



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:23 PM EDT

PDB ID : 7F4S / pdb_00007f4s
Title : Crystal structure of TthMTA1-PteMTA9 complex
Authors : Chen, J.; Liu, L.
Deposited on : 2021-06-21
Resolution : 3.09 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

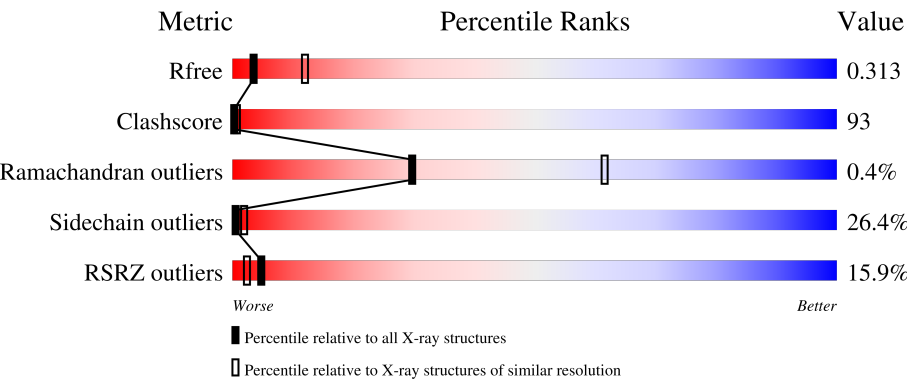
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.09 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	202	
1	B	202	
1	C	202	
2	D	237	
2	E	237	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	237	27% 23% 37% 19% • 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9145 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 MT-a70 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1422	909	244	261	8			
1	B	178	Total	C	N	O	S	0	0	0
			1426	906	249	263	8			
1	C	176	Total	C	N	O	S	0	0	0
			1411	898	244	261	8			

- Molecule 2 is a protein called MTA9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	215	Total	C	N	O	S	0	0	0
			1632	1041	269	315	7			
2	E	213	Total	C	N	O	S	0	0	0
			1608	1034	270	297	7			
2	F	192	Total	C	N	O	S	0	0	0
			1434	927	239	262	6			

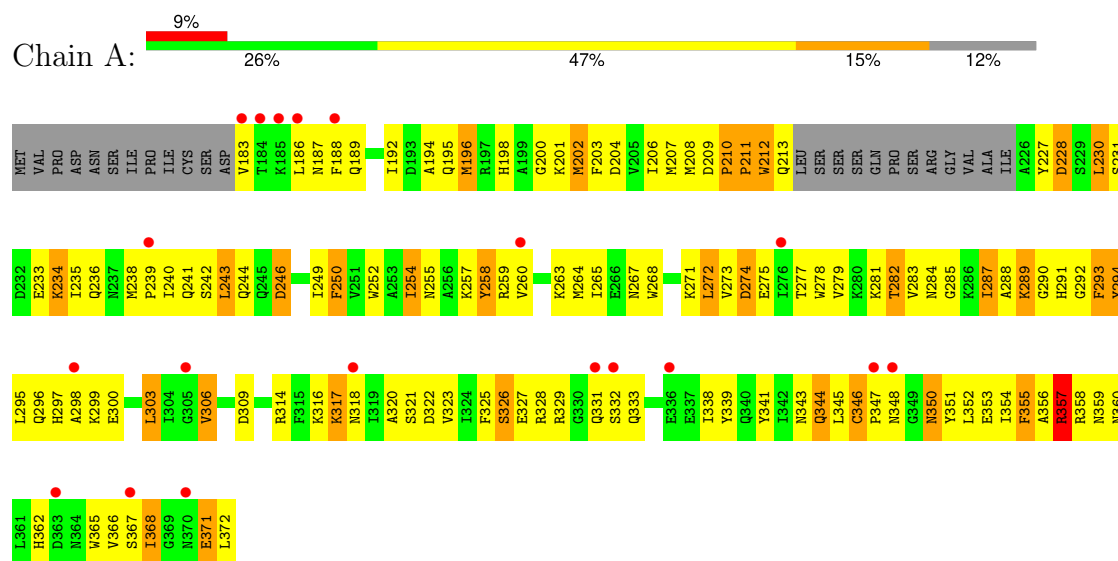
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	28	Total	O	0	0
			28	28		
3	C	24	Total	O	0	0
			24	24		
3	D	43	Total	O	0	0
			43	43		
3	E	43	Total	O	0	0
			43	43		
3	F	42	Total	O	0	0
			42	42		

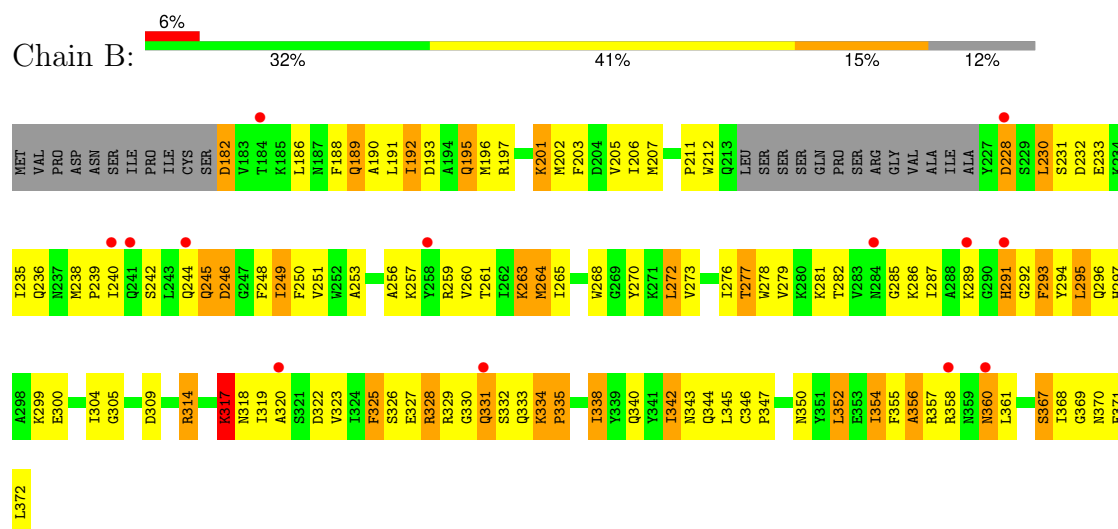
3 Residue-property plots

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.

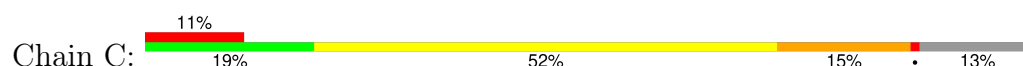
• Molecule 1: MT-a70 family protein

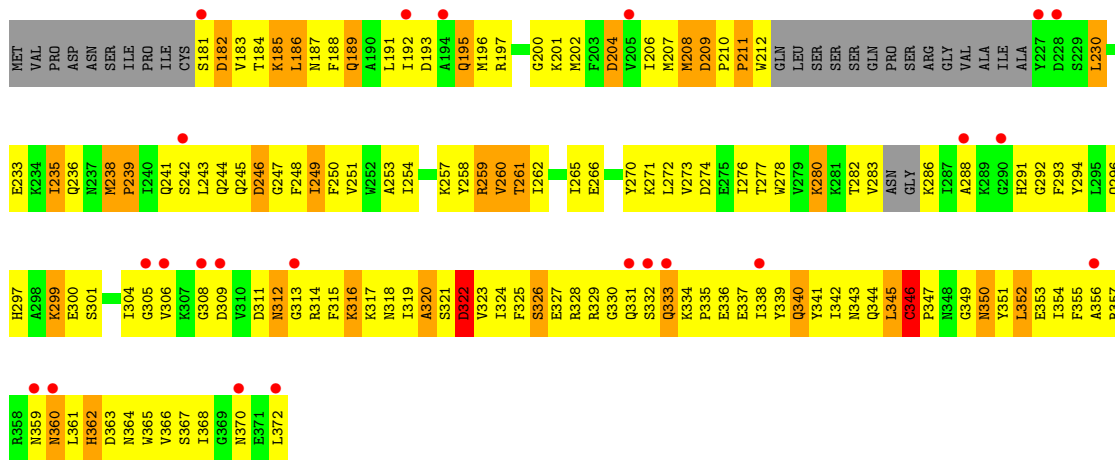


• Molecule 1: MT-a70 family protein

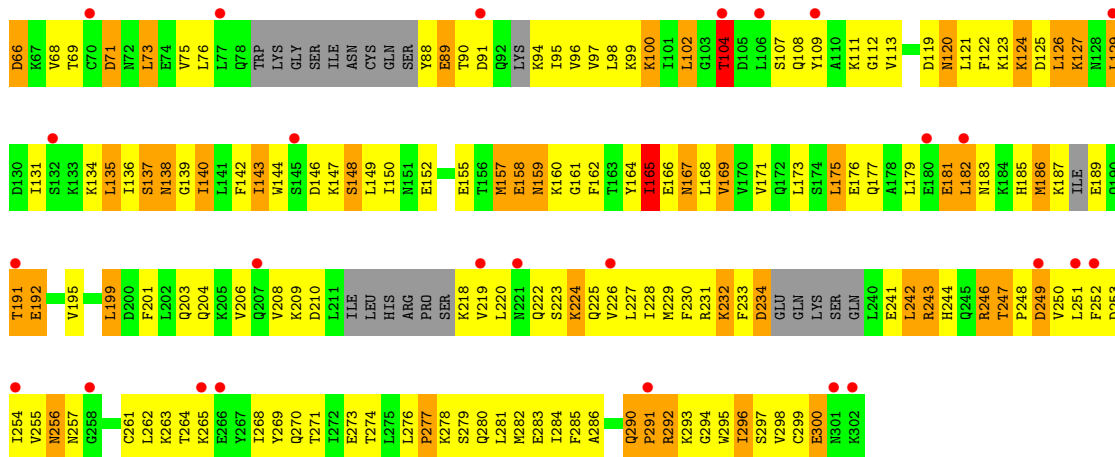


• Molecule 1: MT-a70 family protein

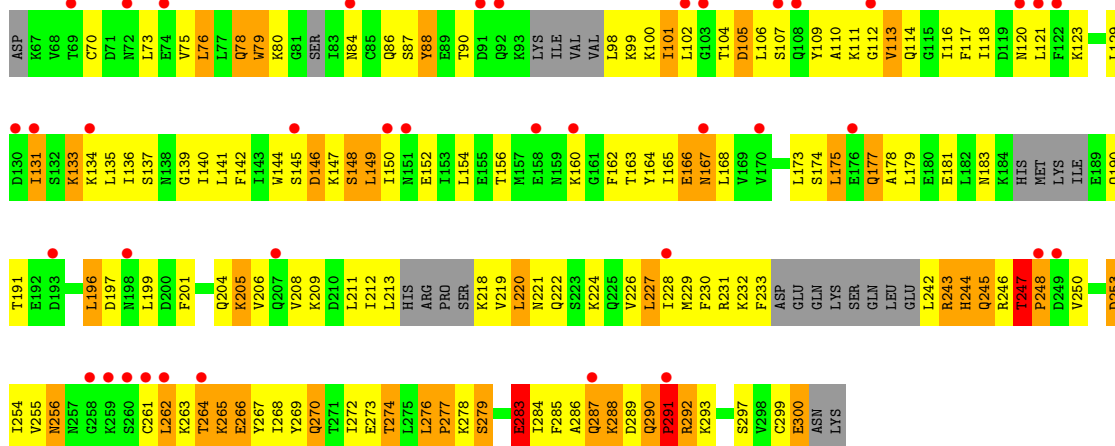




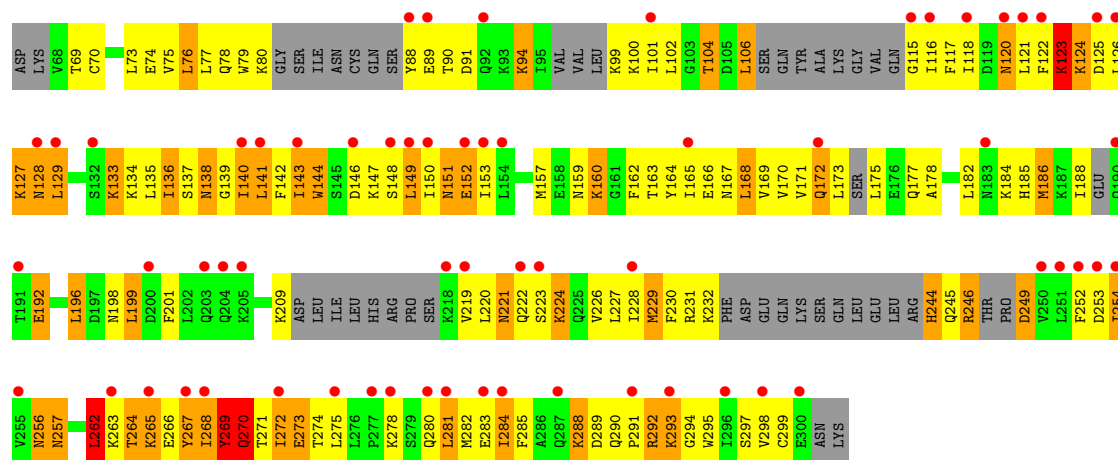
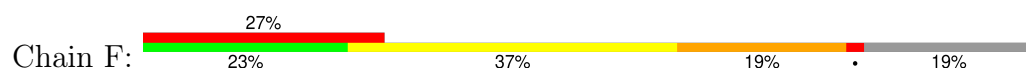
• Molecule 2: MTA9



• Molecule 2: MTA9



• Molecule 2: MTA9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.70Å 75.65Å 142.47Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	44.93 – 3.09 44.93 – 3.09	Depositor EDS
% Data completeness (in resolution range)	57.1 (44.93-3.09) 77.1 (44.93-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.304 , 0.316 0.302 , 0.313	Depositor DCC
R_{free} test set	2000 reflections (6.81%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 109.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	9145	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.74	5/1453 (0.3%)	1.17	14/1962 (0.7%)
1	B	0.67	3/1457 (0.2%)	1.00	7/1967 (0.4%)
1	C	0.78	6/1440 (0.4%)	1.16	16/1943 (0.8%)
2	D	0.76	4/1646 (0.2%)	1.11	14/2223 (0.6%)
2	E	0.64	2/1623 (0.1%)	1.10	14/2186 (0.6%)
2	F	0.59	1/1445 (0.1%)	1.21	18/1943 (0.9%)
All	All	0.70	21/9064 (0.2%)	1.13	83/12224 (0.7%)

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	0	1
2	F	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ASP	C-N	8.35	1.40	1.33
2	D	276	LEU	C-N	7.99	1.40	1.33
1	C	209	ASP	C-N	6.19	1.40	1.33
2	D	247	THR	C-N	6.12	1.41	1.33
1	A	210	PRO	C-N	5.85	1.40	1.33
1	B	334	LYS	C-N	5.66	1.41	1.33
1	C	334	LYS	C-N	5.63	1.41	1.33
2	F	290	GLN	C-N	5.60	1.41	1.33
2	E	277	PRO	N-CD	5.40	1.55	1.47
1	A	239	PRO	N-CD	5.37	1.55	1.47
1	A	347	PRO	N-CD	5.30	1.55	1.47
2	D	248	PRO	N-CD	5.29	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	277	PRO	N-CD	5.29	1.55	1.47
1	B	239	PRO	N-CD	5.20	1.55	1.47
1	C	239	PRO	N-CD	5.18	1.55	1.47
1	C	210	PRO	N-CD	5.18	1.55	1.47
1	A	211	PRO	N-CD	5.17	1.54	1.47
1	C	211	PRO	N-CD	5.15	1.54	1.47
2	E	276	LEU	C-N	5.12	1.40	1.34
1	B	335	PRO	N-CD	5.07	1.54	1.47
1	C	210	PRO	C-N	5.07	1.40	1.34

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	PRO	N-CA-C	-12.29	89.40	112.01
1	A	212	TRP	N-CA-CB	-11.45	90.91	110.83
1	A	212	TRP	N-CA-C	-10.84	91.74	109.40
1	C	319	ILE	N-CA-C	10.37	121.20	110.72
1	A	211	PRO	CB-CA-C	-9.93	94.62	110.21
2	F	123	LYS	N-CA-C	9.01	121.10	111.28
1	A	209	ASP	CA-C-N	-8.63	113.36	119.66
1	A	209	ASP	C-N-CA	-8.63	113.36	119.66
2	D	291	PRO	N-CA-CB	8.49	110.86	103.31
2	D	148	SER	N-CA-C	8.12	120.21	111.36
2	D	201	PHE	N-CA-C	7.80	119.86	111.36
2	F	201	PHE	N-CA-C	7.51	119.46	111.28
2	E	150	ILE	N-CA-C	7.39	118.16	110.62
2	E	291	PRO	N-CA-CB	7.22	110.83	103.25
2	F	270	GLN	N-CA-C	7.07	118.98	111.28
1	C	209	ASP	CA-C-N	-7.06	113.11	120.38
1	C	209	ASP	C-N-CA	-7.06	113.11	120.38
1	B	317	LYS	N-CA-C	7.06	119.05	111.36
2	F	289	ASP	N-CA-C	7.00	118.98	111.36
2	D	247	THR	CA-C-N	-6.86	113.73	120.52
2	D	247	THR	C-N-CA	-6.86	113.73	120.52
2	F	198	ASN	N-CA-C	6.85	118.75	111.28
2	F	192	GLU	N-CA-C	6.83	118.73	111.28
1	C	322	ASP	N-CA-C	6.76	118.30	111.07
1	C	334	LYS	CA-C-N	-6.59	112.98	119.76
1	C	334	LYS	C-N-CA	-6.59	112.98	119.76
2	D	104	THR	N-CA-C	6.54	120.08	110.59
2	F	129	LEU	N-CA-C	6.54	118.41	111.28
2	E	78	GLN	N-CA-C	6.51	118.17	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	254	ILE	N-CA-C	6.50	118.06	108.45
2	F	290	GLN	N-CA-C	6.50	122.38	113.16
2	E	136	ILE	N-CA-C	-6.39	101.31	109.80
2	D	276	LEU	CA-C-N	-6.35	113.20	120.89
2	D	276	LEU	C-N-CA	-6.35	113.20	120.89
2	F	146	ASP	N-CA-C	-6.33	102.17	110.53
2	D	165	ILE	N-CA-C	6.31	117.42	112.12
2	F	284	ILE	N-CA-C	6.30	119.06	112.83
1	B	334	LYS	CA-C-N	-6.27	113.30	119.76
1	B	334	LYS	C-N-CA	-6.27	113.30	119.76
2	E	248	PRO	N-CA-CB	6.14	109.83	103.38
2	F	290	GLN	CA-C-N	-6.09	113.51	119.78
2	F	290	GLN	C-N-CA	-6.09	113.51	119.78
2	E	88	TYR	N-CA-C	6.01	119.92	112.59
2	F	104	THR	N-CA-C	5.92	118.39	110.35
1	C	238	MET	CA-C-N	-5.90	112.47	119.84
1	C	238	MET	C-N-CA	-5.90	112.47	119.84
1	C	320	ALA	N-CA-C	5.88	118.49	108.90
1	A	243	LEU	N-CA-C	5.85	117.66	111.28
1	A	210	PRO	O-C-N	5.83	123.99	121.31
1	A	357	ARG	N-CA-C	-5.82	101.67	110.28
1	C	342	ILE	N-CA-C	5.74	116.52	110.72
2	D	232	LYS	N-CA-C	5.62	120.29	113.38
1	B	356	ALA	N-CA-C	5.61	117.77	110.53
1	C	195	GLN	N-CA-C	5.55	117.14	111.14
1	C	346	CYS	CA-C-N	-5.55	112.90	119.84
1	C	346	CYS	C-N-CA	-5.55	112.90	119.84
1	A	346	CYS	CA-C-N	-5.51	112.93	119.05
1	A	346	CYS	C-N-CA	-5.51	112.93	119.05
2	F	256	ASN	N-CA-C	5.49	117.27	111.28
2	E	276	LEU	CA-C-N	-5.49	113.37	119.19
2	E	276	LEU	C-N-CA	-5.49	113.37	119.19
2	E	279	SER	N-CA-C	5.44	117.29	111.36
1	A	210	PRO	CA-C-N	-5.43	113.67	120.51
1	A	210	PRO	C-N-CA	-5.43	113.67	120.51
2	E	288	LYS	N-CA-C	-5.34	104.91	111.75
2	E	283	GLU	N-CA-C	-5.33	101.07	109.50
1	B	346	CYS	CA-C-N	-5.31	113.20	119.84
1	B	346	CYS	C-N-CA	-5.31	113.20	119.84
2	D	161	GLY	N-CA-C	5.29	123.36	115.64
2	F	262	LEU	N-CA-C	-5.29	107.20	113.97
1	C	235	ILE	N-CA-C	-5.29	105.23	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	GLY	N-CA-C	5.28	117.56	110.43
2	F	160	LYS	N-CA-C	-5.25	103.09	110.50
1	A	258	TYR	N-CA-C	5.23	116.66	111.07
2	F	267	TYR	N-CA-C	5.21	117.71	111.71
2	D	250	VAL	N-CA-C	5.17	116.69	109.55
1	C	340	GLN	N-CA-C	-5.14	105.68	111.28
1	B	190	ALA	N-CA-C	-5.10	105.72	111.28
2	E	247	THR	CA-C-N	5.08	125.06	120.03
2	E	247	THR	C-N-CA	5.08	125.06	120.03
2	E	148	SER	N-CA-C	5.06	119.41	112.88
2	D	290	GLN	CA-C-N	-5.05	114.56	119.76
2	D	290	GLN	C-N-CA	-5.05	114.56	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	ASP	Peptide
2	F	269	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1422	0	1371	296	0
1	B	1426	0	1364	261	1
1	C	1411	0	1357	248	2
2	D	1632	0	1554	316	1
2	E	1608	0	1552	276	0
2	F	1434	0	1364	395	1
3	A	32	0	0	2	0
3	B	28	0	0	4	1
3	C	24	0	0	10	0
3	D	43	0	0	9	0
3	E	43	0	0	9	0
3	F	42	0	0	11	0
All	All	9145	0	8562	1623	3

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 93.

