



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DM0  
Title : SHIGA TOXIN  
Authors : Fraser, M.E.; Chernaia, M.M.; Kozlov, Y.V.; James, M.N.  
Deposited on : 1999-12-13  
Resolution : 2.50 Å(reported)

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

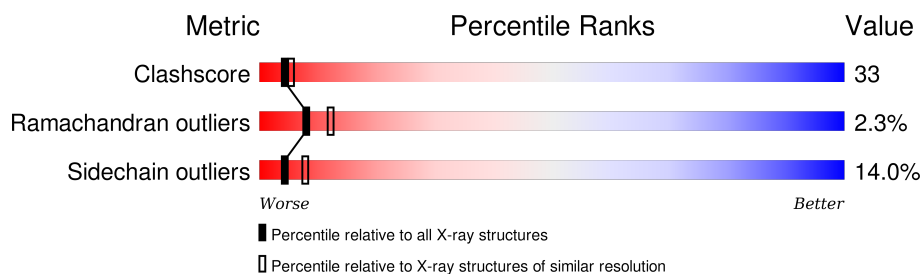
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	
1	L	287	
2	B	69	
2	C	69	
2	D	69	
2	E	69	
2	F	69	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	69	<div><div></div><div>54%41%6%</div></div>
2	H	69	<div><div></div><div>33%51%14%•</div></div>
2	I	69	<div><div></div><div>48%46%6%</div></div>
2	J	69	<div><div></div><div>38%39%22%•</div></div>
2	K	69	<div><div></div><div>58%36%6%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9538 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 SHIGA TOXIN A SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2046	1284	363	390	9			
1	L	262	Total	C	N	O	S	0	0	0
			2030	1276	361	384	9			

- Molecule 2 is a protein called SHIGA TOXIN B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	F	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	G	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	H	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	I	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	J	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	K	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

- Molecule 3 is water.

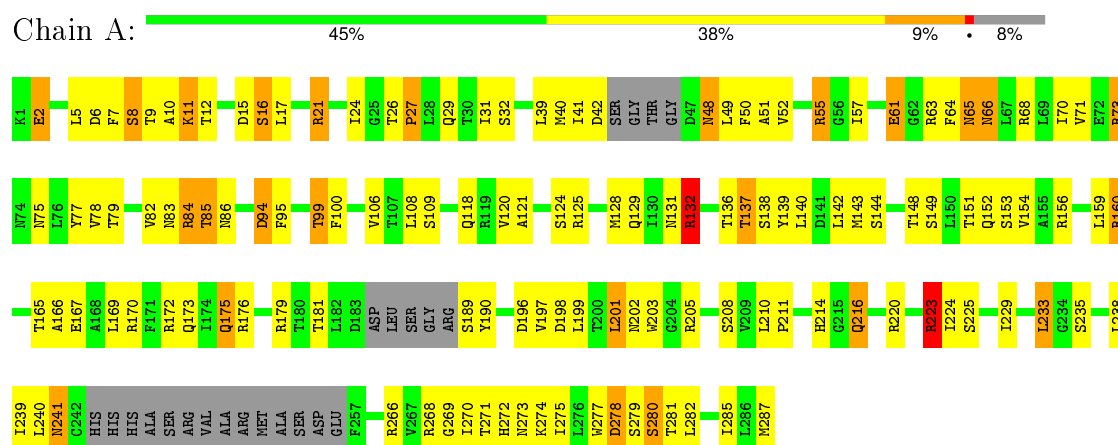
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	1	Total 1	O 1	0	0
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0
3	E	5	Total 5	O 5	0	0
3	F	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0
3	I	2	Total 2	O 2	0	0
3	J	5	Total 5	O 5	0	0
3	K	10	Total 10	O 10	0	0
3	L	11	Total 11	O 11	0	0

### 3 Residue-property plots

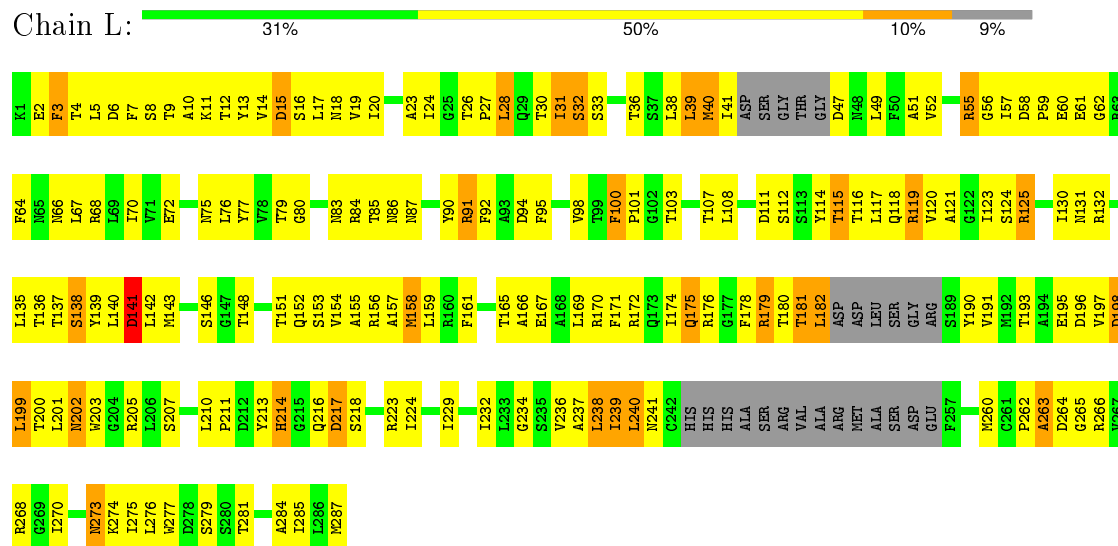
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: SHIGA TOXIN A SUBUNIT



#### • Molecule 1: SHIGA TOXIN A SUBUNIT

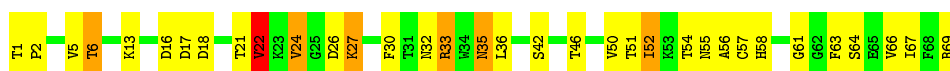


#### • Molecule 2: SHIGA TOXIN B SUBUNIT





• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



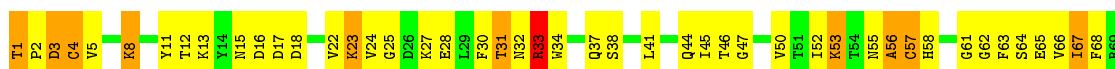
• Molecule 2: SHIGA TOXIN B SUBUNIT



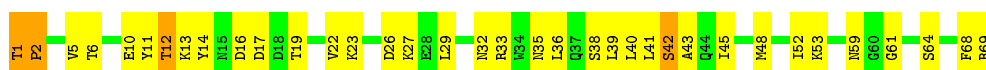
• Molecule 2: SHIGA TOXIN B SUBUNIT



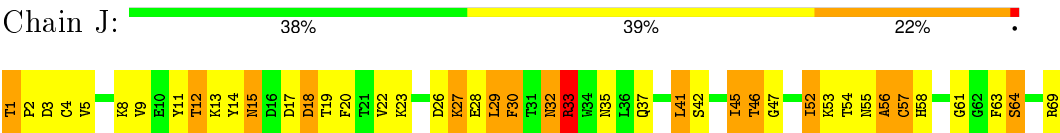
• Molecule 2: SHIGA TOXIN B SUBUNIT



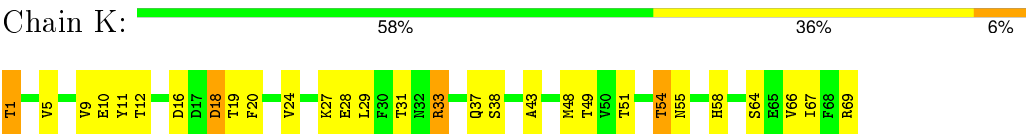
• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



