



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 3DKT / pdb_00003dkt
Title : Crystal structure of Thermotoga maritima encapsulin
Authors : Sutter, M.; Boehringer, D.; Gutmann, S.; Weber-Ban, E.; Ban, N.
Deposited on : 2008-06-26
Resolution : 3.10 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

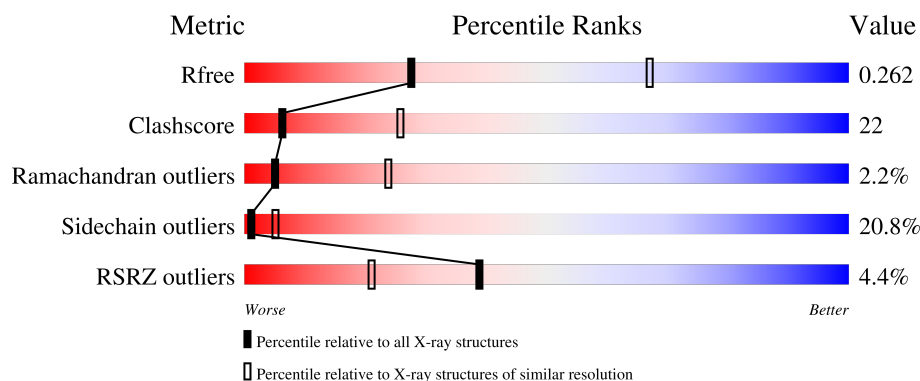
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	265	3% 54% 35% 10%
1	B	265	4% 51% 38% 11%
1	C	265	3% 50% 39% 10%
1	D	265	5% 49% 39% 12%
1	E	265	3% 52% 35% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	265	
1	G	265	
1	H	265	
1	I	265	
1	J	265	
2	K	8	
2	L	8	
2	M	8	
2	N	8	
2	O	8	
2	P	8	
2	Q	8	
2	R	8	
2	S	8	
2	T	8	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22070 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 Maritimacin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	B	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	C	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	D	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	E	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	F	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	G	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	H	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	I	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			
1	J	264	Total	C	N	O	S	0	0	0
			2141	1372	358	407	4			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	L	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	M	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	N	8	Total	C	N	O	0	0	0
			56	34	12	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	P	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	Q	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	R	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	S	8	Total	C	N	O	0	0	0
			56	34	12	10			
2	T	8	Total	C	N	O	0	0	0
			56	34	12	10			

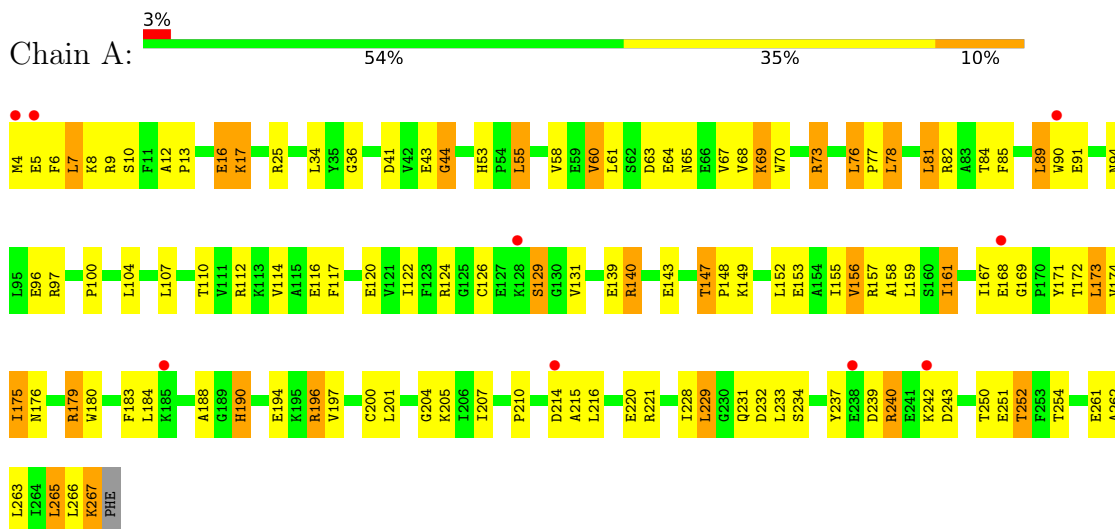
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	11	Total	O	0	0
			11	11		
3	C	9	Total	O	0	0
			9	9		
3	D	12	Total	O	0	0
			12	12		
3	E	9	Total	O	0	0
			9	9		
3	F	11	Total	O	0	0
			11	11		
3	G	9	Total	O	0	0
			9	9		
3	H	11	Total	O	0	0
			11	11		
3	I	9	Total	O	0	0
			9	9		
3	J	10	Total	O	0	0
			10	10		

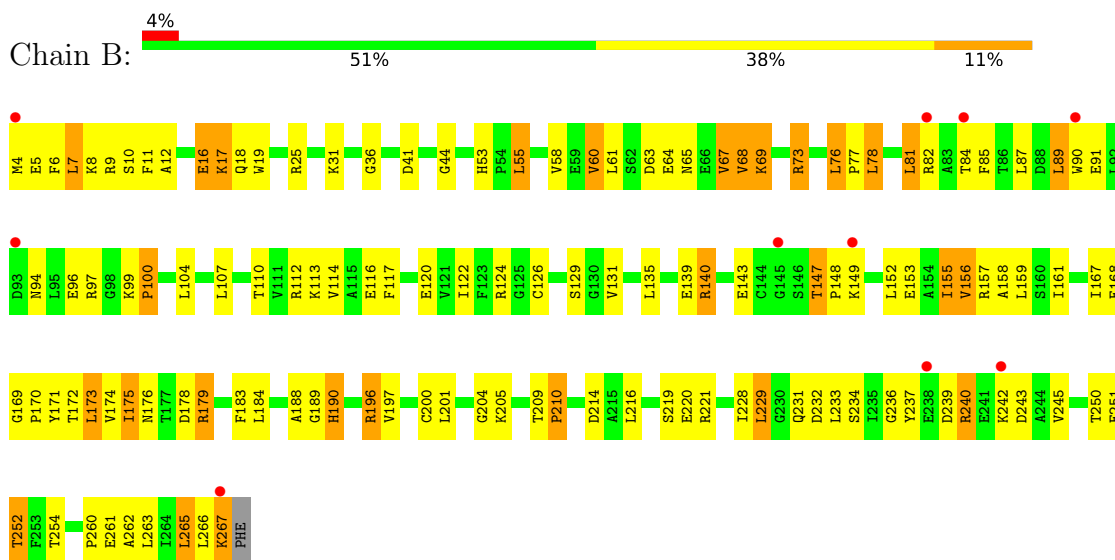
3 Residue-property plots [i](#)