All (1623) 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:292:GLY:HA2	1:A:297:HIS:CE1	1.23	1.68
2:D:134:LYS:HE2	2:D:282:MET:SD	1.14	1.67
2:F:118:ILE:CG1	2:F:284:ILE:HD12	1.29	1.60
2:F:144:TRP:HE1	2:F:264:THR:CG2	1.12	1.59
2:E:79:TRP:CZ3	2:E:190:GLN:NE2	1.68	1.57
1:A:292:GLY:CA	1:A:297:HIS:CE1	1.79	1.56
2:F:118:ILE:HG12	2:F:284:ILE:CD1	1.10	1.55
2:E:242:LEU:CB	2:E:277:PRO:HD2	1.36	1.54
2:D:97:VAL:CG2	2:D:109:TYR:CE1	1.90	1.51
2:F:70:CYS:H	2:F:199:LEU:CD2	1.18	1.51
2:D:97:VAL:CG2	2:D:109:TYR:CZ	1.94	1.50
1:B:272:LEU:CB	2:F:151:ASN:ND2	1.72	1.50
1:B:320:ALA:CB	2:F:220:LEU:CD2	1.87	1.49
1:A:287:ILE:CG2	1:B:371:GLU:HB2	1.41	1.47
1:B:296:GLN:HE21	2:F:246:ARG:C	1.21	1.46
1:A:289:LYS:NZ	1:B:186:LEU:HD13	1.19	1.46
1:C:321:SER:HB2	2:E:208:VAL:CG2	1.41	1.46
2:E:175:LEU:HD21	2:E:191:THR:CB	1.44	1.46
1:B:320:ALA:CB	2:F:220:LEU:HD22	1.43	1.45
2:F:142:PHE:C	2:F:143:ILE:HD12	1.38	1.44
1:B:293:PHE:HE2	2:F:244:HIS:CD2	1.36	1.43
1:C:293:PHE:O	2:E:245:GLN:CB	1.67	1.43
1:C:353:GLU:OE1	1:C:356:ALA:CB	1.64	1.43
1:B:320:ALA:HB3	2:F:220:LEU:CD2	0.99	1.43
2:E:242:LEU:CB	2:E:277:PRO:CD	1.95	1.43
2:F:74:GLU:O	2:F:78:GLN:CB	1.65	1.41
2:F:118:ILE:CG1	2:F:284:ILE:CD1	1.84	1.41
2:D:97:VAL:HG22	2:D:109:TYR:CE1	1.50	1.40
2:F:116:ILE:CD1	2:F:135:LEU:HD21	1.48	1.40
2:D:68:VAL:CB	2:D:199:LEU:HG	1.50	1.40
2:F:144:TRP:NE1	2:F:264:THR:HG21	1.30	1.39
2:D:134:LYS:CE	2:D:282:MET:SD	2.11	1.38
1:A:281:LYS:O	1:A:327:GLU:CB	1.71	1.37
1:A:292:GLY:CA	1:A:297:HIS:HE1	1.19	1.36
1:A:358:ARG:N	1:A:372:LEU:HD22	1.42	1.35
1:B:206:ILE:CG1	1:B:244:GLN:NE2	1.90	1.34
2:F:70:CYS:CB	2:F:199:LEU:CD2	2.04	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HG13	1:B:244:GLN:NE2	1.42	1.34
1:A:356:ALA:O	1:A:372:LEU:CD2	1.74	1.34
2:D:273:GLU:OE2	2:D:292:ARG:NH2	1.59	1.33
2:D:127:LYS:O	2:D:160:LYS:NZ	1.61	1.33
1:B:293:PHE:CE2	2:F:244:HIS:CD2	2.15	1.33
2:D:104:THR:CG2	3:D:418:HOH:O	1.77	1.32
2:F:173:LEU:HD11	2:F:254:ILE:CG2	1.60	1.31
1:C:322:ASP:OD2	2:E:222:GLN:HA	1.21	1.31
2:E:79:TRP:HZ3	2:E:190:GLN:NE2	0.84	1.30
1:A:329:ARG:HH21	1:A:333:GLN:CD	1.36	1.30
1:A:289:LYS:NZ	1:B:186:LEU:CD1	1.92	1.29
2:F:70:CYS:N	2:F:199:LEU:CD2	1.91	1.29
1:A:316:LYS:CE	1:A:344:GLN:OE1	1.81	1.29
1:B:358:ARG:HG2	1:B:372:LEU:O	1.29	1.29
2:D:68:VAL:CB	2:D:199:LEU:CG	2.10	1.29
1:A:263:LYS:O	1:A:267:ASN:ND2	1.66	1.28
1:A:356:ALA:C	1:A:372:LEU:HD21	1.58	1.28
1:A:274:ASP:OD1	2:D:220:LEU:HD12	1.23	1.28
1:B:314:ARG:O	1:B:347:PRO:HD3	1.24	1.28
1:A:357:ARG:CA	1:A:372:LEU:HD23	1.63	1.27
1:A:316:LYS:NZ	1:A:344:GLN:OE1	1.69	1.26
2:D:189:GLU:CB	2:D:192:GLU:OE1	1.83	1.26
1:B:197:ARG:NH2	2:D:231:ARG:HG2	1.50	1.26
1:A:321:SER:OG	1:A:341:TYR:CE1	1.88	1.25
1:B:206:ILE:CD1	1:B:244:GLN:HE21	1.50	1.25
1:B:296:GLN:O	2:F:249:ASP:N	1.68	1.24
1:C:291:HIS:O	2:E:246:ARG:CB	1.86	1.23
1:A:293:PHE:O	2:D:244:HIS:HB3	1.26	1.23
2:D:146:ASP:OD1	2:D:225:GLN:HG2	1.28	1.23
2:F:173:LEU:CD1	2:F:254:ILE:HB	1.68	1.23
1:B:300:GLU:OE2	1:B:334:LYS:NZ	1.70	1.23
2:D:168:LEU:HG	2:D:249:ASP:O	1.06	1.23
2:E:144:TRP:CZ2	2:E:264:THR:OG1	1.89	1.23
2:F:70:CYS:CB	2:F:199:LEU:HD23	1.63	1.23
1:A:281:LYS:O	1:A:327:GLU:HB3	1.08	1.22
1:B:293:PHE:CE2	2:F:244:HIS:HD2	1.52	1.22
2:F:172:GLN:HG3	2:F:223:SER:O	1.34	1.22
2:E:131:ILE:CG1	2:E:160:LYS:HD3	1.69	1.22
2:F:173:LEU:CG	2:F:254:ILE:HB	1.70	1.21
2:F:171:VAL:HB	2:F:252:PHE:CD1	1.75	1.21
2:D:243:ARG:CG	2:D:246:ARG:HD3	1.70	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:LYS:N	2:D:295:TRP:O	1.74	1.20
2:E:165:ILE:HD11	2:E:231:ARG:CB	1.70	1.20
2:F:196:LEU:HD11	3:F:429:HOH:O	1.06	1.20
1:B:272:LEU:HD12	2:F:151:ASN:ND2	1.55	1.20
2:D:137:SER:O	2:D:233:PHE:HB2	1.37	1.20
1:A:357:ARG:C	1:A:372:LEU:CD2	2.15	1.20
1:B:272:LEU:CG	2:F:151:ASN:ND2	2.05	1.19
1:A:357:ARG:CA	1:A:372:LEU:CD2	2.20	1.19
2:F:116:ILE:HD11	2:F:135:LEU:CD2	1.73	1.19
1:B:272:LEU:CD1	2:F:151:ASN:ND2	2.04	1.18
1:B:320:ALA:CA	2:F:220:LEU:HD22	1.72	1.18
1:B:272:LEU:HB2	2:F:151:ASN:ND2	1.57	1.18
1:C:321:SER:CB	2:E:208:VAL:CG2	2.21	1.18
1:A:358:ARG:N	1:A:372:LEU:CD2	2.06	1.18
2:F:70:CYS:N	2:F:199:LEU:HD22	1.52	1.18
2:F:118:ILE:CD1	2:F:284:ILE:HD13	1.75	1.17
2:E:116:ILE:HD11	2:E:134:LYS:CD	1.75	1.17
2:F:142:PHE:O	2:F:143:ILE:HD12	1.41	1.17
2:E:90:THR:HG22	3:E:427:HOH:O	1.37	1.17
1:B:358:ARG:CG	1:B:372:LEU:O	1.92	1.16
1:B:206:ILE:HG13	1:B:244:GLN:CD	1.69	1.16
1:A:323:VAL:CG2	2:D:224:LYS:HE2	1.75	1.16
1:A:356:ALA:O	1:A:372:LEU:HD21	1.01	1.16
2:F:76:LEU:HD12	2:F:77:LEU:H	1.07	1.16
2:E:113:VAL:O	2:E:135:LEU:CD2	1.93	1.15
2:E:265:LYS:HD2	3:E:402:HOH:O	1.01	1.15
1:B:296:GLN:NE2	2:F:246:ARG:C	2.04	1.15
1:A:371:GLU:OE2	3:A:401:HOH:O	1.63	1.15
2:E:269:TYR:OH	2:E:283:GLU:OE1	1.63	1.15
1:C:249:ILE:HG22	1:C:270:TYR:CE1	1.81	1.15
2:D:175:LEU:HD12	2:D:257:ASN:OD1	1.48	1.14
1:A:316:LYS:HE2	1:A:344:GLN:OE1	1.41	1.14
2:D:97:VAL:HG21	2:D:109:TYR:CE1	1.73	1.14
1:B:272:LEU:HB3	2:F:151:ASN:ND2	1.54	1.14
1:C:321:SER:HB2	2:E:208:VAL:HG22	1.17	1.14
1:A:296:GLN:O	2:D:249:ASP:OD1	1.65	1.13
2:D:68:VAL:CB	2:D:199:LEU:CD2	2.26	1.13
1:C:283:VAL:HG21	1:C:327:GLU:OE2	1.46	1.13
1:C:339:TYR:OH	1:C:360:ASN:OD1	1.64	1.13
2:F:172:GLN:CG	2:F:223:SER:O	1.96	1.13
1:B:230:LEU:HB3	1:B:235:ILE:HD11	1.29	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:HH22	2:D:231:ARG:CG	1.61	1.12
2:F:116:ILE:HD11	2:F:135:LEU:HD21	1.16	1.12
1:A:289:LYS:HZ2	1:B:186:LEU:CD1	1.56	1.12
1:A:329:ARG:NH2	1:A:333:GLN:CD	2.07	1.12
2:F:281:LEU:O	2:F:295:TRP:CE3	2.02	1.12
1:A:287:ILE:HG22	1:B:371:GLU:HB2	1.20	1.11
1:C:249:ILE:CG2	1:C:270:TYR:CE1	2.32	1.11
2:E:131:ILE:HD11	2:E:160:LYS:HD2	1.24	1.11
2:D:243:ARG:H	2:D:243:ARG:HD3	1.15	1.11
2:F:173:LEU:CD1	2:F:254:ILE:CG2	2.28	1.11
2:F:118:ILE:HA	2:F:284:ILE:HB	1.32	1.11
1:C:209:ASP:OD1	3:C:401:HOH:O	1.66	1.11
2:D:120:ASN:HB3	2:D:144:TRP:O	1.50	1.11
2:F:144:TRP:HZ3	2:F:226:VAL:C	1.56	1.11
2:D:168:LEU:CG	2:D:249:ASP:O	1.97	1.10
2:D:253:ASP:CB	2:D:265:LYS:HE3	1.81	1.10
2:F:70:CYS:CB	2:F:199:LEU:HD21	1.74	1.10
1:A:287:ILE:HG21	1:B:371:GLU:HB2	1.23	1.10
1:A:329:ARG:HH21	1:A:333:GLN:NE2	1.48	1.10
2:E:107:SER:HA	2:E:133:LYS:NZ	1.64	1.10
2:F:135:LEU:HD11	2:F:141:LEU:HD21	1.29	1.10
1:A:329:ARG:NH2	1:A:333:GLN:NE2	2.00	1.10
2:F:269:TYR:HA	2:F:272:ILE:HD11	1.30	1.10
1:A:292:GLY:HA3	1:A:297:HIS:CE1	1.76	1.10
2:E:113:VAL:O	2:E:135:LEU:HD23	1.51	1.09
2:E:175:LEU:CD2	2:E:191:THR:CB	2.30	1.09
1:B:206:ILE:HD11	1:B:244:GLN:HE21	1.10	1.09
2:E:131:ILE:HG12	2:E:160:LYS:HD3	1.33	1.09
1:A:323:VAL:HG21	2:D:224:LYS:HE2	1.09	1.09
2:D:69:THR:HG22	2:D:195:VAL:HG12	1.10	1.09
2:D:241:GLU:O	2:D:274:THR:O	1.70	1.09
1:B:195:GLN:HG3	1:B:203:PHE:CZ	1.88	1.09
2:F:173:LEU:CD1	2:F:254:ILE:CB	2.30	1.09
1:B:203:PHE:HB2	1:B:244:GLN:HE22	1.17	1.08
1:C:321:SER:HB2	2:E:208:VAL:HG21	1.22	1.08
2:D:146:ASP:OD1	2:D:225:GLN:CG	2.01	1.08
1:B:191:LEU:HD22	1:B:368:ILE:HD11	1.29	1.08
2:D:97:VAL:HG23	2:D:109:TYR:CZ	1.71	1.08
2:F:137:SER:O	2:F:232:LYS:HD2	1.54	1.08
1:C:353:GLU:OE1	1:C:356:ALA:HB2	1.34	1.08
1:C:353:GLU:OE1	1:C:356:ALA:HB1	1.41	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:TRP:CZ3	2:F:226:VAL:O	2.07	1.08
2:D:97:VAL:HG23	2:D:109:TYR:OH	1.53	1.07
2:F:144:TRP:NE1	2:F:264:THR:CG2	1.95	1.07
1:A:274:ASP:OD1	2:D:220:LEU:CD1	2.01	1.07
1:C:242:SER:O	1:C:245:GLN:NE2	1.88	1.07
2:D:243:ARG:HG3	2:D:246:ARG:HD3	1.34	1.06
2:F:168:LEU:HB3	3:F:414:HOH:O	1.55	1.06
2:F:144:TRP:HE1	2:F:264:THR:HG23	1.12	1.06
2:F:168:LEU:CB	3:F:414:HOH:O	2.03	1.06
2:F:281:LEU:HB2	2:F:295:TRP:CE3	1.91	1.06
1:B:320:ALA:C	2:F:220:LEU:HD22	1.80	1.06
2:E:165:ILE:HD11	2:E:231:ARG:HB2	1.31	1.06
1:A:211:PRO:HG2	1:A:211:PRO:O	1.55	1.06
1:B:191:LEU:CD2	1:B:368:ILE:HD11	1.84	1.06
2:D:243:ARG:NH1	3:D:401:HOH:O	1.89	1.06
2:D:223:SER:O	2:D:224:LYS:NZ	1.88	1.05
2:E:116:ILE:CD1	2:E:134:LYS:CD	2.32	1.05
2:E:116:ILE:CD1	2:E:134:LYS:HD2	1.86	1.05
1:A:287:ILE:CG2	1:B:371:GLU:CB	2.34	1.05
2:F:163:THR:O	2:F:230:PHE:HD2	1.39	1.05
2:F:116:ILE:HG21	2:F:284:ILE:HD11	1.36	1.05
1:B:327:GLU:OE2	1:B:328:ARG:NH1	1.88	1.05
2:D:162:PHE:CE1	2:D:232:LYS:HB2	1.90	1.05
2:F:118:ILE:HG12	2:F:284:ILE:HD13	1.24	1.05
2:D:69:THR:HG22	2:D:195:VAL:CG1	1.84	1.05
2:F:173:LEU:HD11	2:F:254:ILE:HG21	1.35	1.04
1:A:354:ILE:HG22	1:A:355:PHE:HD2	1.20	1.04
1:A:354:ILE:HG22	1:A:355:PHE:CD2	1.92	1.04
1:A:230:LEU:HD22	1:A:235:ILE:HG13	1.34	1.04
2:F:118:ILE:HG13	2:F:284:ILE:HD12	1.31	1.04
2:F:173:LEU:HG	2:F:254:ILE:HB	1.32	1.04
1:C:322:ASP:CG	2:E:222:GLN:HA	1.82	1.03
2:F:135:LEU:CD1	2:F:141:LEU:HD21	1.86	1.03
1:B:206:ILE:CG1	1:B:244:GLN:HE21	1.58	1.03
2:F:88:TYR:OH	2:F:293:LYS:N	1.91	1.03
1:B:206:ILE:HD12	1:B:244:GLN:HG2	1.35	1.02
1:B:358:ARG:CD	1:B:372:LEU:O	2.07	1.02
1:C:353:GLU:CD	1:C:356:ALA:HB2	1.83	1.02
2:D:109:TYR:HE2	2:D:296:ILE:CG2	1.70	1.02
2:F:142:PHE:C	2:F:143:ILE:CD1	2.32	1.02
1:A:322:ASP:OD1	2:D:220:LEU:HD13	1.56	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:222:GLN:OE1	2:E:224:LYS:NZ	1.92	1.02
2:F:144:TRP:CE3	2:F:226:VAL:O	2.12	1.02
1:A:290:GLY:HA3	1:B:372:LEU:HD12	1.39	1.02
1:B:256:ALA:CB	3:B:416:HOH:O	2.06	1.02
2:D:149:LEU:HD11	2:D:152:GLU:HB2	1.36	1.02
2:F:122:PHE:HB3	2:F:126:LEU:HG	1.39	1.02
2:E:242:LEU:CB	2:E:277:PRO:HD3	1.86	1.01
1:A:198:HIS:CD2	1:C:294:TYR:OH	2.13	1.01
1:A:202:MET:HG3	1:A:243:LEU:O	1.60	1.01
1:B:320:ALA:CB	2:F:220:LEU:HD21	1.64	1.01
2:E:116:ILE:HD11	2:E:134:LYS:HD2	1.40	1.01
2:D:120:ASN:HD21	2:D:123:LYS:HA	1.24	1.01
2:D:120:ASN:ND2	2:D:120:ASN:O	1.93	1.00
2:D:253:ASP:HB3	2:D:265:LYS:HE3	1.40	1.00
2:F:127:LYS:O	2:F:159:ASN:ND2	1.94	1.00
2:F:76:LEU:HD12	2:F:77:LEU:N	1.76	1.00
2:E:106:LEU:HD13	2:E:134:LYS:HE2	1.41	1.00
1:B:354:ILE:HG22	1:B:355:PHE:CD2	1.95	1.00
2:F:265:LYS:NZ	3:F:401:HOH:O	1.93	1.00
1:B:293:PHE:HE2	2:F:244:HIS:CG	1.80	0.99
2:D:109:TYR:HE2	2:D:296:ILE:HG21	1.24	0.99
1:A:357:ARG:HA	1:A:372:LEU:HD23	1.01	0.99
2:D:253:ASP:OD2	2:D:265:LYS:HE2	1.61	0.99
1:B:206:ILE:CD1	1:B:244:GLN:HG2	1.93	0.99
2:F:281:LEU:HB3	2:F:295:TRP:CH2	1.98	0.99
1:C:293:PHE:C	2:E:245:GLN:HB3	1.87	0.99
2:E:165:ILE:HD11	2:E:231:ARG:HB3	1.45	0.99
1:A:194:ALA:O	1:A:198:HIS:ND1	1.96	0.99
1:A:186:LEU:HD22	1:A:187:ASN:H	1.24	0.98
1:A:265:ILE:HD11	1:A:272:LEU:HD22	1.42	0.98
1:C:293:PHE:O	2:E:245:GLN:HB3	0.82	0.98
2:D:182:LEU:HD22	2:D:183:ASN:H	1.23	0.98
2:F:281:LEU:O	2:F:295:TRP:CZ3	2.16	0.98
1:A:198:HIS:CD2	1:C:294:TYR:HH	1.80	0.98
2:F:118:ILE:CD1	2:F:284:ILE:CD1	2.38	0.98
1:A:289:LYS:HZ1	1:B:186:LEU:CG	1.76	0.98
2:F:144:TRP:CZ3	2:F:226:VAL:C	2.39	0.98
2:F:70:CYS:CA	2:F:199:LEU:CD2	2.41	0.98
1:A:357:ARG:HA	1:A:372:LEU:CD2	1.87	0.98
1:C:325:PHE:CD1	2:E:204:GLN:HG3	1.97	0.98
2:D:253:ASP:OD2	2:D:265:LYS:CE	2.11	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:VAL:CB	2:D:199:LEU:HD21	1.93	0.97
2:F:173:LEU:HD12	2:F:254:ILE:HB	1.43	0.97
1:A:289:LYS:HZ1	1:B:186:LEU:CD2	1.77	0.97
2:F:73:LEU:O	2:F:76:LEU:CD1	2.12	0.97
2:F:136:ILE:HD12	2:F:137:SER:H	1.29	0.97
2:D:104:THR:HG21	3:D:418:HOH:O	1.49	0.97
1:B:314:ARG:O	1:B:347:PRO:CD	2.12	0.97
2:D:146:ASP:CG	2:D:225:GLN:HE21	1.73	0.97
2:F:281:LEU:CB	2:F:295:TRP:CZ3	2.46	0.97
2:D:176:GLU:OE1	2:D:176:GLU:N	1.96	0.97
1:B:328:ARG:HB2	1:B:331:GLN:NE2	1.79	0.97
2:F:136:ILE:HG23	2:F:139:GLY:N	1.80	0.97
1:A:356:ALA:O	1:A:372:LEU:CG	2.13	0.96
1:C:202:MET:CE	1:C:243:LEU:O	2.13	0.96
1:A:322:ASP:OD2	2:D:222:GLN:HA	1.65	0.96
2:F:120:ASN:OD1	2:F:285:PHE:CE2	2.18	0.96
1:C:273:VAL:HG23	1:C:306:VAL:HG12	1.48	0.96
1:C:322:ASP:OD2	2:E:222:GLN:CA	2.13	0.96
2:D:97:VAL:HG21	2:D:109:TYR:CZ	1.83	0.96
1:B:281:LYS:O	1:B:327:GLU:HG3	1.67	0.95
1:C:257:LYS:HB3	1:C:260:VAL:HG21	1.48	0.95
2:F:196:LEU:HD21	3:F:429:HOH:O	1.66	0.95
1:A:289:LYS:HE3	1:B:182:ASP:N	1.79	0.95
1:A:320:ALA:HB3	2:D:220:LEU:CD2	1.96	0.95
1:A:346:CYS:O	1:A:351:TYR:OH	1.83	0.95
1:A:274:ASP:OD2	2:D:218:LYS:HD3	1.65	0.95
1:C:316:LYS:HZ1	1:C:347:PRO:HG2	1.28	0.95
1:C:314:ARG:O	1:C:347:PRO:HD3	1.63	0.95