● Molecule 2: SHIGA TOXIN B SUBUNIT





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.05Å 147.46Å 83.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.1 (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR, TNT	Depositor
R, $R_{free}$	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.07	1/2078 (0.0%)	1.22	7/2815 (0.2%)
1	L	0.91	0/2062	1.14	4/2793 (0.1%)
2	B	1.09	0/549	1.17	1/742 (0.1%)
2	C	1.10	0/549	1.18	2/742 (0.3%)
2	D	1.11	1/549 (0.2%)	1.19	3/742 (0.4%)
2	E	1.29	2/549 (0.4%)	1.35	2/742 (0.3%)
2	F	1.15	2/549 (0.4%)	1.32	3/742 (0.4%)
2	G	1.23	1/549 (0.2%)	1.16	1/742 (0.1%)
2	H	1.04	1/549 (0.2%)	1.07	2/742 (0.3%)
2	I	1.05	0/549	1.13	1/742 (0.1%)
2	J	1.18	0/549	1.31	5/742 (0.7%)
2	K	1.33	3/549 (0.5%)	1.32	4/742 (0.5%)
All	All	1.09	11/9630 (0.1%)	1.21	35/13028 (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
2	F	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	GLU	CG-CD	7.29	1.62	1.51
2	G	22	VAL	CB-CG1	-6.42	1.39	1.52
2	K	10	GLU	CD-OE2	6.20	1.32	1.25
2	K	10	GLU	CD-OE1	6.06	1.32	1.25
2	H	67	ILE	CA-CB	-5.95	1.41	1.54
2	F	9	VAL	CB-CG1	-5.76	1.40	1.52
2	K	24	VAL	CA-CB	-5.73	1.42	1.54
2	D	9	VAL	CB-CG1	-5.60	1.41	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	28	GLU	CB-CG	-5.45	1.41	1.52
2	E	22	VAL	CB-CG2	-5.32	1.41	1.52
1	A	106	VAL	CB-CG2	-5.26	1.41	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	THR	C-N-CD	-10.21	98.13	120.60
2	E	69	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	A	132	ARG	NE-CZ-NH2	-7.71	116.45	120.30
2	J	33	ARG	NE-CZ-NH1	-7.23	116.69	120.30
2	D	36	LEU	CB-CG-CD2	-6.75	99.53	111.00
1	A	201	LEU	CB-CG-CD2	-6.71	99.59	111.00
2	C	22	VAL	CB-CA-C	-6.62	98.82	111.40
2	F	39	LEU	CB-CG-CD1	-6.54	99.89	111.00
2	H	33	ARG	NE-CZ-NH1	-6.37	117.11	120.30
2	F	24	VAL	N-CA-C	-6.19	94.28	111.00
1	A	160	ARG	NE-CZ-NH1	-6.11	117.25	120.30
2	G	26	ASP	CB-CG-OD1	6.08	123.78	118.30
2	K	64	SER	CB-CA-C	-6.07	98.56	110.10
1	A	199	LEU	CA-CB-CG	6.01	129.13	115.30
2	J	41	LEU	CB-CG-CD2	5.85	120.95	111.00
2	I	1	THR	C-N-CD	-5.84	107.76	120.60
2	C	24	VAL	CB-CA-C	-5.72	100.53	111.40
2	J	33	ARG	NE-CZ-NH2	5.71	123.16	120.30
2	D	24	VAL	CB-CA-C	-5.66	100.65	111.40
2	B	39	LEU	CA-CB-CG	5.57	128.12	115.30
1	L	91	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	172	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	L	199	LEU	CB-CG-CD2	-5.47	101.70	111.00
2	D	36	LEU	CB-CG-CD1	5.45	120.27	111.00
1	A	282	LEU	CB-CG-CD1	-5.38	101.85	111.00
2	F	19	THR	N-CA-C	-5.37	96.50	111.00
1	L	68	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	L	28	LEU	N-CA-C	-5.29	96.72	111.00
2	K	1	THR	N-CA-C	-5.27	96.77	111.00
2	J	28	GLU	N-CA-C	-5.26	96.81	111.00
2	H	23	LYS	CD-CE-NZ	-5.14	99.89	111.70
1	A	223	ARG	NE-CZ-NH2	-5.11	117.74	120.30
2	E	67	ILE	N-CA-C	-5.11	97.20	111.00
2	K	10	GLU	OE1-CD-OE2	5.03	129.33	123.30
2	K	19	THR	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	14	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2046	0	2040	126	0
1	L	2030	0	2032	202	0
2	B	540	0	527	35	0
2	C	540	0	527	27	0
2	D	540	0	527	27	0
2	E	540	0	527	20	0
2	F	540	0	527	43	0
2	G	540	0	527	29	0
2	H	540	0	527	53	0
2	I	540	0	527	32	0
2	J	540	0	527	50	0
2	K	540	0	527	18	0
3	A	12	0	0	1	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
3	E	5	0	0	1	0
3	F	3	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	5	0	0	1	0
3	K	10	0	0	0	0
3	L	11	0	0	1	0
All	All	9538	0	9342	620	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 33.

