB	2.04	0.71
1:A:648:ASN:HD22	1:A:660:TYR:HB3	1.56	0.71
2:C:50:LEU:HD21	2:C:197:ILE:CG1	2.21	0.70
1:A:750:THR:HG22	1:A:751:ALA:N	2.06	0.70
1:B:124:ILE:HG23	1:B:131:ILE:HD13	1.71	0.70
1:B:731:GLN:HA	1:B:796:GLN:HE21	1.56	0.70
1:A:1032:THR:HG21	1:A:1036:MET:HB3	1.71	0.70
1:B:449:MET:HA	1:B:449:MET:CE	2.21	0.70
1:B:643:SER:HB3	1:B:706:GLU:HG3	1.73	0.70
1:A:291:MET:HG3	1:A:292:ASP:H	1.57	0.70
1:A:879:LYS:HE2	1:A:902:GLU:OE2	1.91	0.70
2:C:52:THR:CG2	2:C:85:ILE:HG12	2.20	0.70
1:A:16:ASN:HD22	1:A:35:LYS:C	1.94	0.70
1:B:656:PRO:HB2	1:B:671:VAL:HB	1.74	0.70
1:B:665:LYS:HD3	1:B:1138:ARG:NH1	2.07	0.70
2:C:108:THR:O	2:C:110:SER:N	2.24	0.70
2:C:164:GLY:O	2:C:194:CYS:HA	1.91	0.70
2:D:99:PRO:HG2	2:D:106:ASP:HA	1.73	0.70
1:A:289:GLU:C	1:A:290:GLN:O	2.30	0.70
1:B:196:SER:OG	1:B:199:GLU:HG2	1.92	0.70
1:B:63:VAL:HB	1:B:80:LEU:HB3	1.72	0.69
2:D:171:HIS:CD2	2:D:212:PRO:HG2	2.25	0.69
1:A:369:ARG:O	1:A:370:GLN:HB3	1.92	0.69
1:B:419:ARG:NH1	1:B:423:ASP:HB3	2.05	0.69
1:B:1036:MET:O	1:B:1037:ILE:HB	1.92	0.69
2:C:215:CYS:SG	2:C:218:CYS:N	2.64	0.69
1:A:1022:THR:HG22	1:A:1024:THR:H	1.58	0.69
2:C:52:THR:CB	2:C:85:ILE:HA	2.21	0.69
1:A:298:LYS:HD3	1:A:299:ASP:HB2	1.74	0.69
1:A:480:SER:HB3	1:A:487:VAL:HG11	1.74	0.69
1:B:107:ASN:OD1	1:B:109:GLN:HG2	1.91	0.69
1:B:482:GLU:CB	1:B:483:PRO:HD3	2.18	0.69
2:D:82:LYS:C	2:D:83:ILE:HD12	2.12	0.69
1:A:253:ILE:O	1:A:255:GLN:N	2.25	0.69
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.75	0.69
1:A:507:GLN:NE2	1:A:553:SER:H	1.90	0.69
1:B:130:MET:HG2	1:B:197:LEU:HD21	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ARG:HH12	1:B:670:ASN:HB3	1.58	0.69
1:B:456:GLN:OE1	1:B:473:SER:HB3	1.93	0.69
1:B:480:SER:HB3	1:B:485:ALA:N	2.08	0.69
2:C:108:THR:O	2:C:222:THR:HA	1.93	0.69
1:B:1026:GLY:O	1:B:1041:THR:HG22	1.92	0.69
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.74	0.68
1:B:464:ALA:O	1:B:465:HIS:ND1	2.27	0.68
1:B:736:LEU:HD13	1:B:813:ALA:HB1	1.75	0.68
1:A:81:THR:CG2	1:A:83:LYS:H	2.02	0.68
1:B:367:LEU:HD21	1:B:374:GLN:CA	2.23	0.68
2:C:86:VAL:CG1	2:C:198:THR:HA	2.23	0.68
1:A:844:LYS:HG3	1:A:845:GLN:HG3	1.76	0.68
1:B:910:MET:HB2	1:B:926:LEU:HB3	1.75	0.68
1:B:474:ALA:CB	1:B:477:ARG:HH22	1.96	0.68
1:A:372:GLN:HB3	1:A:1014:MET:SD	2.34	0.68
1:B:167:VAL:O	1:B:168:LYS:HB2	1.92	0.68
1:A:977:CYS:HB3	1:A:992:LEU:HD13	1.75	0.68
1:B:582:LEU:HD12	1:B:582:LEU:O	1.93	0.68
2:C:161:PHE:CE1	2:C:163:ARG:HB2	2.29	0.67
1:B:402:ILE:HD12	1:B:402:ILE:N	2.10	0.67
2:D:163:ARG:H	2:D:163:ARG:HD2	1.58	0.67
1:B:112:ILE:HG22	1:B:113:GLY:H	1.58	0.67
1:B:450:GLY:HA2	1:B:479:VAL:HG13	1.75	0.67
1:B:475:SER:HA	1:B:498:ILE:HD11	1.74	0.67
1:A:929:SER:HB3	1:A:952:ASN:HB2	1.76	0.67
1:B:294:THR:HG22	1:B:295:VAL:N	2.05	0.67
2:C:38:LEU:O	2:C:40:LYS:N	2.27	0.67
1:A:839:GLU:CD	1:A:839:GLU:H	1.99	0.67
1:B:1032:THR:HG22	1:B:1033:VAL:N	2.10	0.67
1:A:992:LEU:HD12	1:A:992:LEU:O	1.94	0.67
2:C:161:PHE:HE1	2:C:163:ARG:HB2	1.60	0.67
1:A:663:ASN:O	1:A:664:HIS:HB2	1.95	0.67
1:B:514:ARG:O	1:B:514:ARG:HG2	1.94	0.67
2:C:88:ALA:HA	2:C:199:ALA:HB3	1.76	0.67
2:D:171:HIS:HB2	2:D:215:CYS:HB2	1.76	0.67
1:B:355:ASN:C	1:B:357:GLY:H	1.96	0.66
1:B:704:ILE:HD13	1:B:704:ILE:H	1.60	0.66
1:B:80:LEU:HD22	1:B:133:LEU:HD23	1.76	0.66
2:D:51:LEU:HD12	2:D:142:THR:H	1.60	0.66
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.77	0.66
1:A:275:ASP:HB3	1:A:279:ARG:H	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:ASP:O	1:A:1132:VAL:HG23	1.94	0.66
1:A:388:ARG:HD3	1:A:714:THR:HB	1.76	0.66
1:A:416:ASP:HB3	1:A:419:ARG:CG	2.25	0.66
1:A:23:PHE:N	1:A:30:ASN:HD22	1.84	0.66
1:B:1017:LEU:HD12	1:B:1019:GLU:OE2	1.96	0.66
1:B:232:ILE:CG2	1:B:258:ILE:HD12	2.25	0.66
1:B:690:SER:C	1:B:691:LEU:HD12	2.15	0.66
2:D:113:THR:HB	2:D:186:VAL:HB	1.78	0.66
1:B:270:ARG:HG2	1:B:284:LEU:HD23	1.78	0.66
1:B:743:GLN:HE21	1:B:782:PHE:HA	1.60	0.66
2:D:168:GLY:CA	2:D:208:CYS:SG	2.84	0.66
1:B:275:ASP:CG	1:B:279:ARG:HB2	2.16	0.66
1:B:973:ASN:HD21	1:B:1077:HIS:H	1.42	0.66
1:B:1112:LEU:HD23	1:B:1113:GLN:N	2.11	0.66
1:A:207:TRP:CB	1:A:242:GLY:HA2	2.27	0.65
1:B:742:VAL:HG23	1:B:750:THR:CB	2.25	0.65
1:B:695:ASN:HB2	1:B:698:THR:HG22	1.77	0.65
1:B:707:ILE:HG23	1:B:709:LYS:HE3	1.78	0.65
1:A:648:ASN:HD22	1:A:660:TYR:CB	2.09	0.65
1:A:396:ILE:H	1:A:396:ILE:CD1	2.09	0.65
1:B:465:HIS:CE1	1:B:523:PRO:HD3	2.32	0.65
2:D:163:ARG:HD2	2:D:197:ILE:HD11	1.78	0.65
1:A:611:LEU:C	1:A:611:LEU:HD23	2.17	0.65
1:A:1085:ALA:O	1:A:1086:THR:HG23	1.96	0.65
1:A:1113:GLN:HB3	1:A:1121:LYS:HD2	1.78	0.65
2:D:49:GLY:HA3	2:D:83:ILE:HG13	1.79	0.65
2:D:168:GLY:HA2	2:D:208:CYS:SG	2.37	0.65
2:D:171:HIS:HB2	2:D:215:CYS:HB3	1.79	0.65
1:A:10:GLN:HB2	1:A:1037:ILE:HB	1.78	0.65
1:A:699:LEU:HD13	1:A:700:THR:H	1.58	0.64
1:B:112:ILE:N	1:B:112:ILE:HD12	2.12	0.64
1:B:365:VAL:O	1:B:367:LEU:HD23	1.98	0.64
2:D:163:ARG:CD	2:D:197:ILE:HD11	2.26	0.64
1:B:385:GLY:HA3	1:B:719:GLU:O	1.97	0.64
1:B:894:THR:HG22	1:B:895:THR:N	2.11	0.64
1:A:564:ILE:HG22	1:A:564:ILE:O	1.97	0.64
1:B:16:ASN:ND2	1:B:35:LYS:O	2.23	0.64
1:B:427:LEU:HD13	1:B:429:PHE:HE1	1.62	0.64
1:B:1058:LEU:HD23	1:B:1093:LEU:HD22	1.80	0.64
1:B:407:ILE:HD12	1:B:407:ILE:N	2.11	0.64
1:A:368:GLU:HB3	1:A:370:GLN:HE22	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:HB2	1:A:279:ARG:HB2	1.79	0.64
1:B:208:LYS:HG3	1:B:209:GLN:H	1.62	0.64
1:B:238:THR:HA	1:B:247:ALA:HA	1.79	0.64
2:D:46:GLY:O	2:D:146:GLU:HG3	1.97	0.64
1:B:432:GLN:OE1	1:B:454:ASP:O	2.16	0.64
1:B:451:PHE:O	1:B:451:PHE:HD2	1.81	0.64
2:C:145:ILE:HD11	2:C:174:GLU:CD	2.18	0.64
1:B:317:LEU:O	1:B:318:ASP:HB2	1.96	0.64
1:B:419:ARG:HD3	1:B:421:THR:O	1.97	0.64
2:D:170:PHE:N	2:D:170:PHE:CD1	2.66	0.64
1:A:1051:LEU:HD22	1:A:1094:ILE:HG12	1.79	0.63
1:B:19:VAL:HG22	1:B:20:THR:H	1.63	0.63
1:B:682:LEU:HD13	1:B:683:ASN:N	2.13	0.63
1:B:272:LEU:HD22	1:B:280:LEU:HD11	1.80	0.63
1:B:367:LEU:HD22	1:B:374:GLN:NE2	2.13	0.63
2:D:218:CYS:HB2	2:D:221:ASP:OD1	1.98	0.63
1:A:767:SER:O	1:A:769:LYS:HE3	1.98	0.63
1:B:394:ILE:HD12	1:B:658:VAL:HB	1.81	0.63
1:B:1022:THR:HG22	1:B:1024:THR:OG1	1.99	0.63
1:B:1130:ILE:O	1:B:1134:GLU:HB2	1.97	0.63
1:B:866:VAL:HG12	1:B:884:ILE:HG21	1.80	0.63
1:B:129:ARG:HD3	1:B:176:PRO:HG3	1.81	0.63
1:B:432:GLN:O	1:B:433:THR:OG1	2.17	0.63
1:B:481:GLN:NE2	1:B:484:LYS:NZ	2.47	0.63
1:B:742:VAL:CG2	1:B:750:THR:HG22	2.19	0.62
1:A:580:GLU:HG2	1:A:614:PHE:CZ	2.33	0.62
1:A:706:GLU:C	1:A:707:ILE:HG13	2.19	0.62
1:A:268:GLY:O	1:A:270:ARG:N	2.32	0.62
1:A:780:THR:HB	1:A:784:GLU:HB2	1.81	0.62
1:B:507:GLN:NE2	1:B:553:SER:H	1.96	0.62
2:D:128:LYS:HE2	2:D:146:GLU:OE1	2.00	0.62
1:B:513:GLY:O	1:B:514:ARG:HB3	1.99	0.62
1:B:926:LEU:HG	1:B:927:MET:HG3	1.81	0.62
2:D:102:LEU:HD23	2:D:102:LEU:O	1.99	0.62
1:A:986:ASP:HB2	1:B:1118:SER:HB3	1.81	0.62
1:A:1114:TYR:HB2	1:A:1124:ALA:HB2	1.82	0.62
1:B:803:HIS:CD2	1:B:804:ALA:N	2.67	0.62
1:B:474:ALA:O	1:B:475:SER:HB3	2.00	0.62
1:B:1051:LEU:HA	1:B:1054:MET:HB2	1.80	0.62
1:A:910:MET:HE3	1:A:912:LEU:HD21	1.81	0.62
1:B:414:ARG:HB2	1:B:462:ASN:ND2	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLN:NE2	1:B:473:SER:HB3	2.00	0.62
2:C:164:GLY:HA2	2:C:194:CYS:O	2.00	0.62
2:D:173:ARG:NH1	2:D:218:CYS:HB3	2.14	0.62
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.64	0.61
1:B:739:ARG:NH1	1:B:758:THR:HG23	2.15	0.61
1:B:918:GLY:O	1:B:919:ASP:HB2	1.99	0.61
1:B:629:VAL:HA	1:B:1017:LEU:O	1.99	0.61
1:B:769:LYS:H	1:B:769:LYS:HD2	1.65	0.61
2:D:47:VAL:HG12	2:D:48:THR:N	2.15	0.61
1:B:386:SER:HA	1:B:717:LEU:HG	1.81	0.61
1:B:440:GLY:O	1:B:686:GLY:HA3	2.00	0.61
1:A:986:ASP:H	1:B:1118:SER:HB3	1.65	0.61
1:B:14:ALA:HB1	1:B:327:ARG:HG3	1.82	0.61
1:B:414:ARG:HB2	1:B:462:ASN:HD21	1.64	0.61
2:C:52:THR:HG22	2:C:85:ILE:HG23	1.82	0.61
2:C:119:GLY:O	2:C:120:LYS:HB2	1.99	0.61
1:A:234:GLN:NE2	1:A:257:THR:HA	2.14	0.61
1:A:358:PRO:O	1:A:379:SER:HA	2.01	0.61
1:B:286:GLU:O	1:B:297:LEU:HD12	2.00	0.61
1:B:644:LEU:HD23	1:B:644:LEU:H	1.66	0.61
1:B:740:ILE:N	1:B:740:ILE:HD12	2.16	0.61
1:A:564:ILE:HG22	1:A:582:LEU:CD1	2.29	0.60
2:C:160:ASP:CG	2:C:161:PHE:H	2.04	0.60
1:B:1105:MET:CE	1:B:1126:ALA:HB1	2.31	0.60
1:A:722:ARG:HG3	1:A:722:ARG:HH11	1.65	0.60