2:F:163:THR:O	2:F:230:PHE:CD2	2.19	0.95
2:E:208:VAL:HG13	2:E:209:LYS:CB	1.95	0.94
2:E:284:ILE:HG22	2:E:285:PHE:HD2	1.31	0.94
2:F:74:GLU:O	2:F:78:GLN:CA	2.15	0.94
2:F:70:CYS:N	2:F:199:LEU:HD21	1.80	0.94
2:F:167:ASN:C	2:F:168:LEU:HD13	1.91	0.94
1:B:246:ASP:OD1	1:B:309:ASP:N	1.99	0.94
2:F:118:ILE:HG23	2:F:284:ILE:HG21	1.49	0.94
2:D:137:SER:O	2:D:233:PHE:CB	2.15	0.94
2:F:172:GLN:HG3	2:F:223:SER:C	1.93	0.94
1:B:203:PHE:HB2	1:B:244:GLN:NE2	1.82	0.94
1:B:357:ARG:HH21	1:B:360:ASN:HD21	1.12	0.94
2:F:171:VAL:HB	2:F:252:PHE:HD1	1.31	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:LEU:CD1	2:E:134:LYS:HE2	1.97	0.94
2:E:121:LEU:O	2:E:121:LEU:HD12	1.67	0.94
2:E:131:ILE:HD11	2:E:160:LYS:CD	1.96	0.94
2:E:101:ILE:HA	2:E:104:THR:HG21	1.49	0.93
2:E:284:ILE:HG22	2:E:285:PHE:CD2	2.02	0.93
1:A:316:LYS:HE2	1:A:344:GLN:CD	1.92	0.93
1:B:286:LYS:CB	1:B:325:PHE:HZ	1.80	0.93
1:A:287:ILE:HG22	1:B:371:GLU:CB	1.97	0.93
2:F:281:LEU:HB3	2:F:295:TRP:CZ3	2.04	0.93
1:B:327:GLU:HG2	1:B:328:ARG:H	1.30	0.93
2:D:204:GLN:O	2:D:208:VAL:HG23	1.68	0.93
2:E:245:GLN:H	2:E:245:GLN:HE21	1.17	0.93
2:E:129:LEU:O	2:E:160:LYS:NZ	2.01	0.93
2:E:196:LEU:HD23	2:E:196:LEU:H	1.32	0.93
1:A:208:MET:HE2	1:A:210:PRO:HG3	1.50	0.93
2:F:173:LEU:HD11	2:F:254:ILE:HG22	1.49	0.93
2:F:116:ILE:CD1	2:F:135:LEU:CD2	2.34	0.93
1:B:286:LYS:CB	1:B:325:PHE:CZ	2.51	0.93
2:F:70:CYS:CA	2:F:199:LEU:HD21	1.99	0.93
1:A:288:ALA:HB1	1:A:298:ALA:HA	1.49	0.93
2:D:75:VAL:HG21	2:D:252:PHE:H	1.34	0.92
1:A:289:LYS:HZ1	1:B:186:LEU:HD22	1.31	0.92
1:C:322:ASP:OD1	2:E:222:GLN:CB	2.17	0.92
2:D:138:ASN:O	2:D:138:ASN:ND2	2.03	0.92
2:E:116:ILE:HD11	2:E:134:LYS:HD3	1.46	0.92
2:E:283:GLU:HG2	2:E:286:ALA:HB2	1.47	0.92
2:D:243:ARG:HG2	2:D:246:ARG:HD3	1.47	0.92
2:F:118:ILE:HG12	2:F:284:ILE:CG1	1.98	0.92
2:F:175:LEU:CB	2:F:254:ILE:HG21	1.99	0.92
1:B:206:ILE:CD1	1:B:244:GLN:NE2	2.25	0.92
2:D:127:LYS:C	2:D:160:LYS:HZ2	1.78	0.92
2:E:107:SER:HA	2:E:133:LYS:HZ3	1.29	0.92
1:A:281:LYS:O	1:A:327:GLU:HB2	1.69	0.92
1:B:257:LYS:O	1:B:261:THR:OG1	1.86	0.92
1:C:320:ALA:O	2:E:220:LEU:HB3	1.68	0.92
2:F:116:ILE:CG2	2:F:284:ILE:HD11	1.99	0.91
1:A:265:ILE:HD11	1:A:272:LEU:CD2	1.99	0.91
1:A:274:ASP:OD2	2:D:218:LYS:CD	2.18	0.91
2:F:118:ILE:CG1	2:F:284:ILE:HD13	1.73	0.91
2:F:173:LEU:HD12	2:F:254:ILE:CB	1.98	0.91
2:E:144:TRP:CE2	2:E:264:THR:OG1	2.20	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLY:HA3	1:A:295:LEU:O	1.71	0.91
2:F:73:LEU:O	2:F:76:LEU:HD11	1.69	0.91
2:E:177:GLN:HE22	2:E:206:VAL:HA	1.34	0.91
1:B:326:SER:OG	1:B:335:PRO:HG3	1.71	0.91
1:A:230:LEU:HD22	1:A:235:ILE:CG1	2.01	0.90
1:B:340:GLN:O	1:B:343:ASN:OD1	1.89	0.90
1:C:321:SER:CB	2:E:208:VAL:HG21	1.91	0.90
2:E:137:SER:HG	2:E:233:PHE:HD1	1.03	0.90
2:F:173:LEU:HG	2:F:254:ILE:CB	1.99	0.90
1:A:213:GLN:HG3	1:A:230:LEU:O	1.72	0.90
2:D:147:LYS:CA	2:D:222:GLN:OE1	2.19	0.90
2:E:114:GLN:HG2	2:E:278:LYS:HD2	1.50	0.90
2:D:120:ASN:OD1	2:D:126:LEU:HD11	1.71	0.90
2:F:135:LEU:HD12	2:F:162:PHE:HE2	1.36	0.90
1:A:254:ILE:HG13	1:A:257:LYS:HB2	1.53	0.90
2:E:162:PHE:HB3	2:E:230:PHE:HB3	1.54	0.90
2:D:109:TYR:CE2	2:D:296:ILE:HG21	2.07	0.90
2:E:106:LEU:CD1	2:E:134:LYS:CE	2.50	0.90
2:F:74:GLU:O	2:F:78:GLN:N	2.05	0.90
2:E:174:SER:OG	2:E:177:GLN:HB2	1.72	0.90
2:E:100:LYS:HA	2:E:300:GLU:HG3	1.52	0.89
1:C:246:ASP:OD1	1:C:309:ASP:N	2.04	0.89
2:F:173:LEU:N	2:F:253:ASP:O	2.04	0.89
2:D:147:LYS:HA	2:D:222:GLN:OE1	1.73	0.89
2:E:116:ILE:CD1	2:E:134:LYS:HD3	1.99	0.89
1:C:182:ASP:OD1	1:C:370:ASN:OD1	1.89	0.89
1:C:249:ILE:HG21	1:C:270:TYR:CE1	2.06	0.89
2:F:143:ILE:O	2:F:227:LEU:HG	1.72	0.89
1:B:244:GLN:HB2	1:B:270:TYR:OH	1.73	0.88
1:B:369:GLY:HA3	1:B:372:LEU:HD21	1.55	0.88
1:A:263:LYS:C	1:A:267:ASN:HD22	1.80	0.88
1:A:278:TRP:NE1	1:A:326:SER:O	2.06	0.88
2:F:76:LEU:CD1	2:F:77:LEU:N	2.35	0.88
1:B:314:ARG:HH11	1:B:314:ARG:HG2	1.36	0.88
1:A:288:ALA:CB	1:A:298:ALA:HA	2.03	0.88
2:E:121:LEU:HB3	2:E:144:TRP:O	1.74	0.88
1:B:203:PHE:CB	1:B:244:GLN:HE22	1.87	0.88
2:D:97:VAL:HG22	2:D:109:TYR:HE1	1.16	0.88
2:D:177:GLN:HG3	2:D:209:LYS:CB	2.03	0.88
2:E:131:ILE:CG1	2:E:160:LYS:CD	2.52	0.88
1:A:211:PRO:O	1:A:211:PRO:CG	2.18	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:231:ARG:HH21	2:E:231:ARG:HG3	1.37	0.87
2:F:118:ILE:HG23	2:F:284:ILE:CG2	2.04	0.87
2:D:175:LEU:CD1	2:D:257:ASN:OD1	2.22	0.87
2:E:100:LYS:O	2:E:104:THR:HB	1.74	0.87
2:E:101:ILE:HA	2:E:104:THR:CG2	2.04	0.87
1:B:206:ILE:HD12	1:B:244:GLN:CG	2.05	0.87
2:F:76:LEU:CD1	2:F:77:LEU:H	1.86	0.87
2:D:149:LEU:HD11	2:D:152:GLU:CB	2.04	0.87
2:D:256:ASN:ND2	3:D:402:HOH:O	2.00	0.87
2:F:142:PHE:O	2:F:143:ILE:CD1	2.20	0.87
1:B:272:LEU:HD12	2:F:151:ASN:CG	2.00	0.87
1:C:322:ASP:OD1	2:E:222:GLN:CG	2.21	0.87
2:E:144:TRP:HZ2	2:E:264:THR:OG1	1.54	0.87
2:D:146:ASP:CG	2:D:225:GLN:HG2	1.99	0.86
2:D:120:ASN:ND2	2:D:123:LYS:HA	1.90	0.86
1:A:297:HIS:NE2	2:D:166:GLU:OE2	2.08	0.86
1:B:328:ARG:O	1:B:331:GLN:HG2	1.75	0.86
2:D:109:TYR:CE2	2:D:296:ILE:CG2	2.59	0.86
2:F:281:LEU:O	2:F:295:TRP:HE3	1.57	0.86
2:D:261:CYS:O	2:D:262:LEU:HD23	1.75	0.86
1:B:294:TYR:CE2	2:F:165:ILE:HG12	2.10	0.86
1:C:293:PHE:CE2	1:C:294:TYR:HE2	1.93	0.86
2:E:166:GLU:O	2:E:229:MET:HB3	1.76	0.86
2:F:117:PHE:O	2:F:284:ILE:CG1	2.24	0.86
2:F:168:LEU:HD23	2:F:227:LEU:HD22	1.55	0.86
1:C:280:LYS:O	1:C:288:ALA:HB2	1.75	0.86
2:F:262:LEU:HD23	2:F:262:LEU:H	1.40	0.86
1:C:278:TRP:CE2	1:C:335:PRO:HD3	2.11	0.85
2:F:116:ILE:CG1	2:F:135:LEU:HD21	2.06	0.85
1:B:189:GLN:NE2	1:B:192:ILE:HD11	1.92	0.85
1:C:322:ASP:OD1	2:E:222:GLN:HG3	1.77	0.85
2:D:75:VAL:CG2	2:D:252:PHE:H	1.89	0.85
1:B:285:GLY:HA2	2:F:69:THR:CB	2.07	0.85
1:A:356:ALA:HB3	1:A:367:SER:OG	1.77	0.85
1:A:263:LYS:HG2	1:A:267:ASN:HD21	1.39	0.85
1:A:293:PHE:O	2:D:244:HIS:CB	2.21	0.85
1:B:358:ARG:HD2	1:B:372:LEU:O	1.73	0.85
2:F:173:LEU:CD1	2:F:254:ILE:HG21	2.01	0.85
1:C:322:ASP:OD2	2:E:221:ASN:O	1.95	0.84
2:F:70:CYS:H	2:F:199:LEU:HD22	0.68	0.84
1:C:182:ASP:OD1	1:C:370:ASN:CG	2.20	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:GLU:O	2:F:298:VAL:HG23	1.76	0.84
1:B:338:ILE:O	1:B:342:ILE:HG13	1.75	0.84
1:C:283:VAL:HG13	3:C:421:HOH:O	1.76	0.84
2:D:168:LEU:HG	2:D:249:ASP:C	2.03	0.84
2:E:79:TRP:HZ3	2:E:190:GLN:CD	1.83	0.84
2:E:269:TYR:CD1	2:E:292:ARG:HD2	2.13	0.84
1:A:186:LEU:HD22	1:A:187:ASN:N	1.92	0.84
1:A:246:ASP:OD1	1:A:309:ASP:N	2.11	0.84
1:C:293:PHE:O	2:E:245:GLN:CG	2.25	0.84
2:D:162:PHE:HE1	2:D:232:LYS:HB2	1.38	0.84
1:A:211:PRO:CB	1:A:228:ASP:HB3	2.08	0.84
2:D:127:LYS:C	2:D:160:LYS:NZ	2.33	0.84
2:E:209:LYS:CB	2:E:221:ASN:CB	2.55	0.84
1:B:206:ILE:HD11	1:B:244:GLN:NE2	1.90	0.83
2:E:283:GLU:CG	2:E:286:ALA:HB2	2.08	0.83
2:F:162:PHE:CE1	2:F:232:LYS:HG3	2.13	0.83
2:D:144:TRP:HZ2	2:D:268:ILE:CD1	1.91	0.83
1:A:289:LYS:NZ	1:B:186:LEU:HD22	1.92	0.83
2:F:116:ILE:HD12	2:F:135:LEU:HD21	1.56	0.83
2:D:179:LEU:HD21	2:D:191:THR:HG22	1.60	0.83
1:A:290:GLY:HA3	1:B:372:LEU:CD1	2.09	0.83
1:B:295:LEU:N	2:F:166:GLU:OE2	2.11	0.83
2:F:148:SER:O	2:F:149:LEU:HD23	1.79	0.83
2:E:101:ILE:O	2:E:104:THR:HG22	1.79	0.83
2:F:196:LEU:HD12	2:F:196:LEU:O	1.78	0.82
2:F:159:ASN:OD1	2:F:160:LYS:HG2	1.79	0.82
1:A:183:VAL:HG22	1:A:238:MET:HE3	1.59	0.82
1:A:186:LEU:HG	1:A:368:ILE:HD11	1.59	0.82
1:A:288:ALA:HB3	1:A:298:ALA:CB	2.09	0.82
2:D:179:LEU:CD2	2:D:191:THR:HB	2.09	0.82
2:F:171:VAL:CB	2:F:252:PHE:CD1	2.58	0.82
2:D:253:ASP:CG	2:D:265:LYS:HE3	2.04	0.82
1:A:213:GLN:CG	1:A:230:LEU:O	2.28	0.82
1:A:233:GLU:OE2	3:A:402:HOH:O	1.98	0.81
1:C:294:TYR:O	2:E:246:ARG:N	2.13	0.81
2:E:131:ILE:CD1	2:E:160:LYS:CD	2.58	0.81
2:F:117:PHE:O	2:F:284:ILE:HG13	1.80	0.81
2:E:131:ILE:CD1	2:E:160:LYS:HD2	2.07	0.81
2:F:116:ILE:CG2	2:F:284:ILE:CD1	2.58	0.81
1:B:206:ILE:CD1	1:B:244:GLN:CG	2.56	0.81
2:D:143:ILE:CD1	2:D:157:MET:HE3	2.10	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LYS:HB2	1:C:288:ALA:HB2	1.61	0.81
2:F:125:ASP:O	2:F:128:ASN:ND2	2.13	0.81
2:D:179:LEU:HD21	2:D:191:THR:CG2	2.11	0.81
2:E:131:ILE:HG13	2:E:160:LYS:HD3	1.63	0.81
1:C:296:GLN:CD	2:E:247:THR:O	2.24	0.81
2:F:101:ILE:HA	2:F:104:THR:HB	1.59	0.81
1:A:289:LYS:NZ	1:B:186:LEU:CD2	2.43	0.80
1:B:292:GLY:O	1:B:297:HIS:CD2	2.34	0.80
1:C:322:ASP:OD1	2:E:222:GLN:HB2	1.79	0.80
2:D:273:GLU:CD	2:D:292:ARG:NH2	2.38	0.80
2:E:79:TRP:CE3	2:E:190:GLN:NE2	2.47	0.80
2:F:170:VAL:O	2:F:224:LYS:HB3	1.82	0.80
1:A:357:ARG:C	1:A:372:LEU:HD21	2.06	0.80
2:E:114:GLN:HG2	2:E:278:LYS:CD	2.11	0.80
2:F:165:ILE:O	2:F:166:GLU:HG2	1.80	0.80
1:B:357:ARG:HH21	1:B:360:ASN:ND2	1.80	0.80
2:F:168:LEU:CD2	2:F:227:LEU:HD22	2.11	0.80
2:D:124:LYS:O	2:D:126:LEU:CD2	2.30	0.80
2:D:149:LEU:CD1	2:D:152:GLU:HB2	2.11	0.80
1:A:322:ASP:OD1	2:D:220:LEU:CD1	2.29	0.80
2:F:122:PHE:H	2:F:126:LEU:CD1	1.94	0.80
1:B:281:LYS:HB2	1:B:286:LYS:HA	1.64	0.80
2:D:223:SER:C	2:D:224:LYS:HG2	2.07	0.80
2:E:129:LEU:O	2:E:160:LYS:CE	2.30	0.80
1:C:249:ILE:HG21	1:C:270:TYR:CZ	2.17	0.79
1:B:293:PHE:O	2:F:245:GLN:N	2.14	0.79
1:B:360:ASN:O	1:B:361:LEU:HD23	1.82	0.79
1:B:299:LYS:NZ	3:B:401:HOH:O	2.15	0.79
2:E:174:SER:CB	2:E:177:GLN:HB2	2.12	0.79
2:E:129:LEU:O	2:E:160:LYS:HE2	1.82	0.79
2:F:101:ILE:HA	2:F:104:THR:CB	2.12	0.79
1:B:195:GLN:CG	1:B:203:PHE:CZ	2.65	0.79
1:B:319:ILE:O	1:B:344:GLN:NE2	2.14	0.79
1:C:186:LEU:HD23	1:C:187:ASN:O	1.83	0.79
1:B:297:HIS:HA	2:F:249:ASP:OD1	1.82	0.79
1:C:316:LYS:NZ	1:C:347:PRO:HG2	1.97	0.79
2:E:175:LEU:HG	2:E:254:ILE:HG21	1.63	0.79
2:E:266:GLU:O	2:E:269:TYR:HB2	1.83	0.79
1:C:343:ASN:O	1:C:346:CYS:O	2.01	0.78
1:B:326:SER:OG	1:B:335:PRO:CG	2.30	0.78
1:C:316:LYS:NZ	1:C:347:PRO:CG	2.45	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:ILE:CA	2:F:284:ILE:HB	2.12	0.78
1:A:230:LEU:CD2	1:A:235:ILE:HG13	2.13	0.78
1:A:289:LYS:HD3	1:A:291:HIS:CB	2.12	0.78
2:F:141:LEU:HB2	2:F:230:PHE:HB2	1.64	0.78
2:D:99:LYS:O	2:D:300:GLU:HA	1.83	0.78
1:C:354:ILE:HG22	1:C:355:PHE:CD2	2.18	0.78
2:F:101:ILE:CD1	2:F:106:LEU:HD21	2.12	0.78
1:A:211:PRO:CB	1:A:228:ASP:CB	2.62	0.78
1:B:244:GLN:CB	1:B:270:TYR:OH	2.32	0.78
2:F:135:LEU:HD11	2:F:141:LEU:CD2	2.14	0.78
1:A:358:ARG:CA	1:A:372:LEU:HD22	2.12	0.78
1:B:207:MET:HE1	1:B:342:ILE:HD11	1.64	0.78
1:C:278:TRP:CZ3	1:C:300:GLU:OE2	2.36	0.78
2:D:143:ILE:HD11	2:D:157:MET:HE3	1.66	0.78
2:D:121:LEU:HD11	2:D:144:TRP:CE3	2.18	0.77
1:C:316:LYS:HZ2	1:C:347:PRO:HG3	1.47	0.77
2:F:88:TYR:HH	2:F:293:LYS:N	1.81	0.77
1:A:230:LEU:HB3	1:A:235:ILE:HD11	1.65	0.77
1:A:289:LYS:NZ	1:B:186:LEU:CG	2.41	0.77
1:C:182:ASP:CB	1:C:185:LYS:HB2	2.14	0.77
1:C:273:VAL:CG2	1:C:306:VAL:CG1	2.62	0.77
1:A:258:TYR:OH	1:A:275:GLU:OE1	2.03	0.77
2:E:165:ILE:CD1	2:E:231:ARG:HB2	2.12	0.77
1:C:249:ILE:HG22	1:C:270:TYR:HE1	1.48	0.77
1:C:291:HIS:O	2:E:246:ARG:CA	2.32	0.77
1:C:321:SER:CB	2:E:208:VAL:HG22	1.98	0.76
1:C:353:GLU:CD	1:C:356:ALA:CB	2.48	0.76
1:A:186:LEU:HD13	1:A:187:ASN:N	2.00	0.76
1:A:263:LYS:C	1:A:267:ASN:ND2	2.42	0.76
1:B:230:LEU:CB	1:B:235:ILE:HD11	2.14	0.76
1:C:293:PHE:CD2	1:C:294:TYR:CE2	2.74	0.76
1:C:323:VAL:O	2:E:204:GLN:NE2	2.18	0.76
1:C:278:TRP:HZ3	1:C:300:GLU:OE2	1.69	0.76
2:F:168:LEU:HD21	2:F:229:MET:CE	2.16	0.76
2:E:133:LYS:HG3	2:E:134:LYS:N	2.01	0.76
2:E:245:GLN:HE21	2:E:245:GLN:N	1.82	0.76
1:A:289:LYS:HZ1	1:B:186:LEU:HD13	1.43	0.75
1:C:202:MET:HE3	1:C:243:LEU:O	1.87	0.75
2:D:165:ILE:O	2:D:166:GLU:HG2	1.86	0.75
2:D:179:LEU:HD23	2:D:191:THR:HB	1.68	0.75
1:A:194:ALA:C	1:A:198:HIS:HD1	1.94	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:159:ASN:OD1	2:F:160:LYS:N	2.19	0.75
1:A:353:GLU:HB2	1:A:365:TRP:CE3	2.21	0.75
2:E:131:ILE:HG12	2:E:160:LYS:CD	2.12	0.75
2:D:144:TRP:HZ2	2:D:268:ILE:HD11	1.49	0.75
2:F:262:LEU:HD23	2:F:262:LEU:N	2.01	0.75
1:B:188:PHE:O	1:B:192:ILE:HG23	1.87	0.75
1:C:257:LYS:HB3	1:C:260:VAL:CG2	2.17	0.75
2:D:253:ASP:CB	2:D:265:LYS:CE	2.62	0.75
2:E:177:GLN:NE2	2:E:206:VAL:HA	2.01	0.75
1:A:186:LEU:HD12	1:A:188:PHE:CE2	2.21	0.75
1:B:207:MET:CE	1:B:342:ILE:HD11	2.16	0.75
1:C:280:LYS:O	1:C:288:ALA:CB	2.34	0.75