All (620) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:MET:SD	1:A:40:MET:CE	2.04	1.45
1:L:60:GLU:HG2	1:L:61:GLU:HG2	1.31	1.13
2:J:33:ARG:HH12	2:J:64:SER:HB3	1.07	1.06
1:A:151:THR:HG22	1:A:154:VAL:HG23	1.41	1.02
1:A:121:ALA:HB1	1:A:156:ARG:HG2	1.39	1.02
2:F:14:TYR:HE1	2:F:41:LEU:HD11	1.20	1.01
1:L:125:ARG:HH11	1:L:125:ARG:HG3	1.27	0.99
2:H:67:ILE:HG13	2:I:13:LYS:HG3	1.43	0.99
1:L:285:ILE:HD12	2:J:45:ILE:HG21	1.50	0.92
1:L:123:ILE:HD13	1:L:156:ARG:HG2	1.51	0.91
2:I:48:MET:HE1	2:I:68:PHE:HB3	1.51	0.91
2:J:33:ARG:NH1	2:J:64:SER:HB3	1.85	0.91
1:A:216:GLN:HE21	1:A:216:GLN:H	1.19	0.90
1:L:123:ILE:CD1	1:L:156:ARG:HG2	2.03	0.88
1:L:64:PHE:CE2	1:L:140:LEU:HD21	2.08	0.87
1:L:8:SER:HA	1:L:132:ARG:HH22	1.37	0.87
1:A:31:ILE:HG23	1:A:229:ILE:HD11	1.57	0.86
2:H:67:ILE:CG1	2:I:13:LYS:HG3	2.07	0.85
1:A:214:HIS:H	1:A:216:GLN:HE22	1.23	0.85
2:F:14:TYR:CE1	2:F:41:LEU:HD11	2.10	0.84
1:A:40:MET:HE2	1:A:241:ASN:HA	1.57	0.84
2:F:69:ARG:HH11	2:F:69:ARG:HG2	1.43	0.84
1:L:64:PHE:HE2	1:L:140:LEU:HD21	1.39	0.84
1:L:32:SER:H	1:L:229:ILE:HD11	1.43	0.84
1:A:151:THR:CG2	1:A:154:VAL:HG23	2.09	0.83
1:L:67:LEU:HD11	1:L:142:LEU:HD13	1.60	0.82
1:A:131:ASN:HA	1:A:181:THR:HG21	1.61	0.81
1:L:6:ASP:HA	1:L:55:ARG:O	1.81	0.80
1:L:60:GLU:CG	1:L:61:GLU:HG2	2.10	0.79
2:C:67:ILE:HG13	2:D:13:LYS:HG3	1.63	0.79
2:J:32:ASN:H	2:J:32:ASN:HD22	1.29	0.79
1:L:31:ILE:HD12	1:L:38:LEU:HD22	1.65	0.79
1:L:91:ARG:HD2	1:L:95:PHE:O	1.83	0.79
1:A:216:GLN:HE21	1:A:216:GLN:N	1.80	0.78
1:A:285:ILE:HD12	2:F:45:ILE:HG22	1.66	0.78
1:L:41:ILE:HG13	1:L:238:LEU:HD21	1.66	0.78
1:L:165:THR:O	1:L:169:LEU:HB2	1.84	0.78
1:A:128:MET:HE1	1:A:159:LEU:HB3	1.66	0.78
1:L:40:MET:SD	1:L:241:ASN:HA	2.24	0.77
1:L:285:ILE:CD1	2:J:45:ILE:HG21	2.14	0.77
2:B:8:LYS:HZ3	2:B:8:LYS:HB3	1.49	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HD23	1:A:7:PHE:CE1	2.20	0.76
2:B:8:LYS:HB3	2:B:8:LYS:NZ	2.00	0.75
2:D:22:VAL:CG1	2:D:24:VAL:HG23	2.17	0.75
2:G:5:VAL:HG22	2:G:24:VAL:HG12	1.69	0.75
1:L:95:PHE:HB3	1:L:98:VAL:CG2	2.17	0.75
2:J:56:ALA:HB1	2:J:61:GLY:HA2	1.68	0.74
1:L:138:SER:HB3	1:L:161:PHE:HE2	1.51	0.74
1:A:287:MET:HE2	2:D:38:SER:HB2	1.70	0.74
1:A:7:PHE:O	1:A:132:ARG:NH2	2.20	0.74
1:A:203:TRP:CZ3	1:A:240:LEU:HD21	2.23	0.74
1:L:58:ASP:HB3	1:L:62:GLY:HA2	1.70	0.73
1:L:58:ASP:HB3	1:L:62:GLY:CA	2.18	0.73
1:L:7:PHE:CD2	1:L:135:LEU:HD21	2.24	0.73
2:F:69:ARG:NH1	2:F:69:ARG:HG2	2.03	0.72
2:D:4:CYS:HB2	2:D:54:THR:HG22	1.71	0.72
1:L:8:SER:HA	1:L:132:ARG:NH2	2.03	0.72
2:J:33:ARG:HH11	2:J:33:ARG:CG	2.03	0.72
1:L:95:PHE:HB3	1:L:98:VAL:HG21	1.69	0.72
1:L:83:ASN:OD1	1:L:85:THR:HB	1.88	0.72
2:G:67:ILE:HG12	2:H:13:LYS:HG3	1.72	0.71
2:I:26:ASP:OD1	2:I:27:LYS:HG2	1.89	0.71
1:L:8:SER:CA	1:L:132:ARG:HH22	2.03	0.71
2:H:1:THR:HG23	2:H:2:PRO:CD	2.20	0.71
2:D:22:VAL:HG11	2:D:24:VAL:HG23	1.73	0.71
1:L:175:GLN:HG2	1:L:176:ARG:N	2.04	0.71
1:A:285:ILE:HD12	2:F:45:ILE:CG2	2.21	0.70
1:L:38:LEU:CD1	1:L:236:VAL:HG12	2.21	0.70
1:L:20:ILE:O	1:L:23:ALA:HB3	1.91	0.70
1:A:151:THR:HG22	1:A:154:VAL:CG2	2.21	0.70
1:L:90:TYR:OH	1:L:146:SER:HA	1.92	0.70
2:J:17:ASP:OD1	2:J:19:THR:HG23	1.91	0.70
2:F:12:THR:HG22	2:F:22:VAL:HG12	1.72	0.69
1:A:6:ASP:HA	1:A:55:ARG:O	1.92	0.69
1:L:131:ASN:HA	1:L:181:THR:HG21	1.74	0.69
1:A:61:GLU:HB3	1:A:63:ARG:HG2	1.74	0.69
1:A:131:ASN:HD22	1:A:189:SER:HB2	1.57	0.69
1:L:26:THR:HB	1:L:27:PRO:HD2	1.73	0.69
1:L:154:VAL:O	1:L:158:MET:HB2	1.92	0.69
2:H:18:ASP:HB3	2:H:34:TRP:CH2	2.27	0.69
1:A:287:MET:CE	2:D:38:SER:HB2	2.23	0.69
2:G:20:PHE:CD1	2:G:37:GLN:HG2	2.27	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:121:ALA:HB1	1:L:123:ILE:HG12	1.75	0.68
1:L:85:THR:HG22	1:L:86:ASN:N	2.07	0.68
2:G:42:SER:O	2:G:46:THR:HG23	1.93	0.68
1:L:203:TRP:CH2	1:L:240:LEU:HG	2.28	0.68
1:A:137:THR:HG22	1:A:138:SER:N	2.08	0.68
1:A:108:LEU:HA	1:A:148:THR:O	1.94	0.68
1:L:91:ARG:NH1	1:L:98:VAL:O	2.26	0.68
2:H:5:VAL:HG22	2:H:24:VAL:HG12	1.76	0.68
1:L:51:ALA:HB2	1:L:100:PHE:CE2	2.28	0.68
2:G:41:LEU:HD12	2:G:44:GLN:NE2	2.08	0.68
2:C:26:ASP:OD1	2:C:27:LYS:HD3	1.94	0.68
1:A:68:ARG:HD2	1:A:84:ARG:HD3	1.75	0.68
2:D:17:ASP:OD1	2:D:19:THR:HG23	1.94	0.68
1:L:176:ARG:NH1	1:L:234:GLY:O	2.27	0.67
2:I:10:GLU:HB3	2:I:23:LYS:HG3	1.75	0.67
2:K:51:THR:OG1	2:K:69:ARG:NH1	2.27	0.67
1:L:60:GLU:N	1:L:60:GLU:OE1	2.27	0.67
2:H:1:THR:HG22	2:H:53:LYS:HB3	1.76	0.67
1:A:165:THR:O	1:A:169:LEU:HB2	1.94	0.67
1:A:129:GLN:HA	1:A:190:TYR:O	1.94	0.67
1:A:5:LEU:HD23	1:A:7:PHE:CZ	2.29	0.67
2:C:33:ARG:NH2	2:D:16:ASP:O	2.26	0.67
2:J:27:LYS:HD2	2:J:57:CYS:O	1.95	0.67
2:D:33:ARG:NH2	2:E:16:ASP:O	2.29	0.66
2:J:45:ILE:HG22	2:J:46:THR:N	2.09	0.66
2:B:33:ARG:NH2	2:C:16:ASP:O	2.29	0.66
1:A:173:GLN:HB2	1:A:235:SER:HA	1.78	0.66
1:A:173:GLN:NE2	1:A:196:ASP:OD1	2.28	0.66
2:B:16:ASP:O	2:F:33:ARG:NH2	2.29	0.66
2:G:33:ARG:NH2	2:H:16:ASP:O	2.29	0.65
1:L:210:LEU:N	1:L:211:PRO:HD2	2.11	0.65
1:L:8:SER:O	1:L:132:ARG:NH1	2.27	0.65
1:L:41:ILE:CG1	1:L:238:LEU:HD21	2.27	0.65
1:L:179:ARG:O	1:L:179:ARG:HG2	1.95	0.65
1:L:239:ILE:HG12	1:L:239:ILE:O	1.95	0.65
2:J:11:TYR:CE2	2:J:23:LYS:HD3	2.32	0.65
2:C:1:THR:CG2	2:C:2:PRO:HD2	2.26	0.64
1:L:130:ILE:HG22	1:L:131:ASN:N	2.13	0.64
2:J:35:ASN:ND2	2:K:37:GLN:OE1	2.29	0.64
1:L:125:ARG:HH11	1:L:125:ARG:CG	2.09	0.63
1:L:141:ASP:HB3	1:L:153:SER:OG	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:VAL:CG2	2:F:25:GLY:HA3	2.28	0.63
1:L:202:ASN:ND2	1:L:202:ASN:N	2.46	0.63
1:L:130:ILE:HG22	1:L:131:ASN:H	1.64	0.63
2:J:17:ASP:CG	2:J:19:THR:HG23	2.19	0.63
1:L:152:GLN:O	1:L:155:ALA:HB3	1.98	0.63
2:E:11:TYR:CE2	2:E:23:LYS:HD3	2.34	0.62