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

• Molecule 1: Maritimacin

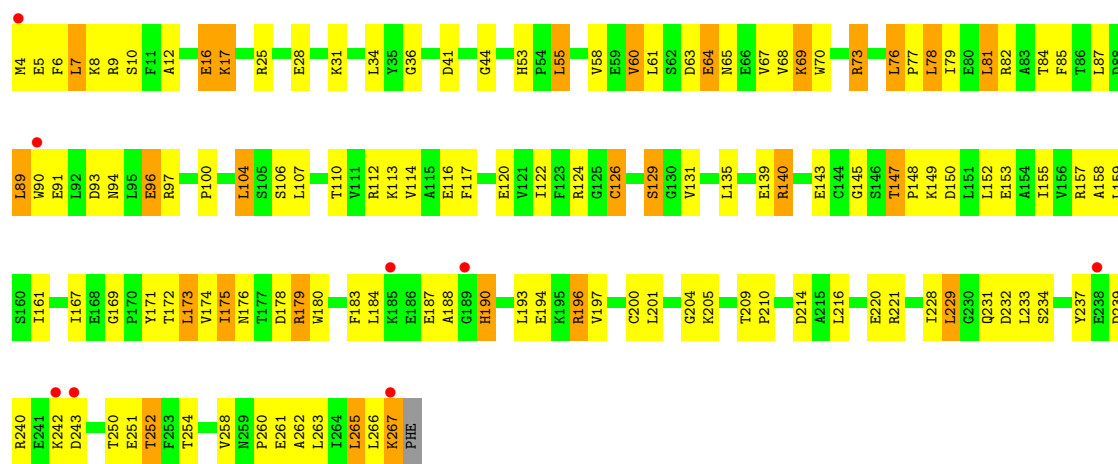


• Molecule 1: Maritimacin

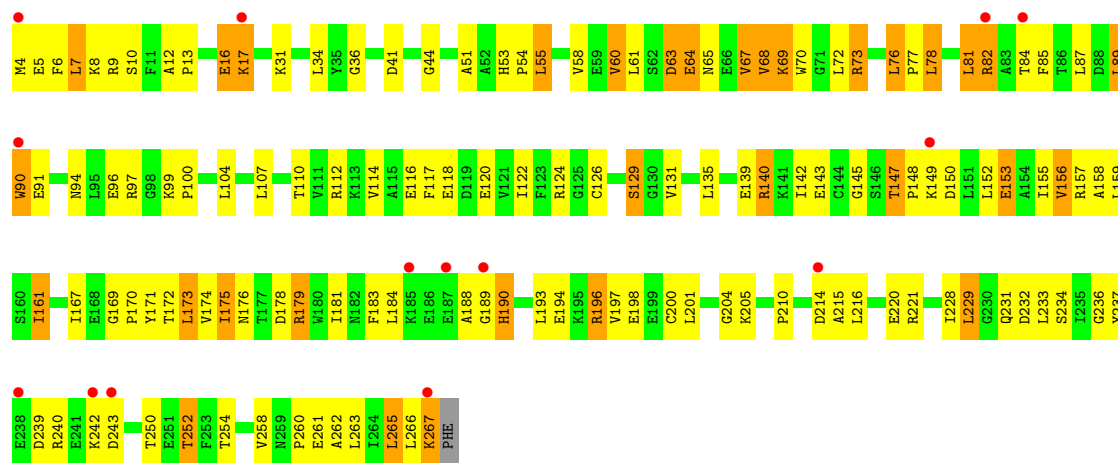


• Molecule 1: Maritimacin

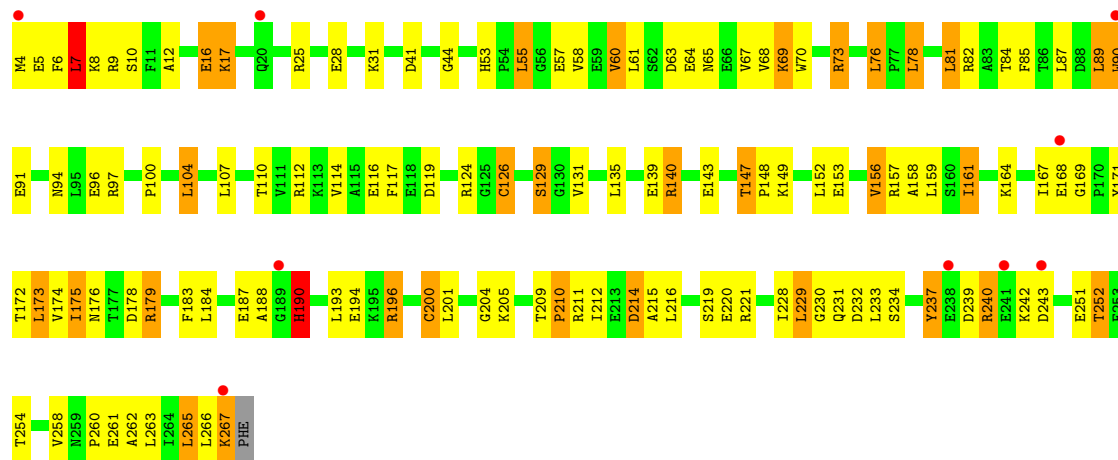




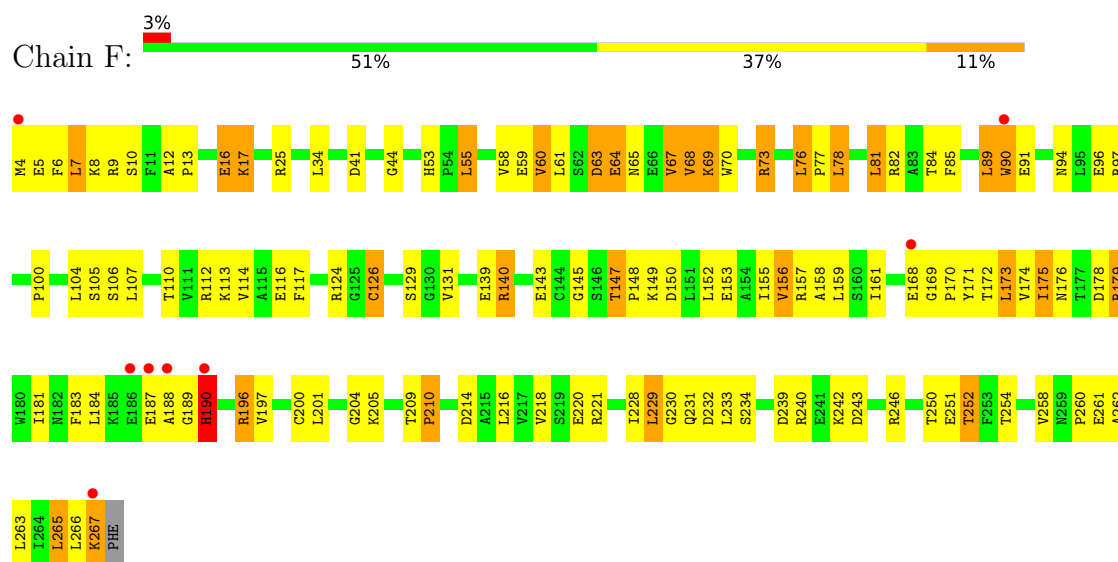
• Molecule 1: Maritimacin



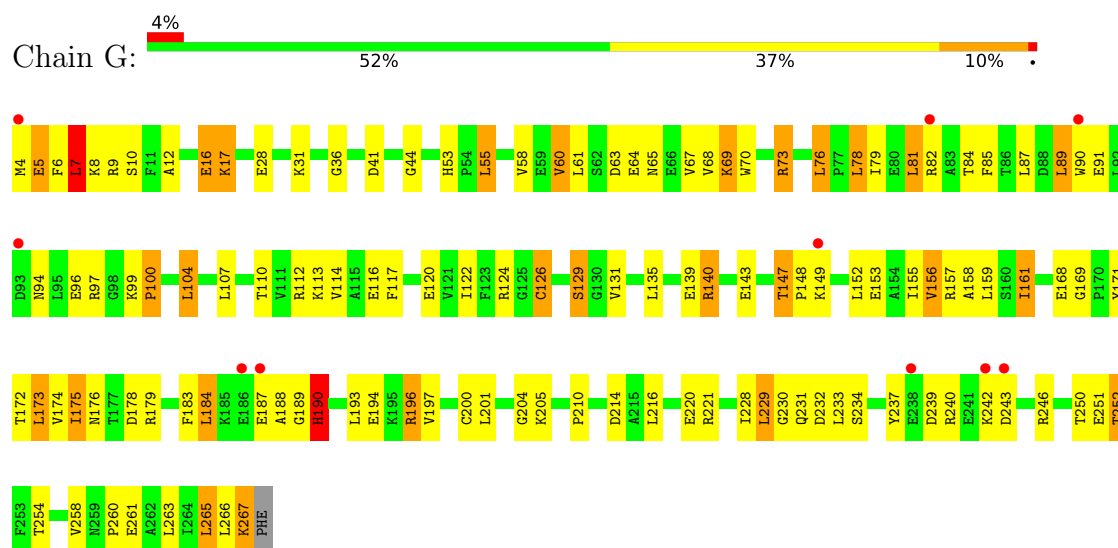
• Molecule 1: Maritimacin



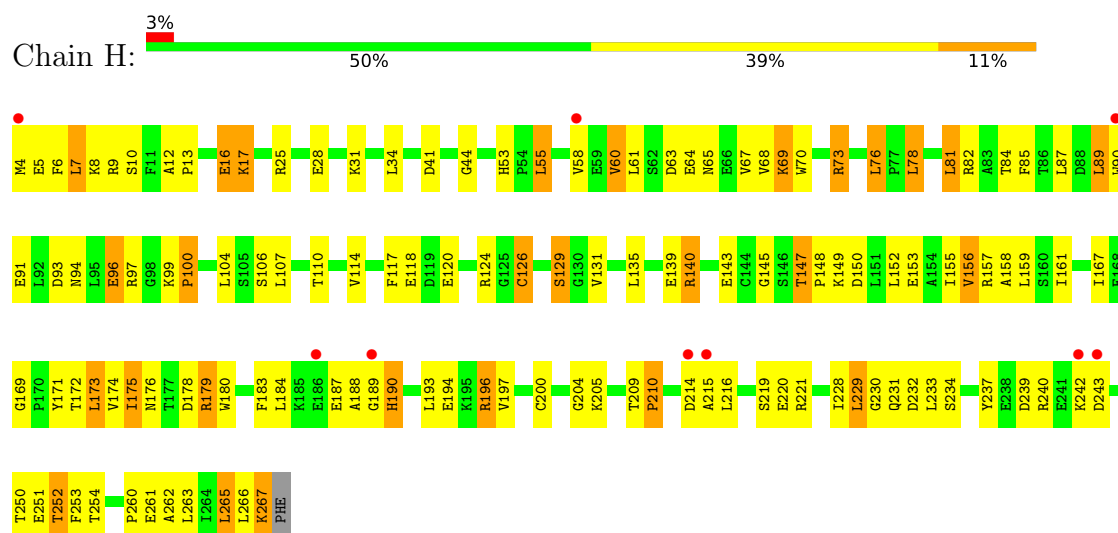
• Molecule 1: Maritimacin



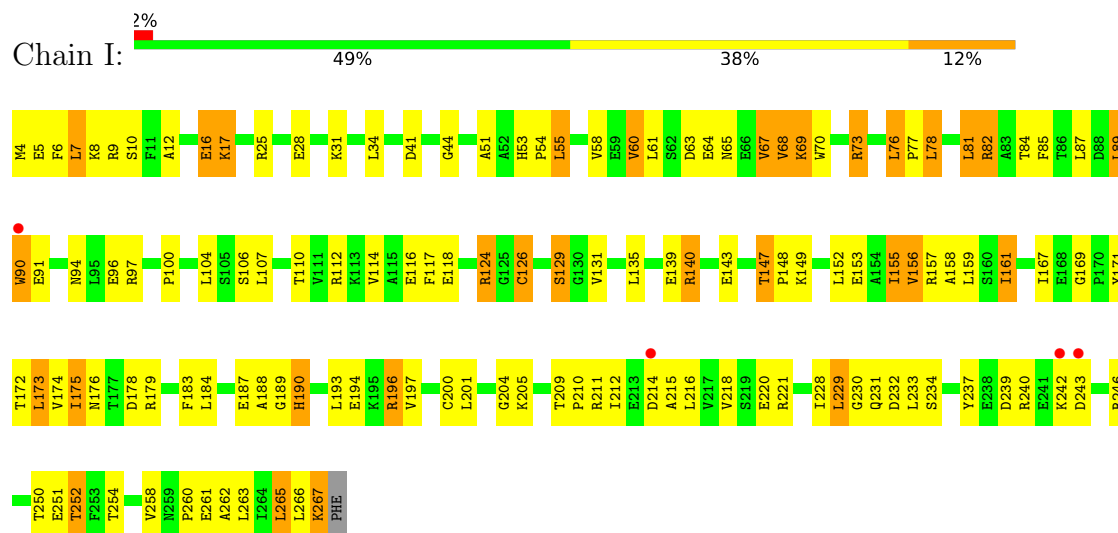
• Molecule 1: Maritimacin



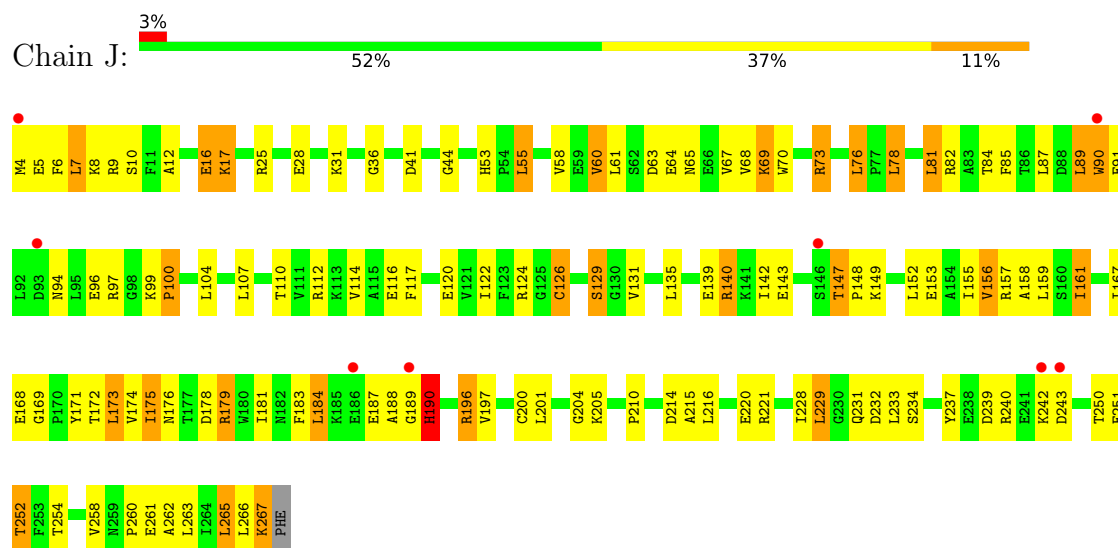
• Molecule 1: Maritimacin



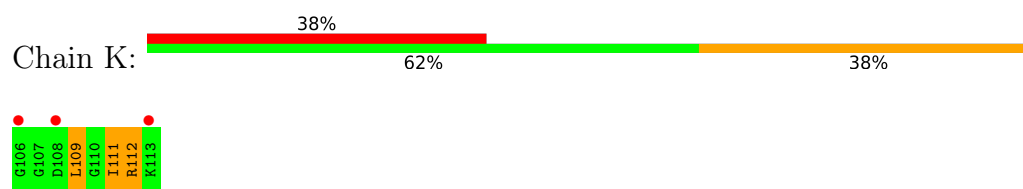
- Molecule 1: Maritimacin



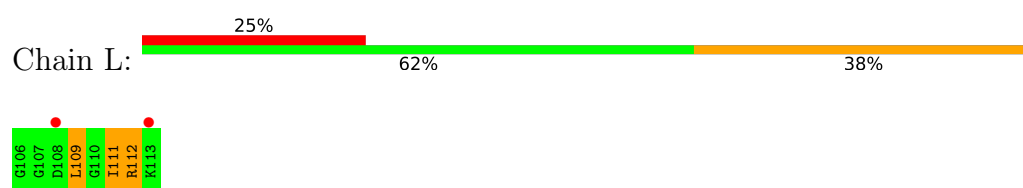
- Molecule 1: Maritimacin



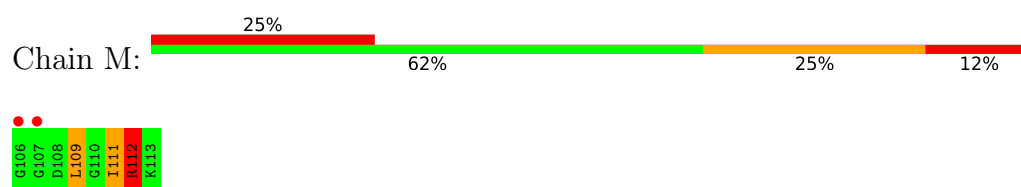
- Molecule 2: Putative uncharacterized protein



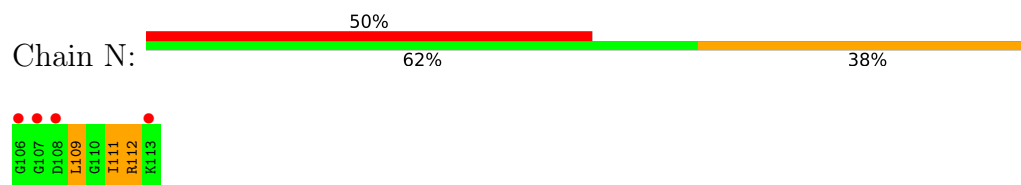
- Molecule 2: Putative uncharacterized protein



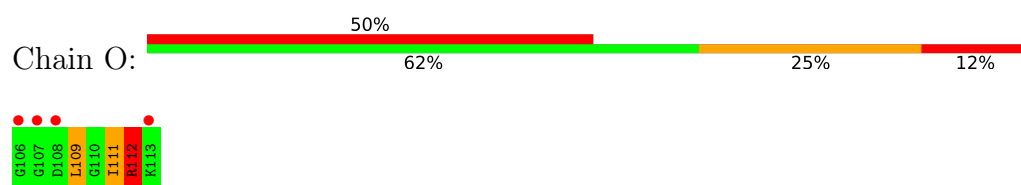
- Molecule 2: Putative uncharacterized protein



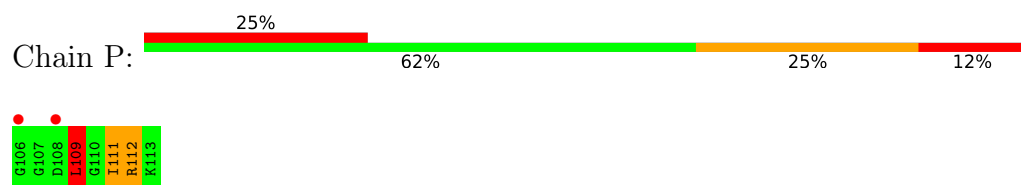
- Molecule 2: Putative uncharacterized protein



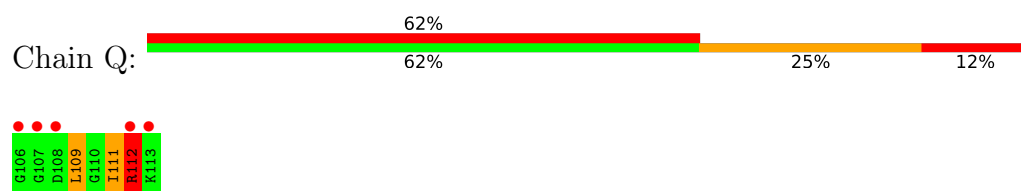
- Molecule 2: Putative uncharacterized protein



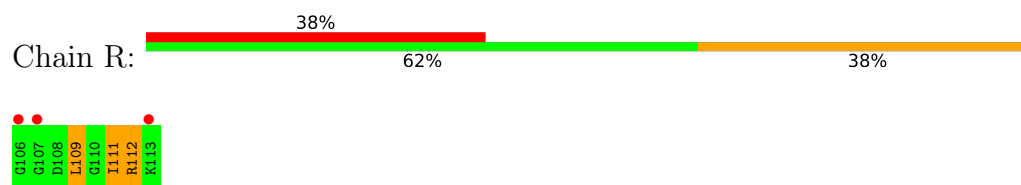
- Molecule 2: Putative uncharacterized protein



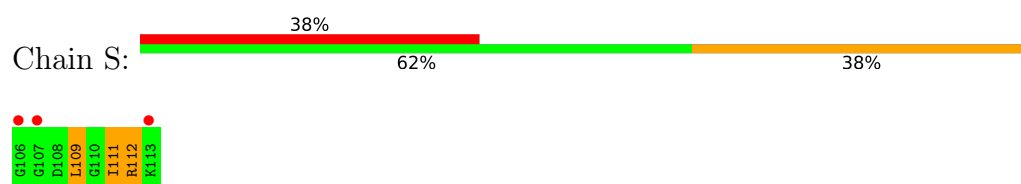
- Molecule 2: Putative uncharacterized protein



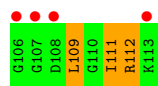
- Molecule 2: Putative uncharacterized protein