2:D:135:LEU:CD2	2:D:139:GLY:HA3	2.17	0.75
2:F:283:GLU:O	2:F:298:VAL:CG2	2.34	0.75
2:F:173:LEU:HG	2:F:254:ILE:N	2.02	0.75
1:A:288:ALA:CB	1:A:298:ALA:CB	2.65	0.75
1:B:256:ALA:HB3	3:B:416:HOH:O	1.77	0.75
1:B:326:SER:OG	1:B:335:PRO:CB	2.35	0.74
1:C:182:ASP:O	1:C:186:LEU:N	2.18	0.74
2:D:171:VAL:HG22	2:D:224:LYS:HE3	1.68	0.74
2:F:269:TYR:HA	2:F:272:ILE:CD1	2.16	0.74
1:A:211:PRO:HB3	1:A:228:ASP:CB	2.16	0.74
2:D:296:ILE:HD12	2:D:296:ILE:N	2.02	0.74
2:F:116:ILE:HD11	2:F:135:LEU:HD23	1.67	0.74
1:C:273:VAL:HG23	1:C:306:VAL:CG1	2.16	0.74
1:C:296:GLN:HG3	2:E:247:THR:N	2.03	0.74
2:F:73:LEU:O	2:F:76:LEU:HD12	1.86	0.74
2:F:74:GLU:C	2:F:78:GLN:CB	2.59	0.74
1:A:282:THR:HG23	1:A:284:ASN:O	1.88	0.74
2:D:165:ILE:O	2:D:165:ILE:HD12	1.87	0.74
2:D:243:ARG:HD3	2:D:243:ARG:N	2.00	0.74
2:F:77:LEU:CB	2:F:252:PHE:O	2.36	0.74
1:A:213:GLN:CG	1:A:230:LEU:C	2.60	0.74
1:A:352:LEU:HD12	1:A:366:VAL:O	1.87	0.74
1:B:291:HIS:ND1	1:B:292:GLY:N	2.36	0.74
2:F:125:ASP:HA	2:F:128:ASN:ND2	2.03	0.74
1:A:314:ARG:NH1	1:A:348:ASN:O	2.20	0.74
1:C:280:LYS:O	1:C:288:ALA:N	2.20	0.74
1:A:292:GLY:N	1:A:297:HIS:CE1	2.54	0.74
2:E:87:SER:OG	3:E:401:HOH:O	2.04	0.74
2:D:104:THR:HG23	3:D:418:HOH:O	1.59	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:284:ILE:O	2:F:284:ILE:HG22	1.87	0.73
1:A:188:PHE:CD1	1:A:243:LEU:HD11	2.23	0.73
1:B:357:ARG:NH2	1:B:360:ASN:HD21	1.86	0.73
1:C:280:LYS:HB2	1:C:288:ALA:CB	2.18	0.73
2:D:121:LEU:CD1	2:D:144:TRP:CE3	2.71	0.73
2:E:163:THR:OG1	2:E:231:ARG:O	2.05	0.73
1:B:326:SER:OG	1:B:335:PRO:HB3	1.88	0.73
2:F:249:ASP:N	2:F:249:ASP:OD1	2.20	0.73
1:A:291:HIS:O	1:A:297:HIS:CE1	2.42	0.73
1:A:357:ARG:N	1:A:372:LEU:HD21	2.04	0.73
1:B:329:ARG:HD3	1:B:329:ARG:C	2.13	0.73
1:B:354:ILE:HG22	1:B:355:PHE:CE2	2.24	0.73
2:F:144:TRP:CD1	2:F:264:THR:HG21	2.21	0.73
1:A:252:TRP:CE3	1:A:300:GLU:HG2	2.24	0.73
1:A:288:ALA:HB3	1:A:298:ALA:HB2	1.70	0.73
1:B:320:ALA:HB3	2:F:220:LEU:HD21	0.74	0.73
2:D:97:VAL:HG21	2:D:109:TYR:CD1	2.23	0.73
2:E:231:ARG:HG3	2:E:231:ARG:NH2	2.02	0.73
2:D:204:GLN:O	2:D:208:VAL:CG2	2.37	0.73
2:F:118:ILE:HG12	2:F:284:ILE:HD12	0.81	0.73
2:F:292:ARG:HB2	2:F:295:TRP:HB2	1.71	0.73
1:C:278:TRP:CZ2	1:C:335:PRO:HD3	2.24	0.73
2:F:168:LEU:HD22	2:F:168:LEU:N	2.03	0.72
1:A:213:GLN:HG2	1:A:230:LEU:C	2.14	0.72
1:B:191:LEU:CD2	1:B:368:ILE:CD1	2.67	0.72
1:B:314:ARG:HG2	1:B:314:ARG:NH1	1.99	0.72
2:F:136:ILE:HG13	2:F:138:ASN:H	1.54	0.72
2:F:173:LEU:HG	2:F:253:ASP:C	2.15	0.72
2:E:196:LEU:HD23	2:E:196:LEU:N	2.03	0.72
2:F:133:LYS:N	2:F:133:LYS:HD2	2.04	0.72
1:C:265:ILE:HD11	1:C:272:LEU:HD11	1.70	0.72
1:C:292:GLY:HA2	1:C:297:HIS:CE1	2.25	0.72
2:D:247:THR:HG22	3:D:407:HOH:O	1.89	0.72
2:E:135:LEU:HD12	2:E:162:PHE:HZ	1.54	0.72
2:F:122:PHE:H	2:F:126:LEU:HD12	1.54	0.72
2:D:149:LEU:HD11	2:D:152:GLU:CG	2.20	0.72
2:F:273:GLU:OE2	2:F:274:THR:N	2.23	0.72
1:A:211:PRO:HB2	1:A:228:ASP:HB3	1.70	0.72
2:D:146:ASP:CG	2:D:225:GLN:NE2	2.48	0.72
2:E:286:ALA:O	2:E:299:CYS:SG	2.48	0.72
2:F:118:ILE:HD11	2:F:284:ILE:HD13	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:281:LEU:C	2:F:295:TRP:CZ3	2.67	0.72
2:F:291:PRO:HG3	2:F:297:SER:OG	1.88	0.72
2:D:249:ASP:OD1	2:D:249:ASP:N	2.22	0.71
2:E:262:LEU:HD23	2:E:262:LEU:C	2.15	0.71
2:F:125:ASP:HA	2:F:128:ASN:HD21	1.55	0.71
2:F:269:TYR:CA	2:F:272:ILE:HD11	2.15	0.71
1:A:201:LYS:NZ	1:A:204:ASP:OD2	2.22	0.71
1:A:231:SER:HB3	1:A:234:LYS:HD2	1.72	0.71
2:D:100:LYS:HE3	2:D:300:GLU:OE1	1.90	0.71
2:E:269:TYR:O	2:E:273:GLU:HG3	1.90	0.71
1:C:296:GLN:HG3	2:E:247:THR:C	2.16	0.71
2:D:120:ASN:H	2:D:144:TRP:HB2	1.55	0.71
2:E:86:GLN:O	2:E:291:PRO:CB	2.38	0.71
2:F:136:ILE:HG23	2:F:139:GLY:CA	2.19	0.71
2:F:144:TRP:HE3	2:F:226:VAL:O	1.72	0.71
2:F:159:ASN:OD1	2:F:160:LYS:NZ	2.22	0.71
2:E:101:ILE:N	2:E:101:ILE:HD12	2.06	0.71
2:D:125:ASP:C	2:D:126:LEU:HD23	2.15	0.71
2:E:113:VAL:O	2:E:135:LEU:HD21	1.87	0.71
1:A:287:ILE:HG21	1:B:371:GLU:CB	2.11	0.71
1:A:353:GLU:HB2	1:A:365:TRP:CZ3	2.25	0.71
2:F:125:ASP:C	2:F:128:ASN:HD22	1.99	0.71
2:F:136:ILE:HD12	2:F:137:SER:N	2.04	0.71
2:F:142:PHE:CZ	2:F:272:ILE:HG21	2.26	0.71
2:F:171:VAL:HG21	2:F:252:PHE:CE1	2.25	0.71
1:A:186:LEU:HD13	1:A:186:LEU:C	2.15	0.70
2:F:281:LEU:CB	2:F:295:TRP:CE3	2.66	0.70
1:C:246:ASP:OD1	1:C:308:GLY:HA3	1.91	0.70
2:D:124:LYS:O	2:D:126:LEU:HD21	1.91	0.70
1:B:251:VAL:CG1	1:B:265:ILE:HD11	2.21	0.70
1:C:191:LEU:HD23	1:C:191:LEU:O	1.92	0.70
2:D:253:ASP:OD2	2:D:265:LYS:HE3	1.92	0.70
1:C:191:LEU:HD23	1:C:191:LEU:C	2.16	0.70
2:D:136:ILE:HG22	2:D:137:SER:N	2.06	0.70
2:E:106:LEU:C	2:E:133:LYS:HE2	2.17	0.70
2:F:127:LYS:HE2	2:F:159:ASN:HB3	1.73	0.70
2:E:100:LYS:HD2	2:E:100:LYS:N	2.06	0.70
1:A:186:LEU:HD12	1:A:188:PHE:CD2	2.26	0.70
1:A:192:ILE:HD11	1:A:242:SER:OG	1.92	0.70
1:B:293:PHE:CZ	2:F:244:HIS:CD2	2.77	0.70
2:D:98:LEU:HA	2:D:299:CYS:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:MET:SD	1:B:202:MET:HG3	2.32	0.70
1:B:197:ARG:HH22	2:D:231:ARG:HG2	0.68	0.70
2:F:117:PHE:HA	2:F:142:PHE:HB2	1.74	0.70
2:F:135:LEU:CD1	2:F:162:PHE:HE2	2.05	0.70
2:F:175:LEU:CA	2:F:254:ILE:HG21	2.22	0.70
2:F:182:LEU:HD23	2:F:182:LEU:O	1.92	0.70
1:B:279:VAL:HG23	1:B:325:PHE:CD2	2.27	0.70
1:B:281:LYS:CB	1:B:286:LYS:HA	2.21	0.70
1:B:296:GLN:O	2:F:249:ASP:OD1	2.10	0.70
1:B:358:ARG:HD2	1:B:372:LEU:C	2.17	0.69
2:F:168:LEU:HD23	2:F:227:LEU:HB3	1.73	0.69
2:E:106:LEU:HD13	2:E:134:LYS:CE	2.15	0.69
1:A:288:ALA:CB	1:A:298:ALA:CA	2.71	0.69
1:B:233:GLU:HA	1:B:236:GLN:OE1	1.91	0.69
2:F:196:LEU:HD12	2:F:196:LEU:C	2.16	0.69
1:A:263:LYS:HG2	1:A:267:ASN:ND2	2.08	0.69
1:B:191:LEU:HD22	1:B:368:ILE:CD1	2.17	0.69
1:A:211:PRO:HB2	1:A:228:ASP:CB	2.22	0.69
1:A:357:ARG:CA	1:A:372:LEU:HD21	2.09	0.69
2:E:129:LEU:C	2:E:160:LYS:HZ3	2.00	0.69
2:E:265:LYS:CD	3:E:402:HOH:O	1.82	0.69
2:F:284:ILE:CG2	2:F:284:ILE:O	2.40	0.69
1:A:230:LEU:HD22	1:A:235:ILE:CD1	2.22	0.69
1:C:293:PHE:CD2	1:C:294:TYR:HE2	2.10	0.69
2:D:179:LEU:HD11	2:D:187:LYS:C	2.17	0.69
2:D:242:LEU:HD13	2:D:277:PRO:HG3	1.74	0.69
2:D:243:ARG:H	2:D:243:ARG:CD	1.97	0.69
2:F:136:ILE:CD1	2:F:137:SER:H	2.05	0.69
2:E:177:GLN:NE2	2:E:206:VAL:C	2.50	0.69
2:F:118:ILE:HD11	2:F:284:ILE:CD1	2.20	0.69
1:A:358:ARG:H	1:A:372:LEU:HD22	1.54	0.69
1:C:299:LYS:HE2	3:C:407:HOH:O	1.92	0.69
2:F:196:LEU:CD1	3:F:429:HOH:O	1.82	0.69
1:C:196:MET:O	1:C:200:GLY:N	2.23	0.68
2:F:142:PHE:HZ	2:F:272:ILE:HG21	1.58	0.68
1:C:296:GLN:CG	2:E:247:THR:O	2.41	0.68
2:D:169:VAL:HG23	2:D:171:VAL:HG23	1.76	0.68
2:F:168:LEU:HB2	3:F:414:HOH:O	1.76	0.68
1:A:259:ARG:HD2	1:A:259:ARG:O	1.93	0.68
1:B:294:TYR:HB2	2:F:166:GLU:OE2	1.93	0.68
1:C:283:VAL:CG1	3:C:421:HOH:O	2.38	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:GLU:O	1:C:340:GLN:HB2	1.93	0.68
2:F:117:PHE:O	2:F:284:ILE:CB	2.41	0.68
1:B:206:ILE:CG1	1:B:244:GLN:CD	2.51	0.68
2:E:245:GLN:H	2:E:245:GLN:NE2	1.88	0.68
2:E:270:GLN:O	2:E:274:THR:HG23	1.92	0.68
2:F:122:PHE:CB	2:F:126:LEU:HG	2.19	0.68
1:C:283:VAL:HG21	1:C:327:GLU:CD	2.19	0.68
2:E:201:PHE:HA	2:E:205:LYS:HD3	1.76	0.68
1:C:322:ASP:CG	2:E:222:GLN:CA	2.63	0.68
1:A:275:GLU:HG3	1:A:303:LEU:HD13	1.75	0.68
1:B:203:PHE:O	1:B:244:GLN:OE1	2.11	0.68
1:C:313:GLY:O	1:C:316:LYS:HE3	1.93	0.68
1:C:349:GLY:O	1:C:351:TYR:CE1	2.46	0.68
2:E:118:ILE:HG22	2:E:120:ASN:H	1.59	0.68
1:B:281:LYS:O	1:B:327:GLU:CG	2.42	0.68
1:C:363:ASP:OD1	3:C:402:HOH:O	2.10	0.67
2:D:136:ILE:HG22	2:D:137:SER:H	1.59	0.67
2:F:116:ILE:CG1	2:F:135:LEU:CD2	2.70	0.67
1:B:282:THR:HG23	1:B:287:ILE:O	1.93	0.67
1:C:361:LEU:CD2	1:C:367:SER:OG	2.42	0.67
2:F:118:ILE:O	2:F:143:ILE:HA	1.94	0.67
2:E:116:ILE:HD13	2:E:134:LYS:CD	2.21	0.67
2:F:115:GLY:HA2	2:F:140:ILE:HG13	1.74	0.67
2:F:167:ASN:OD1	2:F:226:VAL:CG1	2.43	0.67
1:B:206:ILE:HG12	1:B:244:GLN:NE2	2.03	0.67
2:F:168:LEU:HD22	2:F:168:LEU:H	1.60	0.67
2:F:175:LEU:CB	2:F:254:ILE:CG2	2.72	0.67
1:C:188:PHE:HB3	1:C:243:LEU:HD11	1.77	0.67
1:C:196:MET:HG3	1:C:197:ARG:HD3	1.76	0.67
2:D:89:GLU:HG2	2:D:90:THR:N	2.09	0.67
2:E:135:LEU:HD12	2:E:162:PHE:CZ	2.28	0.67
2:F:135:LEU:CD1	2:F:141:LEU:CD2	2.69	0.67
1:B:320:ALA:CA	2:F:220:LEU:CD2	2.52	0.67
2:E:107:SER:HA	2:E:133:LYS:CE	2.24	0.67
1:B:228:ASP:OD2	1:B:228:ASP:N	2.24	0.66
1:A:252:TRP:HE3	1:A:300:GLU:HG2	1.60	0.66
2:E:131:ILE:CD1	2:E:160:LYS:HD3	2.24	0.66
2:F:101:ILE:HD12	2:F:106:LEU:HD21	1.77	0.66
2:E:100:LYS:HA	2:E:300:GLU:CG	2.26	0.66
1:A:186:LEU:HD13	1:A:187:ASN:C	2.21	0.66
1:A:203:PHE:O	1:A:244:GLN:HB2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:PHE:HE1	2:F:232:LYS:HG3	1.61	0.66
2:D:66:ASP:N	2:D:66:ASP:OD1	2.27	0.66
2:D:228:ILE:HG22	2:D:230:PHE:CE1	2.30	0.66
1:C:316:LYS:NZ	1:C:347:PRO:HG3	2.10	0.65
2:F:117:PHE:O	2:F:284:ILE:HB	1.96	0.65
2:D:127:LYS:C	2:D:127:LYS:HD3	2.21	0.65
1:A:238:MET:HE1	1:A:355:PHE:CZ	2.31	0.65
1:C:273:VAL:CG2	1:C:306:VAL:HG11	2.26	0.65
2:D:179:LEU:HD12	2:D:185:HIS:O	1.96	0.65
1:B:292:GLY:HA2	2:F:245:GLN:CB	2.26	0.65
1:B:293:PHE:CZ	2:F:244:HIS:HD2	2.09	0.65
1:C:182:ASP:HB2	1:C:185:LYS:HB2	1.78	0.65
2:D:162:PHE:HB3	2:D:230:PHE:HB3	1.78	0.65
2:D:182:LEU:HD22	2:D:183:ASN:N	2.05	0.65
2:D:284:ILE:HA	2:D:298:VAL:CG2	2.27	0.65
2:E:99:LYS:O	2:E:101:ILE:HD12	1.96	0.65
2:E:121:LEU:HD13	2:E:149:LEU:HD13	1.78	0.65
1:A:368:ILE:HA	1:C:291:HIS:CB	2.27	0.65
1:B:281:LYS:HA	1:B:287:ILE:H	1.62	0.65
1:C:193:ASP:O	1:C:197:ARG:HG2	1.96	0.65
2:E:247:THR:HG23	2:E:248:PRO:N	2.11	0.65
1:A:211:PRO:HA	1:A:227:TYR:CE1	2.32	0.65
1:C:188:PHE:HD1	1:C:243:LEU:HD11	1.61	0.65
1:C:204:ASP:HB3	1:C:315:PHE:CE2	2.31	0.65
2:F:134:LYS:O	2:F:135:LEU:HD23	1.96	0.65
1:B:370:ASN:O	1:B:371:GLU:HG2	1.97	0.65
1:C:291:HIS:O	2:E:246:ARG:HA	1.97	0.65
2:D:140:ILE:HD11	2:D:142:PHE:CZ	2.31	0.65
2:F:159:ASN:CG	2:F:160:LYS:HZ2	2.04	0.65
1:A:213:GLN:HG3	1:A:230:LEU:C	2.21	0.64
1:A:329:ARG:HH21	1:A:333:GLN:CG	2.10	0.64
1:A:357:ARG:C	1:A:372:LEU:HD22	1.99	0.64
2:D:195:VAL:O	2:D:199:LEU:HB2	1.96	0.64
1:C:331:GLN:HA	1:C:332:SER:C	2.20	0.64
2:D:167:ASN:O	2:D:249:ASP:HB3	1.97	0.64
2:D:243:ARG:HG2	2:D:246:ARG:CD	2.23	0.64
2:F:281:LEU:HB2	2:F:295:TRP:CD2	2.32	0.64
2:E:174:SER:HB3	2:E:177:GLN:HB2	1.77	0.64
2:F:116:ILE:HG13	2:F:135:LEU:CD2	2.27	0.64
1:B:201:LYS:HB2	1:B:201:LYS:HZ2	1.61	0.64
1:C:276:ILE:HG23	1:C:322:ASP:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:GLU:CG	1:C:356:ALA:HB2	2.27	0.64
2:F:101:ILE:O	2:F:104:THR:N	2.30	0.64
1:A:367:SER:O	1:C:291:HIS:CB	2.45	0.64
1:A:320:ALA:HB3	2:D:220:LEU:HD21	1.77	0.64
2:E:107:SER:HA	2:E:133:LYS:HZ1	1.60	0.64
1:C:188:PHE:CD1	1:C:243:LEU:HD11	2.33	0.64
2:F:171:VAL:HB	2:F:252:PHE:CE1	2.33	0.64
2:F:173:LEU:HG	2:F:254:ILE:CA	2.27	0.64
1:A:188:PHE:CE1	1:A:243:LEU:HD11	2.32	0.64
2:E:175:LEU:O	2:E:179:LEU:N	2.30	0.64
1:A:183:VAL:CG2	1:A:238:MET:HE3	2.27	0.64
1:A:195:GLN:HG3	1:A:203:PHE:CZ	2.33	0.64
1:C:211:PRO:O	1:C:212:TRP:HB2	1.98	0.63
2:D:144:TRP:CZ2	2:D:268:ILE:CD1	2.79	0.63
1:B:326:SER:CB	1:B:335:PRO:HB3	2.29	0.63
1:C:257:LYS:CB	1:C:260:VAL:HG21	2.27	0.63
1:C:283:VAL:CG2	1:C:327:GLU:OE2	2.37	0.63
2:F:100:LYS:O	2:F:104:THR:OG1	2.13	0.63
1:A:292:GLY:N	1:A:297:HIS:HE1	1.93	0.63
1:C:182:ASP:HB3	1:C:185:LYS:HB2	1.81	0.63
1:C:206:ILE:HA	1:C:352:LEU:O	1.98	0.63
2:F:116:ILE:HG21	2:F:284:ILE:CD1	2.20	0.63
1:B:326:SER:CB	1:B:335:PRO:CB	2.77	0.63
1:C:354:ILE:HG22	1:C:355:PHE:CE2	2.33	0.63
2:D:88:TYR:OH	2:D:293:LYS:CB	2.46	0.63
1:A:318:ASN:OD1	2:D:219:VAL:HA	1.98	0.63
1:B:242:SER:O	1:B:245:GLN:NE2	2.31	0.63
2:D:147:LYS:C	2:D:222:GLN:OE1	2.41	0.63
2:E:134:LYS:HZ3	2:E:284:ILE:HD11	1.63	0.63
1:C:296:GLN:HG3	2:E:247:THR:CA	2.28	0.63
2:E:255:VAL:HG22	2:E:256:ASN:N	2.12	0.63
2:F:168:LEU:HD13	2:F:168:LEU:N	2.11	0.63
1:A:281:LYS:C	1:A:327:GLU:HB3	2.11	0.63
1:C:212:TRP:CE3	1:C:235:ILE:HD12	2.34	0.63
2:F:143:ILE:HD12	2:F:143:ILE:N	2.07	0.63
1:C:359:ASN:ND2	1:C:360:ASN:HD22	1.96	0.62
2:F:101:ILE:HA	2:F:104:THR:OG1	1.98	0.62
1:B:251:VAL:HG11	1:B:265:ILE:HD11	1.80	0.62
2:D:147:LYS:HB3	2:D:222:GLN:OE1	1.99	0.62