1:B:1013:VAL:O	1:B:1014:MET:HB3	2.01	0.60
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.83	0.60
1:A:889:ARG:HD2	1:A:901:THR:HG23	1.84	0.60
1:B:594:THR:CG2	1:B:595:THR:H	2.12	0.60
1:B:43:VAL:HG23	1:B:52:VAL:HG11	1.83	0.60
1:B:232:ILE:HG12	1:B:237:ILE:HG23	1.82	0.60
1:B:432:GLN:OE1	1:B:454:ASP:C	2.39	0.60
1:B:693:LEU:N	1:B:693:LEU:HD23	2.16	0.60
1:B:994:GLU:HG3	1:B:995:VAL:H	1.66	0.60
2:D:111:THR:C	2:D:188:GLU:OE2	2.38	0.60
1:A:564:ILE:N	1:A:564:ILE:HD12	2.16	0.60
1:A:660:TYR:CZ	1:A:708:GLN:OE1	2.50	0.60
1:B:162:LEU:H	1:B:162:LEU:CD2	2.10	0.60
1:B:367:LEU:HD21	1:B:374:GLN:N	2.16	0.60
1:B:498:ILE:CG2	1:B:512:VAL:HG22	2.31	0.60
2:C:180:VAL:HG12	2:C:180:VAL:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LYS:HG2	1:B:575:GLU:OE1	2.02	0.60
1:A:848:ILE:HD11	1:A:870:VAL:HG11	1.83	0.60
1:B:1118:SER:O	1:B:1120:MET:HG3	2.02	0.60
2:D:147:GLU:O	2:D:149:ARG:N	2.34	0.60
1:A:543:ILE:O	1:A:543:ILE:HG13	2.02	0.60
1:B:356:LEU:HD23	1:B:388:ARG:HG3	1.83	0.59
1:B:985:THR:O	1:B:989:ARG:HB3	2.02	0.59
1:B:1108:VAL:O	1:B:1109:VAL:HB	2.02	0.59
1:A:160:GLU:HB3	1:A:161:GLU:OE2	2.02	0.59
1:A:300:LEU:N	1:A:300:LEU:HD23	2.17	0.59
1:B:5:TYR:CE2	1:B:7:VAL:CG2	2.85	0.59
2:D:143:ARG:HA	2:D:175:TYR:O	2.01	0.59
1:B:167:VAL:HG12	1:B:180:PHE:CB	2.26	0.59
1:A:589:ARG:HG2	1:A:589:ARG:HH11	1.66	0.59
1:A:867:LYS:CD	1:A:867:LYS:H	2.15	0.59
2:D:174:GLU:O	2:D:188:GLU:HA	2.03	0.59
2:D:192:PRO:C	2:D:194:CYS:H	2.05	0.59
1:A:492:GLU:CD	1:A:494:GLN:H	2.05	0.59
1:B:472:THR:OG1	1:B:477:ARG:NH2	2.33	0.59
1:A:743:GLN:HB3	1:A:782:PHE:O	2.03	0.59
2:D:22:ASN:O	2:D:24:VAL:N	2.36	0.59
2:D:112:GLN:HE22	2:D:187:THR:HG23	1.67	0.59
1:A:20:THR:HB	1:A:315:THR:HG21	1.84	0.59
1:B:449:MET:O	1:B:451:PHE:N	2.35	0.59
1:B:1032:THR:CG2	1:B:1033:VAL:N	2.66	0.59
2:C:208:CYS:SG	2:C:210:GLN:CG	2.88	0.59
1:A:36:ASN:OD1	1:A:60:LYS:HD2	2.02	0.59
1:A:186:GLN:NE2	1:A:186:GLN:N	2.50	0.59
1:A:532:THR:HG22	1:A:533:GLU:N	2.17	0.59
1:B:192:THR:OG1	1:B:205:GLY:HA3	2.02	0.59
1:B:1062:ILE:HD13	1:B:1100:ILE:HD11	1.85	0.59
2:D:208:CYS:C	2:D:210:GLN:H	2.03	0.59
1:A:1070:HIS:CE1	1:A:1093:LEU:HD12	2.38	0.59
1:A:188:ARG:NH1	1:A:216:ALA:O	2.36	0.58
1:A:507:GLN:HE22	1:A:553:SER:HB3	1.68	0.58
1:A:780:THR:HG22	1:A:781:SER:H	1.68	0.58
1:B:417:PRO:HG3	1:B:481:GLN:OE1	2.03	0.58
2:D:112:GLN:NE2	2:D:187:THR:HG23	2.18	0.58
1:A:288:GLU:HB3	1:A:296:THR:HG23	1.86	0.58
1:A:1118:SER:C	1:A:1120:MET:H	2.07	0.58
1:B:466:GLN:HE21	1:B:466:GLN:N	1.99	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:GLU:O	1:B:707:ILE:HB	2.03	0.58
1:B:795:ASP:HB3	1:B:798:THR:OG1	2.03	0.58
1:B:866:VAL:HG11	1:B:884:ILE:HD12	1.86	0.58
1:B:369:ARG:HH21	1:B:372:GLN:CD	2.06	0.58
1:B:577:LEU:O	1:B:578:HIS:HB2	2.02	0.58
1:B:199:GLU:HG3	1:B:201:GLU:HG2	1.84	0.58
1:B:1014:MET:HG3	1:B:1015:GLN:N	2.17	0.58
1:A:298:LYS:HD3	1:A:298:LYS:C	2.24	0.58
1:B:129:ARG:HD3	1:B:176:PRO:CG	2.33	0.58
1:B:341:ASN:ND2	1:B:342:GLU:HG2	2.19	0.58
2:C:51:LEU:HD23	2:C:141:MET:HA	1.86	0.58
1:A:146:ASP:C	1:A:148:ASP:N	2.56	0.58
1:B:53:LYS:HE3	1:B:98:ILE:HB	1.85	0.58
1:B:356:LEU:O	1:B:357:GLY:O	2.21	0.58
1:B:1070:HIS:NE2	1:B:1093:LEU:HD12	2.19	0.58
1:A:910:MET:HE2	1:A:912:LEU:HD21	1.84	0.58
1:A:1032:THR:HB	1:A:1036:MET:O	2.03	0.58
1:B:367:LEU:HD11	1:B:374:GLN:OE1	1.95	0.58
1:B:368:GLU:HG3	1:B:369:ARG:HG2	1.86	0.58
2:D:172:ARG:HH21	2:D:191:ASN:HD22	1.50	0.58
1:A:766:SER:HB3	1:A:808:LEU:HD23	1.85	0.58
1:A:771:PHE:CE2	1:A:845:GLN:HB3	2.39	0.58
1:B:310:ILE:HG21	1:B:328:LEU:HD12	1.86	0.58
1:B:864:LYS:HE2	1:B:891:TYR:CE2	2.35	0.58
1:B:1065:VAL:C	1:B:1067:LYS:H	2.07	0.58
1:B:368:GLU:CD	1:B:391:ARG:HH21	2.06	0.58
1:B:842:GLU:HG2	2:D:128:LYS:NZ	2.18	0.58
1:A:578:HIS:CD2	1:A:623:LEU:H	2.22	0.58
1:A:864:LYS:HE2	1:A:891:TYR:HE2	1.68	0.58
1:B:143:ILE:HG12	1:B:154:ALA:HB2	1.85	0.58
1:B:437:MET:HB2	1:B:446:THR:HG23	1.85	0.58
1:A:262:ASN:HD21	1:A:316:TYR:H	1.48	0.57
1:B:294:THR:CG2	1:B:295:VAL:H	2.11	0.57
2:D:108:THR:HG22	2:D:109:PRO:N	2.17	0.57
1:B:1039:LEU:HD12	1:B:1040:VAL:H	1.69	0.57
2:D:173:ARG:HH12	2:D:218:CYS:HB3	1.69	0.57
1:B:486:LEU:HG	1:B:486:LEU:O	2.05	0.57
1:B:1028:VAL:O	1:B:1039:LEU:HD12	2.05	0.57
1:B:1108:VAL:HG12	1:B:1109:VAL:N	2.19	0.57
2:D:108:THR:CB	2:D:109:PRO:HD3	2.34	0.57
1:B:433:THR:HG22	1:B:433:THR:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLY:O	1:B:479:VAL:CG2	2.49	0.57
1:B:465:HIS:O	1:B:467:GLN:HG3	2.04	0.57
1:A:117:GLU:O	1:A:119:GLY:N	2.37	0.57
1:B:256:SER:HB3	1:B:277:GLU:OE2	2.04	0.57
1:B:500:VAL:HB	1:B:511:ALA:HB3	1.85	0.57
1:B:550:ASN:O	1:B:552:LEU:N	2.38	0.57
1:B:769:LYS:HD2	1:B:769:LYS:N	2.18	0.57
1:B:24:THR:N	1:B:30:ASN:HD21	1.92	0.57
1:B:365:VAL:O	1:B:367:LEU:CD2	2.52	0.57
1:B:504:ASN:OD1	1:B:507:GLN:N	2.31	0.57
1:A:1032:THR:CG2	1:A:1036:MET:H	2.17	0.57
1:A:507:GLN:HE22	1:A:553:SER:H	1.51	0.57
1:B:743:GLN:NE2	1:B:781:SER:OG	2.30	0.57
1:B:876:PHE:CE1	1:B:921:ILE:HD11	2.40	0.57
1:B:1039:LEU:HD21	1:B:1139:ILE:HG22	1.87	0.57
1:A:894:THR:HG22	1:B:585:GLU:OE1	2.04	0.57
1:B:433:THR:HG21	1:B:457:THR:CB	2.35	0.57
1:A:1101:SER:HB2	1:A:1103:PRO:HD2	1.87	0.56
1:B:731:GLN:CA	1:B:796:GLN:HE21	2.17	0.56
1:B:1057:ARG:CZ	1:B:1112:LEU:HB2	2.35	0.56
2:D:202:ARG:HD2	2:D:204:PHE:CZ	2.39	0.56
1:A:722:ARG:HG3	1:A:722:ARG:NH1	2.19	0.56
1:B:503:CYS:SG	1:B:508:VAL:HG22	2.46	0.56
1:B:731:GLN:O	1:B:796:GLN:HG2	2.05	0.56
1:B:744:ASP:OD2	1:B:747:GLY:N	2.37	0.56
1:B:1014:MET:CG	1:B:1015:GLN:N	2.68	0.56
1:A:225:PRO:HG2	1:A:267:ASN:HB2	1.87	0.56
1:B:159:LEU:CD2	1:B:161:GLU:HB2	2.36	0.56
1:B:334:VAL:HG12	1:B:349:ALA:HA	1.88	0.56
1:B:1075:SER:HB2	1:B:1084:PRO:HA	1.88	0.56
2:C:97:PRO:HA	2:C:202:ARG:HA	1.86	0.56
1:A:417:PRO:CG	1:A:481:GLN:HB3	2.33	0.56
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.86	0.56
1:B:255:GLN:NE2	1:B:255:GLN:N	2.52	0.56
1:B:261:HIS:HA	1:B:272:LEU:O	2.06	0.56
1:B:275:ASP:OD1	1:B:279:ARG:HB2	2.04	0.56
2:C:52:THR:HB	2:C:86:VAL:H	1.71	0.56
1:A:19:VAL:HG22	1:A:20:THR:N	2.21	0.56
1:A:108:VAL:O	1:A:141:LYS:HE2	2.05	0.56
1:A:334:VAL:HG11	1:A:347:VAL:HG13	1.88	0.56
1:A:564:ILE:HD12	1:A:564:ILE:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1125:THR:HG22	1:B:1127:ASP:N	2.15	0.56
2:C:215:CYS:H	2:C:218:CYS:HB2	1.70	0.56
1:A:224:GLU:HB2	1:A:225:PRO:HD3	1.87	0.56
1:B:178:ILE:HG23	1:B:193:TYR:O	2.03	0.56
2:C:99:PRO:HG3	2:C:106:ASP:O	2.05	0.56
1:B:308:THR:OG1	1:B:309:SER:N	2.38	0.56
1:B:560:LEU:HD12	1:B:567:ARG:HH11	1.71	0.56
1:B:1022:THR:C	1:B:1024:THR:H	2.09	0.56
2:D:102:LEU:CD1	2:D:180:VAL:HG22	2.36	0.56
2:D:169:GLY:HA2	2:D:211:CYS:HA	1.87	0.56
1:A:707:ILE:HG23	1:A:708:GLN:HG2	1.87	0.56
1:B:429:PHE:O	1:B:432:GLN:N	2.28	0.56
1:B:511:ALA:HB2	1:B:541:LEU:HD11	1.87	0.56
1:A:589:ARG:HG3	1:A:635:PRO:CB	2.34	0.56
1:A:852:GLN:HG2	1:A:854:SER:H	1.71	0.56
1:B:159:LEU:HD21	1:B:161:GLU:HB2	1.87	0.56
1:B:262:ASN:ND2	1:B:316:TYR:H	2.03	0.56
1:B:367:LEU:CG	1:B:374:GLN:CG	2.66	0.56
2:C:163:ARG:HB3	2:C:195:SER:O	2.04	0.56
1:B:223:PRO:HD3	1:B:271:TYR:OH	2.05	0.55
1:B:662:SER:CB	1:B:1138:ARG:HH21	2.19	0.55
1:A:161:GLU:CD	1:A:161:GLU:H	2.09	0.55
1:B:573:SER:O	1:B:574:PHE:HB2	2.05	0.55
2:C:90:ASP:OD1	2:C:92:THR:HB	2.07	0.55
2:C:100:ASN:HB3	2:C:103:LEU:HG	1.87	0.55
1:A:838:PRO:HD2	1:A:839:GLU:OE2	2.05	0.55
1:B:626:ARG:O	1:B:626:ARG:HG2	2.06	0.55
2:D:159:ILE:HG22	2:D:159:ILE:O	2.07	0.55
1:A:340:SER:HB3	1:A:346:TYR:CE1	2.41	0.55
1:A:537:GLU:HB3	1:A:561:TRP:HB2	1.87	0.55
1:B:206:PRO:HB2	1:B:207:TRP:CE3	2.41	0.55
1:B:498:ILE:HG22	1:B:512:VAL:HG22	1.88	0.55
2:D:113:THR:HG22	2:D:114:VAL:N	2.21	0.55
1:B:235:GLU:H	1:B:253:ILE:CG2	2.19	0.55
1:B:1120:MET:O	1:B:1121:LYS:HB3	2.06	0.55
2:D:51:LEU:HD12	2:D:142:THR:N	2.21	0.55
2:D:87:PRO:HG3	2:D:91:LYS:NZ	2.22	0.55
1:A:250:PRO:HG2	1:A:253:ILE:HG12	1.89	0.55
1:A:634:GLN:HG2	1:A:654:ASP:OD1	2.06	0.55
1:B:235:GLU:O	1:B:236:SER:HB2	2.07	0.55
1:B:389:ILE:N	1:B:389:ILE:HD12	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1002:GLU:HB3	1:B:1032:THR:HG21	1.88	0.55
2:D:19:THR:HG22	2:D:20:GLY:N	2.19	0.55
1:A:811:GLU:HB2	1:A:835:MET:SD	2.47	0.55
1:A:1119:GLY:HA3	1:B:984:THR:HG23	1.89	0.55