- Molecule 2: Putative uncharacterized protein



- Molecule 2: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	669.04Å 669.04Å 669.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 3.10 49.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.87-3.10) 96.5 (49.87-3.10)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.239 0.247 , 0.262	Depositor DCC
R_{free} test set	10961 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 94.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22070	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% 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	0.52	0/2182	0.97	5/2945 (0.2%)
1	B	0.52	0/2182	0.96	3/2945 (0.1%)
1	C	0.55	0/2182	0.97	6/2945 (0.2%)
1	D	0.53	0/2182	0.97	6/2945 (0.2%)
1	E	0.51	0/2182	0.97	7/2945 (0.2%)
1	F	0.64	0/2182	1.02	5/2945 (0.2%)
1	G	0.56	0/2182	0.98	7/2945 (0.2%)
1	H	0.56	0/2182	0.98	5/2945 (0.2%)
1	I	0.58	0/2182	0.99	5/2945 (0.2%)
1	J	0.59	0/2182	0.95	5/2945 (0.2%)
2	K	0.77	0/55	0.91	0/70
2	L	0.86	0/55	0.99	0/70
2	M	0.83	0/55	0.87	0/70
2	N	0.81	0/55	0.92	0/70
2	O	0.84	0/55	0.97	0/70
2	P	0.80	0/55	0.92	0/70
2	Q	0.85	0/55	1.00	0/70
2	R	0.79	0/55	0.99	0/70
2	S	0.92	0/55	0.96	0/70
2	T	0.81	0/55	0.94	0/70
All	All	0.57	0/22370	0.97	54/30150 (0.2%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	LEU	CA-C-N	7.51	129.23	119.84
1	F	76	LEU	C-N-CA	7.51	129.23	119.84
1	I	190	HIS	N-CA-C	-7.42	102.82	112.68
1	H	190	HIS	N-CA-C	-7.31	102.96	112.68
1	I	76	LEU	CA-C-N	7.16	128.79	119.84
1	I	76	LEU	C-N-CA	7.16	128.79	119.84
1	B	76	LEU	CA-C-N	6.99	128.57	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	LEU	C-N-CA	6.99	128.57	119.84
1	F	190	HIS	N-CA-C	-6.84	103.58	112.68
1	J	190	HIS	N-CA-C	-6.83	103.60	112.68
1	A	190	HIS	N-CA-C	-6.82	103.60	112.68
1	C	190	HIS	N-CA-C	-6.80	103.64	112.68
1	G	190	HIS	N-CA-C	-6.79	103.65	112.68
1	J	76	LEU	CA-C-N	6.77	128.31	119.84
1	J	76	LEU	C-N-CA	6.77	128.31	119.84
1	B	190	HIS	N-CA-C	-6.61	103.89	112.68
1	E	190	HIS	N-CA-C	-6.58	103.92	112.68
1	E	76	LEU	CA-C-N	6.45	127.90	119.84
1	E	76	LEU	C-N-CA	6.45	127.90	119.84
1	D	190	HIS	N-CA-C	-6.39	104.19	112.68
1	D	76	LEU	CA-C-N	6.28	127.69	119.84
1	D	76	LEU	C-N-CA	6.28	127.69	119.84
1	C	76	LEU	CA-C-N	6.27	127.68	119.84
1	C	76	LEU	C-N-CA	6.27	127.68	119.84
1	I	70	TRP	N-CA-C	6.16	117.50	108.14
1	F	70	TRP	N-CA-C	6.12	117.43	108.14
1	G	76	LEU	CA-C-N	6.05	127.40	119.84
1	G	76	LEU	C-N-CA	6.05	127.40	119.84
1	H	76	LEU	CA-C-N	6.05	127.40	119.84
1	H	76	LEU	C-N-CA	6.05	127.40	119.84
1	H	70	TRP	N-CA-C	5.87	117.06	108.14
1	E	161	ILE	CB-CA-C	-5.81	104.20	112.22
1	A	76	LEU	CA-C-N	5.79	127.08	119.84
1	A	76	LEU	C-N-CA	5.79	127.08	119.84
1	J	70	TRP	N-CA-C	5.70	116.81	108.14
1	D	70	TRP	N-CA-C	5.65	116.73	108.14
1	J	161	ILE	CB-CA-C	-5.61	104.47	112.22
1	A	70	TRP	N-CA-C	5.56	116.59	108.14
1	G	5	GLU	N-CA-C	5.50	118.20	111.82
1	C	70	TRP	N-CA-C	5.47	116.46	108.14
1	G	161	ILE	CB-CA-C	-5.46	104.68	112.22
1	G	70	TRP	N-CA-C	5.39	116.33	108.14
1	C	79	ILE	CB-CA-C	-5.24	104.34	111.15
1	I	161	ILE	CB-CA-C	-5.23	103.79	112.26
1	A	161	ILE	CB-CA-C	-5.18	105.07	112.22
1	G	79	ILE	CB-CA-C	-5.18	104.41	111.15
1	C	64	GLU	N-CA-C	-5.16	106.95	113.20
1	D	64	GLU	N-CA-C	-5.15	106.97	113.20
1	D	161	ILE	CB-CA-C	-5.14	103.92	112.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	70	TRP	N-CA-C	5.14	115.95	108.14
1	E	214	ASP	CA-C-O	5.13	121.56	118.33
1	H	253	PHE	N-CA-C	5.05	115.81	108.14
1	F	64	GLU	N-CA-C	-5.04	107.10	113.20
1	E	214	ASP	N-CA-C	5.04	113.58	108.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2141	0	2148	91	0
1	B	2141	0	2148	102	0
1	C	2141	0	2148	95	0
1	D	2141	0	2148	114	0
1	E	2141	0	2148	97	0
1	F	2141	0	2148	105	0
1	G	2141	0	2148	105	0
1	H	2141	0	2148	99	0
1	I	2141	0	2148	108	0
1	J	2141	0	2148	98	0
2	K	56	0	60	6	0
2	L	56	0	60	5	0
2	M	56	0	60	5	0
2	N	56	0	60	6	0
2	O	56	0	60	5	0
2	P	56	0	60	6	0
2	Q	56	0	60	8	0
2	R	56	0	60	6	0
2	S	56	0	60	7	0
2	T	56	0	60	6	0
3	A	9	0	0	2	0
3	B	11	0	0	4	0
3	C	9	0	0	2	0
3	D	12	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	9	0	0	2	0
3	F	11	0	0	3	0
3	G	9	0	0	2	0
3	H	11	0	0	2	0
3	I	9	0	0	3	0
3	J	10	0	0	2	0
All	All	22070	0	22080	981	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (981) 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:H:196:ARG:HG3	1:H:196:ARG:HH11	1.11	1.16
1:I:196:ARG:HG3	1:I:196:ARG:HH11	1.12	1.15
1:B:196:ARG:HH11	1:B:196:ARG:HG3	1.12	1.14
1:J:196:ARG:HG3	1:J:196:ARG:HH11	1.12	1.13
2:R:109:LEU:HD12	2:R:111:ILE:HD11	1.27	1.13
2:Q:109:LEU:HD12	2:Q:111:ILE:HD11	1.28	1.11
2:S:109:LEU:HD12	2:S:111:ILE:HD11	1.31	1.11
1:D:196:ARG:HG3	1:D:196:ARG:HH11	1.14	1.11
1:G:196:ARG:HH11	1:G:196:ARG:HG3	1.11	1.10
2:T:109:LEU:HD12	2:T:111:ILE:HD11	1.32	1.09
1:E:196:ARG:HG3	1:E:196:ARG:HH11	1.09	1.09
1:F:196:ARG:HG3	1:F:196:ARG:HH11	1.09	1.09
2:M:109:LEU:HD12	2:M:111:ILE:HD11	1.30	1.09
1:C:196:ARG:HG3	1:C:196:ARG:HH11	1.10	1.08
2:N:109:LEU:HD12	2:N:111:ILE:HD11	1.36	1.08
2:O:109:LEU:HD12	2:O:111:ILE:HD11	1.35	1.08
2:K:109:LEU:HD12	2:K:111:ILE:HD11	1.35	1.06
2:L:109:LEU:HD12	2:L:111:ILE:HD11	1.37	1.06
1:A:196:ARG:HG3	1:A:196:ARG:HH11	1.13	1.04
1:A:176:ASN:HD22	1:A:179:ARG:H	1.09	0.98
1:F:176:ASN:HD22	1:F:179:ARG:H	1.09	0.98
2:P:109:LEU:HD12	2:P:111:ILE:HD11	1.43	0.98
1:E:176:ASN:HD22	1:E:179:ARG:H	1.13	0.96
1:I:188:ALA:HB1	1:J:149:LYS:HG2	1.44	0.96
1:G:252:THR:HG21	3:G:1043:HOH:O	1.65	0.95
1:H:176:ASN:HD22	1:H:179:ARG:H	1.13	0.94
1:G:176:ASN:HD22	1:G:179:ARG:H	1.09	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:ASN:HD22	1:I:179:ARG:H	1.13	0.94
1:E:252:THR:HG21	3:E:1043:HOH:O	1.66	0.94
1:F:252:THR:HG21	3:F:1004:HOH:O	1.69	0.93
1:C:176:ASN:HD22	1:C:179:ARG:H	1.11	0.92
1:D:176:ASN:HD22	1:D:179:ARG:H	1.08	0.92
1:J:176:ASN:HD22	1:J:179:ARG:H	1.10	0.92
1:I:252:THR:HG21	3:I:1043:HOH:O	1.70	0.91
1:D:252:THR:HG21	3:D:1010:HOH:O	1.70	0.90
1:I:16:GLU:OE1	1:I:16:GLU:HA	1.73	0.89
1:B:176:ASN:HD22	1:B:179:ARG:H	1.14	0.89
1:J:252:THR:HG21	3:J:1006:HOH:O	1.73	0.88
1:E:196:ARG:HG3	1:E:196:ARG:NH1	1.89	0.86
1:F:196:ARG:HG3	1:F:196:ARG:NH1	1.89	0.86
1:C:252:THR:HG21	3:C:1043:HOH:O	1.77	0.84
1:F:16:GLU:OE1	1:F:16:GLU:HA	1.77	0.83
1:A:147:THR:HG21	1:A:149:LYS:HE3	1.61	0.82
1:C:196:ARG:HH11	1:C:196:ARG:CG	1.93	0.82
1:C:147:THR:HG21	1:C:149:LYS:HE3	1.62	0.82
1:B:252:THR:HG21	3:B:1009:HOH:O	1.80	0.81
1:H:252:THR:HG21	3:H:1009:HOH:O	1.80	0.81
1:I:196:ARG:HG3	1:I:196:ARG:NH1	1.92	0.81
1:G:196:ARG:HG3	1:G:196:ARG:NH1	1.90	0.81
1:A:252:THR:HG21	3:A:1043:HOH:O	1.80	0.81
1:B:16:GLU:HA	1:B:16:GLU:OE1	1.79	0.81
1:E:16:GLU:HA	1:E:16:GLU:OE1	1.78	0.81
1:A:16:GLU:OE1	1:A:16:GLU:HA	1.81	0.81
1:J:16:GLU:HA	1:J:16:GLU:OE1	1.81	0.81
1:I:188:ALA:CB	1:J:149:LYS:HG2	2.10	0.80
1:H:157:ARG:O	1:H:161:ILE:HD12	1.81	0.80
1:D:157:ARG:O	1:D:161:ILE:HD12	1.80	0.80
1:A:157:ARG:O	1:A:161:ILE:HD12	1.81	0.80
1:D:188:ALA:HB1	1:E:149:LYS:HG2	1.64	0.79
1:G:147:THR:HG21	1:G:149:LYS:HE3	1.62	0.79
1:H:216:LEU:HD11	1:H:263:LEU:HD11	1.64	0.79
1:H:188:ALA:HB1	1:I:149:LYS:HG2	1.64	0.79
1:E:147:THR:HG21	1:E:149:LYS:HE3	1.66	0.78
1:D:16:GLU:OE1	1:D:16:GLU:HA	1.81	0.78
1:G:16:GLU:HA	1:G:16:GLU:OE1	1.84	0.78
1:J:157:ARG:O	1:J:161:ILE:HD12	1.83	0.77
1:I:157:ARG:O	1:I:161:ILE:HD12	1.85	0.77
1:B:188:ALA:HB1	1:C:149:LYS:HG2	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ARG:O	1:E:161:ILE:HD12	1.85	0.77
1:A:196:ARG:HG3	1:A:196:ARG:NH1	1.93	0.76
1:C:16:GLU:HA	1:C:16:GLU:OE1	1.83	0.76
1:F:157:ARG:O	1:F:161:ILE:HD12	1.86	0.76
1:C:157:ARG:O	1:C:161:ILE:HD12	1.86	0.75
1:I:147:THR:HG21	1:I:149:LYS:HE3	1.68	0.74
1:D:196:ARG:HG3	1:D:196:ARG:NH1	1.93	0.74
1:E:196:ARG:HH11	1:E:196:ARG:CG	1.95	0.74
1:G:157:ARG:O	1:G:161:ILE:HD12	1.87	0.74
1:H:16:GLU:OE1	1:H:16:GLU:HA	1.87	0.74
1:J:196:ARG:HH11	1:J:196:ARG:CG	1.97	0.74
1:I:196:ARG:HH11	1:I:196:ARG:CG	1.97	0.74
1:J:147:THR:HG21	1:J:149:LYS:HE3	1.68	0.74
1:H:196:ARG:HH11	1:H:196:ARG:CG	1.96	0.74
1:J:196:ARG:HG3	1:J:196:ARG:NH1	1.92	0.74
1:H:147:THR:HG21	1:H:149:LYS:HE3	1.70	0.73
1:B:147:THR:HG22	1:B:148:PRO:HD2	1.70	0.73
1:A:91:GLU:O	1:A:94:ASN:HB2	1.88	0.73
1:A:216:LEU:HD11	1:A:263:LEU:HD11	1.69	0.73
1:B:157:ARG:O	1:B:161:ILE:HD12	1.88	0.72
1:F:196:ARG:HH11	1:F:196:ARG:CG	1.94	0.72
1:F:188:ALA:HB1	1:G:149:LYS:HG2	1.72	0.72
1:I:216:LEU:HD11	1:I:263:LEU:HD11	1.72	0.72
1:G:216:LEU:HD11	1:G:263:LEU:HD11	1.71	0.71
1:H:196:ARG:HG3	1:H:196:ARG:NH1	1.91	0.71
1:B:196:ARG:HH11	1:B:196:ARG:CG	1.97	0.71
1:B:216:LEU:HD11	1:B:263:LEU:HD11	1.71	0.71
1:D:6:PHE:HB3	1:H:96:GLU:HG2	1.72	0.71
1:F:73:ARG:HH21	1:J:97:ARG:HD3	1.55	0.71
1:G:176:ASN:ND2	1:G:179:ARG:H	1.86	0.70
1:A:174:VAL:HB	1:A:216:LEU:HB3	1.73	0.70
1:G:91:GLU:O	1:G:94:ASN:HB2	1.91	0.70
1:D:216:LEU:HD11	1:D:263:LEU:HD11	1.72	0.70
1:J:216:LEU:HD11	1:J:263:LEU:HD11	1.72	0.70
1:F:147:THR:HG22	1:F:148:PRO:HD2	1.72	0.70
1:C:91:GLU:O	1:C:94:ASN:HB2	1.91	0.69
1:C:196:ARG:HG3	1:C:196:ARG:NH1	1.91	0.69
1:E:17:LYS:HE3	1:E:17:LYS:HA	1.74	0.69
1:G:188:ALA:HB1	1:H:149:LYS:HG2	1.74	0.69
1:E:147:THR:HG22	1:E:148:PRO:HD2	1.74	0.69
1:E:216:LEU:HD11	1:E:263:LEU:HD11	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:ARG:HD3	1:J:73:ARG:HH21	1.57	0.69
1:B:147:THR:HG21	1:B:149:LYS:HE3	1.74	0.69
1:F:174:VAL:HB	1:F:216:LEU:HB3	1.73	0.69
1:A:188:ALA:HB1	1:B:149:LYS:HG2	1.74	0.69
1:D:147:THR:HG21	1:D:149:LYS:HE3	1.74	0.69
1:H:174:VAL:HB	1:H:216:LEU:HB3	1.75	0.69
1:I:147:THR:HG22	1:I:148:PRO:HD2	1.75	0.68
1:H:91:GLU:O	1:H:94:ASN:HB2	1.92	0.68