1:A:289:LYS:HZ3	1:B:186:LEU:CD1	2.08	0.62
1:A:356:ALA:O	1:A:372:LEU:CD1	2.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.13	0.62
1:B:329:ARG:NH1	1:B:333:GLN:OE1	2.32	0.62
2:D:158:GLU:HG3	2:D:159:ASN:N	2.15	0.62
2:E:243:ARG:HH21	2:E:274:THR:HA	1.63	0.62
2:F:173:LEU:CG	2:F:254:ILE:CB	2.54	0.62
1:A:316:LYS:HD3	1:A:344:GLN:O	2.00	0.62
2:D:75:VAL:HG21	2:D:252:PHE:N	2.12	0.62
2:E:114:GLN:CG	2:E:278:LYS:HD2	2.27	0.62
2:F:168:LEU:HD23	2:F:227:LEU:CD2	2.29	0.62
2:F:171:VAL:HG21	2:F:252:PHE:HE1	1.63	0.62
1:B:328:ARG:HB2	1:B:331:GLN:HE21	1.65	0.61
2:D:143:ILE:HD12	2:D:157:MET:CE	2.30	0.61
2:D:146:ASP:O	2:D:225:GLN:HA	2.00	0.61
2:E:140:ILE:HD11	2:E:276:LEU:HD11	1.82	0.61
2:E:177:GLN:NE2	2:E:206:VAL:O	2.33	0.61
2:F:256:ASN:OD1	2:F:257:ASN:OD1	2.18	0.61
2:D:242:LEU:CD2	2:D:242:LEU:H	2.13	0.61
1:A:339:TYR:OH	1:A:360:ASN:ND2	2.33	0.61
2:D:208:VAL:HG12	2:D:208:VAL:O	2.00	0.61
1:A:282:THR:OG1	1:A:283:VAL:N	2.34	0.61
1:A:291:HIS:C	1:A:297:HIS:CE1	2.78	0.61
1:A:356:ALA:O	1:A:372:LEU:HD11	2.00	0.61
1:C:212:TRP:HZ2	1:C:261:THR:HG23	1.65	0.61
1:C:296:GLN:HG3	2:E:246:ARG:C	2.26	0.61
1:C:183:VAL:HB	1:C:188:PHE:HZ	1.64	0.61
2:D:111:LYS:CB	2:D:112:GLY:HA2	2.30	0.61
2:F:171:VAL:CB	2:F:252:PHE:HD1	2.05	0.61
2:F:269:TYR:O	2:F:272:ILE:HG13	2.00	0.61
1:B:329:ARG:HD3	1:B:330:GLY:N	2.15	0.61
1:B:371:GLU:O	1:B:371:GLU:HG3	2.00	0.61
1:A:323:VAL:CG2	2:D:224:LYS:CE	2.67	0.61
2:D:143:ILE:HD12	2:D:157:MET:HE3	1.82	0.61
1:C:329:ARG:HD3	3:C:406:HOH:O	2.01	0.61
2:D:179:LEU:HD21	2:D:191:THR:CB	2.31	0.61
2:D:183:ASN:O	3:D:403:HOH:O	2.15	0.61
1:C:265:ILE:HG13	1:C:266:GLU:N	2.14	0.61
2:D:99:LYS:O	2:D:300:GLU:HB3	2.00	0.61
2:E:262:LEU:HD23	2:E:262:LEU:O	2.01	0.61
2:F:271:THR:O	2:F:271:THR:HG22	2.00	0.61
2:D:138:ASN:HA	2:D:233:PHE:HB3	1.83	0.61
2:D:68:VAL:CB	2:D:199:LEU:CD1	2.79	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:TRP:NE1	2:F:264:THR:HG23	1.91	0.60
1:B:264:MET:SD	1:B:268:TRP:CH2	2.93	0.60
2:D:175:LEU:CD2	2:D:179:LEU:HG	2.31	0.60
2:E:287:GLN:O	2:E:290:GLN:N	2.34	0.60
2:E:76:LEU:C	2:E:76:LEU:HD22	2.27	0.60
2:F:88:TYR:HH	2:F:293:LYS:H	1.35	0.60
2:F:171:VAL:CB	2:F:252:PHE:CE1	2.84	0.60
2:F:178:ALA:O	2:F:182:LEU:HB2	2.01	0.60
1:C:299:LYS:CE	3:C:407:HOH:O	2.48	0.60
2:D:232:LYS:HD2	2:D:232:LYS:O	2.01	0.60
2:E:262:LEU:O	2:E:263:LYS:HD2	2.00	0.60
2:F:118:ILE:CG2	2:F:284:ILE:HG21	2.29	0.60
2:F:143:ILE:HG22	2:F:144:TRP:N	2.17	0.60
1:A:202:MET:HG3	1:A:244:GLN:HA	1.83	0.60
2:E:105:ASP:OD2	2:E:107:SER:OG	2.09	0.60
2:F:144:TRP:HZ3	2:F:226:VAL:CA	2.14	0.60
1:A:354:ILE:HG22	1:A:355:PHE:CE2	2.37	0.60
1:A:274:ASP:OD1	2:D:220:LEU:CG	2.49	0.60
1:C:206:ILE:HD13	1:C:244:GLN:OE1	2.01	0.60
2:D:121:LEU:CD1	2:D:144:TRP:HE3	2.14	0.60
2:D:298:VAL:HG23	2:D:298:VAL:O	2.01	0.60
2:E:167:ASN:O	2:E:167:ASN:ND2	2.35	0.60
2:F:178:ALA:O	2:F:182:LEU:N	2.28	0.60
1:A:294:TYR:CE1	2:D:165:ILE:HG12	2.37	0.60
2:E:274:THR:HG21	3:E:409:HOH:O	2.02	0.60
1:A:211:PRO:HG3	1:A:230:LEU:HD13	1.84	0.59
2:D:147:LYS:CB	2:D:222:GLN:OE1	2.49	0.59
1:C:280:LYS:C	1:C:288:ALA:HB2	2.28	0.59
1:A:202:MET:CG	1:A:243:LEU:O	2.43	0.59
1:C:350:ASN:N	1:C:350:ASN:OD1	2.32	0.59
2:D:284:ILE:HG23	2:D:298:VAL:CG2	2.32	0.59
1:B:322:ASP:OD2	2:F:221:ASN:O	2.21	0.59
2:F:196:LEU:CG	3:F:429:HOH:O	2.29	0.59
1:A:357:ARG:O	1:A:359:ASN:N	2.29	0.59
1:A:358:ARG:H	1:A:372:LEU:CD2	2.08	0.59
2:E:121:LEU:CD1	2:E:149:LEU:HD13	2.32	0.59
1:A:183:VAL:HG23	1:A:183:VAL:O	2.01	0.59
1:A:195:GLN:OE1	1:A:201:LYS:O	2.21	0.59
2:D:162:PHE:CD1	2:D:232:LYS:HB2	2.36	0.59
2:E:76:LEU:HD22	2:E:76:LEU:O	2.02	0.59
2:E:107:SER:N	2:E:133:LYS:HE2	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:MET:O	2:F:160:LYS:O	2.21	0.59
1:C:297:HIS:CD2	2:E:166:GLU:OE1	2.56	0.59
2:D:124:LYS:O	2:D:126:LEU:HD23	2.02	0.59
2:F:79:TRP:HD1	2:F:80:LYS:N	2.01	0.59
2:F:163:THR:HG22	2:F:164:TYR:N	2.17	0.59
2:F:171:VAL:CG2	2:F:252:PHE:CE1	2.86	0.59
1:A:321:SER:OG	1:A:341:TYR:HE1	1.76	0.59
2:E:177:GLN:HE22	2:E:206:VAL:CA	2.12	0.59
2:F:118:ILE:HG12	2:F:284:ILE:CB	2.33	0.59
2:F:135:LEU:CD1	2:F:162:PHE:CE2	2.86	0.59
1:A:186:LEU:CD1	1:A:188:PHE:CD2	2.85	0.58
2:D:68:VAL:C	2:D:69:THR:HG23	2.28	0.58
2:F:125:ASP:C	2:F:128:ASN:ND2	2.59	0.58
1:A:292:GLY:HA2	1:A:297:HIS:HE1	0.48	0.58
1:B:293:PHE:CE2	2:F:244:HIS:CG	2.72	0.58
2:E:117:PHE:HD2	2:E:272:ILE:HD11	1.68	0.58
2:F:162:PHE:CE1	2:F:232:LYS:CG	2.87	0.58
1:A:357:ARG:C	1:A:359:ASN:H	2.11	0.58
1:B:292:GLY:O	1:B:297:HIS:NE2	2.36	0.58
1:C:293:PHE:CE2	1:C:294:TYR:CE2	2.82	0.58
2:D:97:VAL:CG2	2:D:109:TYR:OH	2.25	0.58
2:F:123:LYS:HE3	2:F:123:LYS:H	1.69	0.58
2:F:144:TRP:CD1	2:F:264:THR:HG1	2.21	0.58
1:A:321:SER:OG	1:A:341:TYR:CZ	2.32	0.58
2:E:101:ILE:HD12	2:E:101:ILE:H	1.67	0.58
1:B:191:LEU:HD23	1:B:368:ILE:HD11	1.81	0.58
1:B:212:TRP:CD2	1:B:257:LYS:HG3	2.38	0.58
1:C:296:GLN:OE1	2:E:247:THR:O	2.21	0.58
2:D:246:ARG:HB3	3:D:407:HOH:O	2.03	0.58
2:D:281:LEU:O	2:D:296:ILE:CD1	2.52	0.58
2:E:175:LEU:HD23	2:E:178:ALA:HB3	1.86	0.58
2:E:222:GLN:CD	2:E:224:LYS:NZ	2.62	0.58
2:E:112:GLY:HA2	2:E:134:LYS:O	2.04	0.58
2:F:125:ASP:CA	2:F:128:ASN:ND2	2.66	0.58
1:C:253:ALA:HB2	1:C:261:THR:HG21	1.86	0.58
2:D:182:LEU:CD2	2:D:183:ASN:H	2.08	0.58
2:E:90:THR:CG2	3:E:427:HOH:O	2.14	0.58
2:F:172:GLN:HG2	2:F:223:SER:O	1.98	0.58
1:A:198:HIS:CD2	2:E:231:ARG:CD	2.86	0.57
1:C:282:THR:O	1:C:283:VAL:HB	2.01	0.57
2:E:84:ASN:CB	3:E:417:HOH:O	2.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:ILE:HG22	2:F:284:ILE:CD1	2.33	0.57
2:F:167:ASN:O	2:F:168:LEU:HD13	2.03	0.57
1:B:281:LYS:HA	1:B:287:ILE:N	2.19	0.57
2:D:95:ILE:HG22	2:D:96:VAL:N	2.19	0.57
2:E:253:ASP:OD1	3:E:402:HOH:O	2.17	0.57
2:F:76:LEU:HD13	2:F:77:LEU:N	2.19	0.57
1:B:354:ILE:CG2	1:B:355:PHE:CE2	2.88	0.57
1:C:336:GLU:O	1:C:338:ILE:N	2.38	0.57
2:E:174:SER:O	2:E:177:GLN:HB3	2.03	0.57
2:F:116:ILE:HD11	2:F:282:MET:HE1	1.85	0.57
2:D:179:LEU:CD1	2:D:185:HIS:O	2.52	0.57
2:D:280:GLN:HA	2:D:280:GLN:OE1	2.03	0.57
2:E:75:VAL:HG12	2:E:75:VAL:O	2.05	0.57
2:E:174:SER:HB3	2:E:177:GLN:CB	2.34	0.57
1:A:281:LYS:HG3	1:A:285:GLY:O	2.04	0.57
1:A:211:PRO:CG	1:A:230:LEU:HB2	2.35	0.57
1:B:206:ILE:HG13	1:B:244:GLN:CG	2.33	0.57
2:E:121:LEU:HD12	2:E:121:LEU:C	2.30	0.57
2:E:283:GLU:HG2	2:E:286:ALA:CB	2.29	0.57
1:C:265:ILE:HD11	1:C:272:LEU:CD1	2.35	0.57
1:C:296:GLN:HG3	2:E:247:THR:O	2.04	0.57
1:C:299:LYS:HD3	2:E:250:VAL:CG1	2.34	0.57
2:D:281:LEU:O	2:D:296:ILE:HD13	2.05	0.57
2:E:211:LEU:CB	2:E:221:ASN:HA	2.35	0.57
1:C:293:PHE:O	2:E:245:GLN:HG2	2.02	0.56
2:D:286:ALA:O	2:D:299:CYS:HB3	2.05	0.56
2:D:102:LEU:O	2:D:102:LEU:HD22	2.06	0.56
2:E:116:ILE:HB	2:E:141:LEU:HD12	1.87	0.56
2:E:269:TYR:CD1	2:E:292:ARG:CD	2.85	0.56
2:F:122:PHE:CD1	2:F:123:LYS:N	2.74	0.56
2:F:159:ASN:HD21	2:F:160:LYS:NZ	2.02	0.56
1:A:236:GLN:CG	1:A:264:MET:HE2	2.35	0.56
1:A:250:PHE:CD1	1:A:250:PHE:N	2.73	0.56
1:A:281:LYS:H	1:A:327:GLU:HA	1.70	0.56
1:A:317:LYS:HD2	1:A:317:LYS:N	2.20	0.56
1:C:314:ARG:O	1:C:347:PRO:CD	2.46	0.56
1:C:338:ILE:O	1:C:341:TYR:HB2	2.06	0.56
2:D:94:LYS:O	2:D:95:ILE:HG13	2.04	0.56
2:E:100:LYS:HD2	2:E:100:LYS:H	1.70	0.56
1:A:368:ILE:HG23	1:A:368:ILE:O	2.05	0.56
2:F:167:ASN:OD1	2:F:226:VAL:HG13	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASP:HB3	1:C:315:PHE:HE2	1.70	0.56
1:C:330:GLY:O	1:C:333:GLN:HB2	2.05	0.56
2:D:253:ASP:CG	2:D:265:LYS:CE	2.68	0.56
2:E:168:LEU:HD11	2:E:250:VAL:HA	1.88	0.56
1:A:355:PHE:CD2	1:A:355:PHE:N	2.73	0.56
1:B:360:ASN:C	1:B:361:LEU:HD23	2.30	0.56
2:E:116:ILE:HD13	2:E:134:LYS:HD3	1.81	0.56
1:B:195:GLN:HE22	1:B:350:ASN:ND2	2.04	0.56
2:D:241:GLU:CB	2:D:243:ARG:CZ	2.84	0.56
2:D:242:LEU:N	2:D:242:LEU:HD22	2.21	0.56
2:E:78:GLN:O	2:E:265:LYS:NZ	2.36	0.56
2:E:144:TRP:NE1	2:E:264:THR:OG1	2.37	0.56
2:E:177:GLN:NE2	2:E:206:VAL:CA	2.69	0.56
2:E:253:ASP:HB3	2:E:265:LYS:HE3	1.87	0.56
2:E:286:ALA:O	2:E:299:CYS:HB2	2.06	0.56
2:F:283:GLU:O	2:F:298:VAL:CB	2.54	0.56
1:B:261:THR:O	1:B:265:ILE:HG13	2.05	0.56
1:B:328:ARG:NH1	1:B:328:ARG:HG3	2.20	0.56
2:D:270:GLN:O	2:D:274:THR:HG23	2.06	0.56
1:C:183:VAL:O	1:C:188:PHE:HE2	1.88	0.55
2:D:282:MET:HE3	2:D:298:VAL:HG11	1.88	0.55
1:B:327:GLU:HG2	1:B:328:ARG:N	2.09	0.55
1:A:186:LEU:HG	1:A:368:ILE:CD1	2.34	0.55
1:A:289:LYS:HG3	1:B:182:ASP:N	2.21	0.55
1:C:257:LYS:CA	1:C:260:VAL:CG2	2.84	0.55
1:C:357:ARG:HB2	1:C:359:ASN:OD1	2.06	0.55
2:D:143:ILE:HG22	2:D:144:TRP:N	2.22	0.55
1:B:206:ILE:CG1	1:B:244:GLN:CG	2.84	0.55
2:F:291:PRO:HB3	2:F:297:SER:HB2	1.88	0.55
2:D:126:LEU:HD23	2:D:126:LEU:N	2.20	0.55
1:A:355:PHE:HD2	1:A:355:PHE:N	2.05	0.55
1:B:293:PHE:C	1:B:293:PHE:CD2	2.85	0.55
1:C:315:PHE:CE2	1:C:346:CYS:SG	2.99	0.55
2:F:140:ILE:HG22	2:F:231:ARG:CB	2.36	0.55
2:F:151:ASN:OD1	2:F:151:ASN:N	2.40	0.55
2:F:151:ASN:O	2:F:152:GLU:OE1	2.25	0.55
1:B:232:ASP:HB3	1:B:236:GLN:HE22	1.71	0.55
1:B:264:MET:SD	1:B:268:TRP:CZ2	3.00	0.55
1:C:296:GLN:CG	2:E:246:ARG:C	2.80	0.55
2:D:181:GLU:O	2:D:181:GLU:HG3	2.05	0.55
1:C:202:MET:HE1	1:C:243:LEU:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:ASP:O	2:D:124:LYS:HE2	2.06	0.55
2:D:210:ASP:CB	2:D:223:SER:OG	2.55	0.55
1:A:211:PRO:HB3	1:A:228:ASP:HB3	1.79	0.55
1:B:195:GLN:HE22	1:B:350:ASN:HD22	1.54	0.55
2:E:106:LEU:HD12	2:E:134:LYS:CE	2.34	0.55
1:C:250:PHE:CE2	1:C:304:ILE:HD13	2.42	0.55
2:D:167:ASN:HD21	2:D:226:VAL:CG1	2.20	0.55
2:F:135:LEU:HD12	2:F:162:PHE:CE2	2.28	0.55
2:F:136:ILE:CG2	2:F:139:GLY:CA	2.85	0.55
1:A:292:GLY:CA	1:A:295:LEU:O	2.51	0.54
2:D:179:LEU:HD11	2:D:186:MET:O	2.06	0.54
2:D:134:LYS:CD	2:D:282:MET:SD	2.92	0.54
2:D:187:LYS:O	2:D:191:THR:HG22	2.07	0.54
2:F:134:LYS:HD3	2:F:134:LYS:C	2.31	0.54
1:A:211:PRO:CB	1:A:228:ASP:HB2	2.37	0.54
1:C:318:ASN:N	2:E:219:VAL:O	2.40	0.54
2:D:97:VAL:HG21	2:D:109:TYR:CE2	2.39	0.54
2:F:137:SER:O	2:F:232:LYS:CD	2.44	0.54
2:F:244:HIS:N	2:F:275:LEU:CB	2.71	0.54
1:B:327:GLU:CG	1:B:328:ARG:H	2.10	0.54
1:C:212:TRP:CE3	1:C:212:TRP:HA	2.42	0.54
2:F:100:LYS:C	2:F:104:THR:OG1	2.50	0.54
1:A:230:LEU:CD2	1:A:235:ILE:CD1	2.86	0.54
2:D:149:LEU:HD11	2:D:152:GLU:HG3	1.89	0.54
2:F:118:ILE:HD13	2:F:284:ILE:HD13	1.80	0.54
1:B:278:TRP:CZ2	1:B:335:PRO:HD3	2.42	0.54
1:C:272:LEU:N	1:C:272:LEU:HD22	2.21	0.54
2:D:127:LYS:O	2:D:127:LYS:HD3	2.08	0.54
2:E:110:ALA:HB1	2:E:111:LYS:HG2	1.89	0.54
2:F:94:LYS:NZ	2:F:94:LYS:HB3	2.22	0.54
1:A:323:VAL:HG23	2:D:224:LYS:HE2	1.80	0.54
2:D:126:LEU:O	2:D:129:LEU:HB2	2.07	0.54
2:E:117:PHE:HD2	2:E:272:ILE:CD1	2.20	0.54
2:E:253:ASP:CB	2:E:265:LYS:HE3	2.38	0.54
2:F:116:ILE:HG13	2:F:135:LEU:HD21	1.85	0.54
1:A:201:LYS:HE3	1:A:350:ASN:OD1	2.08	0.54
1:A:211:PRO:HD3	1:A:355:PHE:CD1	2.43	0.54
1:A:320:ALA:HB3	2:D:220:LEU:HD22	1.87	0.54
2:E:141:LEU:HD13	2:E:162:PHE:CE2	2.43	0.54
2:F:136:ILE:HG23	2:F:139:GLY:H	1.70	0.54
1:A:236:GLN:HG3	1:A:264:MET:HE2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:SER:C	2:D:224:LYS:HZ2	2.00	0.54
2:E:174:SER:O	2:E:178:ALA:N	2.40	0.54
1:A:322:ASP:OD1	2:D:220:LEU:HB3	2.08	0.54
1:B:253:ALA:HB2	1:B:261:THR:HG21	1.90	0.54
2:D:284:ILE:HA	2:D:298:VAL:HG22	1.90	0.54
1:A:288:ALA:CB	1:A:298:ALA:HB1	2.38	0.53
1:A:294:TYR:N	1:A:294:TYR:CD2	2.73	0.53
2:E:117:PHE:CD1	2:E:117:PHE:C	2.86	0.53
1:B:249:ILE:HG22	1:B:305:GLY:O	2.09	0.53
1:B:282:THR:H	1:B:287:ILE:H	1.57	0.53
1:C:286:LYS:HA	2:E:70:CYS:SG	2.48	0.53
1:C:297:HIS:NE2	2:E:166:GLU:OE1	2.41	0.53
1:C:321:SER:OG	2:E:208:VAL:CG2	2.56	0.53
1:C:363:ASP:O	1:C:364:ASN:HB2	2.08	0.53
2:D:247:THR:HG21	2:D:271:THR:HG23	1.91	0.53
2:D:282:MET:CE	2:D:298:VAL:HG11	2.38	0.53
2:F:164:TYR:CD1	2:F:164:TYR:C	2.86	0.53
2:F:283:GLU:O	2:F:298:VAL:HB	2.07	0.53
1:B:206:ILE:CD1	1:B:244:GLN:CD	2.79	0.53
1:C:204:ASP:OD1	1:C:204:ASP:N	2.37	0.53
2:F:281:LEU:O	2:F:295:TRP:HZ3	1.86	0.53
1:A:258:TYR:OH	1:A:275:GLU:CD	2.51	0.53
1:B:278:TRP:O	1:B:299:LYS:HA	2.07	0.53
1:C:331:GLN:HA	1:C:333:GLN:N	2.23	0.53
2:F:75:VAL:O	2:F:78:GLN:O	2.27	0.53
2:F:168:LEU:CD2	2:F:227:LEU:CD2	2.84	0.53
2:F:159:ASN:HD21	2:F:160:LYS:HZ1	1.55	0.53