2:F:27:LYS:CE	2:F:58:HIS:HA	2.29	0.62
2:G:5:VAL:HG21	2:G:24:VAL:O	1.99	0.62
2:H:13:LYS:HE3	2:H:15:ASN:OD1	1.99	0.62
2:G:55:ASN:O	2:G:57:CYS:N	2.33	0.62
1:A:223:ARG:NH2	2:E:9:VAL:O	2.31	0.62
2:J:45:ILE:O	2:J:47:GLY:N	2.31	0.62
1:L:172:ARG:O	1:L:176:ARG:HB2	2.00	0.62
1:L:207:SER:OG	1:L:239:ILE:HB	2.00	0.62
2:C:33:ARG:NH1	2:C:64:SER:HB3	2.15	0.62
1:A:64:PHE:C	1:A:65:ASN:HD22	2.02	0.62
1:A:128:MET:CE	1:A:159:LEU:HB3	2.29	0.62
1:A:269:GLY:HA2	1:A:277:TRP:O	2.00	0.62
1:A:66:ASN:HB3	1:A:84:ARG:HB2	1.81	0.62
2:H:12:THR:HG23	2:H:44:GLN:HE21	1.64	0.62
2:B:1:THR:HG21	2:B:53:LYS:O	2.00	0.62
1:L:138:SER:HB3	1:L:161:PHE:CE2	2.33	0.61
2:H:12:THR:HG23	2:H:44:GLN:NE2	2.14	0.61
1:A:9:THR:N	1:A:12:THR:OG1	2.30	0.61
1:A:61:GLU:HA	1:A:61:GLU:OE1	2.00	0.61
2:J:32:ASN:HD22	2:J:32:ASN:N	1.98	0.61
2:B:56:ALA:O	2:B:61:GLY:HA3	2.01	0.61
2:J:56:ALA:O	2:J:61:GLY:HA3	2.01	0.61
1:L:51:ALA:HB2	1:L:100:PHE:HE2	1.65	0.61
1:L:139:TYR:O	1:L:143:MET:HG2	2.00	0.61
1:L:125:ARG:NH1	1:L:125:ARG:HG3	2.07	0.60
1:L:172:ARG:HH21	1:L:237:ALA:HA	1.66	0.60
1:L:9:THR:O	1:L:12:THR:N	2.31	0.60
2:H:65:GLU:HA	2:I:14:TYR:O	2.01	0.60
1:L:67:LEU:CD1	1:L:142:LEU:HD13	2.29	0.60
1:L:24:ILE:HD11	1:L:76:LEU:HD21	1.83	0.60
1:A:270:ILE:HD12	1:A:279:SER:HA	1.82	0.60
1:A:50:PHE:HE1	1:A:52:VAL:CG2	2.15	0.60
2:F:17:ASP:O	2:J:32:ASN:HB2	2.02	0.60
2:B:10:GLU:HB3	2:B:23:LYS:HG2	1.84	0.60
2:B:34:TRP:CZ3	2:F:34:TRP:HD1	2.19	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:LEU:HB3	1:L:238:LEU:HD12	1.83	0.59
1:L:123:ILE:HD11	1:L:156:ARG:HG2	1.84	0.59
2:I:48:MET:CE	2:I:68:PHE:HB3	2.29	0.59
1:A:41:ILE:HG22	1:A:42:ASP:N	2.17	0.59
1:L:30:THR:HG21	1:L:213:TYR:O	2.01	0.59
1:L:136:THR:O	1:L:140:LEU:HG	2.03	0.59
1:L:284:ALA:HB2	2:H:46:THR:HG23	1.84	0.59
1:A:167:GLU:OE1	1:A:167:GLU:HA	2.03	0.59
1:L:41:ILE:HG13	1:L:238:LEU:CD2	2.33	0.59
2:D:24:VAL:HG21	2:D:52:ILE:HD12	1.84	0.59
2:F:52:ILE:HG23	2:F:63:PHE:CD1	2.37	0.59
1:A:148:THR:HG23	1:A:149:SER:N	2.18	0.58
2:F:41:LEU:O	2:F:45:ILE:HD12	2.03	0.58
2:F:21:THR:CG2	2:F:28:GLU:HG2	2.33	0.58
2:E:4:CYS:HB3	2:E:52:ILE:O	2.03	0.58
1:L:223:ARG:O	1:L:223:ARG:HG2	2.03	0.58
2:H:56:ALA:O	2:H:58:HIS:N	2.34	0.58
1:A:10:ALA:HB1	1:A:179:ARG:HG2	1.84	0.58
1:L:167:GLU:OE1	1:L:170:ARG:NH1	2.36	0.58
2:D:1:THR:CG2	2:D:2:PRO:HD2	2.34	0.58
1:A:31:ILE:HG23	1:A:229:ILE:CD1	2.33	0.58
2:B:6:THR:OG1	2:B:51:THR:HG23	2.04	0.58
2:C:1:THR:HG23	2:C:2:PRO:HD2	1.85	0.57
2:I:36:LEU:HD21	2:J:14:TYR:CD2	2.39	0.57
1:L:38:LEU:HD12	1:L:236:VAL:HG12	1.86	0.57
1:L:5:LEU:HD12	1:L:16:SER:CB	2.34	0.57
1:L:180:THR:O	1:L:182:LEU:N	2.36	0.57
1:A:198:ASP:O	1:A:202:ASN:ND2	2.38	0.57
2:H:56:ALA:O	2:H:61:GLY:HA3	2.04	0.57
1:L:4:THR:HG23	1:L:55:ARG:HB3	1.85	0.57
1:A:50:PHE:HE1	1:A:52:VAL:HG23	1.69	0.57
2:F:49:THR:HG22	2:F:69:ARG:HD2	1.87	0.57
1:L:100:PHE:CD1	1:L:101:PRO:HD2	2.40	0.57
2:B:12:THR:HB	2:B:20:PHE:CZ	2.39	0.57
1:A:214:HIS:H	1:A:216:GLN:NE2	1.99	0.57
1:L:120:VAL:HG12	1:L:152:GLN:HA	1.87	0.57
1:L:193:THR:O	1:L:196:ASP:HB2	2.05	0.57
1:A:83:ASN:O	1:A:85:THR:N	2.38	0.56
2:D:30:PHE:O	2:D:62:GLY:HA2	2.05	0.56
2:G:33:ARG:NH1	2:G:64:SER:OG	2.37	0.56
1:L:202:ASN:H	1:L:202:ASN:HD22	1.53	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:270:ILE:HD12	1:L:279:SER:HA	1.86	0.56
1:L:273:ASN:O	1:L:274:LYS:HB2	2.05	0.56
2:D:24:VAL:HG21	2:D:52:ILE:CD1	2.35	0.56
2:H:41:LEU:O	2:H:45:ILE:HG13	2.04	0.56
1:L:14:VAL:O	1:L:18:ASN:ND2	2.38	0.56
2:K:31:THR:OG1	2:K:33:ARG:HG2	2.06	0.56
1:L:7:PHE:CE2	1:L:135:LEU:HD21	2.39	0.56
2:H:1:THR:HG23	2:H:2:PRO:N	2.21	0.56
1:A:152:GLN:O	1:A:156:ARG:HG3	2.06	0.56
2:F:14:TYR:CE1	2:F:20:PHE:CE1	2.94	0.56
1:L:114:TYR:O	1:L:118:GLN:HB2	2.05	0.56
2:J:32:ASN:ND2	2:J:32:ASN:H	2.02	0.56
2:F:16:ASP:O	2:F:18:ASP:N	2.39	0.56
2:I:22:VAL:HG22	2:I:23:LYS:N	2.21	0.56
2:E:33:ARG:NH2	2:F:15:ASN:O	2.38	0.55
1:A:64:PHE:CE1	1:A:140:LEU:HD21	2.41	0.55
2:H:1:THR:HG23	2:H:2:PRO:HD2	1.87	0.55
2:J:32:ASN:ND2	2:J:32:ASN:N	2.53	0.55
1:A:216:GLN:H	1:A:216:GLN:NE2	1.98	0.55
1:L:5:LEU:HD23	1:L:7:PHE:CE1	2.42	0.55
1:L:24:ILE:CD1	1:L:76:LEU:HD21	2.37	0.55
1:A:121:ALA:CB	1:A:156:ARG:HG2	2.25	0.55
2:I:48:MET:HE1	2:I:68:PHE:CD2	2.42	0.55
1:L:20:ILE:HA	1:L:23:ALA:HB3	1.89	0.55
1:L:5:LEU:HG	1:L:7:PHE:CE1	2.42	0.55
1:A:17:LEU:O	1:A:21:ARG:HG3	2.06	0.55
2:C:56:ALA:O	2:C:58:HIS:N	2.37	0.55
2:J:1:THR:CG2	2:J:54:THR:HA	2.37	0.55
1:L:58:ASP:HB3	1:L:62:GLY:HA3	1.87	0.54
2:I:48:MET:HE1	2:I:68:PHE:HD2	1.72	0.54
1:L:217:ASP:OD1	1:L:217:ASP:N	2.39	0.54
1:A:26:THR:HB	1:A:27:PRO:HD2	1.88	0.54
2:E:33:ARG:HH22	2:F:14:TYR:HD2	1.54	0.54
1:A:216:GLN:N	1:A:216:GLN:NE2	2.51	0.54
1:A:64:PHE:HE1	1:A:140:LEU:HD21	1.73	0.54
2:B:5:VAL:HG12	2:B:52:ILE:HB	1.90	0.54
2:F:5:VAL:HG21	2:F:25:GLY:HA3	1.89	0.54
1:L:108:LEU:HA	1:L:148:THR:O	2.06	0.54
2:I:41:LEU:HD23	2:I:41:LEU:O	2.08	0.54
2:D:1:THR:HG21	2:D:54:THR:HA	1.89	0.54
1:L:210:LEU:HD21	1:L:232:ILE:HD13	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:VAL:CG2	2:B:24:VAL:HG12	2.38	0.54
1:L:38:LEU:HD11	1:L:236:VAL:HG12	1.90	0.54
2:C:50:VAL:HA	2:C:67:ILE:O	2.07	0.54
2:E:41:LEU:O	2:E:41:LEU:HG	2.08	0.54
2:K:18:ASP:N	2:K:18:ASP:OD1	2.41	0.54
1:L:67:LEU:HD11	1:L:142:LEU:CD1	2.35	0.54
2:C:66:VAL:HG12	2:C:67:ILE:N	2.23	0.54
1:L:20:ILE:C	1:L:23:ALA:HB3	2.28	0.54
2:B:20:PHE:CD1	2:B:37:GLN:HG2	2.42	0.53
2:D:1:THR:HG22	2:D:2:PRO:HD2	1.90	0.53
1:L:287:MET:HE1	2:H:38:SER:HA	1.90	0.53
2:F:14:TYR:CE1	2:F:20:PHE:HE1	2.27	0.53
1:A:40:MET:CE	1:A:241:ASN:HA	2.33	0.53
1:A:170:ARG:HD3	1:A:203:TRP:CD2	2.43	0.53
1:L:26:THR:HB	1:L:27:PRO:CD	2.37	0.53
2:F:27:LYS:HE2	2:F:58:HIS:HA	1.91	0.53