1:B:329:GLY:HA3	1:B:384:GLU:CG	2.34	0.55
2:C:52:THR:OG1	2:C:85:ILE:HA	2.07	0.55
2:D:143:ARG:HB3	2:D:143:ARG:NH1	2.22	0.55
1:A:369:ARG:O	1:A:370:GLN:CB	2.54	0.55
1:B:427:LEU:HD12	1:B:427:LEU:H	1.72	0.55
1:B:1065:VAL:O	1:B:1067:LYS:N	2.40	0.55
1:A:341:ASN:CG	1:A:342:GLU:N	2.57	0.54
1:A:931:LEU:HD23	1:A:931:LEU:C	2.27	0.54
1:B:494:GLN:O	1:B:494:GLN:HG2	2.05	0.54
2:D:82:LYS:HZ3	2:D:161:PHE:HZ	1.55	0.54
1:B:396:ILE:HD11	1:B:673:LEU:CD1	2.37	0.54
1:B:976:VAL:O	1:B:994:GLU:O	2.24	0.54
1:B:1102:ARG:HB2	1:B:1103:PRO:HD3	1.88	0.54
1:A:117:GLU:C	1:A:119:GLY:H	2.10	0.54
1:B:57:MET:HE3	1:B:1066:GLY:H	1.72	0.54
1:B:475:SER:HB2	1:B:490:TRP:O	2.08	0.54
1:B:1095:GLU:HG2	1:B:1137:THR:HG22	1.89	0.54
1:A:146:ASP:O	1:A:148:ASP:N	2.41	0.54
1:A:969:GLU:HG2	1:A:970:ASN:N	2.23	0.54
1:B:242:GLY:O	1:B:243:ASP:CB	2.56	0.54
1:B:1050:LEU:C	1:B:1050:LEU:HD23	2.28	0.54
2:C:161:PHE:HZ	2:C:196:PRO:HA	1.73	0.54
1:A:982:ALA:C	1:A:984:THR:H	2.11	0.54
1:B:165:ILE:HG21	1:B:217:SER:HA	1.90	0.54
1:B:477:ARG:HD2	1:B:489:GLU:HG3	1.90	0.54
1:B:560:LEU:HD12	1:B:567:ARG:NH1	2.22	0.54
1:B:881:LEU:HD22	1:B:921:ILE:HD12	1.88	0.54
1:B:1065:VAL:HG12	1:B:1066:GLY:N	2.23	0.54
2:C:95:GLY:O	2:C:202:ARG:HD2	2.07	0.54
2:D:18:GLU:OE1	2:D:18:GLU:HA	2.06	0.54
1:B:401:SER:HA	1:B:700:THR:HG22	1.89	0.54
2:C:50:LEU:CD2	2:C:86:VAL:HG21	2.37	0.54
2:D:170:PHE:HD1	2:D:170:PHE:H	1.56	0.54
1:A:396:ILE:CD1	1:A:396:ILE:N	2.69	0.54
1:A:416:ASP:CB	1:A:419:ARG:HG3	2.35	0.54
1:A:665:LYS:HD3	1:A:1138:ARG:CZ	2.37	0.54
1:B:430:VAL:HG13	1:B:456:GLN:CB	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:LEU:CD1	2:D:180:VAL:CG2	2.86	0.54
1:A:189:HIS:HB3	1:A:210:GLU:HA	1.90	0.54
1:A:612:PHE:CE2	1:A:628:LYS:HD2	2.43	0.54
1:B:182:TYR:CZ	1:B:189:HIS:HB2	2.43	0.54
1:B:228:GLY:HA2	1:B:241:ASN:HA	1.90	0.54
1:B:504:ASN:ND2	1:B:507:GLN:HB2	2.22	0.54
1:B:516:LEU:HD13	1:B:534:MET:HG2	1.90	0.54
1:B:717:LEU:HD12	1:B:721:PRO:HG3	1.90	0.54
1:B:1036:MET:O	1:B:1037:ILE:CB	2.56	0.54
1:B:1102:ARG:O	1:B:1106:GLN:HG3	2.08	0.54
1:A:130:MET:HA	1:A:145:LEU:HD13	1.90	0.54
1:B:616:LEU:HD12	1:B:617:ASN:N	2.22	0.54
1:B:866:VAL:CG1	1:B:884:ILE:HG21	2.38	0.54
1:B:1075:SER:HB2	1:B:1083:GLU:O	2.08	0.54
2:C:206:CYS:SG	2:C:211:CYS:HB3	2.48	0.54
2:D:17:ILE:HD11	2:D:139:ASN:ND2	2.23	0.54
1:A:889:ARG:NH1	1:A:904:ASN:ND2	2.49	0.53
1:B:450:GLY:O	1:B:451:PHE:C	2.44	0.53
1:B:652:CYS:HB3	1:B:676:VAL:O	2.09	0.53
1:B:949:PHE:HA	2:D:122:LEU:HD21	1.89	0.53
2:D:98:ILE:HB	2:D:201:ALA:CB	2.36	0.53
2:C:215:CYS:O	2:C:219:GLU:OE1	2.25	0.53
2:D:90:ASP:O	2:D:91:LYS:HG3	2.07	0.53
1:B:248:ILE:C	1:B:250:PRO:HD3	2.29	0.53
2:D:171:HIS:ND1	2:D:215:CYS:HB3	2.23	0.53
1:B:511:ALA:HA	1:B:515:ALA:O	2.09	0.53
1:B:771:PHE:CE2	1:B:845:GLN:HB2	2.43	0.53
2:C:144:PHE:HB2	2:C:175:TYR:HB2	1.91	0.53
1:A:867:LYS:H	1:A:867:LYS:HD2	1.73	0.53
1:B:451:PHE:C	1:B:451:PHE:HD2	2.05	0.53
1:B:564:ILE:HG22	1:B:582:LEU:HD12	1.91	0.53
1:A:354:THR:HG21	1:A:712:ILE:HD12	1.91	0.53
1:B:414:ARG:HH21	1:B:462:ASN:HB2	1.74	0.53
1:A:183:GLN:HB2	1:A:188:ARG:HG2	1.90	0.53
1:B:19:VAL:O	1:B:31:LEU:HD12	2.08	0.53
1:B:170:LEU:HD12	1:B:177:THR:HG22	1.90	0.53
1:B:413:LEU:HD22	1:B:424:THR:HB	1.90	0.53
1:B:644:LEU:HG	1:B:645:SER:N	2.24	0.53
1:B:731:GLN:CA	1:B:796:GLN:NE2	2.71	0.53
2:C:143:ARG:NH2	2:C:174:GLU:OE1	2.42	0.53
2:D:169:GLY:O	2:D:212:PRO:CG	2.51	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:VAL:HG23	1:A:524:GLN:HA	1.91	0.53
1:A:707:ILE:CG2	1:A:708:GLN:HG2	2.39	0.53
1:A:725:CYS:O	1:A:733:PHE:HD2	1.92	0.53
1:B:90:GLU:HB3	1:B:101:ILE:HG12	1.91	0.53
1:B:586:ILE:HG21	1:B:608:ASP:H	1.72	0.53
1:B:1020:THR:O	1:B:1021:SER:HB2	2.08	0.53
1:B:1118:SER:O	1:B:1119:GLY:C	2.47	0.53
1:A:23:PHE:N	1:A:30:ASN:ND2	2.48	0.53
1:B:159:LEU:HD23	1:B:161:GLU:N	2.22	0.53
1:B:340:SER:HB3	1:B:346:TYR:CD1	2.43	0.53
2:D:108:THR:O	2:D:109:PRO:C	2.46	0.53
1:A:686:GLY:C	1:A:688:PRO:HD3	2.29	0.52
1:B:432:GLN:CD	1:B:454:ASP:O	2.47	0.52
1:B:369:ARG:CG	1:B:369:ARG:O	2.56	0.52
1:B:1079:GLU:OE2	1:B:1079:GLU:HA	2.09	0.52
2:C:35:THR:C	2:C:36:SER:O	2.42	0.52
2:C:179:TRP:O	2:C:180:VAL:HB	2.09	0.52
1:B:134:ARG:NH1	1:B:164:VAL:HB	2.25	0.52
1:B:369:ARG:NH1	1:B:670:ASN:HB3	2.22	0.52
2:D:87:PRO:HG3	2:D:91:LYS:CE	2.39	0.52
2:D:110:SER:O	2:D:221:ASP:HA	2.10	0.52
2:D:169:GLY:N	2:D:211:CYS:SG	2.69	0.52
1:A:275:ASP:CB	1:A:279:ARG:HB2	2.38	0.52
1:A:334:VAL:CG1	1:A:347:VAL:HG13	2.39	0.52
1:B:355:ASN:C	1:B:357:GLY:N	2.62	0.52
1:B:1015:GLN:O	1:B:1015:GLN:HG3	2.09	0.52
2:D:202:ARG:HB3	2:D:204:PHE:CE1	2.44	0.52
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.44	0.52
1:B:162:LEU:HG	1:B:163:HIS:H	1.74	0.52
2:D:143:ARG:NH2	2:D:174:GLU:OE1	2.42	0.52
1:B:29:LEU:HB3	1:B:44:VAL:HB	1.91	0.52
1:B:180:PHE:CE1	1:B:182:TYR:HB3	2.45	0.52
1:B:475:SER:OG	1:B:477:ARG:NH1	2.42	0.52
1:B:741:GLU:OE1	1:B:749:THR:HB	2.09	0.52
1:B:973:ASN:ND2	1:B:1077:HIS:H	2.06	0.52
2:D:18:GLU:O	2:D:42:THR:HG23	2.09	0.52
1:A:476:VAL:CG1	1:A:490:TRP:HB3	2.40	0.52
1:A:848:ILE:CD1	1:A:870:VAL:HG11	2.40	0.52
2:C:86:VAL:HG13	2:C:87:PRO:HD2	1.92	0.52
2:D:115:LEU:HD23	2:D:123:PRO:HB3	1.90	0.52
1:A:112:ILE:HD13	1:A:112:ILE:N	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ARG:HG3	1:A:655:ARG:HH11	1.74	0.52
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.91	0.52
1:B:10:GLN:O	1:B:1036:MET:O	2.28	0.52
2:C:161:PHE:O	2:C:162:LYS:HB2	2.10	0.52
1:A:780:THR:HB	1:A:784:GLU:CB	2.39	0.52
1:B:489:GLU:OE2	1:B:491:LYS:HE3	2.10	0.52
1:A:309:SER:HA	1:A:384:GLU:OE2	2.10	0.51
1:B:57:MET:CE	1:B:1066:GLY:H	2.23	0.51
1:B:228:GLY:CA	1:B:241:ASN:HA	2.40	0.51
1:B:237:ILE:O	1:B:248:ILE:HG12	2.09	0.51
1:B:383:LYS:HG3	1:B:384:GLU:OE2	2.10	0.51
2:C:109:PRO:HG2	2:C:203:ARG:NH1	2.24	0.51
2:D:171:HIS:CB	2:D:215:CYS:HB3	2.40	0.51
1:A:837:TYR:HB3	1:A:839:GLU:OE2	2.10	0.51
1:B:281:PHE:CD2	1:B:304:LEU:HA	2.46	0.51
1:B:769:LYS:O	1:B:769:LYS:HG2	2.11	0.51
2:D:86:VAL:HG13	2:D:87:PRO:HD2	1.92	0.51
2:D:104:GLY:O	2:D:105:LEU:HB3	2.11	0.51
2:D:192:PRO:C	2:D:194:CYS:N	2.62	0.51
1:A:780:THR:HG22	1:A:781:SER:N	2.24	0.51
1:B:5:TYR:HB2	1:B:1043:LEU:HD11	1.93	0.51
1:B:1121:LYS:O	1:B:1121:LYS:HG2	2.10	0.51
1:A:1114:TYR:CB	1:A:1124:ALA:HB2	2.41	0.51
1:B:790:ASN:N	1:B:790:ASN:ND2	2.58	0.51
1:B:910:MET:HB2	1:B:926:LEU:CB	2.41	0.51
2:D:21:LEU:HD22	2:D:26:TYR:CD1	2.46	0.51
1:A:912:LEU:HB2	1:A:913:TYR:CE1	2.46	0.51
1:B:355:ASN:OD1	1:B:357:GLY:N	2.43	0.51
1:B:393:GLY:HA2	1:B:708:GLN:HG2	1.92	0.51
1:B:1126:ALA:O	1:B:1130:ILE:HG13	2.10	0.51
2:D:87:PRO:HG3	2:D:91:LYS:HE3	1.93	0.51
1:B:388:ARG:NE	1:B:714:THR:HG23	2.26	0.51
1:B:419:ARG:HD2	1:B:423:ASP:OD1	2.11	0.51
2:C:216:SER:HA	2:C:219:GLU:OE2	2.10	0.51
2:D:98:ILE:HG22	2:D:99:PRO:O	2.11	0.51
2:D:110:SER:N	2:D:221:ASP:HB3	2.25	0.51
1:A:634:GLN:HB3	1:A:635:PRO:HD2	1.93	0.51
1:B:130:MET:HA	1:B:145:LEU:CB	2.41	0.51
1:B:255:GLN:HE21	1:B:255:GLN:N	2.04	0.51
1:B:290:GLN:NE2	1:B:293:GLY:HA3	2.19	0.51
2:C:215:CYS:SG	2:C:217:GLU:HB2	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:HIS:CG	2:D:215:CYS:HB3	2.46	0.51
1:B:861:VAL:HG12	1:B:862:ALA:N	2.26	0.51
2:C:100:ASN:HB3	2:C:103:LEU:CD1	2.40	0.51
2:C:167:THR:O	2:C:193:SER:HB3	2.10	0.51
2:D:109:PRO:HB2	2:D:203:ARG:NH2	2.25	0.51
2:D:163:ARG:NH1	2:D:197:ILE:HD11	2.25	0.51
1:A:537:GLU:HB3	1:A:561:TRP:CB	2.41	0.51
1:A:1026:GLY:O	1:A:1027:SER:HB2	2.10	0.51
1:A:1101:SER:CB	1:A:1103:PRO:HD2	2.41	0.51
1:B:41:ILE:O	1:B:52:VAL:HG22	2.11	0.51
1:B:451:PHE:HE2	1:B:453:ASP:HB3	1.76	0.51
1:B:986:ASP:O	1:B:990:GLN:HB2	2.10	0.51
2:D:82:LYS:O	2:D:83:ILE:HD12	2.10	0.51
2:D:218:CYS:O	2:D:221:ASP:HB2	2.11	0.51
1:B:480:SER:O	1:B:484:LYS:HA	2.11	0.51
2:C:108:THR:O	2:C:222:THR:CA	2.58	0.51
1:B:230:ILE:HD13	1:B:239:TYR:HD1	1.75	0.50
1:B:687:TYR:O	1:B:688:PRO:O	2.29	0.50
1:A:410:LEU:HD23	1:A:410:LEU:N	2.25	0.50
1:B:63:VAL:HB	1:B:80:LEU:CB	2.40	0.50
1:B:161:GLU:HB3	1:B:182:TYR:HB2	1.93	0.50
1:B:342:GLU:C	1:B:344:GLY:H	2.15	0.50
2:C:97:PRO:CD	2:C:202:ARG:HD3	2.42	0.50
1:A:117:GLU:C	1:A:119:GLY:N	2.64	0.50
1:A:256:SER:OG	1:A:277:GLU:HG3	2.11	0.50
2:D:89:ASP:OD1	2:D:90:ASP:N	2.45	0.50