1:B:345:LEU:C	1:B:345:LEU:HD13	2.34	0.53
1:C:238:MET:O	1:C:238:MET:HG3	2.08	0.53
1:C:249:ILE:CG2	1:C:270:TYR:CD1	2.90	0.53
1:C:249:ILE:CG2	1:C:270:TYR:CZ	2.80	0.53
2:E:98:LEU:N	2:E:109:TYR:HH	2.06	0.53
2:F:153:ILE:HD11	2:F:228:ILE:HG13	1.91	0.53
2:F:281:LEU:CB	2:F:295:TRP:CH2	2.80	0.53
1:B:191:LEU:O	1:B:195:GLN:HB2	2.08	0.53
1:C:183:VAL:O	1:C:188:PHE:CE2	2.61	0.53
2:E:226:VAL:HG12	2:E:227:LEU:N	2.23	0.53
2:F:101:ILE:CD1	2:F:106:LEU:CD2	2.86	0.53
1:A:198:HIS:HD2	2:E:231:ARG:NE	2.07	0.53
1:A:265:ILE:HD11	1:A:272:LEU:HD21	1.88	0.52
1:B:232:ASP:OD1	1:B:257:LYS:NZ	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PHE:HD1	1:B:304:ILE:HG23	1.73	0.52
1:C:320:ALA:O	2:E:220:LEU:CB	2.50	0.52
2:E:173:LEU:O	2:E:254:ILE:HG23	2.09	0.52
2:F:88:TYR:HD1	2:F:88:TYR:O	1.92	0.52
2:F:122:PHE:O	2:F:126:LEU:HB2	2.09	0.52
1:A:211:PRO:HD3	1:A:355:PHE:CE1	2.43	0.52
1:B:201:LYS:NZ	1:B:201:LYS:CB	2.73	0.52
2:D:233:PHE:CG	2:D:234:ASP:N	2.78	0.52
2:E:101:ILE:N	2:E:101:ILE:CD1	2.73	0.52
1:A:317:LYS:N	1:A:317:LYS:CD	2.73	0.52
1:B:281:LYS:HB3	1:B:286:LYS:CB	2.40	0.52
1:C:361:LEU:HD23	1:C:367:SER:OG	2.08	0.52
1:A:289:LYS:HZ1	1:B:186:LEU:CB	2.23	0.52
2:E:168:LEU:CD1	2:E:250:VAL:HA	2.39	0.52
1:A:231:SER:CB	1:A:234:LYS:NZ	2.73	0.52
2:D:175:LEU:O	2:D:175:LEU:HD22	2.09	0.52
2:D:242:LEU:CD2	2:D:242:LEU:N	2.73	0.52
2:F:267:TYR:N	2:F:267:TYR:CD2	2.74	0.52
1:A:213:GLN:HG3	1:A:231:SER:HA	1.92	0.52
1:A:238:MET:HE1	1:A:355:PHE:HZ	1.74	0.52
2:D:179:LEU:HD21	2:D:191:THR:HB	1.86	0.52
2:E:101:ILE:H	2:E:101:ILE:CD1	2.23	0.52
2:F:298:VAL:C	2:F:299:CYS:SG	2.93	0.52
2:F:221:ASN:OD1	2:F:221:ASN:N	2.42	0.52
1:A:329:ARG:HH22	1:A:333:GLN:NE2	2.01	0.52
1:C:204:ASP:OD2	1:C:349:GLY:HA3	2.10	0.52
2:E:100:LYS:N	2:E:100:LYS:CD	2.73	0.52
1:B:357:ARG:HB2	1:B:360:ASN:OD1	2.09	0.51
1:A:188:PHE:HD1	1:A:243:LEU:HD11	1.72	0.51
1:A:238:MET:HE1	1:A:355:PHE:CE2	2.45	0.51
2:D:91:ASP:HB2	2:D:291:PRO:O	2.11	0.51
2:D:99:LYS:O	2:D:300:GLU:CB	2.58	0.51
2:D:233:PHE:CD1	2:D:234:ASP:N	2.75	0.51
1:B:207:MET:CE	1:B:342:ILE:CD1	2.86	0.51
1:B:231:SER:O	1:B:235:ILE:HG12	2.10	0.51
2:D:140:ILE:HD11	2:D:142:PHE:HZ	1.72	0.51
2:D:171:VAL:HG22	2:D:224:LYS:CE	2.40	0.51
2:F:141:LEU:HG	2:F:162:PHE:CD2	2.46	0.51
2:F:143:ILE:CG2	2:F:144:TRP:N	2.73	0.51
1:A:207:MET:HA	1:A:250:PHE:O	2.11	0.51
1:A:211:PRO:O	1:A:211:PRO:CD	2.49	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ALA:O	1:A:372:LEU:HG	2.06	0.51
1:B:232:ASP:HB3	1:B:236:GLN:NE2	2.25	0.51
1:C:259:ARG:HA	1:C:262:ILE:HG13	1.92	0.51
1:B:294:TYR:HB2	2:F:166:GLU:HG3	1.92	0.51
1:C:299:LYS:HD3	2:E:250:VAL:HG11	1.92	0.51
2:D:99:LYS:O	2:D:300:GLU:CA	2.56	0.51
2:D:228:ILE:CG2	2:D:230:PHE:CE1	2.93	0.51
2:D:283:GLU:HG2	2:D:286:ALA:HB2	1.91	0.51
2:D:88:TYR:OH	2:D:293:LYS:HB3	2.11	0.51
2:D:223:SER:O	2:D:224:LYS:HG2	2.10	0.51
2:D:286:ALA:O	2:D:299:CYS:CB	2.59	0.51
1:A:198:HIS:CD2	2:E:231:ARG:HD3	2.45	0.51
1:A:240:ILE:HD12	1:A:240:ILE:N	2.25	0.51
1:A:299:LYS:HG2	2:D:249:ASP:OD2	2.10	0.51
1:C:293:PHE:CD2	1:C:294:TYR:CD2	2.98	0.51
2:D:284:ILE:HG23	2:D:298:VAL:HG23	1.93	0.51
1:C:272:LEU:N	1:C:272:LEU:CD2	2.73	0.51
2:D:136:ILE:CG2	2:D:137:SER:N	2.73	0.51
2:D:253:ASP:HB2	2:D:265:LYS:NZ	2.26	0.51
1:A:238:MET:HB2	1:A:240:ILE:CD1	2.40	0.51
1:A:273:VAL:HG13	1:A:274:ASP:N	2.26	0.51
1:A:274:ASP:OD2	2:D:218:LYS:HD2	2.08	0.51
1:A:289:LYS:HG2	1:A:290:GLY:N	2.26	0.51
1:C:296:GLN:N	2:E:248:PRO:O	2.44	0.51
1:C:316:LYS:HZ2	1:C:347:PRO:CG	2.11	0.51
2:D:146:ASP:OD1	2:D:225:GLN:HG3	2.06	0.51
2:D:261:CYS:C	2:D:262:LEU:HD23	2.35	0.51
2:E:253:ASP:HB2	2:E:265:LYS:CE	2.41	0.51
1:A:195:GLN:HE22	1:A:350:ASN:HD22	1.59	0.51
2:F:88:TYR:OH	2:F:292:ARG:CA	2.59	0.51
2:F:122:PHE:CD1	2:F:122:PHE:C	2.89	0.51
2:F:281:LEU:C	2:F:295:TRP:HZ3	2.17	0.51
1:B:328:ARG:HH11	1:B:328:ARG:HG3	1.75	0.50
2:D:280:GLN:O	2:D:281:LEU:HD23	2.11	0.50
1:A:254:ILE:CG1	1:A:257:LYS:HB2	2.36	0.50
1:A:350:ASN:OD1	1:A:350:ASN:N	2.41	0.50
2:D:187:LYS:O	2:D:191:THR:CG2	2.60	0.50
2:D:241:GLU:CB	2:D:243:ARG:NE	2.74	0.50
2:F:163:THR:CG2	2:F:164:TYR:N	2.74	0.50
2:F:165:ILE:C	2:F:166:GLU:HG2	2.37	0.50
1:A:192:ILE:CD1	1:A:242:SER:OG	2.57	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HE22	1:B:192:ILE:HD11	1.71	0.50
2:D:181:GLU:HA	2:D:182:LEU:C	2.35	0.50
2:E:286:ALA:O	2:E:299:CYS:CB	2.60	0.50
1:A:206:ILE:HA	1:A:352:LEU:O	2.12	0.50
1:B:248:PHE:CE1	1:B:304:ILE:CG2	2.95	0.50
1:C:211:PRO:HG2	1:C:230:LEU:HB2	1.92	0.50
2:D:255:VAL:HG23	3:D:404:HOH:O	2.11	0.50
2:F:269:TYR:H	2:F:269:TYR:HD2	1.58	0.50
1:A:358:ARG:N	1:A:372:LEU:HD23	2.09	0.50
1:B:279:VAL:HG23	1:B:325:PHE:HD2	1.76	0.50
1:C:250:PHE:CE2	1:C:304:ILE:CD1	2.95	0.50
2:D:136:ILE:CG2	2:D:137:SER:H	2.23	0.50
2:E:154:LEU:HD23	2:E:230:PHE:CE2	2.47	0.50
1:B:195:GLN:NE2	1:B:350:ASN:ND2	2.60	0.50
1:C:257:LYS:CB	1:C:260:VAL:CG2	2.86	0.50
2:F:244:HIS:N	2:F:244:HIS:ND1	2.60	0.50
1:B:248:PHE:CD1	1:B:304:ILE:HG23	2.47	0.50
1:B:326:SER:HG	1:B:335:PRO:HB3	1.74	0.50
2:D:95:ILE:CG2	2:D:96:VAL:N	2.75	0.50
2:F:101:ILE:CA	2:F:104:THR:HB	2.38	0.50
1:C:315:PHE:CD2	1:C:346:CYS:SG	3.02	0.49
1:C:330:GLY:C	1:C:333:GLN:HB2	2.37	0.49
2:D:127:LYS:C	2:D:127:LYS:CD	2.85	0.49
2:D:176:GLU:H	2:D:176:GLU:CD	2.06	0.49
2:F:101:ILE:O	2:F:104:THR:HB	2.12	0.49
1:A:186:LEU:CD1	1:A:187:ASN:C	2.85	0.49
2:F:256:ASN:C	2:F:257:ASN:OD1	2.55	0.49
1:B:246:ASP:OD1	1:B:309:ASP:O	2.30	0.49
2:D:159:ASN:O	2:D:159:ASN:ND2	2.45	0.49
2:E:76:LEU:C	2:E:76:LEU:CD2	2.85	0.49
2:F:118:ILE:HA	2:F:284:ILE:CB	2.22	0.49
2:F:297:SER:OG	2:F:299:CYS:SG	2.70	0.49
1:A:255:ASN:O	2:D:164:TYR:HE1	1.94	0.49
2:D:173:LEU:O	2:D:254:ILE:HA	2.11	0.49
2:F:79:TRP:CD1	2:F:80:LYS:N	2.80	0.49
1:A:198:HIS:HD2	2:E:231:ARG:CD	2.24	0.49
1:C:233:GLU:O	1:C:236:GLN:HB3	2.12	0.49
2:D:155:GLU:HA	2:D:158:GLU:HG2	1.94	0.49
1:C:250:PHE:HE2	1:C:304:ILE:CD1	2.25	0.49
1:A:289:LYS:CG	1:B:369:GLY:O	2.61	0.49
1:B:340:GLN:C	1:B:343:ASN:OD1	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LYS:CD	2:E:250:VAL:CG1	2.91	0.49
1:C:325:PHE:HB2	3:C:405:HOH:O	2.12	0.49
2:F:170:VAL:O	2:F:224:LYS:CB	2.59	0.49
2:F:262:LEU:O	2:F:263:LYS:C	2.53	0.49
1:B:256:ALA:HB1	3:B:416:HOH:O	1.95	0.49
1:C:211:PRO:CG	1:C:230:LEU:HB2	2.42	0.49
1:A:289:LYS:HZ2	1:B:186:LEU:HD13	0.61	0.49
1:C:354:ILE:CG2	1:C:355:PHE:CE2	2.96	0.49
2:D:88:TYR:OH	2:D:293:LYS:N	2.42	0.49
2:E:262:LEU:C	2:E:262:LEU:CD2	2.85	0.49
1:B:328:ARG:NH1	1:B:328:ARG:CG	2.73	0.49
1:C:340:GLN:O	1:C:344:GLN:HG3	2.13	0.49
2:D:71:ASP:OD1	2:D:71:ASP:N	2.45	0.49
2:F:76:LEU:CD1	2:F:76:LEU:C	2.86	0.49
1:A:353:GLU:HB2	1:A:365:TRP:HE3	1.71	0.48
1:C:212:TRP:HA	1:C:212:TRP:HE3	1.77	0.48
2:D:175:LEU:HD22	2:D:179:LEU:HG	1.94	0.48
2:E:253:ASP:CG	3:E:402:HOH:O	2.56	0.48
1:C:353:GLU:HG2	1:C:356:ALA:HB2	1.95	0.48
2:D:179:LEU:CD2	2:D:191:THR:CG2	2.89	0.48
2:E:219:VAL:HG13	2:E:220:LEU:HG	1.95	0.48
2:E:244:HIS:ND1	2:E:244:HIS:N	2.60	0.48
1:A:252:TRP:CZ3	1:A:300:GLU:HG2	2.48	0.48
1:C:343:ASN:O	1:C:346:CYS:C	2.56	0.48
2:D:242:LEU:CD1	2:D:277:PRO:HG3	2.43	0.48
2:F:122:PHE:HA	2:F:123:LYS:HE3	1.94	0.48
2:F:138:ASN:N	2:F:138:ASN:ND2	2.60	0.48
2:F:159:ASN:ND2	2:F:160:LYS:NZ	2.60	0.48
1:A:271:LYS:O	1:A:306:VAL:HG12	2.13	0.48
1:B:293:PHE:CE2	2:F:244:HIS:CB	2.95	0.48
1:C:207:MET:HA	1:C:250:PHE:O	2.13	0.48
2:F:269:TYR:CD2	2:F:269:TYR:N	2.76	0.48
1:B:314:ARG:H	1:B:314:ARG:HD3	1.77	0.48
2:F:121:LEU:CD1	2:F:153:ILE:CG2	2.92	0.48
2:F:281:LEU:HD12	2:F:294:GLY:O	2.13	0.48
1:C:336:GLU:O	1:C:337:GLU:C	2.52	0.48
1:C:352:LEU:HD12	1:C:366:VAL:HB	1.95	0.48
1:C:359:ASN:ND2	1:C:360:ASN:ND2	2.61	0.48
2:D:144:TRP:CZ2	2:D:268:ILE:HD11	2.39	0.48
2:D:165:ILE:C	2:D:166:GLU:HG2	2.38	0.48
2:E:107:SER:CA	2:E:133:LYS:NZ	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:ILE:HG13	2:F:135:LEU:HD22	1.94	0.48
1:A:249:ILE:C	1:A:250:PHE:CD1	2.92	0.48
1:A:289:LYS:CE	1:B:182:ASP:N	2.67	0.48
1:A:317:LYS:HD2	1:A:317:LYS:H	1.78	0.48
2:D:146:ASP:O	2:D:224:LYS:O	2.32	0.48
2:D:244:HIS:ND1	2:D:244:HIS:N	2.60	0.48
2:F:140:ILE:C	2:F:141:LEU:HD23	2.39	0.48
1:A:227:TYR:O	1:A:228:ASP:HB2	2.12	0.48
1:C:350:ASN:C	1:C:351:TYR:CD1	2.92	0.48
2:D:282:MET:HE3	2:D:298:VAL:CG1	2.43	0.48
2:E:165:ILE:HG22	2:E:166:GLU:HG2	1.96	0.48
2:F:196:LEU:CD2	3:F:429:HOH:O	2.24	0.48
1:A:282:THR:HG21	1:A:287:ILE:HB	1.95	0.48
1:C:325:PHE:HA	3:C:405:HOH:O	2.13	0.48
2:F:151:ASN:C	2:F:152:GLU:OE1	2.56	0.48
1:B:197:ARG:NH2	2:D:231:ARG:CG	2.42	0.48
2:F:122:PHE:N	2:F:126:LEU:CD1	2.73	0.48
2:F:268:ILE:H	2:F:268:ILE:HG12	1.53	0.48
1:A:192:ILE:HG23	1:A:202:MET:HE1	1.96	0.47
1:C:249:ILE:HG22	1:C:270:TYR:CD1	2.43	0.47
1:C:280:LYS:CB	1:C:288:ALA:HB2	2.39	0.47
2:E:232:LYS:O	2:E:233:PHE:CB	2.61	0.47
2:D:90:THR:HG22	2:D:91:ASP:N	2.29	0.47
1:C:317:LYS:HD3	2:E:213:LEU:CB	2.44	0.47
2:D:121:LEU:HG	2:D:146:ASP:HB2	1.96	0.47
1:A:203:PHE:CD1	1:A:352:LEU:HB2	2.49	0.47
2:F:116:ILE:HG22	2:F:284:ILE:HD12	1.97	0.47
2:F:177:GLN:NE2	2:F:209:LYS:CB	2.78	0.47
2:D:168:LEU:CD2	2:D:249:ASP:O	2.58	0.47
2:D:243:ARG:O	2:D:246:ARG:HB2	2.14	0.47
2:E:254:ILE:HG22	2:E:255:VAL:H	1.78	0.47
2:F:229:MET:HE3	2:F:229:MET:HB2	1.63	0.47
1:A:292:GLY:CA	1:A:297:HIS:ND1	2.61	0.47
1:C:315:PHE:HD2	1:C:346:CYS:HG	1.56	0.47
2:D:121:LEU:HD11	2:D:144:TRP:HE3	1.70	0.47
2:D:296:ILE:N	2:D:296:ILE:CD1	2.73	0.47
2:E:142:PHE:CZ	2:E:272:ILE:HG12	2.49	0.47
2:F:79:TRP:HD1	2:F:80:LYS:H	1.60	0.47
1:A:271:LYS:HB3	1:A:271:LYS:HE3	1.62	0.47
1:C:191:LEU:C	1:C:191:LEU:CD2	2.87	0.47
1:C:212:TRP:CE3	1:C:235:ILE:CD1	2.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:LYS:C	2:D:95:ILE:HG13	2.40	0.47
2:D:159:ASN:ND2	2:D:159:ASN:C	2.73	0.47
2:D:189:GLU:CB	2:D:192:GLU:HB2	2.44	0.47
2:E:152:GLU:O	2:E:156:THR:OG1	2.27	0.47
2:F:69:THR:N	2:F:199:LEU:HD22	2.30	0.47
2:F:168:LEU:HD21	2:F:229:MET:HE1	1.95	0.47
2:E:106:LEU:HD12	2:E:134:LYS:HE3	1.96	0.47
2:F:137:SER:OG	2:F:138:ASN:ND2	2.48	0.47
1:A:186:LEU:HD13	1:A:187:ASN:CA	2.43	0.47
1:B:249:ILE:HG12	1:B:250:PHE:N	2.29	0.47
1:B:293:PHE:C	1:B:293:PHE:HD2	2.22	0.47
1:C:293:PHE:HD2	1:C:294:TYR:CE2	2.32	0.47
1:A:231:SER:CB	1:A:234:LYS:HZ2	2.28	0.47
1:B:201:LYS:HZ2	1:B:201:LYS:CB	2.25	0.47
2:E:255:VAL:CG2	2:E:256:ASN:N	2.77	0.46
1:B:291:HIS:ND1	1:B:291:HIS:C	2.73	0.46
2:D:242:LEU:H	2:D:242:LEU:HD22	1.80	0.46
1:B:282:THR:HG23	1:B:287:ILE:C	2.41	0.46
2:F:168:LEU:HD21	2:F:227:LEU:HD22	1.95	0.46
2:F:291:PRO:HB3	2:F:297:SER:CB	2.45	0.46
1:B:189:GLN:NE2	1:B:192:ILE:CD1	2.73	0.46
1:C:183:VAL:HG23	1:C:184:THR:N	2.28	0.46
1:C:353:GLU:OE1	1:C:356:ALA:CA	2.52	0.46
1:C:363:ASP:O	1:C:365:TRP:HD1	1.97	0.46
2:D:138:ASN:ND2	2:D:138:ASN:C	2.73	0.46
2:D:179:LEU:CD1	2:D:186:MET:O	2.64	0.46
2:D:293:LYS:HG2	2:D:294:GLY:N	2.29	0.46
2:F:171:VAL:CG1	2:F:252:PHE:HD1	2.29	0.46
1:A:322:ASP:OD1	2:D:220:LEU:CB	2.63	0.46
1:C:277:THR:HG23	2:E:224:LYS:HE2	1.98	0.46
2:D:171:VAL:HG13	2:D:224:LYS:HE3	1.97	0.46
2:D:179:LEU:CD2	2:D:191:THR:CB	2.83	0.46
2:F:136:ILE:CD1	2:F:137:SER:N	2.73	0.46
2:F:288:LYS:HB2	2:F:288:LYS:HE2	1.70	0.46
1:A:211:PRO:HG3	1:A:230:LEU:HB2	1.98	0.46
1:A:231:SER:HB3	1:A:234:LYS:NZ	2.31	0.46
1:B:192:ILE:HG13	1:B:193:ASP:N	2.31	0.46
1:B:314:ARG:HH11	1:B:314:ARG:CG	2.14	0.46
2:E:100:LYS:H	2:E:100:LYS:CD	2.29	0.46
2:F:159:ASN:CG	2:F:160:LYS:NZ	2.73	0.46
2:F:265:LYS:HD3	2:F:265:LYS:HA	1.76	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASP:CG	2:E:222:GLN:CB	2.85	0.46
2:D:69:THR:HA	2:D:195:VAL:HG11	1.97	0.46
2:D:169:VAL:HG23	2:D:169:VAL:O	2.16	0.46
2:D:284:ILE:HG23	2:D:298:VAL:HG21	1.97	0.46
2:F:171:VAL:CG1	2:F:252:PHE:CD1	2.99	0.46
1:B:246:ASP:CG	1:B:309:ASP:H	2.14	0.46
1:C:321:SER:O	1:C:341:TYR:HE1	1.98	0.46
2:D:135:LEU:HD22	2:D:139:GLY:HA3	1.96	0.46
2:E:123:LYS:HD2	2:E:152:GLU:CB	2.45	0.46
2:F:129:LEU:HA	2:F:129:LEU:HD23	1.77	0.46
1:A:186:LEU:CD2	1:A:187:ASN:N	2.73	0.46
1:B:286:LYS:CB	1:B:325:PHE:CE2	2.99	0.46
2:E:222:GLN:CD	2:E:224:LYS:HZ2	2.13	0.46
2:F:116:ILE:CD1	2:F:282:MET:CE	2.93	0.46