1:A:220:ARG:HD3	3:E:71:HOH:O	2.08	0.53
1:L:121:ALA:CB	1:L:123:ILE:HG12	2.38	0.53
2:C:5:VAL:HG21	2:C:24:VAL:O	2.08	0.53
1:A:94:ASP:OD1	1:A:94:ASP:N	2.41	0.53
2:J:26:ASP:C	2:J:27:LYS:HG2	2.29	0.53
1:L:217:ASP:O	1:L:218:SER:HB2	2.08	0.53
2:E:22:VAL:HG21	2:E:40:LEU:HD13	1.91	0.53
1:L:60:GLU:HG2	1:L:61:GLU:CG	2.23	0.53
2:E:5:VAL:HG13	2:E:24:VAL:HG12	1.91	0.53
1:A:156:ARG:O	1:A:160:ARG:HG3	2.09	0.52
1:L:115:THR:O	1:L:119:ARG:HB2	2.09	0.52
1:L:75:ASN:HB2	1:L:77:TYR:CD2	2.45	0.52
1:A:24:ILE:HG22	1:A:73:ARG:HH11	1.74	0.52
2:F:17:ASP:OD1	2:F:19:THR:OG1	2.26	0.52
1:L:125:ARG:NH2	1:L:200:THR:OG1	2.41	0.52
1:L:140:LEU:O	1:L:142:LEU:N	2.43	0.52
1:A:278:ASP:OD2	1:A:280:SER:HB2	2.10	0.52
2:H:18:ASP:HB3	2:H:34:TRP:CZ2	2.45	0.52
1:L:190:TYR:CD1	1:L:191:VAL:N	2.78	0.52
2:G:23:LYS:HG3	2:G:23:LYS:O	2.10	0.52
2:G:22:VAL:HG12	2:G:22:VAL:O	2.07	0.52
1:L:14:VAL:HG12	1:L:18:ASN:ND2	2.25	0.52
1:L:58:ASP:CB	1:L:62:GLY:HA2	2.38	0.52
2:B:5:VAL:HG22	2:B:24:VAL:HG12	1.91	0.52
1:A:189:SER:N	3:A:293:HOH:O	2.42	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:26:ASP:CG	2:J:27:LYS:HZ2	2.13	0.51
2:F:3:ASP:HA	2:F:53:LYS:HG2	1.92	0.51
2:E:36:LEU:O	2:E:38:SER:N	2.43	0.51
1:L:166:ALA:O	1:L:169:LEU:N	2.41	0.51
2:G:13:LYS:HB3	2:K:67:ILE:HA	1.93	0.51
2:K:66:VAL:HG12	2:K:67:ILE:N	2.24	0.51
2:D:56:ALA:O	2:D:61:GLY:HA3	2.10	0.51
1:A:8:SER:HB2	1:A:12:THR:HG21	1.91	0.51
1:A:29:GLN:O	1:A:29:GLN:HG2	2.10	0.51
2:E:17:ASP:O	2:E:18:ASP:HB2	2.10	0.51
1:A:142:LEU:HD23	1:A:154:VAL:HG13	1.92	0.51
2:H:55:ASN:O	2:H:57:CYS:N	2.33	0.51
2:C:51:THR:HB	2:C:67:ILE:HB	1.92	0.51
2:H:34:TRP:H	2:H:34:TRP:HD1	1.59	0.51
1:A:79:THR:HG22	1:A:95:PHE:CD1	2.46	0.51
2:I:10:GLU:HB3	2:I:23:LYS:O	2.10	0.51
1:A:70:ILE:HD11	1:A:82:VAL:HG21	1.93	0.51
2:G:48:MET:CE	2:G:68:PHE:HB3	2.40	0.51
1:A:181:THR:HG22	1:A:181:THR:O	2.11	0.50
1:L:210:LEU:CD2	1:L:232:ILE:HD13	2.41	0.50
1:L:116:THR:O	1:L:120:VAL:HG23	2.11	0.50
1:L:140:LEU:O	1:L:143:MET:N	2.44	0.50
2:F:9:VAL:HB	2:F:44:GLN:HG3	1.93	0.50
2:H:63:PHE:HE2	2:H:66:VAL:HG21	1.77	0.50
2:G:16:ASP:O	2:G:16:ASP:OD1	2.30	0.50
2:K:1:THR:CG2	2:K:54:THR:HA	2.41	0.50
1:A:271:THR:HG22	1:A:272:HIS:N	2.26	0.50
1:L:180:THR:OG1	1:L:181:THR:N	2.44	0.50
2:J:37:GLN:HG3	3:J:70:HOH:O	2.12	0.50
1:A:75:ASN:HB2	1:A:77:TYR:CD2	2.47	0.50
1:A:120:VAL:HG12	1:A:152:GLN:HA	1.93	0.50
2:C:67:ILE:CG1	2:D:13:LYS:HG3	2.36	0.50
1:L:100:PHE:O	1:L:103:THR:OG1	2.28	0.50
2:H:33:ARG:NH2	2:I:16:ASP:OD1	2.45	0.50
1:A:173:GLN:O	1:A:173:GLN:HG2	2.10	0.49
2:K:49:THR:O	2:K:69:ARG:HB2	2.11	0.49
2:B:11:TYR:CE2	2:B:23:LYS:HD3	2.48	0.49
2:J:20:PHE:CD1	2:J:37:GLN:HG2	2.48	0.49
1:A:175:GLN:HG2	1:A:176:ARG:N	2.28	0.49
2:H:17:ASP:O	2:H:18:ASP:HB2	2.12	0.49
2:J:55:ASN:O	2:J:57:CYS:N	2.37	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:CYS:CB	2:D:54:THR:HG22	2.39	0.49
2:H:1:THR:CB	2:H:2:PRO:HD2	2.43	0.49
1:L:19:VAL:O	1:L:23:ALA:HB2	2.12	0.49
1:L:20:ILE:CA	1:L:23:ALA:HB3	2.43	0.49
2:E:67:ILE:HA	2:F:12:THR:O	2.12	0.49
1:A:27:PRO:HA	1:A:39:LEU:HD23	1.95	0.49
1:L:47:ASP:OD2	1:L:72:GLU:OE2	2.29	0.49
2:J:30:PHE:CD1	2:J:30:PHE:N	2.81	0.49
1:A:170:ARG:HG2	1:A:203:TRP:CE2	2.47	0.49
1:L:130:ILE:CG2	1:L:131:ASN:H	2.25	0.49
2:H:34:TRP:N	2:H:34:TRP:CD1	2.80	0.49
1:L:10:ALA:HB1	1:L:179:ARG:CG	2.41	0.49
2:H:63:PHE:HE2	2:H:66:VAL:CG2	2.26	0.49
2:D:44:GLN:HA	3:D:73:HOH:O	2.12	0.49
1:A:12:THR:O	1:A:16:SER:OG	2.30	0.49
2:G:16:ASP:O	2:K:33:ARG:NH2	2.46	0.49
2:K:9:VAL:HG12	2:K:9:VAL:O	2.13	0.49
1:L:39:LEU:CB	1:L:238:LEU:HD12	2.42	0.49
1:L:13:TYR:CE2	1:L:178:PHE:HD2	2.30	0.49
2:B:1:THR:HG23	2:B:2:PRO:HD2	1.95	0.49
1:L:56:GLY:O	1:L:132:ARG:NH2	2.45	0.49
1:L:205:ARG:NH2	1:L:281:THR:OG1	2.45	0.49
2:F:19:THR:HG22	2:F:20:PHE:H	1.78	0.48
2:J:11:TYR:OH	2:J:23:LYS:HD2	2.13	0.48
2:B:18:ASP:HB3	2:B:34:TRP:CH2	2.48	0.48
1:L:92:PHE:HB3	1:L:94:ASP:OD1	2.13	0.48
1:L:11:LYS:O	1:L:15:ASP:OD2	2.31	0.48
2:I:10:GLU:OE2	2:I:23:LYS:HE3	2.13	0.48
1:L:30:THR:HG21	3:L:298:HOH:O	2.13	0.48
2:F:21:THR:HG21	2:F:28:GLU:HG2	1.95	0.48
1:L:4:THR:CG2	1:L:55:ARG:HB3	2.42	0.48
2:J:17:ASP:O	2:J:18:ASP:HB2	2.14	0.48
2:I:11:TYR:CE2	2:I:23:LYS:HG2	2.49	0.48
2:C:55:ASN:C	2:C:57:CYS:H	2.17	0.48
2:K:54:THR:OG1	2:K:55:ASN:N	2.46	0.48
2:K:43:ALA:HA	2:K:48:MET:HG3	1.96	0.48
1:L:195:GLU:CD	1:L:195:GLU:H	2.16	0.48
1:A:31:ILE:HG22	1:A:233:LEU:HD21	1.96	0.48
1:A:50:PHE:CE1	1:A:52:VAL:HG23	2.47	0.48
1:A:210:LEU:N	1:A:211:PRO:HD2	2.28	0.48
2:J:33:ARG:HH12	2:J:64:SER:CB	2.00	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:LEU:HD11	1:L:236:VAL:CG1	2.44	0.48
2:K:16:ASP:O	2:K:18:ASP:OD1	2.32	0.48
2:E:17:ASP:OD1	2:E:19:THR:HG23	2.14	0.48
2:J:33:ARG:HH11	2:J:33:ARG:HG2	1.77	0.48
2:K:29:LEU:HD23	2:K:58:HIS:O	2.13	0.48
2:H:65:GLU:OE1	2:I:13:LYS:NZ	2.45	0.48
1:A:128:MET:HE1	1:A:159:LEU:HD13	1.96	0.48
2:J:56:ALA:HB1	2:J:61:GLY:CA	2.41	0.48
2:J:12:THR:CG2	2:J:22:VAL:HG23	2.44	0.48
2:H:31:THR:OG1	2:H:32:ASN:N	2.47	0.48
1:L:203:TRP:HE1	1:L:239:ILE:HA	1.79	0.47
1:A:27:PRO:HA	1:A:39:LEU:HA	1.96	0.47
2:C:36:LEU:HA	2:C:36:LEU:HD23	1.63	0.47
1:A:11:LYS:O	1:A:15:ASP:HB2	2.14	0.47
2:F:16:ASP:O	2:F:18:ASP:OD1	2.32	0.47
1:L:130:ILE:CG2	1:L:178:PHE:HE1	2.27	0.47
1:L:202:ASN:N	1:L:202:ASN:HD22	2.11	0.47
2:B:17:ASP:OD1	2:B:19:THR:HG23	2.14	0.47
2:H:8:LYS:HE3	2:H:47:GLY:O	2.15	0.47
1:L:8:SER:C	1:L:132:ARG:HH22	2.18	0.47
1:A:170:ARG:HG2	1:A:203:TRP:CZ2	2.50	0.47
2:I:16:ASP:O	2:I:16:ASP:OD1	2.31	0.47
1:L:75:ASN:HB3	1:L:260:MET:HG3	1.96	0.47
1:A:201:LEU:HA	1:A:201:LEU:HD23	1.44	0.47
2:B:27:LYS:HD3	2:B:27:LYS:HA	1.56	0.47
1:A:285:ILE:HD11	2:F:46:THR:HG22	1.97	0.47