1:D:174:VAL:HB	1:D:216:LEU:HB3	1.75	0.68
1:F:149:LYS:HG2	1:J:188:ALA:HB1	1.74	0.68
1:G:196:ARG:HH11	1:G:196:ARG:CG	1.97	0.68
1:B:229:LEU:HD12	1:B:232:ASP:HA	1.76	0.67
1:D:91:GLU:O	1:D:94:ASN:HB2	1.94	0.67
1:I:179:ARG:O	1:I:183:PHE:HD1	1.77	0.67
1:H:179:ARG:O	1:H:183:PHE:HD1	1.78	0.67
1:F:97:ARG:HD3	1:G:73:ARG:HH21	1.59	0.67
1:C:176:ASN:ND2	1:C:179:ARG:H	1.91	0.67
1:F:179:ARG:O	1:F:183:PHE:HD1	1.77	0.67
1:J:91:GLU:O	1:J:94:ASN:HB2	1.95	0.67
1:J:174:VAL:HB	1:J:216:LEU:HB3	1.75	0.67
1:D:196:ARG:HH11	1:D:196:ARG:CG	1.99	0.67
1:C:179:ARG:O	1:C:183:PHE:HD1	1.77	0.67
1:F:55:LEU:HD12	1:F:76:LEU:HB2	1.77	0.67
1:F:147:THR:HG21	1:F:149:LYS:HE3	1.75	0.67
1:B:196:ARG:HG3	1:B:196:ARG:NH1	1.92	0.67
1:C:174:VAL:HB	1:C:216:LEU:HB3	1.76	0.67
1:C:229:LEU:HD12	1:C:232:ASP:HA	1.77	0.67
1:D:176:ASN:ND2	1:D:179:ARG:H	1.88	0.67
1:H:129:SER:HB2	3:H:1013:HOH:O	1.94	0.66
1:G:85:PHE:CZ	1:G:107:LEU:HD13	2.30	0.66
1:D:179:ARG:O	1:D:183:PHE:HD1	1.78	0.66
1:E:64:GLU:HA	1:E:69:LYS:NZ	2.10	0.66
1:C:216:LEU:HD11	1:C:263:LEU:HD11	1.77	0.66
1:G:174:VAL:HB	1:G:216:LEU:HB3	1.77	0.66
1:H:78:LEU:HD12	1:H:252:THR:CG2	2.26	0.66
1:I:91:GLU:O	1:I:94:ASN:HB2	1.95	0.66
1:E:91:GLU:O	1:E:94:ASN:HB2	1.97	0.65
1:F:176:ASN:ND2	1:F:179:ARG:H	1.90	0.65
1:A:229:LEU:HD12	1:A:232:ASP:HA	1.76	0.65
1:F:188:ALA:CB	1:G:149:LYS:HG2	2.26	0.65
1:F:216:LEU:HD11	1:F:263:LEU:HD11	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:VAL:O	1:F:61:LEU:HD12	1.96	0.65
1:F:189:GLY:HA3	1:G:187:GLU:OE2	1.96	0.65
1:J:176:ASN:ND2	1:J:179:ARG:H	1.89	0.65
1:B:174:VAL:HB	1:B:216:LEU:HB3	1.79	0.65
1:I:176:ASN:ND2	1:I:179:ARG:H	1.91	0.65
1:G:64:GLU:HA	1:G:69:LYS:NZ	2.12	0.65
1:J:147:THR:HG22	1:J:148:PRO:HD2	1.79	0.65
1:B:91:GLU:O	1:B:94:ASN:HB2	1.97	0.65
1:F:17:LYS:HE3	1:F:17:LYS:HA	1.79	0.65
1:F:91:GLU:O	1:F:94:ASN:HB2	1.96	0.65
1:B:179:ARG:HG2	1:B:179:ARG:HH11	1.61	0.65
1:B:60:VAL:O	1:B:61:LEU:HD12	1.97	0.64
1:B:85:PHE:CZ	1:B:107:LEU:HD13	2.33	0.64
1:J:179:ARG:O	1:J:183:PHE:HD1	1.80	0.64
1:A:196:ARG:HH11	1:A:196:ARG:CG	2.00	0.64
1:C:78:LEU:HD12	1:C:252:THR:CG2	2.28	0.64
1:E:174:VAL:HB	1:E:216:LEU:HB3	1.77	0.64
1:H:60:VAL:O	1:H:61:LEU:HD12	1.98	0.64
1:A:179:ARG:O	1:A:183:PHE:HD1	1.80	0.64
1:D:147:THR:HG22	1:D:148:PRO:HD2	1.79	0.64
1:D:179:ARG:HG2	1:D:179:ARG:HH11	1.63	0.64
1:E:229:LEU:HD12	1:E:232:ASP:HA	1.80	0.64
1:G:229:LEU:HD12	1:G:232:ASP:HA	1.80	0.64
1:G:97:ARG:HD3	1:H:73:ARG:HH21	1.63	0.63
1:A:176:ASN:ND2	1:A:179:ARG:H	1.89	0.63
1:F:78:LEU:HD12	1:F:252:THR:CG2	2.28	0.63
1:I:174:VAL:HB	1:I:216:LEU:HB3	1.80	0.63
1:J:229:LEU:HD12	1:J:232:ASP:HA	1.80	0.63
1:B:78:LEU:HD12	1:B:252:THR:CG2	2.29	0.63
1:B:64:GLU:HA	1:B:69:LYS:NZ	2.13	0.63
1:E:179:ARG:O	1:E:183:PHE:HD1	1.82	0.62
1:C:97:ARG:HD3	1:D:73:ARG:HH21	1.65	0.62
1:I:64:GLU:HA	1:I:69:LYS:NZ	2.15	0.62
1:B:179:ARG:O	1:B:183:PHE:HD1	1.82	0.62
1:D:82:ARG:NH2	1:H:90:TRP:CZ3	2.68	0.62
1:C:64:GLU:HA	1:C:69:LYS:NZ	2.14	0.62
1:D:229:LEU:HD12	1:D:232:ASP:HA	1.82	0.62
1:F:229:LEU:HD12	1:F:232:ASP:HA	1.82	0.62
1:G:129:SER:HB2	3:G:1053:HOH:O	1.99	0.62
1:H:147:THR:HG22	1:H:148:PRO:HD2	1.82	0.62
1:C:96:GLU:HG2	1:I:6:PHE:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:ARG:O	1:G:183:PHE:HD1	1.83	0.62
1:H:179:ARG:HG2	1:H:179:ARG:HH11	1.65	0.62
1:A:78:LEU:HD12	1:A:252:THR:CG2	2.30	0.61
1:D:85:PHE:CZ	1:D:107:LEU:HD13	2.35	0.61
1:G:78:LEU:HD12	1:G:252:THR:CG2	2.30	0.61
1:D:6:PHE:O	1:D:8:LYS:HG2	2.00	0.61
1:D:17:LYS:HE3	1:D:17:LYS:HA	1.82	0.61
1:I:229:LEU:HD12	1:I:232:ASP:HA	1.81	0.61
1:A:149:LYS:HG2	1:E:188:ALA:HB1	1.81	0.61
1:C:147:THR:HG22	1:C:148:PRO:HD2	1.83	0.60
1:J:179:ARG:HG2	1:J:179:ARG:HH11	1.66	0.60
1:H:229:LEU:HD12	1:H:232:ASP:HA	1.83	0.60
1:E:176:ASN:ND2	1:E:179:ARG:H	1.91	0.60
1:J:78:LEU:HD12	1:J:252:THR:CG2	2.31	0.60
1:D:189:GLY:HA3	1:E:187:GLU:OE2	2.02	0.60
1:H:6:PHE:O	1:H:8:LYS:HG2	2.01	0.60
1:B:17:LYS:HE3	1:B:17:LYS:HA	1.83	0.60
1:J:64:GLU:HA	1:J:69:LYS:NZ	2.16	0.60
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.65	0.60
1:G:12:ALA:HB2	1:G:237:TYR:CD1	2.36	0.60
1:C:76:LEU:HD22	1:C:254:THR:OG1	2.02	0.60
1:H:173:LEU:HD13	1:H:175:ILE:HB	1.83	0.60
1:I:189:GLY:HA3	1:J:187:GLU:OE2	2.02	0.60
1:D:64:GLU:HA	1:D:69:LYS:NZ	2.16	0.59
1:C:110:THR:O	1:C:114:VAL:HG23	2.02	0.59
1:E:6:PHE:O	1:E:8:LYS:HG2	2.01	0.59
1:A:147:THR:HG22	1:A:148:PRO:HD2	1.84	0.59
1:A:6:PHE:O	1:A:8:LYS:HG2	2.03	0.59
1:F:73:ARG:NH2	1:J:97:ARG:HD3	2.18	0.59
1:H:85:PHE:CZ	1:H:107:LEU:HD13	2.37	0.59
1:I:60:VAL:O	1:I:61:LEU:HD12	2.02	0.59
1:F:6:PHE:O	1:F:8:LYS:HG2	2.03	0.59
1:E:81:LEU:C	1:E:81:LEU:HD23	2.28	0.59
1:I:6:PHE:O	1:I:8:LYS:HG2	2.02	0.59
1:B:176:ASN:ND2	1:B:179:ARG:H	1.93	0.58
1:G:60:VAL:O	1:G:61:LEU:HD12	2.03	0.58
1:E:90:TRP:O	1:E:90:TRP:CD1	2.56	0.58
1:D:60:VAL:O	1:D:61:LEU:HD12	2.02	0.58
1:G:205:LYS:HE2	1:G:220:GLU:OE1	2.04	0.58
1:J:60:VAL:O	1:J:61:LEU:HD12	2.04	0.58
1:I:12:ALA:HB2	1:I:237:TYR:CD1	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:LYS:HE3	1:I:17:LYS:HA	1.86	0.58
1:A:53:HIS:CG	1:A:228:ILE:HD13	2.39	0.58
1:F:179:ARG:HH11	1:F:179:ARG:HG2	1.69	0.58
1:E:76:LEU:HD22	1:E:254:THR:OG1	2.04	0.58
1:J:17:LYS:HE3	1:J:17:LYS:HA	1.85	0.58
1:A:231:GLN:H	1:A:252:THR:HB	1.69	0.57
1:C:179:ARG:HG2	1:C:179:ARG:HH11	1.68	0.57
1:B:196:ARG:CG	1:B:196:ARG:NH1	2.64	0.57
1:A:64:GLU:HA	1:A:69:LYS:HZ1	1.70	0.57
1:G:17:LYS:HE3	1:G:17:LYS:HA	1.85	0.57
1:A:64:GLU:HA	1:A:69:LYS:NZ	2.18	0.57
1:G:76:LEU:HD22	1:G:254:THR:OG1	2.04	0.57
1:G:147:THR:HG22	1:G:148:PRO:HD2	1.86	0.57
1:G:231:GLN:H	1:G:252:THR:HB	1.69	0.57
1:B:188:ALA:CB	1:C:149:LYS:HG2	2.35	0.57
1:C:239:ASP:CG	1:C:240:ARG:H	2.13	0.57
1:D:76:LEU:HD22	1:D:254:THR:OG1	2.04	0.57
1:H:97:ARG:HD3	1:I:73:ARG:HH21	1.70	0.57
1:I:78:LEU:HD12	1:I:252:THR:CG2	2.34	0.57
1:C:6:PHE:O	1:C:8:LYS:HG2	2.04	0.57
1:I:205:LYS:HE2	1:I:220:GLU:OE1	2.04	0.57
1:C:17:LYS:HE3	1:C:17:LYS:HA	1.87	0.57
1:F:189:GLY:O	1:G:190:HIS:HB2	2.05	0.57
1:I:85:PHE:CZ	1:I:107:LEU:HD13	2.40	0.57
2:P:111:ILE:N	2:P:111:ILE:HD12	2.20	0.57
1:D:205:LYS:HE2	1:D:220:GLU:OE1	2.05	0.57
1:A:97:ARG:HD3	1:B:73:ARG:HH21	1.70	0.57
1:D:129:SER:HB2	3:D:1014:HOH:O	2.05	0.57
1:E:205:LYS:HE2	1:E:220:GLU:OE1	2.04	0.57
1:A:129:SER:HB2	3:A:1053:HOH:O	2.05	0.56
1:B:173:LEU:HD13	1:B:175:ILE:HB	1.86	0.56
1:G:90:TRP:CD1	1:G:90:TRP:O	2.59	0.56
1:H:188:ALA:CB	1:I:149:LYS:HG2	2.33	0.56
1:F:64:GLU:HA	1:F:69:LYS:NZ	2.20	0.56
1:H:81:LEU:C	1:H:81:LEU:HD23	2.31	0.56
1:I:155:ILE:HG22	1:I:156:VAL:N	2.20	0.56
1:J:6:PHE:O	1:J:8:LYS:HG2	2.04	0.56
1:B:81:LEU:C	1:B:81:LEU:HD23	2.30	0.56
1:C:231:GLN:H	1:C:252:THR:HB	1.69	0.56
1:D:64:GLU:HA	1:D:69:LYS:HZ1	1.69	0.56
1:D:78:LEU:HD12	1:D:252:THR:CG2	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:111:ILE:C	2:S:112:ARG:HG2	2.29	0.56
1:H:176:ASN:ND2	1:H:179:ARG:H	1.94	0.56
1:A:152:LEU:O	1:A:156:VAL:HG13	2.05	0.56
1:G:196:ARG:NH1	1:G:196:ARG:CG	2.63	0.56
1:H:12:ALA:HB2	1:H:237:TYR:CD1	2.40	0.56
1:G:53:HIS:CG	1:G:228:ILE:HD13	2.40	0.56
1:H:231:GLN:H	1:H:252:THR:HB	1.70	0.56
1:A:81:LEU:C	1:A:81:LEU:HD23	2.31	0.56
1:D:53:HIS:CG	1:D:228:ILE:HD13	2.41	0.56
1:E:179:ARG:HG2	1:E:179:ARG:HH11	1.71	0.56
1:I:64:GLU:HA	1:I:69:LYS:HZ1	1.69	0.56
2:Q:111:ILE:C	2:Q:112:ARG:HG2	2.31	0.56
1:D:188:ALA:CB	1:E:149:LYS:HG2	2.34	0.56
1:E:231:GLN:H	1:E:252:THR:HB	1.70	0.56
1:G:64:GLU:HA	1:G:69:LYS:HZ1	1.70	0.55
2:O:111:ILE:C	2:O:112:ARG:HG2	2.30	0.55
1:A:85:PHE:CZ	1:A:107:LEU:HD13	2.41	0.55
1:J:76:LEU:HD22	1:J:254:THR:OG1	2.06	0.55
1:C:188:ALA:HB1	1:D:149:LYS:HG2	1.87	0.55
1:E:173:LEU:HD13	1:E:175:ILE:HB	1.88	0.55
1:H:64:GLU:HA	1:H:69:LYS:HZ1	1.71	0.55
1:A:196:ARG:NH1	1:A:196:ARG:CG	2.66	0.55
1:I:76:LEU:HD22	1:I:254:THR:OG1	2.06	0.55
1:G:152:LEU:HD12	1:G:200:CYS:SG	2.47	0.55
1:C:90:TRP:O	1:C:90:TRP:CD1	2.60	0.55
1:D:63:ASP:HB2	1:D:65:ASN:HB2	1.89	0.55
1:E:78:LEU:HD12	1:E:252:THR:CG2	2.36	0.55
1:F:155:ILE:HG22	1:F:156:VAL:N	2.22	0.55
1:H:17:LYS:HE3	1:H:17:LYS:HA	1.88	0.55
1:A:76:LEU:HD22	1:A:254:THR:OG1	2.06	0.55
1:I:173:LEU:HD13	1:I:175:ILE:HB	1.87	0.55
1:B:6:PHE:O	1:B:8:LYS:HG2	2.06	0.55
1:G:233:LEU:O	2:Q:109:LEU:CB	2.55	0.55
1:J:85:PHE:CZ	1:J:107:LEU:HD13	2.40	0.55
1:I:81:LEU:HD23	1:I:81:LEU:C	2.32	0.55
1:J:173:LEU:HD13	1:J:175:ILE:HB	1.89	0.54
1:I:90:TRP:O	1:I:90:TRP:CD1	2.60	0.54
1:C:233:LEU:O	2:M:109:LEU:CB	2.56	0.54
1:C:90:TRP:CZ3	1:I:82:ARG:NH2	2.75	0.54
1:D:158:ALA:HA	1:D:161:ILE:HD13	1.88	0.54
1:F:76:LEU:HD22	1:F:254:THR:OG1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:SER:HB2	3:J:1009:HOH:O	2.06	0.54
1:J:205:LYS:HE2	1:J:220:GLU:OE1	2.08	0.54
2:R:111:ILE:C	2:R:112:ARG:HG2	2.32	0.54
1:F:110:THR:O	1:F:114:VAL:HG23	2.08	0.54
1:J:231:GLN:H	1:J:252:THR:HB	1.73	0.54
1:I:110:THR:O	1:I:114:VAL:HG23	2.07	0.54
1:J:196:ARG:CG	1:J:196:ARG:NH1	2.64	0.54
1:A:173:LEU:HD13	1:A:175:ILE:HB	1.90	0.54
1:B:231:GLN:H	1:B:252:THR:HB	1.72	0.54
1:G:173:LEU:HD13	1:G:175:ILE:HB	1.90	0.54
1:C:60:VAL:O	1:C:61:LEU:HD12	2.07	0.54
1:D:110:THR:O	1:D:114:VAL:HG23	2.08	0.54
1:D:239:ASP:CG	1:D:240:ARG:H	2.16	0.54
1:H:126:CYS:HB2	1:H:129:SER:OG	2.08	0.54
1:D:97:ARG:HD3	1:E:73:ARG:HH21	1.73	0.54
1:F:173:LEU:HD13	1:F:175:ILE:HB	1.90	0.54
1:J:53:HIS:CG	1:J:228:ILE:HD13	2.43	0.54
1:A:55:LEU:HD12	1:A:76:LEU:HB2	1.88	0.54
1:E:12:ALA:HB2	1:E:237:TYR:CD1	2.42	0.54
2:N:111:ILE:C	2:N:112:ARG:HG2	2.33	0.54
1:A:239:ASP:CG	1:A:240:ARG:H	2.16	0.53
1:F:90:TRP:O	1:F:90:TRP:CD1	2.61	0.53
1:A:205:LYS:HE2	1:A:220:GLU:OE1	2.08	0.53
1:D:173:LEU:HD13	1:D:175:ILE:HB	1.90	0.53
1:G:233:LEU:O	2:Q:109:LEU:HB3	2.08	0.53
1:J:90:TRP:O	1:J:90:TRP:CD1	2.62	0.53