1:B:232:ASP:CG	1:B:257:LYS:HZ2	2.21	0.46
2:E:167:ASN:ND2	2:E:167:ASN:C	2.73	0.46
2:F:192:GLU:CB	3:F:409:HOH:O	2.64	0.46
2:F:227:LEU:CD1	2:F:268:ILE:HG21	2.46	0.46
1:C:183:VAL:HB	1:C:188:PHE:CZ	2.48	0.45
1:C:315:PHE:HE2	1:C:346:CYS:SG	2.39	0.45
1:A:196:MET:O	1:A:200:GLY:N	2.48	0.45
1:A:277:THR:O	1:A:323:VAL:HA	2.16	0.45
1:B:189:GLN:HA	1:B:192:ILE:HG12	1.98	0.45
1:B:343:ASN:OD1	1:B:343:ASN:N	2.49	0.45
2:F:117:PHE:O	2:F:284:ILE:CD1	2.64	0.45
1:C:242:SER:HA	1:C:245:GLN:HE22	1.80	0.45
1:C:277:THR:CG2	2:E:224:LYS:HE2	2.46	0.45
2:E:175:LEU:HA	2:E:178:ALA:HB3	1.99	0.45
1:A:288:ALA:O	1:B:371:GLU:HA	2.16	0.45
1:B:317:LYS:O	2:F:219:VAL:O	2.35	0.45
1:C:239:PRO:O	1:C:243:LEU:HD13	2.16	0.45
1:C:357:ARG:HD2	3:C:409:HOH:O	2.16	0.45
2:E:135:LEU:HD23	2:E:135:LEU:HA	1.84	0.45
2:E:206:VAL:O	2:E:206:VAL:HG12	2.16	0.45
2:F:173:LEU:HG	2:F:253:ASP:O	2.16	0.45
2:F:262:LEU:N	2:F:262:LEU:CD2	2.73	0.45
1:A:188:PHE:HD1	1:A:243:LEU:HD21	1.82	0.45
1:A:202:MET:HG3	1:A:243:LEU:C	2.37	0.45
1:A:289:LYS:HG3	1:B:369:GLY:O	2.17	0.45
1:A:329:ARG:HE	1:A:333:GLN:HG2	1.82	0.45
1:B:230:LEU:HG	1:B:235:ILE:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLN:C	1:C:195:GLN:CD	2.85	0.45
2:D:146:ASP:OD1	2:D:146:ASP:O	2.35	0.45
2:E:114:GLN:O	2:E:139:GLY:CA	2.64	0.45
1:A:273:VAL:CG1	1:A:274:ASP:N	2.80	0.45
1:A:357:ARG:C	1:A:359:ASN:N	2.73	0.45
1:B:327:GLU:OE2	1:B:328:ARG:HG3	2.17	0.45
2:D:284:ILE:HA	2:D:298:VAL:HG23	1.97	0.45
2:F:101:ILE:C	2:F:104:THR:H	2.24	0.45
1:A:260:VAL:O	1:A:263:LYS:HB3	2.17	0.45
1:C:248:PHE:CD2	1:C:345:LEU:HD21	2.52	0.45
2:D:97:VAL:HB	2:D:298:VAL:HA	1.99	0.45
1:B:248:PHE:CD1	1:B:304:ILE:CG2	3.00	0.45
1:C:317:LYS:O	1:C:318:ASN:CB	2.64	0.45
2:D:122:PHE:O	2:D:122:PHE:HD1	2.00	0.45
2:F:79:TRP:CD1	2:F:80:LYS:H	2.33	0.45
2:F:88:TYR:O	2:F:88:TYR:CD1	2.70	0.45
2:F:266:GLU:O	2:F:270:GLN:NE2	2.50	0.45
1:A:201:LYS:NZ	1:A:204:ASP:CG	2.75	0.45
1:A:297:HIS:CD2	2:D:166:GLU:OE2	2.69	0.45
1:C:196:MET:HE3	1:C:196:MET:HB2	1.67	0.45
1:C:201:LYS:HB2	1:C:201:LYS:HE2	1.84	0.45
1:C:206:ILE:CG1	1:C:249:ILE:HG13	2.47	0.45
1:C:258:TYR:O	1:C:261:THR:OG1	2.30	0.45
1:C:265:ILE:HD11	1:C:272:LEU:HD21	1.98	0.45
1:A:329:ARG:NH2	1:A:333:GLN:OE1	2.47	0.44
1:B:264:MET:HG3	1:B:265:ILE:N	2.32	0.44
1:C:322:ASP:OD2	1:C:322:ASP:N	2.50	0.44
1:A:236:GLN:HG2	1:A:264:MET:HE2	1.98	0.44
1:A:287:ILE:CG2	1:B:371:GLU:CA	2.93	0.44
1:B:279:VAL:CG2	1:B:325:PHE:CD2	2.99	0.44
1:B:320:ALA:C	2:F:220:LEU:CD2	2.72	0.44
2:D:88:TYR:CE1	2:D:90:THR:O	2.70	0.44
2:D:143:ILE:HG22	2:D:144:TRP:H	1.81	0.44
1:A:210:PRO:O	1:A:212:TRP:CD1	2.71	0.44
1:B:276:ILE:O	1:B:276:ILE:HG22	2.17	0.44
1:C:257:LYS:C	1:C:260:VAL:CG2	2.90	0.44
1:C:336:GLU:C	1:C:338:ILE:N	2.74	0.44
2:D:246:ARG:HD2	2:D:246:ARG:HA	1.57	0.44
2:F:173:LEU:HD12	2:F:254:ILE:CG1	2.48	0.44
1:A:325:PHE:O	1:A:325:PHE:CD1	2.71	0.44
1:C:248:PHE:HD1	1:C:305:GLY:O	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASN:O	1:C:351:TYR:CD1	2.70	0.44
2:E:268:ILE:O	2:E:272:ILE:HG13	2.18	0.44
1:B:211:PRO:HB2	1:B:228:ASP:O	2.18	0.44
1:B:230:LEU:HG	1:B:235:ILE:CD1	2.47	0.44
1:C:181:SER:OG	1:C:182:ASP:N	2.50	0.44
1:C:350:ASN:O	1:C:351:TYR:HD1	2.01	0.44
2:D:120:ASN:ND2	2:D:123:LYS:CA	2.73	0.44
1:A:211:PRO:CD	1:A:355:PHE:CE1	3.00	0.44
1:A:289:LYS:CD	1:A:291:HIS:CB	2.89	0.44
1:B:295:LEU:CD1	1:B:296:GLN:H	2.31	0.44
1:A:331:GLN:HA	1:A:332:SER:HA	1.62	0.44
1:A:353:GLU:HB2	1:A:365:TRP:HZ3	1.79	0.44
1:B:331:GLN:HA	1:B:332:SER:HA	1.71	0.44
2:E:196:LEU:H	2:E:196:LEU:CD2	2.02	0.44
2:F:219:VAL:O	2:F:220:LEU:HD23	2.18	0.44
1:B:295:LEU:HG	2:F:168:LEU:HD12	1.99	0.44
2:D:100:LYS:HD2	2:D:100:LYS:HA	1.73	0.44
2:F:118:ILE:HG23	2:F:284:ILE:HG22	1.94	0.44
1:B:203:PHE:CZ	1:B:352:LEU:HD13	2.53	0.44
2:E:146:ASP:HB3	2:E:147:LYS:H	1.66	0.44
2:E:253:ASP:CB	2:E:265:LYS:CE	2.96	0.44
2:F:128:ASN:ND2	2:F:128:ASN:H	2.15	0.44
2:F:136:ILE:CG1	2:F:137:SER:N	2.80	0.44
1:A:277:THR:CG2	1:A:299:LYS:HE2	2.48	0.43
1:C:204:ASP:HB3	1:C:315:PHE:CZ	2.53	0.43
2:E:174:SER:O	2:E:177:GLN:CB	2.66	0.43
2:E:267:TYR:CD1	2:E:267:TYR:C	2.96	0.43
2:F:123:LYS:HE3	2:F:123:LYS:N	2.33	0.43
2:F:280:GLN:C	2:F:281:LEU:HG	2.43	0.43
1:A:211:PRO:CD	1:A:355:PHE:HE1	2.32	0.43
1:B:295:LEU:HD12	2:F:249:ASP:HA	1.99	0.43
2:F:88:TYR:OH	2:F:292:ARG:C	2.58	0.43
1:A:210:PRO:HB3	1:A:235:ILE:HG21	2.00	0.43
2:E:105:ASP:OD2	2:E:107:SER:CB	2.66	0.43
2:F:141:LEU:O	2:F:142:PHE:CD1	2.70	0.43
1:A:354:ILE:O	1:A:355:PHE:HB2	2.18	0.43
1:B:259:ARG:HA	1:B:259:ARG:HD2	1.80	0.43
2:D:113:VAL:O	2:D:113:VAL:HG23	2.19	0.43
2:D:124:LYS:H	2:D:124:LYS:CD	2.31	0.43
2:D:251:LEU:C	2:D:252:PHE:HD1	2.26	0.43
2:F:274:THR:O	2:F:275:LEU:CB	2.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PRO:HB2	1:A:228:ASP:HB2	1.94	0.43
1:A:240:ILE:N	1:A:240:ILE:CD1	2.81	0.43
2:D:124:LYS:H	2:D:124:LYS:HD2	1.83	0.43
2:F:167:ASN:OD1	2:F:227:LEU:O	2.36	0.43
2:F:298:VAL:C	2:F:299:CYS:HG	2.26	0.43
2:D:88:TYR:OH	2:D:293:LYS:HB2	2.18	0.43
2:E:243:ARG:NH2	2:E:274:THR:HA	2.31	0.43
2:E:254:ILE:HG22	2:E:255:VAL:N	2.33	0.43
2:F:184:LYS:HA	2:F:185:HIS:HA	1.76	0.43
2:F:227:LEU:HD23	2:F:228:ILE:N	2.34	0.43
1:B:273:VAL:HG22	1:B:273:VAL:O	2.18	0.43
1:C:299:LYS:CD	2:E:250:VAL:HG11	2.48	0.43
2:D:146:ASP:HA	2:D:225:GLN:HG2	2.00	0.43
2:D:175:LEU:HB2	2:D:254:ILE:HG22	2.00	0.43
2:E:242:LEU:CB	2:E:277:PRO:CG	2.87	0.43
2:E:242:LEU:O	2:E:243:ARG:C	2.62	0.43
2:F:123:LYS:H	2:F:123:LYS:CE	2.30	0.43
1:B:197:ARG:O	1:B:197:ARG:HG2	2.19	0.43
1:B:261:THR:HA	1:B:264:MET:HG2	2.00	0.43
2:D:91:ASP:OD1	2:D:91:ASP:O	2.36	0.43
2:D:277:PRO:HD2	2:D:278:LYS:NZ	2.33	0.43
2:F:88:TYR:OH	2:F:292:ARG:HA	2.19	0.43
1:A:212:TRP:O	1:A:213:GLN:C	2.62	0.43
1:B:277:THR:HG21	2:F:169:VAL:HG21	2.01	0.43
1:C:283:VAL:CG2	1:C:327:GLU:CD	2.89	0.43
2:E:218:LYS:HA	2:E:218:LYS:HD3	1.86	0.43
1:A:241:GLN:HG2	1:A:268:TRP:O	2.19	0.42
1:A:250:PHE:N	1:A:250:PHE:HD1	2.14	0.42
1:A:263:LYS:CG	1:A:267:ASN:HD21	2.21	0.42
1:A:289:LYS:HD3	1:A:291:HIS:H	1.84	0.42
1:B:322:ASP:CB	2:F:224:LYS:HE3	2.49	0.42
1:C:189:GLN:HA	1:C:192:ILE:HD12	2.00	0.42
1:C:333:GLN:HG2	1:C:359:ASN:HD22	1.83	0.42
1:A:211:PRO:HG2	1:A:235:ILE:HD11	2.01	0.42
1:A:299:LYS:HE2	1:A:299:LYS:HB2	1.68	0.42
1:C:208:MET:HE2	1:C:355:PHE:HE2	1.84	0.42
2:E:269:TYR:HD1	2:E:292:ARG:CD	2.31	0.42
1:A:293:PHE:C	1:A:294:TYR:HD2	2.27	0.42
1:C:271:LYS:O	1:C:306:VAL:HG12	2.20	0.42
2:E:144:TRP:CZ2	2:E:268:ILE:HG13	2.54	0.42
2:F:94:LYS:HB3	2:F:94:LYS:HZ3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:PHE:O	2:F:245:GLN:CA	2.67	0.42
1:B:356:ALA:HB2	1:B:367:SER:OG	2.20	0.42
2:E:154:LEU:HD23	2:E:230:PHE:HE2	1.84	0.42
2:F:182:LEU:HD23	2:F:182:LEU:C	2.44	0.42
2:F:256:ASN:CG	2:F:257:ASN:OD1	2.61	0.42
1:B:193:ASP:O	1:B:197:ARG:HB3	2.19	0.42
1:C:325:PHE:CE1	2:E:204:GLN:HG3	2.50	0.42
1:C:325:PHE:HD1	2:E:204:GLN:HG3	1.73	0.42
2:E:140:ILE:CD1	2:E:276:LEU:HD11	2.49	0.42
2:F:226:VAL:CG1	2:F:227:LEU:N	2.83	0.42
1:B:289:LYS:O	1:B:297:HIS:O	2.38	0.42
1:C:324:ILE:HG22	1:C:326:SER:H	1.85	0.42
2:D:127:LYS:CA	2:D:160:LYS:NZ	2.81	0.42
2:D:203:GLN:O	2:D:206:VAL:N	2.37	0.42
2:D:284:ILE:O	2:D:285:PHE:HB2	2.19	0.42
2:E:76:LEU:HD23	2:E:80:LYS:HD2	2.01	0.42
1:C:183:VAL:HG21	1:C:355:PHE:CE1	2.55	0.42
1:C:322:ASP:CG	2:E:222:GLN:HG3	2.42	0.42
2:D:109:TYR:HE2	2:D:296:ILE:HG23	1.71	0.42
2:E:99:LYS:O	2:E:101:ILE:CD1	2.66	0.42
2:F:99:LYS:HD2	2:F:106:LEU:HB3	2.02	0.42
2:F:162:PHE:HB3	2:F:230:PHE:HB3	2.02	0.42
2:F:266:GLU:O	2:F:269:TYR:HD2	2.02	0.42
2:F:293:LYS:O	2:F:293:LYS:HG3	2.20	0.42
1:B:259:ARG:NH2	1:B:263:LYS:HG2	2.35	0.42
2:F:124:LYS:O	2:F:127:LYS:HB2	2.20	0.42
2:F:147:LYS:CB	2:F:222:GLN:CD	2.92	0.42
1:B:205:VAL:CG1	1:B:250:PHE:CE1	3.02	0.42
1:B:293:PHE:CD2	2:F:244:HIS:HB2	2.54	0.42
1:C:242:SER:C	1:C:245:GLN:NE2	2.73	0.42
2:D:122:PHE:HB3	2:D:124:LYS:HG3	2.02	0.42
2:D:144:TRP:NE1	2:D:227:LEU:HD13	2.34	0.42
1:B:276:ILE:CG1	1:B:304:ILE:HD11	2.50	0.41
1:C:317:LYS:HA	2:E:219:VAL:HG23	2.02	0.41
1:A:211:PRO:HG2	1:A:230:LEU:HB2	2.01	0.41
1:A:230:LEU:HD22	1:A:235:ILE:HD11	1.99	0.41
1:A:288:ALA:HB2	1:A:298:ALA:HB1	2.00	0.41
1:A:291:HIS:C	1:A:297:HIS:HE1	2.23	0.41
1:C:183:VAL:CG2	1:C:184:THR:N	2.82	0.41
2:E:110:ALA:HA	2:E:111:LYS:HA	1.69	0.41
2:F:116:ILE:CD1	2:F:282:MET:HE2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:CD1	1:A:187:ASN:N	2.79	0.41
2:D:251:LEU:HD23	2:D:251:LEU:HA	1.89	0.41
2:F:122:PHE:H	2:F:126:LEU:HD11	1.80	0.41
1:A:259:ARG:HD2	1:A:259:ARG:C	2.46	0.41
1:A:338:ILE:O	1:A:341:TYR:HB2	2.20	0.41
1:A:356:ALA:C	1:A:372:LEU:CD2	2.48	0.41
2:F:185:HIS:HA	2:F:186:MET:HA	1.86	0.41
1:B:206:ILE:HD11	1:B:244:GLN:HG2	1.92	0.41
1:B:235:ILE:HG12	1:B:235:ILE:H	1.64	0.41
1:B:326:SER:HB2	1:B:335:PRO:HB3	1.99	0.41
2:F:283:GLU:HB3	2:F:297:SER:HA	2.02	0.41
1:B:201:LYS:HB2	1:B:201:LYS:NZ	2.26	0.41
1:C:294:TYR:HA	2:E:245:GLN:HA	2.02	0.41
1:C:312:ASN:OD1	1:C:312:ASN:N	2.53	0.41
1:C:337:GLU:O	1:C:341:TYR:HD2	2.04	0.41
2:D:173:LEU:O	2:D:255:VAL:HG13	2.21	0.41
2:E:154:LEU:HD21	2:E:164:TYR:CD2	2.55	0.41
2:E:283:GLU:HG3	2:E:284:ILE:N	2.35	0.41
1:B:292:GLY:O	1:B:297:HIS:HD2	1.95	0.41
1:C:193:ASP:O	1:C:197:ARG:CG	2.65	0.41
1:C:257:LYS:HA	1:C:260:VAL:CG2	2.50	0.41
1:C:327:GLU:CG	1:C:328:ARG:N	2.84	0.41
2:D:75:VAL:HG22	2:D:251:LEU:HD22	2.03	0.41
2:D:243:ARG:HE	2:D:246:ARG:HG2	1.86	0.41
2:D:269:TYR:CD1	2:D:292:ARG:HD3	2.55	0.41
1:A:206:ILE:O	1:A:249:ILE:HG13	2.20	0.41
1:B:338:ILE:O	1:B:342:ILE:CG1	2.59	0.41
2:D:73:LEU:O	2:D:76:LEU:O	2.39	0.41
2:E:101:ILE:CG2	2:E:129:LEU:HD11	2.51	0.41
2:E:121:LEU:HD22	2:E:145:SER:C	2.45	0.41
2:F:196:LEU:HG	3:F:413:HOH:O	2.20	0.41
1:B:188:PHE:HZ	1:B:238:MET:HE3	1.86	0.41
1:B:278:TRP:NE1	1:B:326:SER:OG	2.54	0.41
2:D:76:LEU:HD23	2:D:76:LEU:HA	1.88	0.41
2:D:144:TRP:CD1	2:D:227:LEU:HD12	2.56	0.41
2:D:284:ILE:HG12	2:D:298:VAL:HG21	2.02	0.41
2:E:106:LEU:C	2:E:133:LYS:CE	2.92	0.41
2:E:196:LEU:N	2:E:196:LEU:CD2	2.73	0.41
2:F:117:PHE:O	2:F:284:ILE:HD12	2.21	0.41
2:F:281:LEU:CA	2:F:295:TRP:CZ3	3.03	0.41
1:B:232:ASP:CG	1:B:257:LYS:NZ	2.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:O	1:B:327:GLU:CD	2.64	0.41
1:C:246:ASP:OD1	1:C:308:GLY:CA	2.66	0.41
1:C:330:GLY:O	1:C:332:SER:O	2.39	0.41
2:D:147:LYS:O	2:D:222:GLN:OE1	2.39	0.41
2:F:168:LEU:CD2	2:F:168:LEU:N	2.73	0.41
1:A:235:ILE:O	1:A:238:MET:SD	2.79	0.40
2:D:75:VAL:HG22	2:D:252:PHE:H	1.78	0.40
2:D:138:ASN:C	2:D:138:ASN:HD22	2.22	0.40
1:B:338:ILE:HD12	1:B:338:ILE:HA	1.80	0.40
2:E:134:LYS:NZ	2:E:284:ILE:HD11	2.33	0.40
1:A:282:THR:CG2	1:A:287:ILE:HB	2.51	0.40
1:C:277:THR:OG1	1:C:323:VAL:HG12	2.22	0.40
2:D:95:ILE:HB	2:D:296:ILE:HG23	2.03	0.40
2:E:129:LEU:HD23	2:E:129:LEU:HA	1.76	0.40
2:E:261:CYS:O	2:E:261:CYS:SG	2.78	0.40
2:F:94:LYS:NZ	2:F:94:LYS:CB	2.83	0.40
1:A:295:LEU:HD12	2:D:166:GLU:HB3	2.03	0.40
1:C:321:SER:OG	2:E:208:VAL:HG23	2.22	0.40
2:D:167:ASN:HD22	2:D:167:ASN:HA	1.74	0.40
2:F:142:PHE:CA	2:F:143:ILE:HD12	2.34	0.40
2:F:143:ILE:CD1	2:F:143:ILE:N	2.73	0.40
2:F:226:VAL:HG12	2:F:227:LEU:N	2.35	0.40
1:B:207:MET:HA	1:B:250:PHE:O	2.22	0.40
1:B:293:PHE:O	1:B:293:PHE:HD2	2.04	0.40
2:D:144:TRP:HE1	2:D:227:LEU:HD13	1.86	0.40
2:D:146:ASP:CA	2:D:225:GLN:HG2	2.51	0.40
2:E:231:ARG:NH2	2:E:231:ARG:CG	2.73	0.40
2:F:136:ILE:O	2:F:232:LYS:HE3	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:HIS:O	2:F:246:ARG:NH2[1_545]	1.87	0.33
2:D:102:LEU:CD1	3:B:422:HOH:O[2_646]	2.07	0.13
1:B:291:HIS:O	1:C:367:SER:O[1_565]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	174/202 (86%)	163 (94%)	11 (6%)	0	100	100
1	B	174/202 (86%)	168 (97%)	6 (3%)	0	100	100
1	C	170/202 (84%)	162 (95%)	8 (5%)	0	100	100
2	D	203/237 (86%)	187 (92%)	15 (7%)	1 (0%)	24	57
2	E	201/237 (85%)	189 (94%)	9 (4%)	3 (2%)	8	32
2	F	174/237 (73%)	166 (95%)	8 (5%)	0	100	100
All	All	1096/1317 (83%)	1035 (94%)	57 (5%)	4 (0%)	30	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	247	THR
2	E	290	GLN
2	E	291	PRO
2	D	290	GLN