1:L:203:TRP:CZ2	1:L:240:LEU:HG	2.49	0.47
1:L:210:LEU:N	1:L:211:PRO:CD	2.78	0.47
1:L:72:GLU:HB3	1:L:77:TYR:HB2	1.97	0.46
1:A:108:LEU:HD23	1:A:148:THR:O	2.15	0.46
2:H:12:THR:CG2	2:H:44:GLN:NE2	2.78	0.46
2:H:1:THR:CG2	2:H:2:PRO:N	2.78	0.46
2:C:1:THR:HG22	2:C:2:PRO:HD2	1.97	0.46
1:A:48:ASN:OD1	1:A:73:ARG:HB3	2.16	0.46
2:G:23:LYS:HE2	2:G:25:GLY:O	2.16	0.46
2:J:12:THR:CG2	2:J:20:PHE:CE2	2.98	0.46
2:G:39:LEU:HD23	2:G:39:LEU:N	2.30	0.46
2:C:35:ASN:N	2:C:35:ASN:OD1	2.43	0.46
2:H:34:TRP:O	2:H:37:GLN:HG3	2.16	0.46
2:F:52:ILE:CG2	2:F:63:PHE:CD1	2.98	0.46
1:A:39:LEU:HB2	1:A:238:LEU:HD12	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:ASP:CG	1:L:111:ASP:HB2	2.36	0.46
1:L:201:LEU:HD23	1:L:201:LEU:HA	1.51	0.46
1:L:5:LEU:HD12	1:L:16:SER:HB3	1.97	0.46
1:L:191:VAL:HG23	1:L:191:VAL:O	2.16	0.46
2:I:27:LYS:HA	2:I:59:ASN:HD21	1.80	0.46
1:L:130:ILE:CG2	1:L:131:ASN:N	2.78	0.46
1:A:203:TRP:CH2	1:A:240:LEU:CD2	2.99	0.46
2:B:33:ARG:NH1	2:B:64:SER:OG	2.49	0.46
1:L:213:TYR:CG	1:L:214:HIS:N	2.84	0.46
2:B:8:LYS:CB	2:B:8:LYS:NZ	2.76	0.46
2:J:29:LEU:HD23	2:J:61:GLY:HA3	1.98	0.46
2:J:42:SER:O	2:J:46:THR:HG23	2.17	0.46
2:H:55:ASN:C	2:H:57:CYS:H	2.17	0.46
1:A:5:LEU:CD2	1:A:7:PHE:CZ	2.97	0.45
2:H:12:THR:OG1	2:H:44:GLN:NE2	2.43	0.45
2:F:52:ILE:CG2	2:F:63:PHE:CG	2.99	0.45
2:C:56:ALA:O	2:C:61:GLY:HA3	2.16	0.45
1:L:100:PHE:CD1	1:L:101:PRO:CD	2.99	0.45
1:L:270:ILE:HD12	1:L:279:SER:CA	2.46	0.45
2:H:18:ASP:CB	2:H:34:TRP:CH2	2.97	0.45
2:J:9:VAL:HG13	2:J:22:VAL:HG22	1.99	0.45
2:B:36:LEU:CD2	2:B:66:VAL:HG21	2.47	0.45
1:A:118:GLN:OE1	1:A:124:SER:HA	2.15	0.45
1:A:99:THR:HG23	1:A:100:PHE:N	2.32	0.45
2:F:17:ASP:O	2:F:18:ASP:HB2	2.16	0.45
1:L:5:LEU:CD2	1:L:7:PHE:CE1	2.99	0.45
2:J:1:THR:HG21	2:J:54:THR:HA	1.97	0.45
1:A:148:THR:CG2	1:A:149:SER:N	2.79	0.45
2:B:16:ASP:OD1	2:B:16:ASP:O	2.34	0.45
1:L:10:ALA:HB1	1:L:179:ARG:HG2	1.98	0.45
2:C:22:VAL:HG23	2:C:63:PHE:HE2	1.81	0.45
1:L:41:ILE:HG22	1:L:41:ILE:O	2.17	0.45
2:G:51:THR:HB	2:G:67:ILE:HB	1.97	0.45
2:B:34:TRP:CE3	2:F:34:TRP:HD1	2.35	0.45
1:A:10:ALA:HB1	1:A:179:ARG:CG	2.46	0.45
2:H:11:TYR:CD1	2:H:11:TYR:C	2.90	0.45
2:E:6:THR:HA	2:E:51:THR:HA	1.99	0.45
2:I:36:LEU:CD2	2:I:39:LEU:HD12	2.47	0.45
2:I:17:ASP:OD1	2:I:19:THR:OG1	2.29	0.45
2:K:11:TYR:OH	2:K:28:GLU:OE1	2.28	0.45
1:L:130:ILE:CG2	1:L:178:PHE:CE1	3.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:CYS:O	2:J:57:CYS:SG	2.75	0.45
1:L:14:VAL:HG12	1:L:18:ASN:HD22	1.82	0.44
1:A:281:THR:O	1:A:285:ILE:HG23	2.18	0.44
1:L:31:ILE:O	1:L:32:SER:HB2	2.18	0.44
1:L:260:MET:HB3	1:L:260:MET:HE2	1.93	0.44
2:G:48:MET:HE1	2:G:68:PHE:HB3	1.99	0.44
1:L:159:LEU:HA	1:L:159:LEU:HD23	1.73	0.44
1:L:262:PRO:O	1:L:263:ALA:O	2.35	0.44
1:L:40:MET:CG	1:L:241:ASN:HB2	2.48	0.44
2:E:36:LEU:O	2:E:39:LEU:N	2.43	0.44
1:A:70:ILE:HD11	1:A:82:VAL:CG2	2.48	0.44
1:L:92:PHE:CD2	1:L:112:SER:HB3	2.51	0.44
2:D:65:GLU:HA	2:E:14:TYR:O	2.16	0.44
1:L:40:MET:HE2	1:L:40:MET:HB2	1.80	0.44
2:H:1:THR:HG23	2:H:2:PRO:CG	2.47	0.44
1:L:213:TYR:CD1	1:L:214:HIS:N	2.86	0.44
1:A:270:ILE:HD11	1:A:279:SER:CB	2.48	0.44
1:A:83:ASN:HB3	1:A:86:ASN:OD1	2.17	0.44
1:L:171:PHE:CE1	1:L:199:LEU:HG	2.53	0.44
1:L:3:PHE:N	1:L:3:PHE:CD1	2.84	0.44
2:C:30:PHE:CD1	2:C:30:PHE:C	2.91	0.44
1:A:139:TYR:CE1	1:A:143:MET:HG3	2.53	0.44
1:A:71:VAL:HG22	1:A:78:VAL:HG22	2.00	0.44
2:J:15:ASN:ND2	2:J:19:THR:OG1	2.50	0.44
1:L:107:THR:HG22	1:L:108:LEU:O	2.17	0.44
2:I:1:THR:HA	2:I:2:PRO:HD3	1.35	0.44
1:A:202:ASN:ND2	1:A:224:ILE:HD12	2.32	0.44
1:A:99:THR:CG2	1:A:100:PHE:N	2.80	0.44
2:E:56:ALA:O	2:E:61:GLY:HA3	2.17	0.44
2:H:12:THR:CG2	2:H:44:GLN:HE21	2.29	0.44
2:B:36:LEU:HD22	2:B:66:VAL:HG21	1.99	0.44
2:F:17:ASP:OD1	2:F:19:THR:N	2.50	0.44
2:D:1:THR:CG2	2:D:54:THR:HA	2.48	0.44
1:L:3:PHE:O	1:L:52:VAL:HA	2.18	0.44
2:E:30:PHE:O	2:E:62:GLY:HA2	2.18	0.44
2:H:5:VAL:CG2	2:H:24:VAL:HG12	2.46	0.43
1:A:2:GLU:HA	1:A:51:ALA:O	2.18	0.43
2:F:23:LYS:HA	2:F:27:LYS:O	2.19	0.43
1:A:79:THR:HG22	1:A:95:PHE:CE1	2.53	0.43
1:A:142:LEU:CD2	1:A:154:VAL:HG13	2.49	0.43
1:L:66:ASN:HB3	1:L:143:MET:HE1	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:LEU:HB3	2:J:61:GLY:O	2.19	0.43
2:C:24:VAL:HG21	2:C:52:ILE:HG13	2.00	0.43
2:B:41:LEU:HD22	2:F:39:LEU:HD23	2.01	0.43
2:B:69:ARG:HB2	2:B:69:ARG:HE	1.58	0.43
2:I:48:MET:CE	2:I:68:PHE:HD2	2.32	0.43
2:C:33:ARG:NH2	2:D:18:ASP:OD1	2.49	0.43
1:L:75:ASN:HB2	1:L:77:TYR:CE2	2.53	0.43
2:G:13:LYS:HE3	2:G:13:LYS:HB2	1.63	0.43
1:A:273:ASN:O	1:A:274:LYS:HB2	2.18	0.43
2:C:1:THR:HG21	2:C:54:THR:HA	2.00	0.43
1:L:167:GLU:HA	1:L:167:GLU:OE1	2.18	0.43
2:G:23:LYS:HD2	2:G:27:LYS:O	2.19	0.43
1:A:271:THR:CG2	1:A:272:HIS:N	2.81	0.43
2:H:30:PHE:O	2:H:62:GLY:HA2	2.19	0.43
1:L:66:ASN:CB	1:L:143:MET:CE	2.97	0.43
2:J:11:TYR:CE2	2:J:23:LYS:CD	3.00	0.43
1:A:65:ASN:HD22	1:A:65:ASN:N	2.17	0.43
2:F:4:CYS:CB	2:F:54:THR:HG22	2.49	0.43
2:H:23:LYS:HD2	2:H:28:GLU:HB2	2.01	0.43
2:D:41:LEU:HA	2:D:41:LEU:HD12	1.68	0.43
2:E:53:LYS:HZ3	2:E:53:LYS:HG2	1.65	0.43
1:L:203:TRP:NE1	1:L:239:ILE:HA	2.34	0.43
1:L:217:ASP:OD2	1:L:274:LYS:HD2	2.18	0.43
1:A:225:SER:O	1:A:225:SER:OG	2.25	0.43
2:F:13:LYS:HG3	2:F:13:LYS:HZ2	1.48	0.43
2:J:45:ILE:C	2:J:47:GLY:H	2.21	0.43
1:L:8:SER:HA	1:L:56:GLY:O	2.19	0.43
2:I:27:LYS:HA	2:I:59:ASN:ND2	2.34	0.43
2:J:11:TYR:CZ	2:J:23:LYS:HD2	2.54	0.43
1:L:70:ILE:HD12	1:L:100:PHE:CE2	2.53	0.42
1:A:270:ILE:HD12	1:A:279:SER:CA	2.49	0.42
1:L:79:THR:OG1	1:L:98:VAL:HG11	2.20	0.42
1:L:130:ILE:HG21	1:L:178:PHE:CE1	2.54	0.42
1:A:57:ILE:HG21	1:A:136:THR:HA	2.01	0.42
1:L:58:ASP:OD1	1:L:60:GLU:OE1	2.37	0.42
1:L:213:TYR:CD1	1:L:213:TYR:C	2.92	0.42