2:T:111:ILE:C	2:T:112:ARG:HG2	2.32	0.53
1:B:112:ARG:O	1:B:116:GLU:HG3	2.09	0.53
1:B:76:LEU:HD22	1:B:254:THR:OG1	2.08	0.53
1:B:205:LYS:HE2	1:B:220:GLU:OE1	2.07	0.53
1:D:126:CYS:HB2	1:D:129:SER:OG	2.08	0.53
1:G:81:LEU:C	1:G:81:LEU:HD23	2.33	0.53
1:F:85:PHE:CZ	1:F:107:LEU:HD13	2.44	0.53
1:F:181:ILE:HG12	1:G:156:VAL:HG21	1.90	0.53
1:I:229:LEU:CD1	1:I:232:ASP:HA	2.39	0.53
1:E:89:LEU:C	1:E:91:GLU:H	2.16	0.53
1:F:53:HIS:CG	1:F:228:ILE:HD13	2.43	0.53
1:G:229:LEU:CD1	1:G:232:ASP:HA	2.39	0.53
1:I:129:SER:HB2	3:I:1053:HOH:O	2.08	0.53
1:A:229:LEU:CD1	1:A:232:ASP:HA	2.39	0.53
1:F:129:SER:HB2	3:F:1008:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:PHE:O	1:G:8:LYS:HG2	2.07	0.53
1:H:55:LEU:HD12	1:H:76:LEU:HB2	1.91	0.53
1:I:53:HIS:CG	1:I:228:ILE:HD13	2.44	0.53
1:C:112:ARG:O	1:C:116:GLU:HG3	2.09	0.53
1:E:64:GLU:HA	1:E:69:LYS:HZ2	1.73	0.53
1:G:55:LEU:HD12	1:G:76:LEU:HB2	1.91	0.53
1:H:53:HIS:CG	1:H:228:ILE:HD13	2.44	0.53
1:B:97:ARG:HD3	1:C:73:ARG:HH21	1.74	0.53
1:I:215:ALA:HB3	1:I:266:LEU:HD12	1.90	0.53
1:E:233:LEU:O	2:O:109:LEU:CB	2.57	0.52
1:J:81:LEU:C	1:J:81:LEU:HD23	2.33	0.52
1:F:149:LYS:HG2	1:J:188:ALA:CB	2.38	0.52
1:H:233:LEU:O	2:R:109:LEU:CB	2.58	0.52
1:I:179:ARG:HG2	1:I:179:ARG:HH11	1.73	0.52
1:A:233:LEU:O	2:K:109:LEU:CB	2.57	0.52
2:M:111:ILE:C	2:M:112:ARG:HG2	2.33	0.52
1:C:229:LEU:CD1	1:C:232:ASP:HA	2.38	0.52
1:E:129:SER:HB2	3:E:1053:HOH:O	2.09	0.52
1:D:258:VAL:O	1:D:260:PRO:HD3	2.10	0.52
1:J:64:GLU:HA	1:J:69:LYS:HZ2	1.73	0.52
1:E:60:VAL:O	1:E:61:LEU:HD12	2.10	0.52
1:A:250:THR:HG22	1:A:251:GLU:N	2.24	0.52
1:B:53:HIS:CG	1:B:228:ILE:HD13	2.43	0.52
1:B:64:GLU:HA	1:B:69:LYS:HZ1	1.75	0.52
1:F:205:LYS:HE2	1:F:220:GLU:OE1	2.10	0.52
1:F:229:LEU:CD1	1:F:232:ASP:HA	2.40	0.52
1:H:64:GLU:HA	1:H:69:LYS:NZ	2.24	0.52
1:D:233:LEU:O	2:N:109:LEU:CB	2.57	0.52
1:E:196:ARG:NH1	1:E:196:ARG:CG	2.61	0.52
1:H:229:LEU:CD1	1:H:232:ASP:HA	2.40	0.52
2:P:111:ILE:C	2:P:112:ARG:HG2	2.35	0.51
1:A:17:LYS:HA	1:A:17:LYS:HE3	1.92	0.51
1:H:81:LEU:HD23	1:H:81:LEU:O	2.09	0.51
1:J:126:CYS:HB2	1:J:129:SER:OG	2.10	0.51
1:A:90:TRP:O	1:A:90:TRP:CD1	2.63	0.51
1:B:90:TRP:CD1	1:B:90:TRP:O	2.63	0.51
1:B:189:GLY:HA3	1:C:187:GLU:OE2	2.10	0.51
1:E:233:LEU:O	2:O:109:LEU:HB2	2.10	0.51
1:I:231:GLN:H	1:I:252:THR:HB	1.75	0.51
1:J:158:ALA:HA	1:J:161:ILE:HD13	1.92	0.51
1:A:73:ARG:HH21	1:E:97:ARG:HD3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:239:ASP:CG	1:I:240:ARG:H	2.19	0.51
1:C:81:LEU:C	1:C:81:LEU:HD23	2.36	0.51
1:C:89:LEU:C	1:C:91:GLU:H	2.19	0.51
1:E:110:THR:O	1:E:114:VAL:HG23	2.11	0.51
1:E:265:LEU:O	1:E:266:LEU:HD23	2.11	0.51
1:F:126:CYS:HB2	1:F:129:SER:OG	2.10	0.51
1:J:110:THR:O	1:J:114:VAL:HG23	2.10	0.51
1:E:214:ASP:OD2	1:E:267:LYS:HG2	2.10	0.51
1:I:230:GLY:HA3	1:I:252:THR:HG22	1.93	0.51
1:C:152:LEU:HD12	1:C:200:CYS:SG	2.51	0.51
1:E:229:LEU:CD1	1:E:232:ASP:HA	2.41	0.51
1:F:258:VAL:O	1:F:260:PRO:HD3	2.10	0.51
1:H:110:THR:O	1:H:114:VAL:HG23	2.11	0.51
1:H:214:ASP:OD2	1:H:267:LYS:HG2	2.10	0.51
1:J:233:LEU:O	2:T:109:LEU:CB	2.58	0.51
1:C:129:SER:HB2	3:C:1053:HOH:O	2.11	0.51
1:E:53:HIS:CG	1:E:228:ILE:HD13	2.46	0.51
1:E:140:ARG:HH22	1:E:161:ILE:CG2	2.24	0.51
1:H:205:LYS:HE2	1:H:220:GLU:OE1	2.11	0.51
1:I:89:LEU:C	1:I:91:GLU:H	2.19	0.51
1:I:233:LEU:O	2:S:109:LEU:CB	2.59	0.51
1:C:173:LEU:HD13	1:C:175:ILE:HB	1.92	0.51
1:C:214:ASP:OD2	1:C:267:LYS:HG2	2.11	0.51
1:E:55:LEU:HD12	1:E:76:LEU:HB2	1.92	0.51
1:E:239:ASP:CG	1:E:240:ARG:H	2.19	0.50
1:H:155:ILE:HG22	1:H:156:VAL:N	2.25	0.50
1:I:176:ASN:HD21	1:I:178:ASP:HB2	1.76	0.50
1:C:12:ALA:HB2	1:C:237:TYR:CD1	2.45	0.50
1:C:167:ILE:HG21	1:C:262:ALA:HA	1.94	0.50
1:D:189:GLY:O	1:E:190:HIS:HB2	2.10	0.50
1:H:196:ARG:CG	1:H:196:ARG:NH1	2.64	0.50
1:B:110:THR:O	1:B:114:VAL:HG23	2.12	0.50
1:B:214:ASP:OD2	1:B:267:LYS:HG2	2.10	0.50
1:E:179:ARG:NE	1:E:267:LYS:HE3	2.26	0.50
1:J:12:ALA:HB2	1:J:237:TYR:CD1	2.46	0.50
1:F:140:ARG:HD3	1:F:263:LEU:O	2.11	0.50
2:L:111:ILE:C	2:L:112:ARG:HG2	2.35	0.50
1:G:81:LEU:O	1:G:250:THR:HG23	2.11	0.50
1:H:76:LEU:HD22	1:H:254:THR:OG1	2.11	0.50
1:B:31:LYS:NZ	3:B:1015:HOH:O	2.43	0.50
1:D:31:LYS:NZ	3:D:1016:HOH:O	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ALA:CB	1:H:149:LYS:HG2	2.42	0.50
1:H:158:ALA:HA	1:H:161:ILE:HD13	1.93	0.50
1:J:229:LEU:CD1	1:J:232:ASP:HA	2.41	0.50
1:C:53:HIS:CG	1:C:228:ILE:HD13	2.47	0.50
1:F:64:GLU:HA	1:F:69:LYS:HZ2	1.76	0.50
1:F:112:ARG:O	1:F:116:GLU:HG3	2.12	0.50
1:J:89:LEU:C	1:J:91:GLU:H	2.19	0.50
1:C:158:ALA:HA	1:C:161:ILE:HD13	1.92	0.50
1:F:89:LEU:C	1:F:91:GLU:H	2.19	0.50
1:C:233:LEU:O	2:M:109:LEU:HB2	2.12	0.49
1:A:140:ARG:HH22	1:A:161:ILE:CG2	2.25	0.49
1:B:126:CYS:HB2	1:B:129:SER:OG	2.12	0.49
1:D:54:PRO:HB3	1:I:51:ALA:HB2	1.94	0.49
1:E:258:VAL:O	1:E:260:PRO:HD3	2.11	0.49
1:I:112:ARG:O	1:I:116:GLU:HG3	2.13	0.49
1:C:7:LEU:O	1:C:9:ARG:N	2.41	0.49
1:C:85:PHE:CZ	1:C:107:LEU:HD13	2.46	0.49
1:H:90:TRP:O	1:H:90:TRP:CD1	2.65	0.49
1:A:126:CYS:HB2	1:A:129:SER:OG	2.13	0.49
1:B:140:ARG:HD3	1:B:263:LEU:O	2.11	0.49
1:B:233:LEU:O	2:L:109:LEU:CB	2.60	0.49
1:E:7:LEU:O	1:E:9:ARG:N	2.44	0.49
1:J:239:ASP:CG	1:J:240:ARG:H	2.19	0.49
1:B:229:LEU:CD1	1:B:232:ASP:HA	2.41	0.49
1:F:233:LEU:O	2:P:109:LEU:CB	2.60	0.49
1:G:89:LEU:C	1:G:91:GLU:H	2.21	0.49
1:H:233:LEU:HG	1:H:251:GLU:OE2	2.12	0.49
1:I:63:ASP:HB2	1:I:65:ASN:HB2	1.94	0.49
1:C:78:LEU:HD12	1:C:252:THR:HG22	1.95	0.49
1:D:167:ILE:HG21	1:D:262:ALA:HA	1.94	0.49
1:D:231:GLN:H	1:D:252:THR:HB	1.77	0.49
1:E:64:GLU:HA	1:E:69:LYS:HZ1	1.77	0.49
1:F:78:LEU:HD12	1:F:252:THR:HG23	1.95	0.49
1:I:126:CYS:HB2	1:I:129:SER:OG	2.12	0.49
1:F:231:GLN:H	1:F:252:THR:HB	1.78	0.49
1:B:167:ILE:HG21	1:B:262:ALA:HA	1.94	0.49
1:C:140:ARG:HH22	1:C:161:ILE:CG2	2.25	0.49
1:F:55:LEU:CD1	1:F:76:LEU:HB2	2.42	0.49
1:G:250:THR:HG22	1:G:251:GLU:H	1.78	0.49
1:H:176:ASN:HD21	1:H:178:ASP:HB2	1.78	0.49
1:A:167:ILE:HG21	1:A:262:ALA:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:CG	1:B:240:ARG:H	2.20	0.49
1:C:64:GLU:HA	1:C:69:LYS:HZ1	1.78	0.49
1:D:179:ARG:HH11	1:D:179:ARG:CG	2.26	0.49
1:E:7:LEU:O	1:E:9:ARG:HG3	2.13	0.49
1:F:158:ALA:HA	1:F:161:ILE:HD13	1.95	0.49
1:F:187:GLU:OE2	1:J:189:GLY:HA3	2.13	0.49
1:J:55:LEU:HD12	1:J:76:LEU:HB2	1.95	0.48
1:A:110:THR:O	1:A:114:VAL:HG23	2.13	0.48
1:B:179:ARG:HH11	1:B:179:ARG:CG	2.26	0.48
1:C:93:ASP:OD1	1:I:8:LYS:NZ	2.45	0.48
1:B:129:SER:HB2	3:B:1013:HOH:O	2.14	0.48
1:C:7:LEU:O	1:C:9:ARG:HG3	2.13	0.48
1:F:152:LEU:HD12	1:F:200:CYS:SG	2.54	0.48
1:A:7:LEU:O	1:A:9:ARG:N	2.45	0.48
1:F:196:ARG:NH1	1:F:196:ARG:CG	2.62	0.48
1:G:158:ALA:HA	1:G:161:ILE:HD13	1.95	0.48
1:I:97:ARG:HD3	1:J:73:ARG:NH2	2.27	0.48
1:C:63:ASP:HB2	1:C:65:ASN:HB2	1.96	0.48
1:F:265:LEU:O	1:F:266:LEU:HD23	2.13	0.48
1:E:167:ILE:HG21	1:E:262:ALA:HA	1.95	0.48
1:C:205:LYS:HE2	1:C:220:GLU:OE1	2.13	0.48
1:D:8:LYS:NZ	1:H:93:ASP:OD1	2.45	0.48
1:D:90:TRP:O	1:D:90:TRP:CD1	2.67	0.48
1:I:214:ASP:OD2	1:I:267:LYS:HG2	2.13	0.48
1:J:7:LEU:O	1:J:9:ARG:N	2.45	0.48
1:B:233:LEU:HG	1:B:251:GLU:OE2	2.13	0.48
1:D:233:LEU:O	2:N:109:LEU:HB2	2.14	0.48
1:F:266:LEU:O	1:F:267:LYS:C	2.56	0.48
1:G:63:ASP:HB2	1:G:65:ASN:HB2	1.96	0.48
1:H:63:ASP:HB2	1:H:65:ASN:HB2	1.95	0.48
1:I:135:LEU:HD23	1:I:265:LEU:HD21	1.95	0.48
2:S:111:ILE:HD12	2:S:111:ILE:N	2.28	0.48
1:A:233:LEU:O	2:K:109:LEU:HB2	2.12	0.48
1:C:233:LEU:O	2:M:109:LEU:HB3	2.14	0.48
1:F:145:GLY:HA3	1:F:150:ASP:HB3	1.96	0.48
1:G:28:GLU:O	1:G:31:LYS:HG2	2.13	0.48
1:H:78:LEU:HD12	1:H:252:THR:HG22	1.96	0.48
1:I:28:GLU:O	1:I:31:LYS:HG2	2.14	0.48
1:B:81:LEU:HD23	1:B:81:LEU:O	2.14	0.47
1:F:63:ASP:HB2	1:F:65:ASN:HB2	1.96	0.47
1:I:176:ASN:HD22	1:I:179:ARG:N	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:111:ILE:N	2:N:111:ILE:HD12	2.29	0.47
1:B:7:LEU:O	1:B:9:ARG:N	2.45	0.47
1:D:229:LEU:CD1	1:D:232:ASP:HA	2.44	0.47
1:E:266:LEU:O	1:E:267:LYS:C	2.57	0.47
1:F:176:ASN:HD22	1:F:179:ARG:N	1.92	0.47
1:F:250:THR:HG22	1:F:251:GLU:N	2.30	0.47
1:G:110:THR:O	1:G:114:VAL:HG23	2.14	0.47
1:G:233:LEU:HG	1:G:251:GLU:OE2	2.13	0.47
1:E:63:ASP:HB2	1:E:65:ASN:HB2	1.96	0.47
1:H:55:LEU:HD11	1:H:76:LEU:HD12	1.96	0.47
1:H:233:LEU:O	2:R:109:LEU:HB2	2.14	0.47
1:J:214:ASP:OD2	1:J:267:LYS:HG2	2.14	0.47
1:B:176:ASN:HD21	1:B:178:ASP:HB2	1.79	0.47
1:F:73:ARG:HH21	1:J:97:ARG:CD	2.27	0.47
1:G:112:ARG:O	1:G:116:GLU:HG3	2.14	0.47
1:H:89:LEU:C	1:H:91:GLU:H	2.23	0.47
1:H:99:LYS:HA	1:H:100:PRO:HD3	1.74	0.47
1:H:215:ALA:HB3	1:H:266:LEU:HD12	1.96	0.47
1:B:179:ARG:NE	1:B:267:LYS:HE3	2.30	0.47
1:H:135:LEU:HD23	1:H:265:LEU:HD21	1.97	0.47
1:A:60:VAL:O	1:A:61:LEU:HD12	2.14	0.47
1:A:112:ARG:O	1:A:116:GLU:HG3	2.15	0.47
1:E:158:ALA:HA	1:E:161:ILE:HD13	1.95	0.47
1:E:168:GLU:HA	1:E:171:TYR:OH	2.15	0.47
1:E:215:ALA:HB3	1:E:266:LEU:HD12	1.97	0.47
1:F:189:GLY:H	1:G:196:ARG:HH12	1.62	0.47
1:F:233:LEU:O	2:P:109:LEU:HB3	2.14	0.47
1:F:239:ASP:CG	1:F:240:ARG:H	2.23	0.47
1:H:126:CYS:CB	1:H:129:SER:OG	2.63	0.47
1:I:117:PHE:CD2	1:I:117:PHE:C	2.93	0.47
1:B:89:LEU:C	1:B:91:GLU:H	2.22	0.47
1:C:64:GLU:HA	1:C:69:LYS:HZ2	1.79	0.47
1:G:126:CYS:HB2	1:G:129:SER:OG	2.15	0.47
1:G:173:LEU:HB2	1:G:201:LEU:HD11	1.96	0.47
1:H:117:PHE:C	1:H:117:PHE:CD2	2.93	0.47
1:H:239:ASP:CG	1:H:240:ARG:H	2.23	0.47
1:B:12:ALA:HB2	1:B:237:TYR:CD1	2.50	0.47
1:C:173:LEU:HB2	1:C:201:LEU:HD11	1.96	0.47
1:H:179:ARG:NE	1:H:267:LYS:HE3	2.30	0.47
1:I:7:LEU:O	1:I:9:ARG:N	2.46	0.47
1:B:158:ALA:HA	1:B:161:ILE:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:CYS:HB2	1:C:129:SER:OG	2.14	0.47
1:H:140:ARG:HD3	1:H:263:LEU:O	2.15	0.47
1:J:25:ARG:HD2	1:J:25:ARG:HA	1.57	0.47