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	148/178 (83%)	117 (79%)	31 (21%)	1	5
1	B	149/178 (84%)	118 (79%)	31 (21%)	1	5
1	C	149/178 (84%)	116 (78%)	33 (22%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	169/225 (75%)	119 (70%)	50 (30%)	0	1
2	E	162/225 (72%)	114 (70%)	48 (30%)	0	1
2	F	140/225 (62%)	91 (65%)	49 (35%)	0	0
All	All	917/1209 (76%)	675 (74%)	242 (26%)	0	2

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	196	MET
1	A	202	MET
1	A	228	ASP
1	A	230	LEU
1	A	234	LYS
1	A	246	ASP
1	A	250	PHE
1	A	254	ILE
1	A	272	LEU
1	A	274	ASP
1	A	279	VAL
1	A	282	THR
1	A	287	ILE
1	A	289	LYS
1	A	293	PHE
1	A	294	TYR
1	A	303	LEU
1	A	306	VAL
1	A	317	LYS
1	A	326	SER
1	A	328	ARG
1	A	343	ASN
1	A	344	GLN
1	A	345	LEU
1	A	350	ASN
1	A	355	PHE
1	A	357	ARG
1	A	362	HIS
1	A	368	ILE
1	A	371	GLU
1	B	189	GLN
1	B	192	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	GLN
1	B	201	LYS
1	B	228	ASP
1	B	230	LEU
1	B	240	ILE
1	B	245	GLN
1	B	246	ASP
1	B	249	ILE
1	B	260	VAL
1	B	263	LYS
1	B	264	MET
1	B	272	LEU
1	B	277	THR
1	B	291	HIS
1	B	293	PHE
1	B	295	LEU
1	B	314	ARG
1	B	317	LYS
1	B	318	ASN
1	B	323	VAL
1	B	325	PHE
1	B	328	ARG
1	B	331	GLN
1	B	338	ILE
1	B	342	ILE
1	B	352	LEU
1	B	354	ILE
1	B	360	ASN
1	B	367	SER
1	C	182	ASP
1	C	185	LYS
1	C	186	LEU
1	C	189	GLN
1	C	204	ASP
1	C	208	MET
1	C	230	LEU
1	C	241	GLN
1	C	246	ASP
1	C	249	ILE
1	C	251	VAL
1	C	254	ILE
1	C	259	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	260	VAL
1	C	261	THR
1	C	274	ASP
1	C	280	LYS
1	C	299	LYS
1	C	301	SER
1	C	311	ASP
1	C	312	ASN
1	C	316	LYS
1	C	322	ASP
1	C	326	SER
1	C	333	GLN
1	C	345	LEU
1	C	346	CYS
1	C	350	ASN
1	C	352	LEU
1	C	360	ASN
1	C	362	HIS
1	C	368	ILE
1	C	372	LEU
2	D	66	ASP
2	D	71	ASP
2	D	73	LEU
2	D	89	GLU
2	D	100	LYS
2	D	102	LEU
2	D	104	THR
2	D	107	SER
2	D	108	GLN
2	D	120	ASN
2	D	124	LYS
2	D	126	LEU
2	D	127	LYS
2	D	129	LEU
2	D	131	ILE
2	D	135	LEU
2	D	137	SER
2	D	138	ASN
2	D	140	ILE
2	D	143	ILE
2	D	148	SER
2	D	150	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	157	MET
2	D	158	GLU
2	D	159	ASN
2	D	165	ILE
2	D	167	ASN
2	D	169	VAL
2	D	175	LEU
2	D	181	GLU
2	D	182	LEU
2	D	186	MET
2	D	191	THR
2	D	192	GLU
2	D	199	LEU
2	D	224	LYS
2	D	229	MET
2	D	234	ASP
2	D	242	LEU
2	D	243	ARG
2	D	246	ARG
2	D	249	ASP
2	D	256	ASN
2	D	263	LYS
2	D	264	THR
2	D	279	SER
2	D	292	ARG
2	D	296	ILE
2	D	297	SER
2	D	300	GLU
2	E	73	LEU
2	E	76	LEU
2	E	79	TRP
2	E	88	TYR
2	E	101	ILE
2	E	102	LEU
2	E	105	ASP
2	E	113	VAL
2	E	131	ILE
2	E	133	LYS
2	E	146	ASP
2	E	148	SER
2	E	149	LEU
2	E	166	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	167	ASN
2	E	175	LEU
2	E	177	GLN
2	E	181	GLU
2	E	183	ASN
2	E	196	LEU
2	E	197	ASP
2	E	199	LEU
2	E	205	LYS
2	E	212	ILE
2	E	220	LEU
2	E	227	LEU
2	E	228	ILE
2	E	243	ARG
2	E	244	HIS
2	E	245	GLN
2	E	247	THR
2	E	253	ASP
2	E	256	ASN
2	E	262	LEU
2	E	264	THR
2	E	265	LYS
2	E	266	GLU
2	E	270	GLN
2	E	274	THR
2	E	279	SER
2	E	283	GLU
2	E	287	GLN
2	E	288	LYS
2	E	289	ASP
2	E	292	ARG
2	E	293	LYS
2	E	297	SER
2	E	300	GLU
2	F	76	LEU
2	F	89	GLU
2	F	90	THR
2	F	91	ASP
2	F	94	LYS
2	F	102	LEU
2	F	106	LEU
2	F	120	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	123	LYS
2	F	124	LYS
2	F	127	LYS
2	F	128	ASN
2	F	133	LYS
2	F	136	ILE
2	F	138	ASN
2	F	140	ILE
2	F	141	LEU
2	F	143	ILE
2	F	144	TRP
2	F	149	LEU
2	F	150	ILE
2	F	151	ASN
2	F	152	GLU
2	F	168	LEU
2	F	172	GLN
2	F	186	MET
2	F	188	ILE
2	F	196	LEU
2	F	199	LEU
2	F	221	ASN
2	F	224	LYS
2	F	229	MET
2	F	244	HIS
2	F	246	ARG
2	F	249	ASP
2	F	257	ASN
2	F	262	LEU
2	F	264	THR
2	F	265	LYS
2	F	268	ILE
2	F	269	TYR
2	F	270	GLN
2	F	272	ILE
2	F	273	GLU
2	F	278	LYS
2	F	281	LEU
2	F	288	LYS
2	F	292	ARG
2	F	293	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	267	ASN
1	A	333	GLN
1	A	360	ASN
1	B	189	GLN
1	B	195	GLN
1	B	244	GLN
1	B	267	ASN
1	B	296	GLN
1	B	297	HIS
1	B	312	ASN
1	B	331	GLN
1	B	350	ASN
1	C	189	GLN
1	C	236	GLN
1	C	241	GLN
1	C	245	GLN
1	C	255	ASN
1	C	333	GLN
1	C	359	ASN
2	D	114	GLN
2	D	159	ASN
2	D	167	ASN
2	D	225	GLN
2	D	290	GLN
2	E	72	ASN
2	E	114	GLN
2	E	177	GLN
2	E	183	ASN
2	E	225	GLN
2	E	245	GLN
2	F	128	ASN
2	F	138	ASN
2	F	244	HIS
2	F	270	GLN
2	F	290	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	178/202 (88%)	0.86	19 (10%) 11 6	37, 57, 85, 115	0
1	B	178/202 (88%)	0.83	13 (7%) 21 11	36, 57, 81, 101	0
1	C	176/202 (87%)	1.10	23 (13%) 7 4	43, 68, 95, 111	0
2	D	215/237 (90%)	0.94	26 (12%) 8 5	31, 54, 81, 111	0
2	E	213/237 (89%)	1.35	39 (18%) 3 1	45, 73, 99, 125	0
2	F	192/237 (81%)	1.78	63 (32%) 1 0	53, 83, 104, 120	0
All	All	1152/1317 (87%)	1.15	183 (15%) 5 2	31, 65, 97, 125	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	284	ILE	11.6
2	F	115	GLY	7.6
2	F	118	ILE	7.3
2	F	150	ILE	6.6
2	F	116	ILE	6.3
1	A	185	LYS	6.0
2	E	259	LYS	5.7
2	F	126	LEU	5.4
2	E	261	CYS	5.1
2	F	149	LEU	5.0
2	E	112	GLY	4.8
2	E	69	THR	4.7
2	E	102	LEU	4.7
1	C	308	GLY	4.6
2	F	205	LYS	4.5
1	C	309	ASP	4.4
1	B	244	GLN	4.4
2	F	204	GLN	4.3
2	F	228	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	241	GLN	4.1
2	D	302	LYS	4.1
1	A	239	PRO	4.1
2	D	221	ASN	3.9
2	F	154	LEU	3.9
1	C	332	SER	3.9
2	E	120	ASN	3.8
1	C	306	VAL	3.8
1	A	298	ALA	3.8
2	F	300	GLU	3.7
2	E	145	SER	3.7
2	F	191	THR	3.7
1	C	205	VAL	3.7
1	A	186	LEU	3.6
2	F	125	ASP	3.6
2	F	122	PHE	3.5
2	E	291	PRO	3.5
2	D	301	ASN	3.5
1	A	184	THR	3.4
2	F	190	GLN	3.4
1	B	358	ARG	3.3
2	E	260	SER	3.3
1	B	258	TYR	3.3
2	D	258	GLY	3.3
2	E	158	GLU	3.3
2	F	143	ILE	3.3
1	C	192	ILE	3.2
2	F	251	LEU	3.2
2	E	74	GLU	3.2
2	F	267	TYR	3.2
2	F	121	LEU	3.1
2	F	129	LEU	3.1
1	A	276	ILE	3.1
1	B	240	ILE	3.1
2	F	252	PHE	3.1
2	F	140	ILE	3.1
2	F	219	VAL	3.0
2	F	296	ILE	3.0
2	F	128	ASN	3.0
1	C	181	SER	3.0
2	F	120	ASN	3.0
2	F	293	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	258	GLY	2.9
2	E	170	VAL	2.9
2	E	107	SER	2.9
1	C	359	ASN	2.9
1	C	360	ASN	2.8
2	E	167	ASN	2.8
2	F	200	ASP	2.8
2	F	298	VAL	2.8
2	E	121	LEU	2.8
2	E	262	LEU	2.8
1	A	305	GLY	2.8
2	D	265	LYS	2.8
1	C	290	GLY	2.8
1	C	305	GLY	2.8
1	A	370	ASN	2.8
2	D	266	GLU	2.8
1	A	367	SER	2.7
2	D	109	TYR	2.7
1	B	320	ALA	2.7
2	F	253	ASP	2.7
2	D	182	LEU	2.7
2	F	165	ILE	2.6
2	E	108	GLN	2.6
2	D	70	CYS	2.6
1	C	194	ALA	2.6
2	F	291	PRO	2.6
2	E	287	GLN	2.6
2	D	226	VAL	2.6
2	F	183	ASN	2.6
1	A	331	GLN	2.5
2	D	106	LEU	2.5
2	D	219	VAL	2.5
2	F	89	GLU	2.5
1	C	333	GLN	2.5
2	D	104	THR	2.5
2	F	278	LYS	2.5
2	E	92	GLN	2.5
1	B	360	ASN	2.5
2	E	264	THR	2.5
2	F	222	GLN	2.5
2	F	277	PRO	2.5
2	F	268	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	249	ASP	2.4
2	F	141	LEU	2.4
2	D	254	ILE	2.4
2	D	132	SER	2.4
2	E	134	LYS	2.4
1	A	318	ASN	2.4
2	E	84	ASN	2.4
2	E	198	ASN	2.4
1	B	228	ASP	2.4
2	F	287	GLN	2.4
2	F	148	SER	2.4
2	F	92	GLN	2.4
2	D	129	LEU	2.4
1	A	260	VAL	2.4
2	F	250	VAL	2.4
1	A	348	ASN	2.4
2	E	131	ILE	2.4
2	F	132	SER	2.4
1	C	228	ASP	2.3
2	D	91	ASP	2.3
2	F	146	ASP	2.3
2	E	122	PHE	2.3
2	E	176	GLU	2.3
1	C	242	SER	2.3
2	F	153	ILE	2.3
1	C	288	ALA	2.3
2	E	91	ASP	2.3
2	E	150	ILE	2.3
1	B	184	THR	2.3
1	B	291	HIS	2.3
2	F	281	LEU	2.3
1	B	284	ASN	2.3
1	B	289	LYS	2.3
1	A	332	SER	2.3
2	D	145	SER	2.3
2	E	193	ASP	2.3
2	F	255	VAL	2.3
2	F	152	GLU	2.2
1	C	313	GLY	2.2
2	E	248	PRO	2.2
2	D	252	PHE	2.2
2	E	160	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	372	LEU	2.2
2	D	251	LEU	2.2
2	F	265	LYS	2.2
2	D	207	GLN	2.2
2	E	207	GLN	2.2
1	A	336	GLU	2.2
2	E	228	ILE	2.2
2	F	101	ILE	2.2
1	A	188	PHE	2.2
2	E	151	ASN	2.2
1	B	331	GLN	2.2
2	D	191	THR	2.1
2	D	77	LEU	2.1
2	F	172	GLN	2.1
2	F	203	GLN	2.1
1	C	370	ASN	2.1
2	D	291	PRO	2.1
2	E	130	ASP	2.1
2	F	280	GLN	2.1
2	F	223	SER	2.1
2	F	283	GLU	2.1
2	F	263	LYS	2.1
1	C	227	TYR	2.1
2	E	103	GLY	2.1
1	A	183	VAL	2.1
2	E	72	ASN	2.1
2	F	218	LYS	2.1
2	F	88	TYR	2.1
1	C	331	GLN	2.1
1	C	338	ILE	2.0
2	D	249	ASP	2.0
2	D	180	GLU	2.0
2	F	254	ILE	2.0
1	C	356	ALA	2.0
1	A	363	ASP	2.0
1	A	347	PRO	2.0
2	F	275	LEU	2.0
2	F	272	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.