2:K:1:THR:HG21	2:K:54:THR:HA	2.00	0.42
1:L:198:ASP:O	1:L:201:LEU:N	2.50	0.42
1:L:171:PHE:CD1	1:L:199:LEU:HG	2.55	0.42
2:C:42:SER:O	2:C:46:THR:HG23	2.19	0.42
1:L:57:ILE:HG22	1:L:57:ILE:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:PRO:O	2:H:3:ASP:O	2.38	0.42
1:L:151:THR:OG1	1:L:154:VAL:HG23	2.18	0.42
2:B:3:ASP:OD1	2:B:53:LYS:NZ	2.52	0.42
2:I:38:SER:O	2:I:42:SER:HB2	2.19	0.42
2:H:68:PHE:HB2	2:I:12:THR:OG1	2.19	0.42
1:L:137:THR:O	1:L:140:LEU:N	2.52	0.42
1:L:55:ARG:O	1:L:55:ARG:HG2	2.20	0.42
1:L:80:GLY:HA3	1:L:90:TYR:O	2.19	0.42
2:K:12:THR:HB	2:K:20:PHE:CZ	2.54	0.42
2:B:9:VAL:H	2:B:9:VAL:HG23	1.65	0.42
1:L:24:ILE:HG13	1:L:24:ILE:O	2.20	0.42
2:E:53:LYS:HE2	2:E:67:ILE:HD11	2.01	0.42
1:L:193:THR:O	1:L:197:VAL:HG23	2.20	0.42
1:L:32:SER:HA	1:L:36:THR:O	2.19	0.42
2:H:1:THR:CG2	2:H:2:PRO:HD2	2.50	0.42
1:A:109:SER:HB3	1:A:149:SER:HA	2.02	0.42
2:B:18:ASP:HB3	2:B:34:TRP:HH2	1.84	0.42
1:A:70:ILE:HG12	1:A:82:VAL:HG23	2.02	0.42
2:B:22:VAL:HG21	2:B:40:LEU:HD13	2.01	0.42
2:B:30:PHE:C	2:B:30:PHE:CD2	2.93	0.42
2:I:5:VAL:O	2:I:6:THR:OG1	2.34	0.42
2:I:29:LEU:HD23	2:I:61:GLY:CA	2.50	0.42
2:J:58:HIS:O	2:J:61:GLY:N	2.47	0.42
2:B:1:THR:HG22	2:B:53:LYS:HB3	2.01	0.42
1:L:217:ASP:OD1	1:L:274:LYS:HD2	2.20	0.42
1:L:14:VAL:CG1	1:L:18:ASN:ND2	2.82	0.42
2:H:23:LYS:HG2	2:H:23:LYS:HZ2	1.60	0.42
1:L:40:MET:SD	1:L:241:ASN:CB	3.08	0.42
1:L:100:PHE:HD1	1:L:100:PHE:HA	1.73	0.42
1:A:165:THR:HG22	1:A:166:ALA:N	2.35	0.42
1:A:270:ILE:CD1	1:A:279:SER:CB	2.97	0.42
2:C:5:VAL:HG22	2:C:6:THR:N	2.34	0.42
2:G:48:MET:HE2	2:G:68:PHE:HB3	2.02	0.42
2:D:11:TYR:C	2:D:11:TYR:CD1	2.93	0.42
2:J:3:ASP:OD1	2:J:53:LYS:NZ	2.44	0.42
1:L:275:ILE:HG22	1:L:277:TRP:CD1	2.54	0.42
1:A:142:LEU:HA	1:A:142:LEU:HD23	1.87	0.41
1:A:285:ILE:HD13	1:A:285:ILE:HG21	1.79	0.41
2:H:67:ILE:HG12	2:I:13:LYS:HG3	1.95	0.41
2:G:12:THR:HB	2:G:20:PHE:CE2	2.55	0.41
2:F:30:PHE:O	2:F:62:GLY:HA2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:ALA:HB2	1:L:179:ARG:O	2.21	0.41
1:A:41:ILE:HG13	1:A:239:ILE:O	2.20	0.41
2:G:30:PHE:C	2:G:30:PHE:CD1	2.94	0.41
2:D:36:LEU:HD23	2:D:36:LEU:HA	1.51	0.41
2:I:43:ALA:HB1	2:I:48:MET:HB2	2.02	0.41
2:H:1:THR:HG23	2:H:2:PRO:HG2	2.01	0.41
1:L:172:ARG:NH2	1:L:237:ALA:CB	2.83	0.41
2:H:24:VAL:HG21	2:H:52:ILE:HD12	2.02	0.41
2:C:33:ARG:NH1	2:C:64:SER:CB	2.83	0.41
1:L:216:GLN:C	1:L:218:SER:H	2.22	0.41
1:A:125:ARG:NH2	1:A:197:VAL:HG13	2.36	0.41
2:I:40:LEU:HD23	2:I:40:LEU:HA	1.83	0.41
1:A:216:GLN:HB3	1:A:274:LYS:O	2.21	0.41
1:L:138:SER:OG	1:L:157:ALA:HA	2.20	0.41
2:D:33:ARG:CZ	2:D:64:SER:OG	2.69	0.41
2:B:1:THR:HG21	2:B:53:LYS:C	2.41	0.41
2:J:20:PHE:CG	2:J:37:GLN:HG2	2.55	0.41
1:L:266:ARG:NH2	2:G:48:MET:HA	2.36	0.41
2:J:69:ARG:HG2	2:J:69:ARG:HH11	1.86	0.41
1:A:121:ALA:HB2	1:A:156:ARG:N	2.36	0.41
1:A:205:ARG:NH1	1:A:278:ASP:OD2	2.52	0.41
1:L:7:PHE:CD2	1:L:135:LEU:CD2	3.00	0.41
1:L:172:ARG:HB2	1:L:237:ALA:HB2	2.01	0.41
2:B:34:TRP:CZ3	2:F:34:TRP:CD1	3.05	0.41
2:G:27:LYS:HE2	2:G:58:HIS:HA	2.03	0.41
2:G:11:TYR:C	2:G:11:TYR:CD1	2.94	0.41
2:G:45:ILE:HG12	2:K:48:MET:HE2	2.03	0.41
2:D:36:LEU:O	2:D:40:LEU:HB2	2.21	0.41
2:C:17:ASP:O	2:C:18:ASP:HB2	2.20	0.41
2:H:1:THR:OG1	2:H:2:PRO:HD2	2.20	0.40
2:F:58:HIS:O	2:F:61:GLY:N	2.43	0.40
1:A:41:ILE:CG2	1:A:42:ASP:N	2.82	0.40
1:L:5:LEU:HD23	1:L:7:PHE:CZ	2.56	0.40
2:G:55:ASN:C	2:G:57:CYS:N	2.75	0.40
1:L:284:ALA:HB2	2:H:46:THR:CG2	2.51	0.40
2:H:22:VAL:O	2:H:22:VAL:HG13	2.21	0.40
1:L:58:ASP:O	1:L:62:GLY:HA3	2.20	0.40
1:L:13:TYR:O	1:L:17:LEU:HG	2.21	0.40
1:L:217:ASP:CG	1:L:274:LYS:HD2	2.41	0.40
2:I:41:LEU:O	2:I:45:ILE:HG13	2.21	0.40
2:J:12:THR:HG21	2:J:20:PHE:CE2	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:LEU:CD1	1:L:142:LEU:CD1	2.99	0.40
1:A:197:VAL:O	1:A:201:LEU:HG	2.21	0.40
1:L:224:ILE:HG21	1:L:224:ILE:HD13	1.85	0.40
1:L:20:ILE:O	1:L:24:ILE:N	2.32	0.40
2:J:52:ILE:HD13	2:J:63:PHE:CD2	2.57	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	256/287 (89%)	232 (91%)	20 (8%)	4 (2%)	12	21
1	L	254/287 (88%)	211 (83%)	34 (13%)	9 (4%)	4	6
2	B	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
2	C	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
2	D	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
2	E	67/69 (97%)	63 (94%)	3 (4%)	1 (2%)	13	22
2	F	67/69 (97%)	61 (91%)	5 (8%)	1 (2%)	13	22
2	G	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
2	H	67/69 (97%)	55 (82%)	7 (10%)	5 (8%)	1	1
2	I	67/69 (97%)	59 (88%)	7 (10%)	1 (2%)	13	22
2	J	67/69 (97%)	57 (85%)	4 (6%)	6 (9%)	1	1
2	K	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
All	All	1180/1264 (93%)	1053 (89%)	100 (8%)	27 (2%)	8	12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	L	141	ASP
1	L	181	THR
1	L	263	ALA
2	F	17	ASP
2	J	2	PRO
2	J	56	ALA
1	L	32	SER
1	L	179	ARG
2	H	3	ASP
2	H	56	ALA
2	J	45	ILE
2	J	46	THR
1	A	48	ASN
2	H	4	CYS
2	H	25	GLY
2	J	18	ASP
2	J	57	CYS
1	L	214	HIS
2	E	37	GLN
2	H	57	CYS
1	A	266	ARG
1	L	264	ASP
1	A	8	SER
1	L	265	GLY
1	L	59	PRO
2	I	2	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/246 (93%)	200 (87%)	29 (13%)	5	10
1	L	227/246 (92%)	194 (86%)	33 (14%)	4	7
2	B	61/61 (100%)	49 (80%)	12 (20%)	1	3
2	C	61/61 (100%)	51 (84%)	10 (16%)	3	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	61/61 (100%)	56 (92%)	5 (8%)	14	27
2	E	61/61 (100%)	53 (87%)	8 (13%)	5	9
2	F	61/61 (100%)	52 (85%)	9 (15%)	4	7
2	G	61/61 (100%)	55 (90%)	6 (10%)	10	19
2	H	61/61 (100%)	52 (85%)	9 (15%)	4	7
2	I	61/61 (100%)	52 (85%)	9 (15%)	4	7
2	J	61/61 (100%)	48 (79%)	13 (21%)	1	2
2	K	61/61 (100%)	55 (90%)	6 (10%)	10	19
All	All	1066/1102 (97%)	917 (86%)	149 (14%)	4	8