1:A:34:ALA:HB2	1:A:64:MET:CE	2.41	0.50
1:B:391:ARG:HG2	1:B:392:ASN:N	2.26	0.50
1:B:769:LYS:N	1:B:769:LYS:CD	2.74	0.50
2:C:83:ILE:O	2:C:84:ALA:HB3	2.12	0.50
1:A:465:HIS:CE1	1:A:523:PRO:HD3	2.47	0.50
1:A:762:SER:HB2	1:A:803:HIS:HA	1.93	0.50
1:A:794:ILE:HG23	1:A:799:PHE:HA	1.92	0.50
1:A:1080:ARG:HD2	2:C:119:GLY:HA3	1.93	0.50
1:B:84:TYR:CG	1:B:109:GLN:HB3	2.46	0.50
1:B:304:LEU:C	1:B:304:LEU:HD23	2.32	0.50
1:B:413:LEU:C	1:B:413:LEU:HD23	2.32	0.50
1:B:568:ILE:O	1:B:569:LEU:HD23	2.11	0.50
1:B:571:LEU:HB3	1:B:572:PRO:HD3	1.93	0.50
2:D:114:VAL:HG22	2:D:185:LYS:CD	2.39	0.50
2:D:165:ARG:HG2	2:D:165:ARG:HH11	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG12	1:B:213:GLU:N	2.27	0.50
1:B:223:PRO:HG2	1:B:268:GLY:CA	2.42	0.50
1:B:432:GLN:NE2	1:B:454:ASP:O	2.44	0.50
1:B:921:ILE:HB	1:B:933:LEU:HB2	1.94	0.50
2:C:162:LYS:O	2:C:162:LYS:HG3	2.11	0.50
1:A:855:ASP:CG	1:A:856:GLY:N	2.65	0.50
1:B:55:VAL:HG21	1:B:100:ILE:HG13	1.93	0.50
1:B:410:LEU:HA	1:B:426:VAL:O	2.11	0.50
1:B:476:VAL:CG1	1:B:490:TRP:HB3	2.38	0.50
1:B:724:ILE:HA	1:B:734:GLY:O	2.12	0.50
1:B:744:ASP:OD2	1:B:746:SER:C	2.50	0.50
1:B:1022:THR:C	1:B:1024:THR:N	2.65	0.50
2:C:108:THR:HA	2:C:222:THR:O	2.11	0.50
2:C:116:ASP:OD2	2:C:119:GLY:O	2.28	0.50
2:D:95:GLY:O	2:D:202:ARG:NH1	2.38	0.50
1:A:580:GLU:HG2	1:A:614:PHE:CE2	2.47	0.50
1:B:553:SER:O	1:B:571:LEU:HG	2.11	0.50
1:B:969:GLU:HG2	1:B:970:ASN:N	2.26	0.50
1:B:994:GLU:HG3	1:B:995:VAL:N	2.26	0.50
1:B:1108:VAL:C	1:B:1110:ALA:H	2.16	0.50
2:C:97:PRO:HD3	2:C:202:ARG:HD3	1.94	0.50
2:D:171:HIS:NE2	2:D:212:PRO:CG	2.68	0.50
1:A:704:ILE:CG2	1:A:705:ASP:N	2.73	0.50
1:B:133:LEU:N	1:B:133:LEU:HD12	2.26	0.50
1:A:597:GLU:OE2	1:A:664:HIS:N	2.41	0.49
1:B:377:THR:O	1:B:387:LEU:HA	2.12	0.49
1:B:468:LEU:HD13	1:B:481:GLN:HG2	1.94	0.49
1:B:675:GLU:HG2	1:B:676:VAL:N	2.27	0.49
1:B:91:TYR:OH	1:B:98:ILE:HD12	2.12	0.49
1:A:1032:THR:HG22	1:A:1036:MET:N	2.25	0.49
1:B:47:GLU:H	1:B:47:GLU:CD	2.14	0.49
1:B:170:LEU:HD12	1:B:177:THR:CG2	2.40	0.49
1:B:1080:ARG:NE	1:B:1080:ARG:HA	2.28	0.49
2:D:48:THR:HB	2:D:145:ILE:CD1	2.42	0.49
1:A:125:ASP:OD2	1:A:127:GLU:HB2	2.12	0.49
1:A:356:LEU:O	1:A:379:SER:HB3	2.12	0.49
1:A:594:THR:HG23	1:A:595:THR:N	2.26	0.49
1:A:1057:ARG:NH1	1:A:1112:LEU:HB2	2.28	0.49
1:B:262:ASN:ND2	1:B:315:THR:HA	2.26	0.49
1:B:359:ILE:HG13	1:B:1035:GLY:HA2	1.95	0.49
1:B:548:ASP:O	1:B:550:ASN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:GLN:HB2	1:B:783:GLY:H	1.78	0.49
1:B:546:LEU:HD11	1:B:593:MET:HB3	1.95	0.49
1:B:614:PHE:N	1:B:614:PHE:CD1	2.79	0.49
1:B:896:GLU:O	1:B:897:LYS:HB2	2.12	0.49
1:A:29:LEU:HG	1:A:44:VAL:HG21	1.94	0.49
1:B:467:GLN:CD	1:B:478:LEU:HD21	2.33	0.49
1:B:467:GLN:HB3	1:B:478:LEU:HD21	1.94	0.49
1:A:337:ASN:O	1:A:346:TYR:HB3	2.12	0.49
1:A:794:ILE:CG2	1:A:799:PHE:HA	2.43	0.49
1:B:910:MET:CE	1:B:912:LEU:HD21	2.43	0.49
2:D:22:ASN:O	2:D:23:THR:C	2.51	0.49
1:A:2:SER:HB2	1:A:995:VAL:CG2	2.42	0.49
1:A:365:VAL:CG1	1:A:367:LEU:HG	2.43	0.49
1:A:576:LEU:HD22	1:A:578:HIS:H	1.77	0.49
1:A:1113:GLN:HA	1:A:1113:GLN:OE1	2.12	0.49
1:B:224:GLU:O	1:B:225:PRO:C	2.50	0.49
1:B:226:PHE:HD2	1:B:297:LEU:HB2	1.76	0.49
2:C:97:PRO:N	2:C:202:ARG:HD3	2.28	0.49
2:D:102:LEU:HD23	2:D:102:LEU:C	2.33	0.49
2:D:103:LEU:O	2:D:105:LEU:HD23	2.12	0.49
1:B:114:ARG:HG3	1:B:137:ASP:OD2	2.12	0.49
1:B:257:THR:HG22	1:B:258:ILE:N	2.28	0.49
1:B:358:PRO:O	1:B:379:SER:HA	2.13	0.49
1:B:477:ARG:HB3	1:B:489:GLU:HG3	1.95	0.49
1:B:485:ALA:O	1:B:487:VAL:HG13	2.13	0.49
1:B:876:PHE:HD1	1:B:916:THR:HG21	1.78	0.49
2:D:208:CYS:C	2:D:210:GLN:N	2.65	0.49
1:A:44:VAL:HG11	1:A:317:LEU:HB3	1.94	0.49
1:A:564:ILE:N	1:A:564:ILE:CD1	2.75	0.49
1:A:582:LEU:O	1:A:583:GLY:C	2.51	0.49
1:A:903:CYS:CB	1:A:941:ASN:HA	2.43	0.49
1:B:267:ASN:HD21	1:B:269:SER:CB	2.13	0.49
1:B:451:PHE:CE2	1:B:453:ASP:HB3	2.48	0.49
1:B:665:LYS:HD3	1:B:1138:ARG:CZ	2.43	0.49
1:B:771:PHE:HE2	1:B:845:GLN:HB2	1.76	0.49
2:C:179:TRP:O	2:C:183:GLU:O	2.30	0.49
1:A:446:THR:HG22	1:A:447:GLU:N	2.28	0.48
1:A:657:THR:HG23	1:A:669:SER:O	2.12	0.48
1:A:926:LEU:O	1:A:953:TRP:HA	2.12	0.48
2:C:40:LYS:HG2	2:C:42:THR:HG23	1.95	0.48
1:A:177:THR:CG2	1:A:194:GLU:HG2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:CD1	1:B:188:ARG:HH12	2.25	0.48
2:C:136:GLY:O	2:C:139:ASN:O	2.31	0.48
2:D:50:LEU:O	2:D:51:LEU:C	2.51	0.48
2:D:177:ILE:HG23	2:D:186:VAL:HG22	1.95	0.48
1:A:385:GLY:HA3	1:A:719:GLU:O	2.13	0.48
1:A:589:ARG:HG2	1:A:589:ARG:NH1	2.28	0.48
1:A:594:THR:CG2	1:A:595:THR:N	2.75	0.48
1:A:876:PHE:HD1	1:A:916:THR:HG21	1.78	0.48
1:A:1121:LYS:HZ3	1:A:1121:LYS:HB2	1.78	0.48
1:B:843:PRO:HD3	2:D:22:ASN:HD21	1.78	0.48
1:A:95:GLY:C	1:A:97:SER:H	2.15	0.48
1:A:288:GLU:HB3	1:A:296:THR:CG2	2.42	0.48
1:A:413:LEU:HD23	1:A:462:ASN:OD1	2.14	0.48
1:A:487:VAL:O	1:A:488:SER:HB2	2.13	0.48
1:B:423:ASP:O	1:B:438:LEU:HB2	2.12	0.48
1:B:437:MET:CB	1:B:446:THR:HG23	2.43	0.48
1:B:612:PHE:CE2	1:B:628:LYS:HD2	2.49	0.48
1:B:1047:TRP:HZ3	1:B:1132:VAL:HG13	1.79	0.48
2:C:48:THR:HG23	2:C:82:LYS:HG2	1.94	0.48
2:C:160:ASP:OD2	2:C:161:PHE:N	2.47	0.48
2:C:192:PRO:HB3	2:C:206:CYS:SG	2.53	0.48
2:D:163:ARG:NH1	2:D:197:ILE:CD1	2.76	0.48
1:A:81:THR:CG2	1:A:82:ALA:N	2.75	0.48
1:A:239:TYR:CE2	1:A:241:ASN:HB2	2.48	0.48
1:A:741:GLU:CD	1:A:750:THR:O	2.52	0.48
1:B:52:VAL:HG23	1:B:53:LYS:N	2.29	0.48
2:D:89:ASP:CG	2:D:202:ARG:HH21	2.17	0.48
2:D:140:LEU:N	2:D:140:LEU:HD23	2.29	0.48
1:A:475:SER:HB2	1:A:490:TRP:O	2.13	0.48
1:B:239:TYR:CE2	1:B:241:ASN:HB2	2.48	0.48
1:B:824:ASP:OD2	1:B:828:TYR:OH	2.28	0.48
1:B:1102:ARG:HD2	1:B:1105:MET:HE1	1.96	0.48
2:C:50:LEU:HD22	2:C:86:VAL:HG21	1.95	0.48
2:D:173:ARG:NH1	2:D:190:CYS:SG	2.87	0.48
1:A:16:ASN:ND2	1:A:35:LYS:C	2.56	0.48
1:B:80:LEU:CD2	1:B:133:LEU:HD23	2.43	0.48
1:B:480:SER:OG	1:B:483:PRO:HD2	2.13	0.48
1:B:655:ARG:HG2	1:B:655:ARG:HH11	1.77	0.48
2:D:198:THR:HG21	2:D:204:PHE:HZ	1.78	0.48
1:A:542:ASP:OD1	1:A:593:MET:N	2.45	0.48
1:B:617:ASN:OD1	1:B:619:GLU:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:VAL:HG23	1:B:786:VAL:O	2.14	0.48
2:D:19:THR:HA	2:D:43:ILE:HG23	1.96	0.48
1:A:537:GLU:O	1:A:561:TRP:HB2	2.14	0.48
1:A:729:VAL:HG23	1:A:730:SER:N	2.28	0.48
1:B:286:GLU:HB3	1:B:298:LYS:HD3	1.95	0.48
1:B:1007:PHE:CD2	1:B:1030:PHE:HB3	2.49	0.48
2:C:18:GLU:OE1	2:C:40:LYS:HD2	2.14	0.48
2:D:108:THR:CB	2:D:109:PRO:CD	2.92	0.48
1:B:162:LEU:HD23	1:B:162:LEU:N	2.17	0.48
1:B:459:PHE:CD2	1:B:503:CYS:HB3	2.48	0.48
1:B:476:VAL:C	1:B:477:ARG:HD3	2.34	0.48
1:B:835:MET:HB2	1:B:845:GLN:HG3	1.95	0.48
1:B:1015:GLN:O	1:B:1016:ASN:C	2.52	0.48
2:D:115:LEU:HG	2:D:130:VAL:HG13	1.96	0.48
1:B:32:LEU:HD12	1:B:32:LEU:N	2.28	0.47
1:B:81:THR:HG22	1:B:83:LYS:N	2.06	0.47
1:B:456:GLN:O	1:B:472:THR:HG22	2.14	0.47
1:B:731:GLN:C	1:B:796:GLN:HE21	2.17	0.47
1:B:794:ILE:HG22	1:B:799:PHE:HA	1.96	0.47
1:B:1014:MET:O	1:B:1015:GLN:HB3	2.14	0.47
2:D:103:LEU:O	2:D:105:LEU:N	2.47	0.47
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.95	0.47
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.78	0.47
1:B:427:LEU:HD13	1:B:429:PHE:CE1	2.48	0.47
1:B:532:THR:HB	1:B:574:PHE:CD1	2.49	0.47
2:C:177:ILE:N	2:C:177:ILE:HD12	2.29	0.47
1:A:112:ILE:H	1:A:112:ILE:CD1	2.20	0.47
2:C:215:CYS:H	2:C:218:CYS:CB	2.27	0.47
1:A:520:GLN:HG3	1:A:529:ILE:HD12	1.97	0.47
1:A:1051:LEU:CB	1:A:1089:ILE:HD13	2.44	0.47
1:B:68:ARG:HB2	1:B:75:ASP:OD2	2.14	0.47
1:B:199:GLU:HG3	1:B:201:GLU:CG	2.45	0.47
1:B:207:TRP:CZ3	1:B:241:ASN:O	2.68	0.47
1:B:458:PHE:CD1	1:B:458:PHE:N	2.82	0.47
1:B:847:ARG:NH1	1:B:849:VAL:HG22	2.29	0.47
1:B:991:HIS:HB3	1:B:993:GLN:NE2	2.29	0.47
2:C:16:LEU:O	2:C:41:ASN:HB2	2.14	0.47
2:D:21:LEU:HD22	2:D:26:TYR:HD1	1.78	0.47
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.48	0.47
1:A:256:SER:HB3	1:A:275:ASP:OD1	2.13	0.47
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.75	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LYS:HG3	1:A:572:PRO:HD2	1.97	0.47
1:B:242:GLY:O	1:B:243:ASP:HB2	2.14	0.47
1:B:571:LEU:HD13	1:B:571:LEU:C	2.34	0.47
1:A:213:GLU:OE1	1:A:236:SER:HB3	2.14	0.47
1:B:886:SER:O	1:B:908:ASN:ND2	2.48	0.47
1:B:1048:TYR:HE2	1:B:1052:LEU:HD12	1.79	0.47