1:B:169:GLY:HA3	1:B:221:ARG:HB3	1.97	0.46
1:C:89:LEU:C	1:C:91:GLU:N	2.73	0.46
1:D:117:PHE:CD2	1:D:117:PHE:C	2.93	0.46
1:E:117:PHE:C	1:E:117:PHE:CD2	2.93	0.46
1:B:233:LEU:O	2:L:109:LEU:HB2	2.15	0.46
1:E:89:LEU:O	1:E:91:GLU:N	2.48	0.46
1:I:67:VAL:HG13	1:I:68:VAL:HG22	1.98	0.46
1:A:158:ALA:HA	1:A:161:ILE:HD13	1.97	0.46
1:E:140:ARG:HD3	1:E:263:LEU:O	2.16	0.46
1:F:81:LEU:C	1:F:81:LEU:HD23	2.40	0.46
2:P:111:ILE:HD12	2:P:111:ILE:H	1.79	0.46
1:B:67:VAL:HG13	1:B:68:VAL:HG22	1.98	0.46
1:B:78:LEU:HD12	1:B:252:THR:HG22	1.97	0.46
1:B:140:ARG:HH22	1:B:161:ILE:CG2	2.28	0.46
1:F:117:PHE:C	1:F:117:PHE:CD2	2.94	0.46
1:I:126:CYS:CB	1:I:129:SER:OG	2.64	0.46
1:J:7:LEU:O	1:J:9:ARG:HG3	2.16	0.46
1:J:63:ASP:HB2	1:J:65:ASN:HB2	1.96	0.46
1:J:155:ILE:HG22	1:J:156:VAL:N	2.30	0.46
1:A:63:ASP:HB2	1:A:65:ASN:HB2	1.98	0.46
1:A:97:ARG:HD3	1:B:73:ARG:NH2	2.30	0.46
1:D:112:ARG:O	1:D:116:GLU:HG3	2.16	0.46
1:F:233:LEU:HG	1:F:251:GLU:OE2	2.15	0.46
1:G:7:LEU:O	1:G:9:ARG:HG3	2.16	0.46
1:C:239:ASP:CG	1:C:240:ARG:N	2.73	0.46
1:E:173:LEU:HB2	1:E:201:LEU:HD11	1.98	0.46
1:G:179:ARG:HG2	1:G:179:ARG:HH11	1.81	0.46
1:J:233:LEU:O	2:T:109:LEU:HB3	2.15	0.46
1:J:233:LEU:O	2:T:109:LEU:HB2	2.14	0.46
2:R:111:ILE:N	2:R:111:ILE:HD12	2.30	0.46
1:A:25:ARG:HA	1:A:25:ARG:HD2	1.60	0.46
1:D:89:LEU:C	1:D:91:GLU:H	2.23	0.46
1:E:25:ARG:HD2	1:E:25:ARG:HA	1.58	0.46
1:G:36:GLY:HA3	1:G:122:ILE:HD13	1.97	0.46
1:H:167:ILE:HG21	1:H:262:ALA:HA	1.97	0.46
1:B:63:ASP:HB2	1:B:65:ASN:HB2	1.98	0.46
1:B:189:GLY:H	1:C:196:ARG:HH12	1.63	0.46
1:C:55:LEU:HD12	1:C:76:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:LEU:O	1:D:267:LYS:C	2.59	0.46
1:G:7:LEU:O	1:G:9:ARG:N	2.46	0.46
1:I:55:LEU:HD12	1:I:76:LEU:HB2	1.96	0.46
1:A:214:ASP:OD2	1:A:267:LYS:HG2	2.16	0.46
1:E:85:PHE:CZ	1:E:107:LEU:HD13	2.51	0.46
1:E:89:LEU:C	1:E:91:GLU:N	2.73	0.46
1:F:76:LEU:HA	1:F:77:PRO:HD2	1.73	0.46
1:I:189:GLY:O	1:J:190:HIS:HB2	2.16	0.46
1:D:69:LYS:H	1:D:69:LYS:HG2	1.58	0.46
1:E:230:GLY:HA3	1:E:252:THR:HG22	1.98	0.46
1:H:7:LEU:O	1:H:9:ARG:N	2.47	0.46
1:I:87:LEU:HD23	1:I:87:LEU:HA	1.74	0.46
1:J:266:LEU:O	1:J:267:LYS:C	2.59	0.46
1:A:152:LEU:HD12	1:A:200:CYS:SG	2.56	0.45
1:D:81:LEU:HD23	1:D:81:LEU:C	2.41	0.45
1:E:171:TYR:O	1:E:204:GLY:HA3	2.17	0.45
1:F:209:THR:HA	1:F:210:PRO:HD3	1.82	0.45
1:G:140:ARG:HH22	1:G:161:ILE:CG2	2.29	0.45
1:G:250:THR:HG22	1:G:251:GLU:N	2.31	0.45
1:H:176:ASN:HD22	1:H:179:ARG:N	1.97	0.45
1:H:233:LEU:O	2:R:109:LEU:HB3	2.15	0.45
1:J:140:ARG:HD3	1:J:263:LEU:O	2.16	0.45
1:D:7:LEU:O	1:D:9:ARG:N	2.46	0.45
1:G:168:GLU:HA	1:G:171:TYR:OH	2.15	0.45
2:Q:109:LEU:HD12	2:Q:111:ILE:CD1	2.21	0.45
1:A:188:ALA:CB	1:B:149:LYS:HG2	2.45	0.45
1:C:69:LYS:H	1:C:69:LYS:HG2	1.59	0.45
1:C:158:ALA:HA	1:C:161:ILE:CD1	2.46	0.45
1:C:196:ARG:CG	1:C:196:ARG:NH1	2.61	0.45
1:D:173:LEU:HB2	1:D:201:LEU:HD11	1.98	0.45
1:D:214:ASP:OD2	1:D:267:LYS:HG2	2.16	0.45
1:F:7:LEU:O	1:F:9:ARG:N	2.47	0.45
1:F:149:LYS:H	1:F:149:LYS:HG3	1.55	0.45
1:G:193:LEU:O	1:G:194:GLU:C	2.60	0.45
1:I:89:LEU:C	1:I:91:GLU:N	2.75	0.45
1:J:167:ILE:HG21	1:J:262:ALA:HA	1.98	0.45
1:J:176:ASN:HD21	1:J:178:ASP:HB2	1.81	0.45
1:A:140:ARG:HD3	1:A:263:LEU:O	2.15	0.45
1:I:215:ALA:CB	1:I:266:LEU:HD12	2.47	0.45
1:J:112:ARG:O	1:J:116:GLU:HG3	2.16	0.45
2:K:111:ILE:C	2:K:112:ARG:HG2	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ALA:HB2	1:D:237:TYR:CD1	2.51	0.45
1:G:149:LYS:H	1:G:149:LYS:HG3	1.57	0.45
1:G:258:VAL:O	1:G:260:PRO:HD3	2.17	0.45
1:I:233:LEU:O	2:S:109:LEU:HB3	2.16	0.45
1:J:126:CYS:CB	1:J:129:SER:OG	2.65	0.45
1:B:36:GLY:HA3	1:B:122:ILE:HD13	1.99	0.45
1:D:152:LEU:HD12	1:D:200:CYS:SG	2.57	0.45
1:E:28:GLU:O	1:E:31:LYS:HG2	2.16	0.45
1:E:231:GLN:HA	1:E:231:GLN:OE1	2.17	0.45
1:F:176:ASN:HD21	1:F:178:ASP:HB2	1.81	0.45
1:I:171:TYR:O	1:I:204:GLY:HA3	2.16	0.45
1:I:209:THR:HA	1:I:210:PRO:HD3	1.80	0.45
1:J:117:PHE:C	1:J:117:PHE:CD2	2.95	0.45
1:J:233:LEU:HG	1:J:251:GLU:OE2	2.17	0.45
1:B:170:PRO:HA	3:B:1008:HOH:O	2.17	0.45
1:C:155:ILE:HD11	1:C:197:VAL:HG13	1.99	0.45
1:C:179:ARG:NE	1:C:267:LYS:HE3	2.32	0.45
1:D:135:LEU:HD23	1:D:265:LEU:HD21	1.98	0.45
1:F:89:LEU:C	1:F:91:GLU:N	2.74	0.45
1:F:97:ARG:HD3	1:G:73:ARG:NH2	2.26	0.45
1:F:173:LEU:HB2	1:F:201:LEU:HD11	1.99	0.45
1:G:117:PHE:C	1:G:117:PHE:CD2	2.95	0.45
1:H:25:ARG:HD2	1:H:25:ARG:HA	1.58	0.45
1:I:34:LEU:HD23	1:I:34:LEU:HA	1.79	0.45
1:J:89:LEU:C	1:J:91:GLU:N	2.74	0.45
1:D:117:PHE:O	1:D:120:GLU:HB2	2.16	0.45
1:D:155:ILE:HG22	1:D:156:VAL:N	2.32	0.45
1:E:233:LEU:HG	1:E:251:GLU:OE2	2.16	0.45
1:F:12:ALA:HA	1:F:13:PRO:HD3	1.74	0.45
1:I:7:LEU:O	1:I:9:ARG:HG3	2.16	0.45
1:I:239:ASP:HB3	1:I:246:ARG:NH2	2.32	0.45
1:G:214:ASP:OD2	1:G:267:LYS:HG2	2.17	0.45
1:D:233:LEU:O	2:N:109:LEU:HB3	2.15	0.45
1:F:7:LEU:O	1:F:9:ARG:HG3	2.18	0.45
1:G:78:LEU:HD12	1:G:252:THR:HG22	1.98	0.45
1:G:117:PHE:O	1:G:120:GLU:HB2	2.17	0.45
1:H:171:TYR:O	1:H:204:GLY:HA3	2.17	0.45
1:I:258:VAL:O	1:I:260:PRO:HD3	2.17	0.45
1:J:152:LEU:HD12	1:J:200:CYS:SG	2.57	0.45
1:A:7:LEU:O	1:A:9:ARG:HG3	2.17	0.44
1:A:155:ILE:HD11	1:A:197:VAL:HG13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:PHE:C	1:C:117:PHE:CD2	2.95	0.44
1:C:169:GLY:HA3	1:C:221:ARG:HB3	2.00	0.44
1:D:36:GLY:HA3	1:D:122:ILE:CD1	2.47	0.44
1:D:176:ASN:HD21	1:D:178:ASP:HB2	1.82	0.44
1:I:135:LEU:HD11	1:I:212:ILE:HG22	1.98	0.44
1:I:266:LEU:O	1:I:267:LYS:C	2.59	0.44
1:J:140:ARG:HH22	1:J:161:ILE:CG2	2.30	0.44
1:A:12:ALA:HB2	1:A:237:TYR:CD1	2.52	0.44
1:D:55:LEU:HD12	1:D:76:LEU:HB2	1.99	0.44
1:D:179:ARG:NE	1:D:267:LYS:HE3	2.32	0.44
1:F:55:LEU:HD11	1:F:76:LEU:HD12	1.99	0.44
1:I:89:LEU:O	1:I:91:GLU:N	2.50	0.44
1:B:55:LEU:HD12	1:B:76:LEU:HB2	1.99	0.44
1:B:64:GLU:HA	1:B:69:LYS:HZ2	1.81	0.44
1:B:99:LYS:HA	1:B:100:PRO:HD3	1.82	0.44
1:B:117:PHE:O	1:B:120:GLU:HB2	2.18	0.44
1:C:25:ARG:HD2	1:C:25:ARG:HA	1.62	0.44
1:C:135:LEU:HD23	1:C:265:LEU:HD21	1.99	0.44
1:G:126:CYS:CB	1:G:129:SER:OG	2.65	0.44
1:G:230:GLY:HA3	1:G:252:THR:HG22	1.99	0.44
2:T:111:ILE:HD12	2:T:111:ILE:N	2.32	0.44
1:D:99:LYS:HE3	1:E:57:GLU:OE1	2.18	0.44
1:H:89:LEU:C	1:H:91:GLU:N	2.76	0.44
1:J:179:ARG:NE	1:J:267:LYS:HE3	2.32	0.44
1:J:265:LEU:O	1:J:266:LEU:HD23	2.17	0.44
1:A:76:LEU:HA	1:A:77:PRO:HD2	1.78	0.44
1:D:196:ARG:NH1	1:D:196:ARG:CG	2.66	0.44
1:G:140:ARG:HD3	1:G:263:LEU:O	2.17	0.44
1:G:233:LEU:O	2:Q:109:LEU:HB2	2.17	0.44
1:I:233:LEU:O	2:S:109:LEU:HB2	2.17	0.44
1:J:179:ARG:HH11	1:J:179:ARG:CG	2.30	0.44
1:A:180:TRP:HH2	1:A:194:GLU:HG3	1.83	0.44
1:D:78:LEU:HD12	1:D:252:THR:HG22	1.99	0.44
1:F:230:GLY:HA3	1:F:252:THR:HG22	2.00	0.44
1:I:233:LEU:HG	1:I:251:GLU:OE2	2.17	0.44
1:I:265:LEU:O	1:I:266:LEU:HD23	2.18	0.44
1:A:233:LEU:O	2:K:109:LEU:HB3	2.17	0.44
1:A:265:LEU:O	1:A:266:LEU:HD23	2.18	0.44
1:C:266:LEU:O	1:C:267:LYS:C	2.61	0.44
1:J:135:LEU:HD23	1:J:265:LEU:HD21	2.00	0.44
1:A:12:ALA:HA	1:A:13:PRO:HD3	1.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD12	1:B:200:CYS:SG	2.57	0.44
1:C:87:LEU:HD23	1:C:87:LEU:HA	1.74	0.44
1:E:126:CYS:HB2	1:E:129:SER:OG	2.17	0.44
1:G:78:LEU:HD12	1:G:252:THR:HG23	2.00	0.44
1:I:167:ILE:HG21	1:I:262:ALA:HA	2.00	0.44
1:J:173:LEU:HB2	1:J:201:LEU:HD11	2.00	0.44
1:A:179:ARG:HH11	1:A:179:ARG:CG	2.29	0.44
1:B:155:ILE:HG22	1:B:156:VAL:N	2.33	0.44
1:C:140:ARG:HD3	1:C:263:LEU:O	2.18	0.44
1:D:239:ASP:CG	1:D:240:ARG:N	2.76	0.44
1:E:233:LEU:O	2:O:109:LEU:HB3	2.18	0.44
1:F:190:HIS:HB2	1:J:189:GLY:O	2.18	0.44
1:H:265:LEU:O	1:H:266:LEU:HD23	2.17	0.44
1:J:258:VAL:O	1:J:260:PRO:HD3	2.18	0.44
1:D:176:ASN:HB3	1:D:179:ARG:HB2	1.99	0.43
1:E:104:LEU:HD12	1:E:104:LEU:H	1.82	0.43
1:F:239:ASP:HB3	1:F:246:ARG:NH2	2.33	0.43
1:I:152:LEU:HD12	1:I:200:CYS:SG	2.58	0.43
1:B:135:LEU:HD23	1:B:265:LEU:HD21	2.00	0.43
1:B:260:PRO:O	1:B:263:LEU:HB3	2.18	0.43
1:G:158:ALA:HA	1:G:161:ILE:CD1	2.49	0.43
1:G:239:ASP:CG	1:G:240:ARG:H	2.26	0.43
1:A:89:LEU:C	1:A:91:GLU:H	2.25	0.43
1:B:36:GLY:HA3	1:B:122:ILE:CD1	2.48	0.43
1:D:140:ARG:HD3	1:D:263:LEU:O	2.17	0.43
1:I:155:ILE:HD11	1:I:197:VAL:HG13	2.00	0.43
2:K:111:ILE:N	2:K:111:ILE:HD12	2.34	0.43
1:A:78:LEU:HD12	1:A:252:THR:HG22	1.98	0.43
1:A:180:TRP:CH2	1:A:194:GLU:HG3	2.54	0.43
1:A:266:LEU:O	1:A:267:LYS:C	2.61	0.43
1:B:8:LYS:HB3	1:B:11:PHE:CD1	2.54	0.43
1:B:89:LEU:C	1:B:91:GLU:N	2.76	0.43
1:B:155:ILE:HD11	1:B:197:VAL:HG13	2.01	0.43
1:E:81:LEU:HD23	1:E:81:LEU:O	2.18	0.43
1:F:25:ARG:HD2	1:F:25:ARG:HA	1.55	0.43
1:F:53:HIS:ND1	1:F:228:ILE:HD13	2.33	0.43
1:F:168:GLU:HA	1:F:171:TYR:OH	2.19	0.43
1:H:193:LEU:O	1:H:194:GLU:C	2.61	0.43
1:J:89:LEU:O	1:J:91:GLU:N	2.51	0.43
2:Q:111:ILE:HD12	2:Q:111:ILE:N	2.33	0.43
1:A:215:ALA:HB3	1:A:266:LEU:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HA	1:B:77:PRO:HD2	1.76	0.43
1:E:135:LEU:HD23	1:E:265:LEU:HD21	1.99	0.43
1:H:180:TRP:HH2	1:H:194:GLU:HG3	1.84	0.43
1:I:169:GLY:HA3	1:I:221:ARG:HB3	2.00	0.43
1:B:239:ASP:CG	1:B:240:ARG:N	2.76	0.43
1:D:12:ALA:HA	1:D:13:PRO:HD3	1.76	0.43
1:D:81:LEU:O	1:D:250:THR:HG23	2.19	0.43
1:G:135:LEU:HD23	1:G:265:LEU:HD21	2.00	0.43
1:A:155:ILE:HG22	1:A:156:VAL:N	2.33	0.43
1:A:239:ASP:CG	1:A:240:ARG:N	2.77	0.43
1:D:89:LEU:O	1:D:91:GLU:N	2.51	0.43
1:E:239:ASP:CG	1:E:240:ARG:N	2.77	0.43
1:F:89:LEU:O	1:F:91:GLU:N	2.51	0.43
1:G:87:LEU:HD23	1:G:87:LEU:HA	1.69	0.43
1:G:89:LEU:C	1:G:91:GLU:N	2.76	0.43
1:B:168:GLU:HA	1:B:171:TYR:OH	2.19	0.43
1:D:89:LEU:C	1:D:91:GLU:N	2.76	0.43
1:I:81:LEU:O	1:I:250:THR:HG23	2.18	0.43
1:E:119:ASP:OD2	1:E:211:ARG:NE	2.43	0.43
1:G:12:ALA:CB	1:G:237:TYR:CD1	3.01	0.43
1:G:266:LEU:O	1:G:267:LYS:C	2.61	0.43
1:H:34:LEU:HD22	1:H:118:GLU:OE2	2.19	0.43