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	11	LYS
1	A	16	SER
1	A	21	ARG
1	A	27	PRO
1	A	32	SER
1	A	49	LEU
1	A	55	ARG
1	A	61	GLU
1	A	65	ASN
1	A	66	ASN
1	A	73	ARG
1	A	85	THR
1	A	94	ASP
1	A	99	THR
1	A	132	ARG
1	A	137	THR
1	A	144	SER
1	A	153	SER
1	A	175	GLN
1	A	208	SER
1	A	216	GLN
1	A	223	ARG
1	A	233	LEU
1	A	241	ASN
1	A	268	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	275	ILE
1	A	278	ASP
1	A	280	SER
1	L	2	GLU
1	L	3	PHE
1	L	15	ASP
1	L	28	LEU
1	L	31	ILE
1	L	33	SER
1	L	39	LEU
1	L	40	MET
1	L	49	LEU
1	L	55	ARG
1	L	84	ARG
1	L	87	ASN
1	L	100	PHE
1	L	115	THR
1	L	117	LEU
1	L	119	ARG
1	L	124	SER
1	L	125	ARG
1	L	138	SER
1	L	141	ASP
1	L	158	MET
1	L	174	ILE
1	L	175	GLN
1	L	182	LEU
1	L	198	ASP
1	L	202	ASN
1	L	217	ASP
1	L	238	LEU
1	L	239	ILE
1	L	240	LEU
1	L	268	ARG
1	L	273	ASN
1	L	276	LEU
2	B	4	CYS
2	B	8	LYS
2	B	13	LYS
2	B	23	LYS
2	B	27	LYS
2	B	29	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	33	ARG
2	B	35	ASN
2	B	38	SER
2	B	53	LYS
2	B	64	SER
2	B	69	ARG
2	C	6	THR
2	C	13	LYS
2	C	21	THR
2	C	22	VAL
2	C	27	LYS
2	C	32	ASN
2	C	33	ARG
2	C	35	ASN
2	C	52	ILE
2	C	69	ARG
2	D	12	THR
2	D	13	LYS
2	D	22	VAL
2	D	33	ARG
2	D	69	ARG
2	E	1	THR
2	E	5	VAL
2	E	13	LYS
2	E	15	ASN
2	E	28	GLU
2	E	33	ARG
2	E	53	LYS
2	E	69	ARG
2	F	1	THR
2	F	13	LYS
2	F	14	TYR
2	F	23	LYS
2	F	27	LYS
2	F	33	ARG
2	F	36	LEU
2	F	41	LEU
2	F	69	ARG
2	G	4	CYS
2	G	23	LYS
2	G	26	ASP
2	G	29	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	G	38	SER
2	G	46	THR
2	H	1	THR
2	H	4	CYS
2	H	8	LYS
2	H	27	LYS
2	H	31	THR
2	H	33	ARG
2	H	50	VAL
2	H	53	LYS
2	H	64	SER
2	I	12	THR
2	I	32	ASN
2	I	33	ARG
2	I	35	ASN
2	I	42	SER
2	I	52	ILE
2	I	53	LYS
2	I	64	SER
2	I	69	ARG
2	J	5	VAL
2	J	8	LYS
2	J	12	THR
2	J	13	LYS
2	J	15	ASN
2	J	27	LYS
2	J	29	LEU
2	J	30	PHE
2	J	32	ASN
2	J	33	ARG
2	J	41	LEU
2	J	52	ILE
2	J	64	SER
2	K	5	VAL
2	K	18	ASP
2	K	27	LYS
2	K	33	ARG
2	K	38	SER
2	K	54	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	65	ASN
1	A	216	GLN
1	A	241	ASN
1	A	272	HIS
1	L	18	ASN
1	L	66	ASN
1	L	74	ASN
1	L	87	ASN
1	L	202	ASN
2	B	35	ASN
2	C	32	ASN
2	D	55	ASN
2	F	15	ASN
2	G	35	ASN
2	G	44	GLN
2	H	44	GLN
2	I	32	ASN
2	I	35	ASN
2	I	59	ASN
2	J	15	ASN
2	J	32	ASN
2	J	59	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.