1:B:1115:ASP:HB2	1:B:1120:MET:CB	2.45	0.47
2:D:16:LEU:O	2:D:41:ASN:HB3	2.14	0.47
1:A:364:VAL:HG21	1:A:1010:GLY:HA3	1.97	0.47
1:A:367:LEU:HD12	1:A:374:GLN:NE2	2.30	0.47
1:A:518:TYR:CD1	1:A:571:LEU:HD22	2.49	0.47
1:A:597:GLU:HG3	1:A:661:SER:HB3	1.95	0.47
1:A:771:PHE:CD1	1:A:835:MET:HE2	2.50	0.47
1:A:889:ARG:CD	1:A:901:THR:HG23	2.44	0.47
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.63	0.47
1:B:147:ARG:HA	1:B:147:ARG:NE	2.26	0.47
1:B:253:ILE:HG22	1:B:253:ILE:O	2.15	0.47
1:B:289:GLU:OE2	1:B:289:GLU:HA	2.14	0.47
1:B:449:MET:HA	1:B:449:MET:HE2	1.97	0.47
1:B:722:ARG:NH1	2:D:28:THR:HG21	2.30	0.47
2:D:90:ASP:CG	2:D:91:LYS:H	2.18	0.47
1:A:550:ASN:O	1:A:552:LEU:N	2.48	0.47
1:A:867:LYS:CE	1:A:889:ARG:NH2	2.77	0.47
1:A:969:GLU:OE2	1:A:971:ALA:HB3	2.14	0.47
1:B:131:ILE:HB	1:B:143:ILE:HB	1.96	0.47
1:B:290:GLN:HG3	1:B:293:GLY:H	1.80	0.47
1:B:458:PHE:N	1:B:458:PHE:HD1	2.13	0.47
1:B:514:ARG:HB2	1:B:537:GLU:HA	1.96	0.47
1:B:739:ARG:NH1	1:B:757:SER:OG	2.47	0.47
1:B:976:VAL:HG22	1:B:996:GLY:CA	2.35	0.47
1:B:1125:THR:HG22	1:B:1126:ALA:N	2.30	0.47
1:A:19:VAL:HG22	1:A:20:THR:H	1.78	0.47
1:A:213:GLU:OE2	1:A:215:GLU:HB2	2.14	0.47
1:A:235:GLU:O	1:A:249:ALA:HA	2.15	0.47
1:B:275:ASP:HB3	1:B:277:GLU:H	1.80	0.47
2:D:47:VAL:HG12	2:D:48:THR:H	1.79	0.47
2:D:108:THR:HB	2:D:109:PRO:CD	2.41	0.47
2:D:116:ASP:O	2:D:118:SER:N	2.45	0.47
1:A:479:VAL:HG12	1:A:480:SER:O	2.15	0.47
1:B:832:GLY:N	1:B:873:MET:HE2	2.30	0.47
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:HIS:O	1:A:467:GLN:HG3	2.15	0.46
1:A:741:GLU:HB3	1:A:750:THR:O	2.14	0.46
1:A:870:VAL:HG22	1:A:884:ILE:HG13	1.96	0.46
1:B:390:ILE:HG22	1:B:710:LEU:HD22	1.96	0.46
1:B:498:ILE:HG23	1:B:512:VAL:HG22	1.97	0.46
1:B:1044:SER:HG	1:B:1047:TRP:HD1	1.62	0.46
2:C:172:ARG:CZ	2:C:197:ILE:HG22	2.44	0.46
1:A:465:HIS:HB2	1:A:467:GLN:HE21	1.79	0.46
1:A:717:LEU:O	1:A:718:TYR:HB2	2.15	0.46
1:B:124:ILE:HG23	1:B:131:ILE:CD1	2.42	0.46
1:B:309:SER:O	1:B:310:ILE:C	2.54	0.46
1:B:1065:VAL:C	1:B:1067:LYS:N	2.69	0.46
2:D:90:ASP:CG	2:D:91:LYS:N	2.68	0.46
1:B:368:GLU:O	1:B:369:ARG:C	2.53	0.46
2:C:147:GLU:HG2	2:C:172:ARG:HG3	1.96	0.46
1:A:360:VAL:O	1:A:360:VAL:HG12	2.16	0.46
1:A:927:MET:CE	2:C:130:VAL:HG11	2.46	0.46
1:B:408:LYS:CB	1:B:430:VAL:HG23	2.44	0.46
1:B:436:LEU:HA	1:B:445:GLU:HA	1.97	0.46
1:B:475:SER:HA	1:B:498:ILE:CD1	2.42	0.46
1:B:789:HIS:ND1	1:B:812:TYR:HA	2.31	0.46
2:C:161:PHE:CD1	2:C:197:ILE:HD12	2.51	0.46
1:A:1097:PHE:CZ	1:A:1105:MET:HG2	2.50	0.46
1:A:1121:LYS:HD3	1:A:1122:ARG:H	1.81	0.46
1:B:226:PHE:CD1	1:B:226:PHE:N	2.84	0.46
1:B:466:GLN:H	1:B:466:GLN:NE2	2.07	0.46
1:A:234:GLN:O	1:A:235:GLU:CG	2.63	0.46
1:A:745:THR:HG23	1:A:782:PHE:CE1	2.51	0.46
1:A:750:THR:CG2	1:A:751:ALA:H	2.17	0.46
1:B:683:ASN:HA	1:B:688:PRO:O	2.14	0.46
1:B:790:ASN:HA	1:B:807:PHE:CD1	2.51	0.46
2:D:43:ILE:HG23	2:D:43:ILE:O	2.15	0.46
1:A:839:GLU:CD	1:A:839:GLU:N	2.69	0.46
1:B:59:GLY:HA2	1:B:1073:TRP:CZ3	2.50	0.46
1:B:63:VAL:CB	1:B:80:LEU:HB3	2.43	0.46
1:B:518:TYR:CZ	1:B:571:LEU:HD11	2.50	0.46
1:B:699:LEU:C	1:B:699:LEU:HD13	2.35	0.46
1:B:983:ALA:O	1:B:985:THR:N	2.44	0.46
1:B:1002:GLU:HB3	1:B:1032:THR:CG2	2.45	0.46
2:C:178:GLY:C	2:C:179:TRP:HE3	2.19	0.46
1:A:587:ILE:HD13	1:A:587:ILE:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:C	1:B:134:ARG:HD2	2.36	0.46
1:B:142:VAL:O	1:B:154:ALA:HB1	2.15	0.46
1:B:881:LEU:CD2	1:B:921:ILE:HD12	2.46	0.46
1:B:984:THR:HG22	1:B:984:THR:O	2.15	0.46
1:A:342:GLU:C	1:A:344:GLY:H	2.20	0.46
1:A:665:LYS:HB3	1:A:1138:ARG:NH2	2.31	0.46
1:A:1098:LEU:HD11	1:A:1133:VAL:HG12	1.97	0.46
1:B:311:ALA:HB2	1:B:324:VAL:HG13	1.98	0.46
1:B:414:ARG:HG2	1:B:414:ARG:HH11	1.81	0.46
1:B:447:GLU:O	1:B:448:LEU:HD12	2.15	0.46
1:B:662:SER:HB2	1:B:1138:ARG:HH21	1.79	0.46
1:B:1014:MET:CG	1:B:1015:GLN:H	2.28	0.46
2:D:17:ILE:HG22	2:D:17:ILE:O	2.16	0.46
2:D:28:THR:HA	2:D:31:GLN:HE21	1.80	0.46
2:D:52:THR:OG1	2:D:85:ILE:HA	2.15	0.46
1:A:234:GLN:O	1:A:235:GLU:CB	2.64	0.46
1:A:269:SER:O	1:A:284:LEU:HA	2.15	0.46
1:A:594:THR:HG23	1:A:595:THR:H	1.80	0.46
1:B:124:ILE:HG12	1:B:131:ILE:CD1	2.46	0.46
1:B:151:GLU:CD	1:B:151:GLU:N	2.70	0.46
1:B:250:PRO:C	1:B:252:ILE:H	2.18	0.46
1:B:289:GLU:OE2	1:B:295:VAL:HG12	2.16	0.46
2:D:149:ARG:O	2:D:150:GLU:O	2.33	0.46
2:D:171:HIS:HA	2:D:193:SER:H	1.81	0.46
2:D:206:CYS:SG	2:D:208:CYS:O	2.74	0.46
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.98	0.45
1:B:905:HIS:CD2	1:B:933:LEU:HD21	2.50	0.45
1:B:1048:TYR:CE2	1:B:1052:LEU:HD12	2.51	0.45
2:D:208:CYS:O	2:D:208:CYS:SG	2.75	0.45
1:A:116:SER:C	1:A:117:GLU:O	2.51	0.45
1:A:334:VAL:HG22	1:A:349:ALA:HA	1.98	0.45
1:B:367:LEU:CG	1:B:374:GLN:CD	2.80	0.45
1:B:412:PRO:HB2	1:B:422:TYR:CD2	2.51	0.45
1:B:422:TYR:HD1	1:B:422:TYR:H	1.63	0.45
1:B:426:VAL:HG22	1:B:435:VAL:HG13	1.99	0.45
1:B:706:GLU:O	1:B:707:ILE:CB	2.64	0.45
1:B:994:GLU:CG	1:B:995:VAL:H	2.29	0.45
1:A:18:CYS:N	1:A:313:CYS:SG	2.89	0.45
1:A:396:ILE:HD13	1:A:396:ILE:N	2.11	0.45
1:A:576:LEU:HD22	1:A:578:HIS:N	2.31	0.45
1:A:652:CYS:HB3	1:A:676:VAL:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:GLN:O	1:A:810:ASN:HB2	2.16	0.45
1:A:892:GLU:O	1:A:899:VAL:HA	2.16	0.45
1:B:6:VAL:HG22	1:B:1088:PHE:HD2	1.80	0.45
1:B:23:PHE:N	1:B:30:ASN:ND2	2.53	0.45
1:B:52:VAL:CG2	1:B:53:LYS:N	2.80	0.45
1:B:1029:LEU:HD23	1:B:1039:LEU:HD13	1.97	0.45
2:C:97:PRO:HA	2:C:202:ARG:HG2	1.97	0.45
2:D:100:ASN:HB3	2:D:103:LEU:HD12	1.97	0.45
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.98	0.45
1:B:5:TYR:HE2	1:B:7:VAL:HG21	1.82	0.45
1:B:250:PRO:O	1:B:252:ILE:N	2.49	0.45
1:B:430:VAL:C	1:B:431:GLY:O	2.52	0.45
1:B:679:MET:HE2	1:B:691:LEU:HD23	1.98	0.45
2:D:116:ASP:C	2:D:118:SER:H	2.19	0.45
2:D:172:ARG:NH2	2:D:191:ASN:HD22	2.14	0.45
1:A:166:ASP:HB3	1:A:219:VAL:HG23	1.98	0.45
1:B:424:THR:HG22	1:B:425:LEU:N	2.32	0.45
2:C:35:THR:CG2	2:C:36:SER:O	2.33	0.45
1:A:410:LEU:N	1:A:410:LEU:CD2	2.80	0.45
1:A:864:LYS:HE2	1:A:891:TYR:CE2	2.49	0.45
1:B:263:ARG:HB2	1:B:271:TYR:CE2	2.51	0.45
1:B:539:ALA:HB2	1:B:561:TRP:CD1	2.51	0.45
1:B:690:SER:O	1:B:691:LEU:HD12	2.16	0.45
1:B:853:TYR:HB2	1:B:858:LEU:HD23	1.99	0.45
2:C:50:LEU:O	2:C:143:ARG:HB2	2.17	0.45
1:A:520:GLN:HG3	1:A:529:ILE:CD1	2.47	0.45
1:B:10:GLN:NE2	1:B:11:LYS:N	2.64	0.45
1:B:196:SER:O	1:B:200:LYS:HA	2.16	0.45
1:B:317:LEU:HD12	1:B:321:VAL:HG12	1.99	0.45
1:B:402:ILE:HD13	1:B:699:LEU:HD12	1.99	0.45
1:B:728:GLU:C	1:B:730:SER:H	2.20	0.45
2:C:52:THR:O	2:C:53:ASN:C	2.45	0.45
2:C:89:ASP:OD1	2:C:90:ASP:N	2.37	0.45
2:C:161:PHE:CE1	2:C:197:ILE:HG23	2.51	0.45
2:D:109:PRO:HB2	2:D:203:ARG:HH21	1.81	0.45
2:D:168:GLY:HA3	2:D:208:CYS:SG	2.55	0.45
1:A:308:THR:O	1:A:383:LYS:NZ	2.49	0.45
1:A:860:THR:HG22	1:A:860:THR:O	2.17	0.45
1:B:29:LEU:HG	1:B:44:VAL:HG21	1.99	0.45
1:B:397:HIS:O	1:B:702:GLY:HA3	2.16	0.45
1:B:569:LEU:CD2	1:B:576:LEU:HA	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:CYS:HB2	1:B:794:ILE:O	2.17	0.45
1:B:1066:GLY:O	1:B:1067:LYS:HB2	2.16	0.45
2:D:169:GLY:C	2:D:212:PRO:HD2	2.24	0.45
1:A:584:GLY:O	1:B:900:ARG:NH2	2.49	0.45
1:A:837:TYR:HB2	1:A:840:GLU:HG3	1.98	0.45
1:B:63:VAL:CG2	1:B:80:LEU:HD23	2.47	0.45
1:B:529:ILE:N	1:B:529:ILE:HD13	2.32	0.45
1:B:644:LEU:HD23	1:B:645:SER:H	1.81	0.45
2:D:17:ILE:HD11	2:D:139:ASN:HD22	1.80	0.45
2:D:42:THR:HG22	2:D:43:ILE:N	2.31	0.45
2:D:169:GLY:CA	2:D:211:CYS:HA	2.46	0.45
1:A:1118:SER:C	1:A:1120:MET:N	2.70	0.45
1:B:42:TYR:CD2	1:B:49:LEU:HB3	2.52	0.45
1:B:451:PHE:HB2	1:B:486:LEU:HD13	1.98	0.45
1:B:1127:ASP:HA	1:B:1130:ILE:HD12	1.98	0.45
2:C:102:LEU:C	2:C:104:GLY:H	2.21	0.45
1:A:304:LEU:HD12	1:A:305:LEU:H	1.82	0.44
1:A:487:VAL:CG2	1:A:524:GLN:HA	2.46	0.44
1:A:587:ILE:H	1:A:587:ILE:CD1	2.30	0.44
1:B:37:THR:HG22	1:B:59:GLY:O	2.18	0.44
1:B:63:VAL:HG21	1:B:80:LEU:HD23	1.98	0.44
1:B:81:THR:OG1	1:B:85:ASN:HB2	2.16	0.44
1:B:192:THR:CB	1:B:206:PRO:HD2	2.47	0.44
1:B:449:MET:HA	1:B:449:MET:HE3	1.98	0.44
2:C:109:PRO:CG	2:C:203:ARG:NH1	2.80	0.44
2:C:147:GLU:CG	2:C:172:ARG:HG3	2.47	0.44
1:A:546:LEU:HD11	1:A:593:MET:HB3	1.99	0.44
1:A:762:SER:HB3	1:A:803:HIS:ND1	2.32	0.44
1:A:865:GLU:HG2	1:A:866:VAL:N	2.32	0.44