1:J:87:LEU:HD23	1:J:87:LEU:HA	1.73	0.43
1:C:36:GLY:HA3	1:C:122:ILE:CD1	2.49	0.43
1:D:231:GLN:OE1	1:D:231:GLN:HA	2.19	0.43
1:E:152:LEU:O	1:E:156:VAL:HG13	2.19	0.43
1:H:155:ILE:HD11	1:H:197:VAL:HG13	2.00	0.43
1:I:76:LEU:HA	1:I:77:PRO:HD2	1.78	0.43
1:A:169:GLY:HA3	1:A:221:ARG:HB3	2.01	0.42
1:B:171:TYR:O	1:B:204:GLY:HA3	2.19	0.42
1:D:7:LEU:O	1:D:9:ARG:HG3	2.18	0.42
1:F:69:LYS:H	1:F:69:LYS:HG2	1.65	0.42
1:H:250:THR:HG22	1:H:251:GLU:N	2.34	0.42
1:I:158:ALA:HA	1:I:161:ILE:HD13	1.99	0.42
1:J:250:THR:HG22	1:J:251:GLU:N	2.33	0.42
1:A:117:PHE:O	1:A:120:GLU:HB2	2.19	0.42
1:A:147:THR:CG2	1:A:149:LYS:HE3	2.42	0.42
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.75	0.42
1:B:209:THR:HA	1:B:210:PRO:HD3	1.78	0.42
1:C:250:THR:HG22	1:C:251:GLU:N	2.34	0.42
1:I:34:LEU:HD22	1:I:118:GLU:OE2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:ARG:NE	1:I:267:LYS:HE3	2.34	0.42
1:C:76:LEU:HA	1:C:77:PRO:HD2	1.79	0.42
1:G:155:ILE:HD11	1:G:197:VAL:HG13	2.01	0.42
1:H:169:GLY:HA3	1:H:221:ARG:HB3	2.01	0.42
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.80	0.42
1:C:147:THR:CG2	1:C:149:LYS:HE3	2.41	0.42
1:D:158:ALA:HA	1:D:161:ILE:CD1	2.49	0.42
1:E:87:LEU:HD23	1:E:87:LEU:HA	1.74	0.42
1:B:7:LEU:HB3	1:B:236:GLY:HA3	2.00	0.42
1:C:28:GLU:O	1:C:31:LYS:HG2	2.19	0.42
1:E:193:LEU:O	1:E:194:GLU:C	2.62	0.42
1:F:126:CYS:CB	1:F:129:SER:OG	2.68	0.42
1:F:155:ILE:HD11	1:F:197:VAL:HG13	2.00	0.42
1:F:179:ARG:NE	1:F:267:LYS:HE3	2.34	0.42
1:G:64:GLU:HA	1:G:69:LYS:HZ2	1.81	0.42
1:I:173:LEU:HB2	1:I:201:LEU:HD11	2.01	0.42
1:A:43:GLU:O	1:A:44:GLY:O	2.37	0.42
1:B:266:LEU:O	1:B:267:LYS:C	2.62	0.42
1:C:193:LEU:O	1:C:194:GLU:C	2.62	0.42
1:E:152:LEU:HD12	1:E:200:CYS:SG	2.59	0.42
1:F:97:ARG:CD	1:G:73:ARG:HH21	2.29	0.42
1:G:189:GLY:HA3	1:H:187:GLU:OE2	2.20	0.42
1:I:152:LEU:O	1:I:156:VAL:HG13	2.20	0.42
1:A:36:GLY:HA3	1:A:122:ILE:CD1	2.49	0.42
1:B:250:THR:HG22	1:B:251:GLU:N	2.35	0.42
1:C:89:LEU:O	1:C:91:GLU:N	2.53	0.42
1:D:153:GLU:O	1:D:156:VAL:HG22	2.19	0.42
1:D:170:PRO:HA	3:D:1009:HOH:O	2.20	0.42
1:G:99:LYS:HA	1:G:100:PRO:HD3	1.79	0.42
1:I:124:ARG:NH2	1:I:211:ARG:O	2.51	0.42
1:J:117:PHE:O	1:J:120:GLU:HB2	2.20	0.42
1:J:142:ILE:HD12	1:J:142:ILE:HA	1.95	0.42
1:J:176:ASN:HD22	1:J:179:ARG:N	1.94	0.42
1:B:233:LEU:O	2:L:109:LEU:HB3	2.19	0.42
1:C:104:LEU:H	1:C:104:LEU:HD12	1.84	0.42
1:D:112:ARG:NE	1:E:164:LYS:O	2.51	0.42
1:D:142:ILE:HD12	1:D:142:ILE:HA	1.93	0.42
1:F:171:TYR:O	1:F:204:GLY:HA3	2.20	0.42
1:G:85:PHE:CE1	1:G:107:LEU:HB2	2.54	0.42
1:G:104:LEU:H	1:G:104:LEU:HD12	1.84	0.42
1:I:140:ARG:HD2	1:I:260:PRO:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:ASP:CG	1:J:240:ARG:N	2.78	0.42
1:A:176:ASN:HB3	1:A:179:ARG:HB2	2.01	0.42
1:B:85:PHE:CE1	1:B:107:LEU:HB2	2.55	0.42
1:F:216:LEU:HA	1:F:216:LEU:HD12	1.77	0.42
1:I:31:LYS:NZ	3:I:1049:HOH:O	2.53	0.42
1:J:78:LEU:HD12	1:J:252:THR:HG22	2.01	0.42
1:A:89:LEU:C	1:A:91:GLU:N	2.78	0.42
1:B:126:CYS:CB	1:B:129:SER:OG	2.67	0.42
1:C:209:THR:HA	1:C:210:PRO:HD3	1.80	0.42
1:I:16:GLU:O	1:I:17:LYS:C	2.63	0.42
1:A:168:GLU:HA	1:A:171:TYR:OH	2.20	0.41
1:D:193:LEU:O	1:D:194:GLU:C	2.63	0.41
1:D:198:GLU:HG2	1:D:204:GLY:O	2.20	0.41
1:E:6:PHE:O	1:E:8:LYS:CG	2.67	0.41
1:E:112:ARG:O	1:E:116:GLU:HG3	2.20	0.41
1:F:34:LEU:HD23	1:F:34:LEU:HA	1.87	0.41
1:F:140:ARG:HH22	1:F:161:ILE:CG2	2.33	0.41
1:G:184:LEU:HD22	1:G:184:LEU:HA	1.95	0.41
1:H:12:ALA:CB	1:H:237:TYR:CD1	3.03	0.41
1:H:87:LEU:HD23	1:H:87:LEU:HA	1.75	0.41
1:I:25:ARG:HD2	1:I:25:ARG:HA	1.56	0.41
1:J:155:ILE:HD11	1:J:197:VAL:HG13	2.01	0.41
1:J:168:GLU:HA	1:J:171:TYR:OH	2.20	0.41
1:J:169:GLY:HA3	1:J:221:ARG:HB3	2.01	0.41
1:B:117:PHE:C	1:B:117:PHE:CD2	2.98	0.41
1:C:117:PHE:O	1:C:120:GLU:HB2	2.20	0.41
1:E:126:CYS:CB	1:E:129:SER:OG	2.68	0.41
1:G:36:GLY:HA3	1:G:122:ILE:CD1	2.50	0.41
1:G:55:LEU:HD11	1:G:76:LEU:HD12	2.02	0.41
1:H:7:LEU:O	1:H:9:ARG:HG3	2.20	0.41
1:B:179:ARG:CG	1:B:179:ARG:NH1	2.83	0.41
1:C:258:VAL:O	1:C:260:PRO:HD3	2.20	0.41
1:G:7:LEU:H	1:G:7:LEU:HG	1.75	0.41
1:I:161:ILE:O	1:I:161:ILE:HG22	2.19	0.41
1:A:117:PHE:C	1:A:117:PHE:CD2	2.99	0.41
1:A:171:TYR:O	1:A:204:GLY:HA3	2.20	0.41
1:C:145:GLY:HA3	1:C:150:ASP:HB3	2.02	0.41
1:G:239:ASP:HB3	1:G:246:ARG:NH2	2.35	0.41
1:H:117:PHE:O	1:H:120:GLU:HB2	2.19	0.41
1:J:171:TYR:O	1:J:204:GLY:HA3	2.20	0.41
1:A:126:CYS:CB	1:A:129:SER:OG	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:HD2	1:B:260:PRO:O	2.21	0.41
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.90	0.41
1:D:7:LEU:HB3	1:D:236:GLY:HA3	2.02	0.41
1:D:97:ARG:CD	1:E:73:ARG:HH21	2.34	0.41
1:D:155:ILE:CD1	1:D:197:VAL:HG13	2.50	0.41
1:F:170:PRO:HA	3:F:1003:HOH:O	2.21	0.41
1:G:265:LEU:O	1:G:266:LEU:HD23	2.21	0.41
1:H:69:LYS:H	1:H:69:LYS:HG2	1.60	0.41
1:H:180:TRP:CH2	1:H:194:GLU:HG3	2.56	0.41
2:Q:111:ILE:HD12	2:Q:111:ILE:H	1.84	0.41
1:B:231:GLN:OE1	1:B:231:GLN:HA	2.21	0.41
1:C:69:LYS:HE3	1:C:69:LYS:HB3	1.94	0.41
1:H:152:LEU:HD12	1:H:200:CYS:SG	2.60	0.41
1:C:180:TRP:HH2	1:C:194:GLU:HG3	1.85	0.41
1:D:34:LEU:HD22	1:D:118:GLU:OE2	2.20	0.41
1:D:97:ARG:HD3	1:E:73:ARG:NH2	2.36	0.41
1:F:59:GLU:O	1:F:61:LEU:HD13	2.20	0.41
1:G:169:GLY:HA3	1:G:221:ARG:HB3	2.02	0.41
1:G:179:ARG:NE	1:G:267:LYS:HE3	2.35	0.41
1:H:266:LEU:O	1:H:267:LYS:C	2.63	0.41
1:A:250:THR:HG22	1:A:251:GLU:H	1.85	0.41
1:D:72:LEU:HD11	1:I:129:SER:HB3	2.03	0.41
1:D:155:ILE:HD11	1:D:197:VAL:HG13	2.01	0.41
1:D:169:GLY:HA3	1:D:221:ARG:HB3	2.01	0.41
1:D:265:LEU:O	1:D:266:LEU:HD23	2.21	0.41
1:E:135:LEU:HD11	1:E:212:ILE:HG22	2.03	0.41
1:F:250:THR:HG22	1:F:251:GLU:H	1.85	0.41
1:H:209:THR:HA	1:H:210:PRO:HD3	1.84	0.41
1:I:140:ARG:HD3	1:I:263:LEU:O	2.21	0.41
1:I:239:ASP:CG	1:I:240:ARG:N	2.79	0.41
1:J:28:GLU:O	1:J:31:LYS:HG2	2.21	0.41
1:B:173:LEU:HB2	1:B:201:LEU:HD11	2.02	0.41
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.90	0.41
1:C:126:CYS:CB	1:C:129:SER:OG	2.68	0.41
1:C:176:ASN:HD21	1:C:178:ASP:HB2	1.85	0.41
1:D:140:ARG:HD2	1:D:260:PRO:O	2.21	0.41
1:D:179:ARG:CG	1:D:179:ARG:NH1	2.83	0.41
1:E:7:LEU:H	1:E:7:LEU:HG	1.75	0.41
1:E:169:GLY:HA3	1:E:221:ARG:HB3	2.01	0.41
1:E:209:THR:HA	1:E:210:PRO:HD3	1.80	0.41
1:F:67:VAL:HG13	1:F:68:VAL:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:LEU:O	1:G:91:GLU:N	2.54	0.41
1:G:176:ASN:HD21	1:G:178:ASP:HB2	1.85	0.41
1:H:34:LEU:HD23	1:H:34:LEU:HA	1.91	0.41
1:H:78:LEU:HD12	1:H:252:THR:HG23	2.01	0.41
1:I:152:LEU:N	1:I:152:LEU:HD22	2.35	0.41
1:J:215:ALA:HB3	1:J:266:LEU:HD12	2.03	0.41
1:A:173:LEU:HB2	1:A:201:LEU:HD11	2.02	0.41
1:B:89:LEU:HD12	1:B:245:VAL:HG23	2.03	0.41
1:D:161:ILE:HD12	1:D:161:ILE:H	1.86	0.41
1:G:53:HIS:ND1	1:G:228:ILE:HD13	2.36	0.41
1:I:196:ARG:NH1	1:I:196:ARG:CG	2.65	0.41
1:I:218:VAL:HA	1:I:262:ALA:O	2.21	0.41
1:A:55:LEU:HD11	1:A:76:LEU:HD12	2.04	0.40
1:A:97:ARG:CD	1:B:73:ARG:HH21	2.35	0.40
1:H:140:ARG:HH22	1:H:161:ILE:CG2	2.34	0.40
1:J:36:GLY:HA3	1:J:122:ILE:CD1	2.51	0.40
1:A:175:ILE:HD12	1:A:180:TRP:HB2	2.04	0.40
1:C:171:TYR:O	1:C:204:GLY:HA3	2.21	0.40
1:D:51:ALA:HB2	1:I:54:PRO:HB3	2.02	0.40
1:D:126:CYS:CB	1:D:129:SER:OG	2.69	0.40
1:D:145:GLY:HA3	1:D:150:ASP:HB3	2.04	0.40
1:D:171:TYR:O	1:D:204:GLY:HA3	2.21	0.40
1:D:215:ALA:HB3	1:D:266:LEU:HD12	2.03	0.40
1:E:176:ASN:HD22	1:E:179:ARG:N	1.97	0.40
1:F:218:VAL:HA	1:F:262:ALA:O	2.22	0.40
1:H:189:GLY:HA3	1:I:187:GLU:OE2	2.21	0.40
1:J:149:LYS:H	1:J:149:LYS:HG3	1.54	0.40
1:A:179:ARG:NE	1:A:267:LYS:HE3	2.36	0.40
1:B:18:GLN:O	1:B:19:TRP:C	2.61	0.40
1:D:87:LEU:HD23	1:D:87:LEU:HA	1.76	0.40
1:E:176:ASN:HD21	1:E:178:ASP:HB2	1.86	0.40
1:F:169:GLY:HA3	1:F:221:ARG:HB3	2.02	0.40
1:G:216:LEU:HD12	1:G:216:LEU:HA	1.83	0.40
1:H:12:ALA:HA	1:H:13:PRO:HD3	1.73	0.40
1:H:28:GLU:O	1:H:31:LYS:HG2	2.21	0.40
1:H:140:ARG:HD2	1:H:260:PRO:O	2.21	0.40
1:J:184:LEU:HD22	1:J:184:LEU:HA	1.95	0.40
1:D:67:VAL:HG13	1:D:68:VAL:HG22	2.03	0.40
1:D:76:LEU:HA	1:D:77:PRO:HD2	1.79	0.40
1:D:140:ARG:HH22	1:D:161:ILE:CG2	2.34	0.40
1:D:152:LEU:O	1:D:156:VAL:HG13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:ASP:OD2	1:F:267:LYS:HG2	2.20	0.40
1:G:171:TYR:O	1:G:204:GLY:HA3	2.22	0.40
1:H:145:GLY:HA3	1:H:150:ASP:OD2	2.21	0.40
1:H:230:GLY:HA3	1:H:252:THR:HG22	2.04	0.40
1:J:99:LYS:HA	1:J:100:PRO:HD3	1.79	0.40
1:B:7:LEU:O	1:B:9:ARG:HG3	2.22	0.40
1:D:181:ILE:HG12	1:E:156:VAL:HG21	2.04	0.40
1:F:140:ARG:HD2	1:F:260:PRO:O	2.22	0.40
1:F:156:VAL:HG21	1:J:181:ILE:HG12	2.04	0.40
1:I:193:LEU:O	1:I:194:GLU:C	2.64	0.40
2:S:111:ILE:O	2:S:112:ARG:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/265 (99%)	232 (88%)	26 (10%)	4 (2%)	8	32
1	B	262/265 (99%)	233 (89%)	24 (9%)	5 (2%)	6	27
1	C	262/265 (99%)	232 (88%)	27 (10%)	3 (1%)	11	39
1	D	262/265 (99%)	231 (88%)	26 (10%)	5 (2%)	6	27
1	E	262/265 (99%)	232 (88%)	24 (9%)	6 (2%)	5	23
1	F	262/265 (99%)	235 (90%)	22 (8%)	5 (2%)	6	27
1	G	262/265 (99%)	231 (88%)	26 (10%)	5 (2%)	6	27
1	H	262/265 (99%)	232 (88%)	26 (10%)	4 (2%)	8	32
1	I	262/265 (99%)	234 (89%)	23 (9%)	5 (2%)	6	27
1	J	262/265 (99%)	233 (89%)	24 (9%)	5 (2%)	6	27
2	K	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	M	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	N	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	O	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	P	6/8 (75%)	3 (50%)	1 (17%)	2 (33%)	0	0
2	Q	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	R	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	S	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	T	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
All	All	2680/2730 (98%)	2355 (88%)	267 (10%)	58 (2%)	5	24