1:B:139:LEU:HD22	1:B:156:ASN:HB3	1.99	0.44
1:B:384:GLU:OE2	1:B:384:GLU:N	2.50	0.44
1:B:894:THR:CG2	1:B:895:THR:N	2.78	0.44
2:C:33:THR:HG22	2:C:35:THR:H	1.81	0.44
2:C:98:ILE:HG13	2:C:189:TRP:CZ2	2.53	0.44
1:A:582:LEU:O	1:A:583:GLY:O	2.35	0.44
1:B:10:GLN:HE21	1:B:11:LYS:N	2.16	0.44
1:B:538:VAL:HG22	1:B:558:ILE:HD11	1.98	0.44
2:D:116:ASP:O	2:D:182:ASP:CB	2.62	0.44
1:A:282:MET:CG	1:A:305:LEU:HD11	2.44	0.44
1:A:346:TYR:CD1	1:A:346:TYR:N	2.85	0.44
1:B:573:SER:O	1:B:574:PHE:CB	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:LEU:C	1:B:602:LEU:HD13	2.38	0.44
2:C:113:THR:HA	2:C:124:SER:O	2.17	0.44
1:A:738:SER:OG	1:A:787:GLU:HG2	2.17	0.44
1:A:1121:LYS:HZ2	1:A:1121:LYS:HA	1.83	0.44
1:B:124:ILE:HG12	1:B:131:ILE:HD12	1.99	0.44
2:D:47:VAL:CG1	2:D:48:THR:N	2.80	0.44
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	2.00	0.44
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.98	0.44
1:A:874:VAL:HG13	1:A:881:LEU:HB3	2.00	0.44
1:B:704:ILE:H	1:B:704:ILE:CD1	2.29	0.44
1:B:984:THR:O	1:B:986:ASP:N	2.51	0.44
2:C:102:LEU:O	2:C:104:GLY:N	2.50	0.44
1:A:704:ILE:HG23	1:A:705:ASP:N	2.32	0.44
1:B:222:VAL:CG1	1:B:223:PRO:HD2	2.47	0.44
1:B:342:GLU:O	1:B:344:GLY:N	2.51	0.44
2:C:119:GLY:O	2:C:120:LYS:CB	2.66	0.44
1:A:29:LEU:HG	1:A:44:VAL:CG2	2.47	0.44
1:A:291:MET:HG3	1:A:292:ASP:N	2.29	0.44
1:A:931:LEU:HD12	1:A:947:ARG:HH22	1.83	0.44
1:B:47:GLU:HG2	1:B:48:GLY:N	2.25	0.44
1:B:246:LEU:HD11	1:B:299:ASP:HA	1.99	0.44
1:B:286:GLU:O	1:B:298:LYS:N	2.45	0.44
1:B:416:ASP:HA	1:B:417:PRO:HD3	1.86	0.44
1:B:482:GLU:HB2	1:B:483:PRO:CD	2.32	0.44
1:B:482:GLU:CB	1:B:483:PRO:CD	2.92	0.44
1:B:1017:LEU:C	1:B:1019:GLU:H	2.20	0.44
2:C:145:ILE:HD11	2:C:174:GLU:OE2	2.18	0.44
2:D:147:GLU:HA	2:D:148:PRO:HD3	1.83	0.44
1:A:663:ASN:O	1:A:664:HIS:CB	2.64	0.44
1:A:745:THR:C	1:A:747:GLY:H	2.21	0.44
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.53	0.44
1:B:140:PHE:CZ	1:B:178:ILE:HD12	2.53	0.44
1:B:355:ASN:CG	1:B:357:GLY:H	2.21	0.44
1:B:644:LEU:CG	1:B:645:SER:N	2.81	0.44
1:B:1080:ARG:HG3	1:B:1081:LYS:N	2.32	0.44
2:C:89:ASP:OD2	2:C:202:ARG:NH2	2.51	0.44
2:D:22:ASN:C	2:D:22:ASN:HD22	2.20	0.44
2:D:172:ARG:NE	2:D:174:GLU:OE2	2.50	0.44
1:A:95:GLY:C	1:A:97:SER:N	2.71	0.43
1:A:275:ASP:HB3	1:A:279:ARG:N	2.30	0.43
1:A:587:ILE:HD13	1:A:587:ILE:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:VAL:HA	1:B:388:ARG:O	2.18	0.43
1:B:616:LEU:HD12	1:B:617:ASN:H	1.80	0.43
2:C:52:THR:HG21	2:C:85:ILE:HA	2.00	0.43
1:A:1:MET:HA	1:A:1:MET:CE	2.48	0.43
1:A:23:PHE:CE2	1:A:91:TYR:HB2	2.53	0.43
1:A:78:PHE:O	1:A:79:ILE:HG12	2.18	0.43
1:A:480:SER:HB3	1:A:487:VAL:CG1	2.46	0.43
1:A:705:ASP:OD2	1:A:709:LYS:CE	2.59	0.43
1:A:734:GLY:HA3	1:A:829:PHE:CE1	2.53	0.43
1:B:130:MET:HA	1:B:145:LEU:HB2	2.00	0.43
1:B:192:THR:HB	1:B:206:PRO:HD2	2.00	0.43
1:B:358:PRO:HA	1:B:1033:VAL:O	2.18	0.43
1:B:821:LEU:O	1:B:822:GLY:C	2.57	0.43
1:B:1115:ASP:HB2	1:B:1120:MET:HB2	2.00	0.43
1:A:90:GLU:HB3	1:A:101:ILE:HG13	2.00	0.43
1:A:405:PRO:HA	1:A:697:SER:HA	2.00	0.43
1:A:516:LEU:HD23	1:A:574:PHE:CE2	2.53	0.43
1:B:9:ALA:HB3	1:B:1037:ILE:HG22	2.01	0.43
1:B:81:THR:HG22	1:B:82:ALA:N	2.34	0.43
1:B:456:GLN:CD	1:B:473:SER:CB	2.64	0.43
1:B:514:ARG:O	1:B:514:ARG:CG	2.63	0.43
1:B:843:PRO:HG2	2:D:24:VAL:HG21	2.00	0.43
1:A:177:THR:HG22	1:A:194:GLU:HA	2.00	0.43
1:A:744:ASP:HA	1:A:782:PHE:CE1	2.53	0.43
1:A:936:LYS:HB3	1:A:939:GLU:HB2	2.00	0.43
1:B:112:ILE:N	1:B:112:ILE:CD1	2.78	0.43
1:B:150:LYS:HB2	1:B:151:GLU:OE2	2.18	0.43
1:B:570:LYS:HE2	1:B:577:LEU:HD11	2.00	0.43
1:B:694:ALA:HA	1:B:698:THR:O	2.18	0.43
1:B:782:PHE:N	1:B:782:PHE:CD2	2.86	0.43
1:B:941:ASN:C	1:B:941:ASN:HD22	2.22	0.43
1:B:1115:ASP:HA	1:B:1120:MET:HB3	2.00	0.43
2:D:115:LEU:CD1	2:D:130:VAL:HG13	2.48	0.43
1:A:401:SER:C	1:A:402:ILE:HD13	2.39	0.43
1:A:679:MET:SD	1:A:680:CYS:N	2.92	0.43
1:A:1032:THR:CG2	1:A:1034:ASN:H	2.23	0.43
1:A:1039:LEU:HD12	1:A:1040:VAL:H	1.83	0.43
1:B:263:ARG:HG2	1:B:263:ARG:HH11	1.83	0.43
1:B:356:LEU:O	1:B:357:GLY:C	2.57	0.43
1:B:543:ILE:N	1:B:543:ILE:HD13	2.33	0.43
1:B:874:VAL:HG22	1:B:875:GLU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:CYS:SG	1:B:941:ASN:HA	2.59	0.43
2:D:211:CYS:HA	2:D:212:PRO:HD2	1.81	0.43
1:A:256:SER:HB3	1:A:275:ASP:CG	2.39	0.43
1:A:318:ASP:O	1:A:319:ASN:C	2.57	0.43
1:A:762:SER:CB	1:A:803:HIS:ND1	2.82	0.43
1:A:931:LEU:HD12	1:A:947:ARG:NH2	2.33	0.43
1:B:222:VAL:HA	1:B:223:PRO:HD3	1.82	0.43
1:B:237:ILE:HD11	1:B:253:ILE:HD11	2.00	0.43
2:D:104:GLY:C	2:D:105:LEU:HD23	2.39	0.43
1:A:614:PHE:CD1	1:A:614:PHE:N	2.86	0.43
1:B:248:ILE:O	1:B:250:PRO:HD3	2.19	0.43
1:B:728:GLU:O	1:B:730:SER:N	2.51	0.43
1:B:740:ILE:HD12	1:B:740:ILE:H	1.82	0.43
1:B:832:GLY:N	1:B:873:MET:CE	2.82	0.43
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	2.01	0.43
1:A:522:HIS:HB3	1:A:523:PRO:CD	2.49	0.43
1:A:532:THR:CG2	1:A:533:GLU:N	2.81	0.43
1:A:948:ASP:N	1:A:992:LEU:HD11	2.33	0.43
1:B:155:PHE:HE1	1:B:157:ILE:HD11	1.83	0.43
1:B:518:TYR:OH	1:B:571:LEU:HD11	2.18	0.43
2:C:143:ARG:HH11	2:C:143:ARG:HG3	1.84	0.43
2:D:80:ARG:HB2	2:D:81:PRO:CD	2.36	0.43
1:A:10:GLN:HG2	1:A:710:LEU:HD12	1.99	0.43
1:A:518:TYR:CE1	1:A:571:LEU:HD22	2.53	0.43
1:B:170:LEU:HD11	1:B:179:CYS:HB2	2.00	0.43
1:B:191:LYS:HD3	1:B:193:TYR:CE2	2.54	0.43
1:B:226:PHE:HB2	1:B:227:GLY:H	1.65	0.43
1:B:281:PHE:O	1:B:305:LEU:HD12	2.18	0.43
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.85	0.43
1:B:380:GLY:O	1:B:381:ALA:HB2	2.18	0.43
1:B:452:VAL:HG22	1:B:453:ASP:N	2.34	0.43
1:B:463:VAL:HG23	1:B:467:GLN:HB2	2.01	0.43
1:B:523:PRO:C	1:B:524:GLN:NE2	2.72	0.43
2:D:44:PRO:HA	2:D:45:PRO:HD3	1.94	0.43
2:D:89:ASP:O	2:D:90:ASP:O	2.37	0.43
2:D:192:PRO:CG	2:D:206:CYS:HB2	2.48	0.43
2:D:218:CYS:CB	2:D:221:ASP:OD1	2.67	0.43
1:A:295:VAL:HG23	1:A:295:VAL:O	2.18	0.43
1:A:504:ASN:OD1	1:A:507:GLN:HG3	2.18	0.43
1:A:946:ALA:HB2	1:A:989:ARG:O	2.19	0.43
1:A:1032:THR:HG22	1:A:1035:GLY:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:HB3	1:B:47:GLU:OE1	2.19	0.43
1:B:194:GLU:OE2	1:B:204:LYS:O	2.36	0.43
1:B:894:THR:HG22	1:B:895:THR:H	1.82	0.43
1:B:919:ASP:O	1:B:934:ALA:HA	2.19	0.43
1:B:948:ASP:N	1:B:992:LEU:HD12	2.33	0.43
1:B:1109:VAL:O	1:B:1110:ALA:O	2.37	0.43
1:A:370:GLN:O	1:A:372:GLN:N	2.52	0.42
1:A:391:ARG:HD2	1:A:392:ASN:O	2.19	0.42
1:A:1097:PHE:CZ	1:A:1105:MET:CG	3.02	0.42
1:B:183:GLN:HG2	1:B:184:ASP:N	2.34	0.42
1:B:275:ASP:HB2	1:B:279:ARG:N	2.25	0.42
1:B:355:ASN:O	1:B:357:GLY:N	2.52	0.42
1:B:843:PRO:HG2	2:D:24:VAL:CG2	2.49	0.42
1:B:1108:VAL:HG12	1:B:1109:VAL:H	1.84	0.42
2:C:100:ASN:HB3	2:C:103:LEU:CG	2.49	0.42
2:D:172:ARG:NH1	2:D:197:ILE:HG12	2.34	0.42
2:D:173:ARG:HH12	2:D:218:CYS:CB	2.31	0.42
1:A:403:ASP:HA	1:A:698:THR:HG22	2.02	0.42
1:A:576:LEU:HD22	1:A:577:LEU:N	2.34	0.42
1:A:745:THR:O	1:A:747:GLY:N	2.50	0.42
1:A:912:LEU:HB2	1:A:913:TYR:CD1	2.54	0.42
1:B:129:ARG:HH11	1:B:176:PRO:HD3	1.81	0.42
1:B:1029:LEU:CD2	1:B:1039:LEU:HD13	2.49	0.42
1:A:127:GLU:O	1:A:128:CYS:HB2	2.20	0.42
1:A:634:GLN:HG2	1:A:654:ASP:CG	2.40	0.42
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.34	0.42
1:A:780:THR:HB	1:A:784:GLU:HG3	2.01	0.42
1:B:181:VAL:HG23	1:B:219:VAL:CG2	2.49	0.42
1:B:553:SER:HA	1:B:554:PRO:HD3	1.82	0.42
1:B:655:ARG:NH1	1:B:655:ARG:HG2	2.35	0.42
1:B:961:ASP:C	1:B:961:ASP:OD2	2.58	0.42
2:C:145:ILE:HA	2:C:145:ILE:HD13	1.74	0.42
2:D:22:ASN:C	2:D:22:ASN:ND2	2.72	0.42
2:D:127:TYR:CE1	2:D:131:LYS:HD3	2.54	0.42
1:A:68:ARG:HD2	1:A:74:LYS:C	2.40	0.42
1:A:570:LYS:HD2	1:A:570:LYS:HA	1.66	0.42
1:A:660:TYR:CE2	1:A:708:GLN:OE1	2.72	0.42
1:A:866:VAL:HA	1:A:867:LYS:NZ	2.34	0.42
1:B:19:VAL:HG22	1:B:20:THR:N	2.33	0.42
1:B:130:MET:HG2	1:B:197:LEU:HD11	2.01	0.42
1:B:130:MET:HA	1:B:145:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1059:ASN:HD21	1:B:1070:HIS:CD2	2.36	0.42
2:C:48:THR:HG22	2:C:83:ILE:O	2.18	0.42
1:A:296:THR:OG1	1:A:297:LEU:N	2.53	0.42
1:A:811:GLU:OE2	1:A:847:ARG:NE	2.53	0.42
1:A:867:LYS:HD2	1:A:867:LYS:N	2.32	0.42
1:A:1032:THR:HG23	1:A:1034:ASN:N	2.25	0.42
1:B:235:GLU:HB2	1:B:254:LYS:HE3	2.00	0.42
1:B:308:THR:OG1	1:B:324:VAL:HG11	2.19	0.42
1:B:324:VAL:HB	1:B:332:GLN:HG2	2.02	0.42
1:B:407:ILE:HG22	1:B:408:LYS:N	2.35	0.42
1:B:414:ARG:NH2	1:B:462:ASN:HB2	2.34	0.42
1:B:516:LEU:HD11	1:B:538:VAL:HG21	2.01	0.42
1:B:603:LEU:N	1:B:603:LEU:HD23	2.35	0.42
1:B:662:SER:HB3	1:B:1138:ARG:HH21	1.85	0.42
1:B:1030:PHE:O	1:B:1037:ILE:HA	2.19	0.42
1:A:305:LEU:HD13	1:A:336:LEU:HD22	2.00	0.42
1:A:549:SER:OG	1:A:550:ASN:N	2.53	0.42
1:A:876:PHE:CD1	1:A:916:THR:HG21	2.55	0.42
1:A:1053:ASP:O	1:A:1057:ARG:HG3	2.20	0.42
1:B:130:MET:CE	1:B:195:VAL:HG11	2.50	0.42
1:B:147:ARG:O	1:B:148:ASP:C	2.58	0.42
1:B:407:ILE:H	1:B:407:ILE:CD1	2.28	0.42
1:B:458:PHE:HE2	1:B:499:SER:O	2.02	0.42
1:B:818:SER:HA	1:B:828:TYR:O	2.19	0.42
2:C:113:THR:HB	2:C:186:VAL:HB	2.00	0.42
2:D:177:ILE:HG12	2:D:186:VAL:HG22	2.02	0.42
1:A:910:MET:HG2	1:A:912:LEU:HD21	2.01	0.42
1:A:931:LEU:C	1:A:931:LEU:CD2	2.87	0.42
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	2.00	0.42
1:B:162:LEU:HG	1:B:163:HIS:N	2.34	0.42
1:B:182:TYR:CE1	1:B:189:HIS:HD2	2.38	0.42
1:B:412:PRO:HD3	1:B:680:CYS:HB2	2.02	0.42
1:B:463:VAL:HG11	1:B:469:ILE:HB	2.01	0.42
1:B:575:GLU:O	1:B:576:LEU:C	2.58	0.42
1:A:170:LEU:HD13	1:A:207:TRP:CH2	2.55	0.42
1:A:854:SER:O	1:A:855:ASP:HB2	2.19	0.42
1:B:4:ASN:ND2	1:B:976:VAL:HG11	2.34	0.42
1:B:43:VAL:HG23	1:B:52:VAL:CG1	2.47	0.42
1:B:394:ILE:HG13	1:B:669:SER:HB3	2.00	0.42
1:B:467:GLN:CB	1:B:478:LEU:HD21	2.49	0.42
1:B:512:VAL:O	1:B:513:GLY:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ILE:HD11	1:B:733:PHE:CD2	2.54	0.42
1:A:177:THR:HG22	1:A:194:GLU:HG2	2.01	0.42
1:A:964:ASN:OD1	1:A:978:GLN:HG3	2.20	0.42
1:B:451:PHE:HD1	1:B:486:LEU:HD22	1.85	0.42
1:B:915:LYS:HD3	1:B:915:LYS:HA	1.84	0.42
2:D:22:ASN:O	2:D:25:GLU:N	2.50	0.42
1:A:429:PHE:O	1:A:430:VAL:C	2.56	0.41
1:B:235:GLU:O	1:B:236:SER:CB	2.68	0.41
1:B:262:ASN:HD21	1:B:316:TYR:H	1.67	0.41
1:B:381:ALA:O	1:B:382:PHE:HB2	2.20	0.41
1:B:437:MET:HB2	1:B:446:THR:CG2	2.49	0.41
1:B:503:CYS:HB2	1:B:508:VAL:HG22	2.02	0.41
1:B:613:TYR:CZ	1:B:627:LYS:HB2	2.55	0.41
1:A:410:LEU:HA	1:A:426:VAL:O	2.20	0.41
1:A:679:MET:CE	1:A:691:LEU:HG	2.50	0.41
1:A:1113:GLN:CB	1:A:1121:LYS:HD2	2.49	0.41
1:A:1114:TYR:CE2	1:A:1128:ASP:HB3	2.56	0.41
1:B:63:VAL:O	1:B:79:ILE:HA	2.19	0.41
1:B:130:MET:CG	1:B:197:LEU:HD11	2.51	0.41
1:B:361:ASP:OD2	1:B:723:LYS:HD3	2.20	0.41
1:B:396:ILE:CD1	1:B:673:LEU:HD11	2.42	0.41
1:B:932:LEU:CD2	1:B:979:LYS:HD3	2.50	0.41
1:B:1063:LYS:HG3	1:B:1063:LYS:O	2.20	0.41
2:C:221:ASP:O	2:C:222:THR:HG23	2.20	0.41
2:D:139:ASN:O	2:D:140:LEU:C	2.58	0.41
1:A:494:GLN:O	1:A:495:ALA:HB3	2.19	0.41
1:A:982:ALA:O	1:A:984:THR:N	2.50	0.41
1:B:167:VAL:O	1:B:168:LYS:HE2	2.20	0.41
1:B:399:HIS:HB2	1:B:701:ILE:O	2.20	0.41
1:B:1058:LEU:HD23	1:B:1093:LEU:CD2	2.48	0.41
1:B:1115:ASP:CB	1:B:1120:MET:HB2	2.50	0.41
1:A:391:ARG:HB3	1:A:391:ARG:HH11	1.85	0.41
1:A:597:GLU:HG3	1:A:661:SER:CB	2.50	0.41
1:A:818:SER:O	1:A:819:CYS:HB3	2.20	0.41
1:B:29:LEU:HD23	1:B:44:VAL:HG11	2.01	0.41
1:B:342:GLU:C	1:B:344:GLY:N	2.73	0.41
1:B:754:PRO:HB2	1:B:759:GLN:OE1	2.20	0.41
2:C:111:THR:HB	2:C:188:GLU:CG	2.50	0.41
2:C:112:GLN:HE22	2:C:187:THR:CG2	2.15	0.41
2:C:170:PHE:HB2	2:C:193:SER:OG	2.20	0.41
2:D:49:GLY:HA2	2:D:144:PHE:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HA	1:A:223:PRO:HD3	1.83	0.41
1:B:203:ASN:O	1:B:204:LYS:HB2	2.21	0.41
1:B:314:LEU:HD12	1:B:314:LEU:C	2.40	0.41
1:B:483:PRO:O	1:B:484:LYS:CB	2.69	0.41
1:B:644:LEU:H	1:B:644:LEU:CD2	2.32	0.41
1:A:81:THR:HG21	1:A:85:ASN:OD1	2.21	0.41
1:A:90:GLU:OE1	1:A:103:ARG:NE	2.53	0.41
1:A:362:MET:HB3	1:A:377:THR:HG22	2.03	0.41
1:A:1013:VAL:HG12	1:A:1014:MET:O	2.21	0.41
1:B:433:THR:OG1	1:B:455:GLN:O	2.24	0.41
1:B:492:GLU:O	1:B:493:PRO:C	2.59	0.41
1:B:617:ASN:O	1:B:621:GLY:N	2.52	0.41
2:D:147:GLU:OE2	2:D:163:ARG:CZ	2.69	0.41
1:A:372:GLN:NE2	1:A:372:GLN:O	2.53	0.41
1:A:388:ARG:CD	1:A:714:THR:HB	2.46	0.41
1:B:459:PHE:HE2	1:B:503:CYS:SG	2.44	0.41
1:B:548:ASP:O	1:B:549:SER:C	2.59	0.41
1:B:1022:THR:O	1:B:1024:THR:N	2.54	0.41
2:C:160:ASP:CG	2:C:161:PHE:N	2.72	0.41
2:D:48:THR:HA	2:D:82:LYS:O	2.21	0.41
1:A:7:VAL:HG11	1:A:1095:GLU:OE2	2.20	0.41
1:A:847:ARG:NH1	1:A:849:VAL:HG22	2.35	0.41
1:B:383:LYS:CG	1:B:384:GLU:OE2	2.69	0.41
1:B:473:SER:O	1:B:497:ASN:HA	2.21	0.41
1:B:474:ALA:O	1:B:475:SER:CB	2.67	0.41
2:C:215:CYS:SG	2:C:217:GLU:N	2.84	0.41
1:A:16:ASN:HB2	1:A:35:LYS:O	2.21	0.41
1:A:125:ASP:OD1	1:A:126:PRO:HD2	2.21	0.41
1:A:181:VAL:HG23	1:A:219:VAL:CG2	2.50	0.41
1:A:358:PRO:HD2	1:A:380:GLY:HA2	2.03	0.41
1:A:622:LEU:HD23	1:A:622:LEU:H	1.86	0.41
1:A:725:CYS:SG	1:A:817:VAL:HA	2.60	0.41
1:A:889:ARG:HD2	1:A:901:THR:CG2	2.51	0.41
1:B:277:GLU:HB3	1:B:279:ARG:NH1	2.35	0.41
1:B:287:LYS:HD3	1:B:287:LYS:O	2.20	0.41
1:B:318:ASP:O	1:B:319:ASN:HB2	2.20	0.41
1:B:392:ASN:C	1:B:392:ASN:ND2	2.75	0.41
1:B:408:LYS:HG3	1:B:430:VAL:HG23	2.03	0.41
1:B:436:LEU:HD11	1:B:443:VAL:O	2.20	0.41
1:B:724:ILE:HD11	1:B:733:PHE:HD2	1.86	0.41
1:B:869:ALA:N	1:B:885:ASN:OD1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:LEU:HD23	1:B:944:GLU:HA	2.02	0.41
1:B:947:ARG:C	1:B:992:LEU:HD12	2.41	0.41
1:B:1039:LEU:CD2	1:B:1139:ILE:HG22	2.50	0.41
2:C:110:SER:N	2:C:221:ASP:HB3	2.35	0.41
2:D:82:LYS:HE2	2:D:161:PHE:CZ	2.56	0.41
2:D:142:THR:O	2:D:143:ARG:C	2.59	0.41
1:A:18:CYS:HA	1:A:32:LEU:O	2.21	0.41
1:A:226:PHE:CD1	1:A:226:PHE:N	2.89	0.41
1:A:537:GLU:HG3	1:A:561:TRP:CD1	2.56	0.41
1:A:730:SER:HB2	1:A:732:CYS:SG	2.61	0.41
1:A:841:ALA:HA	2:C:45:PRO:HG2	2.02	0.41
1:B:450:GLY:CA	1:B:479:VAL:HG11	2.27	0.41
1:B:676:VAL:HG22	1:B:693:LEU:HD12	2.03	0.41
1:B:768:SER:C	1:B:769:LYS:HE2	2.41	0.41
1:B:836:VAL:HG13	2:D:22:ASN:OD1	2.21	0.41
2:C:147:GLU:OE2	2:C:163:ARG:HD3	2.21	0.41
2:C:219:GLU:O	2:C:221:ASP:N	2.53	0.41
2:D:142:THR:O	2:D:143:ARG:O	2.39	0.41
1:A:90:GLU:HB3	1:A:101:ILE:CG1	2.51	0.40
1:A:676:VAL:HG11	1:A:693:LEU:HD22	2.03	0.40
1:B:5:TYR:CE2	1:B:7:VAL:HG21	2.56	0.40
1:B:213:GLU:OE1	1:B:234:GLN:O	2.38	0.40
1:B:456:GLN:O	1:B:472:THR:HB	2.21	0.40
1:A:22:HIS:CD2	1:A:28:ASP:O	2.74	0.40
1:A:125:ASP:HA	1:A:126:PRO:HD3	1.97	0.40
1:A:1109:VAL:O	1:A:1109:VAL:HG12	2.22	0.40
1:B:991:HIS:HB3	1:B:993:GLN:HE22	1.86	0.40
1:B:994:GLU:O	1:B:995:VAL:CG2	2.60	0.40
1:B:1110:ALA:C	1:B:1112:LEU:H	2.25	0.40
2:C:107:SER:O	2:C:109:PRO:HD2	2.21	0.40
1:A:263:ARG:HD2	1:A:265:ASP:O	2.22	0.40
1:A:439:ASN:O	1:A:442:GLU:N	2.47	0.40
1:A:439:ASN:O	1:A:441:GLU:N	2.55	0.40
1:A:542:ASP:HB3	1:A:557:ALA:HB3	2.03	0.40
1:B:2:SER:CB	1:B:995:VAL:HG23	2.51	0.40
1:B:254:LYS:HD2	1:B:254:LYS:N	2.36	0.40
1:B:554:PRO:C	1:B:571:LEU:HB3	2.42	0.40
1:B:628:LYS:HG2	1:B:629:VAL:N	2.36	0.40
1:B:740:ILE:HG22	1:B:741:GLU:N	2.36	0.40
1:B:949:PHE:CE1	1:B:991:HIS:CD2	3.10	0.40
1:A:484:LYS:O	1:A:485:ALA:HB2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ILE:O	1:A:569:LEU:HD23	2.20	0.40
1:A:607:GLY:HA2	1:A:635:PRO:HA	2.04	0.40
1:A:679:MET:HE2	1:A:691:LEU:HG	2.04	0.40
1:B:284:LEU:CD1	1:B:301:ARG:NH2	2.84	0.40
2:C:52:THR:HG21	2:C:85:ILE:CA	2.50	0.40
1:A:166:ASP:O	1:A:180:PHE:HB2	2.21	0.40
1:A:234:GLN:O	1:A:235:GLU:HG2	2.20	0.40
1:A:471:ILE:HG23	1:A:476:VAL:HB	2.04	0.40
1:A:492:GLU:OE2	1:A:494:GLN:N	2.54	0.40
1:A:837:TYR:HA	1:A:838:PRO:HD3	1.95	0.40
1:B:281:PHE:HB3	1:B:282:MET:H	1.67	0.40
1:B:378:CYS:SG	1:B:724:ILE:HB	2.60	0.40
1:B:507:GLN:NE2	1:B:552:LEU:HA	2.37	0.40
1:B:569:LEU:HD23	1:B:576:LEU:HA	2.03	0.40
1:B:1120:MET:HB2	1:B:1121:LYS:H	1.72	0.40
2:C:102:LEU:C	2:C:104:GLY:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1126/1140 (99%)	960 (85%)	128 (11%)	38 (3%)	3 12
1	B	1130/1140 (99%)	892 (79%)	145 (13%)	93 (8%)	1 1
2	C	168/222 (76%)	123 (73%)	33 (20%)	12 (7%)	1 2
2	D	169/222 (76%)	115 (68%)	32 (19%)	22 (13%)	0 0
All	All	2593/2724 (95%)	2090 (81%)	338 (13%)	165 (6%)	1 3

All (165) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LYS
1	A	269	SER
1	A	290	GLN
1	A	341	ASN
1	A	370	GLN
1	A	371	GLY
1	A	708	GLN
1	A	772	SER
1	A	781	SER
1	A	856	GLY
1	A	929	SER
1	B	46	ALA
1	B	223	PRO
1	B	275	ASP
1	B	310	ILE
1	B	341	ASN
1	B	357	GLY
1	B	430	VAL
1	B	434	ARG
1	B	450	GLY
1	B	466	GLN
1	B	493	PRO
1	B	549	SER
1	B	551	GLY
1	B	576	LEU
1	B	688	PRO
1	B	707	ILE
1	B	751	ALA
1	B	782	PHE
1	B	985	THR
1	B	1015	GLN
1	B	1016	ASN
1	B	1021	SER
1	B	1065	VAL
1	B	1109	VAL
1	B	1110	ALA
2	C	39	GLY
2	C	108	THR
2	C	162	LYS
2	D	23	THR
2	D	51	LEU
2	D	89	ASP
2	D	90	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	104	GLY
2	D	108	THR
2	D	109	PRO
2	D	143	ARG
2	D	193	SER
2	D	209	HIS
1	A	118	THR
1	A	147	ARG
1	A	203	ASN
1	A	294	THR
1	A	449	MET
1	A	524	GLN
1	A	551	GLY
1	A	583	GLY
1	A	643	SER
1	A	646	THR
1	A	706	GLU
1	A	746	SER
1	A	983	ALA
1	A	987	GLU
1	B	26	ALA
1	B	35	LYS
1	B	113	GLY
1	B	146	ASP
1	B	149	ASN
1	B	168	LYS
1	B	214	ALA
1	B	276	MET
1	B	318	ASP
1	B	369	ARG
1	B	451	PHE
1	B	524	GLN
1	B	564	ILE
1	B	626	ARG
1	B	729	VAL
1	B	748	GLY
1	B	986	ASP
1	B	995	VAL
1	B	1037	ILE
1	B	1066	GLY
1	B	1119	GLY
2	C	148	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	180	VAL
2	C	220	ARG
2	D	105	LEU
2	D	148	PRO
2	D	149	ARG
2	D	216	SER
1	A	367	LEU
1	A	368	GLU
1	A	817	VAL
1	A	1015	GLN
1	A	1027	SER
1	B	147	ARG
1	B	148	ASP
1	B	236	SER
1	B	343	GLN
1	B	432	GLN
1	B	433	THR
1	B	440	GLY
1	B	444	GLU
1	B	465	HIS
1	B	475	SER
1	B	484	LYS
1	B	578	HIS
1	B	884	ILE
1	B	1080	ARG
2	C	103	LEU
2	C	107	SER
2	D	39	GLY
2	D	91	LYS
2	D	117	LEU
1	A	319	ASN
1	B	226	PHE
1	B	251	PRO
1	B	253	ILE
1	B	255	GLN
1	B	340	SER
1	B	706	GLU
1	B	761	LEU
1	B	783	GLY
1	B	864	LYS
1	B	918	GLY
1	B	984	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	50	LEU
2	D	19	THR
2	D	99	PRO
1	A	184	ASP
1	A	224	GLU
1	A	440	GLY
1	A	937	PRO
1	B	47	GLU
1	B	203	ASN
1	B	208	LYS
1	B	241	ASN
1	B	243	ASP
1	B	356	LEU
1	B	381	ALA
1	B	572	PRO
1	B	575	GLU
1	B	643	SER
1	B	861	VAL
1	B	1036	MET
2	C	195	SER
2	D	212	PRO
1	A	253	ILE
1	B	204	LYS
1	B	486	LEU
1	B	1111	ASN
2	D	192	PRO
1	A	584	GLY
1	B	513	GLY
1	B	822	GLY
2	C	164	GLY
2	D	180	VAL
1	B	571	LEU
1	B	1013	VAL
2	C	20	GLY
1	A	119	GLY
1	B	144	PRO
1	B	224	GLU
1	B	848	ILE

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	992/999 (99%)	900 (91%)	92 (9%)	9 24
1	B	994/999 (100%)	925 (93%)	69 (7%)	15 38
2	C	151/191 (79%)	134 (89%)	17 (11%)	6 16
2	D	151/191 (79%)	133 (88%)	18 (12%)	5 13
All	All	2288/2380 (96%)	2092 (91%)	196 (9%)	10 27

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	VAL
1	A	10	GLN
1	A	47	GLU
1	A	68	ARG
1	A	103	ARG
1	A	112	ILE
1	A	117	GLU
1	A	146	ASP
1	A	147	ARG
1	A	167	VAL
1	A	178	ILE
1	A	186	GLN
1	A	202	PHE
1	A	206	PRO
1	A	235	GLU
1	A	241	ASN
1	A	282	MET
1	A	291	MET
1	A	298	LYS
1	A	300	LEU
1	A	318	ASP
1	A	319	ASN
1	A	365	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	GLN
1	A	391	ARG
1	A	392	ASN
1	A	396	ILE
1	A	410	LEU
1	A	414	ARG
1	A	419	ARG
1	A	449	MET
1	A	455	GLN
1	A	468	LEU
1	A	476	VAL
1	A	507	GLN
1	A	518	TYR
1	A	525	GLU
1	A	531	HIS
1	A	550	ASN
1	A	552	LEU
1	A	567	ARG
1	A	571	LEU
1	A	576	LEU
1	A	579	LYS
1	A	582	LEU
1	A	587	ILE
1	A	589	ARG
1	A	594	THR
1	A	599	SER
1	A	624	SER
1	A	647	THR
1	A	648	ASN
1	A	680	CYS
1	A	682	LEU
1	A	685	ASP
1	A	696	ASN
1	A	700	THR
1	A	704	ILE
1	A	705	ASP
1	A	708	GLN
1	A	713	ARG
1	A	714	THR
1	A	759	GLN
1	A	781	SER
1	A	796	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	817	VAL
1	A	823	LYS
1	A	835	MET
1	A	858	LEU
1	A	866	VAL
1	A	867	LYS
1	A	874	VAL
1	A	902	GLU
1	A	907	ASN
1	A	925	ASP
1	A	931	LEU
1	A	939	GLU
1	A	957	VAL
1	A	966	LEU
1	A	969	GLU
1	A	990	GLN
1	A	992	LEU
1	A	1000	LEU
1	A	1032	THR
1	A	1036	MET
1	A	1041	THR
1	A	1062	ILE
1	A	1069	GLU
1	A	1093	LEU
1	A	1121	LYS
1	A	1135	GLU
1	B	6	VAL
1	B	47	GLU
1	B	67	PHE
1	B	92	LYS
1	B	109	GLN
1	B	112	ILE
1	B	130	MET
1	B	147	ARG
1	B	185	PRO
1	B	255	GLN
1	B	275	ASP
1	B	277	GLU
1	B	287	LYS
1	B	307	GLU
1	B	354	THR
1	B	367	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	392	ASN
1	B	402	ILE
1	B	414	ARG
1	B	427	LEU
1	B	449	MET
1	B	466	GLN
1	B	477	ARG
1	B	493	PRO
1	B	498	ILE
1	B	524	GLN
1	B	529	ILE
1	B	543	ILE
1	B	563	ASP
1	B	567	ARG
1	B	581	MET
1	B	585	GLU
1	B	597	GLU
1	B	614	PHE
1	B	693	LEU
1	B	699	LEU
1	B	704	ILE
1	B	706	GLU
1	B	713	ARG
1	B	746	SER
1	B	749	THR
1	B	750	THR
1	B	769	LYS
1	B	780	THR
1	B	781	SER
1	B	790	ASN
1	B	815	SER
1	B	839	GLU
1	B	852	GLN
1	B	899	VAL
1	B	901	THR
1	B	908	ASN
1	B	931	LEU
1	B	941	ASN
1	B	943	GLU
1	B	957	VAL
1	B	969	GLU
1	B	980	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	990	GLN
1	B	995	VAL
1	B	1000	LEU
1	B	1036	MET
1	B	1052	LEU
1	B	1078	THR
1	B	1080	ARG
1	B	1086	THR
1	B	1093	LEU
1	B	1120	MET
1	B	1131	LYS
2	C	37	SER
2	C	50	LEU
2	C	106	ASP
2	C	121	THR
2	C	137	LYS
2	C	145	ILE
2	C	163	ARG
2	C	176	SER
2	C	179	TRP
2	C	190	CYS
2	C	194	CYS
2	C	197	ILE
2	C	206	CYS
2	C	208	CYS
2	C	211	CYS
2	C	218	CYS
2	C	222	THR
2	D	18	GLU
2	D	22	ASN
2	D	25	GLU
2	D	51	LEU
2	D	101	PRO
2	D	105	LEU
2	D	111	THR
2	D	122	LEU
2	D	140	LEU
2	D	143	ARG
2	D	145	ILE
2	D	163	ARG
2	D	188	GLU
2	D	192	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	194	CYS
2	D	208	CYS
2	D	213	VAL
2	D	215	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	10	GLN
1	A	22	HIS
1	A	30	ASN
1	A	93	GLN
1	A	156	ASN
1	A	186	GLN
1	A	234	GLN
1	A	241	ASN
1	A	262	ASN
1	A	319	ASN
1	A	341	ASN
1	A	343	GLN
1	A	372	GLN
1	A	374	GLN
1	A	455	GLN
1	A	467	GLN
1	A	481	GLN
1	A	507	GLN
1	A	520	GLN
1	A	578	HIS
1	A	634	GLN
1	A	648	ASN
1	A	711	HIS
1	A	743	GLN
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	810	ASN
1	A	904	ASN
1	A	907	ASN
1	A	950	ASN
1	A	990	GLN
1	A	991	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1016	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1070	HIS
1	A	1140	HIS
1	B	4	ASN
1	B	22	HIS
1	B	30	ASN
1	B	109	GLN
1	B	189	HIS
1	B	255	GLN
1	B	262	ASN
1	B	267	ASN
1	B	290	GLN
1	B	343	GLN
1	B	372	GLN
1	B	392	ASN
1	B	399	HIS
1	B	456	GLN
1	B	466	GLN
1	B	481	GLN
1	B	497	ASN
1	B	507	GLN
1	B	524	GLN
1	B	743	GLN
1	B	790	ASN
1	B	796	GLN
1	B	803	HIS
1	B	826	ASN
1	B	904	ASN
1	B	941	ASN
1	B	973	ASN
1	B	991	HIS
1	B	993	GLN
1	B	1015	GLN
1	B	1034	ASN
1	B	1070	HIS
1	B	1140	HIS
2	C	30	GLN
2	C	112	GLN
2	C	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	22	ASN
2	D	31	GLN
2	D	41	ASN
2	D	100	ASN
2	D	112	GLN
2	D	191	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	189:TRP	C	190:CYS	N	0.99

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1132/1140 (99%)	-0.29	10 (0%)	84	84	18, 47, 99, 160	0
1	B	1134/1140 (99%)	0.01	35 (3%)	49	44	29, 68, 122, 173	0
2	C	174/222 (78%)	0.22	12 (6%)	16	12	32, 62, 118, 183	0
2	D	175/222 (78%)	0.56	19 (10%)	5	4	39, 81, 138, 168	0
All	All	2615/2724 (95%)	-0.07	76 (2%)	51	47	18, 59, 117, 183	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1018	GLY	5.9
1	B	750	THR	5.2
1	B	746	SER	5.0
1	B	780	THR	4.9
2	D	16	LEU	4.8
1	B	744	ASP	4.5
1	B	453	ASP	4.3
2	D	92	THR	4.2
2	D	104	GLY	4.1
1	A	548	ASP	3.9
1	B	571	LEU	3.9
1	B	450	GLY	3.8
1	B	1016	ASN	3.6
1	B	748	GLY	3.4
2	D	35	THR	3.3
2	C	162	LYS	3.3
2	D	161	PHE	3.3
1	A	984	THR	3.3
1	B	294	THR	3.3
1	B	295	VAL	3.1
1	B	781	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	782	PHE	3.0
2	D	83	ILE	3.0
2	D	20	GLY	3.0
2	D	17	ILE	3.0
1	B	174	GLN	2.9
1	B	464	ALA	2.9
1	A	983	ALA	2.9
2	D	160	ASP	2.9
1	A	708	GLN	2.8
1	B	419	ARG	2.7
2	D	80	ARG	2.7
1	A	571	LEU	2.7
1	B	455	GLN	2.7
1	B	1118	SER	2.6
2	C	222	THR	2.6
2	C	164	GLY	2.6
2	C	180	VAL	2.6
2	C	160	ASP	2.6
2	C	16	LEU	2.6
1	B	202	PHE	2.5
1	B	209	GLN	2.5
1	B	292	ASP	2.5
2	D	159	ILE	2.5
1	B	367	LEU	2.5
1	B	1017	LEU	2.5
1	A	644	LEU	2.5
1	B	1119	GLY	2.4
1	B	456	GLN	2.4
2	C	52	THR	2.4
1	B	684	SER	2.3
1	B	234	GLN	2.3
2	D	198	THR	2.3
1	B	236	SER	2.3
2	C	50	LEU	2.3
1	B	1114	TYR	2.3
1	A	924	GLY	2.3
2	D	34	GLY	2.2
2	D	165	ARG	2.2
2	C	36	SER	2.2
2	D	209	HIS	2.2
1	A	289	GLU	2.2
2	D	33	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1121	LYS	2.1
1	B	286	GLU	2.1
1	B	1032	THR	2.1
2	C	161	PHE	2.1
1	B	291	MET	2.1
2	D	105	LEU	2.1
2	C	33	THR	2.1
1	A	981	SER	2.1
2	D	163	ARG	2.1
2	C	53	ASN	2.1
1	A	1121	LYS	2.0
1	B	1015	GLN	2.0
2	D	38	LEU	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	ZN	C	3001	1/1	0.83	0.09	35,35,35,35	0
3	ZN	C	3002	1/1	0.89	0.07	35,35,35,35	0
3	ZN	D	3003	1/1	0.96	0.05	35,35,35,35	0
3	ZN	D	3004	1/1	0.96	0.08	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.