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLY
1	B	44	GLY
1	C	44	GLY
1	D	44	GLY
1	F	44	GLY
1	G	44	GLY
1	J	44	GLY
1	E	44	GLY
1	H	44	GLY
1	I	44	GLY
2	K	112	ARG
2	L	112	ARG
2	M	112	ARG
2	N	112	ARG
2	O	112	ARG
2	P	112	ARG
2	Q	112	ARG
2	R	112	ARG
2	S	112	ARG
2	T	112	ARG
1	A	242	LYS
1	E	242	LYS
1	F	242	LYS
1	B	242	LYS
1	C	242	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	90	TRP
1	D	242	LYS
1	E	90	TRP
1	F	90	TRP
1	G	242	LYS
1	H	242	LYS
1	I	90	TRP
1	I	242	LYS
1	J	242	LYS
1	E	7	LEU
1	G	7	LEU
1	J	90	TRP
2	P	109	LEU
1	A	100	PRO
1	B	100	PRO
1	B	210	PRO
1	F	100	PRO
1	G	100	PRO
1	J	100	PRO
1	C	100	PRO
1	D	100	PRO
1	D	210	PRO
1	F	210	PRO
1	H	100	PRO
1	H	210	PRO
1	I	100	PRO
1	A	210	PRO
1	B	155	ILE
1	E	100	PRO
1	G	210	PRO
1	J	210	PRO
1	E	210	PRO
1	I	155	ILE

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	233/234 (100%)	186 (80%)	47 (20%)	1	5
1	B	233/234 (100%)	185 (79%)	48 (21%)	1	5
1	C	233/234 (100%)	186 (80%)	47 (20%)	1	5
1	D	233/234 (100%)	187 (80%)	46 (20%)	1	6
1	E	233/234 (100%)	183 (78%)	50 (22%)	1	5
1	F	233/234 (100%)	184 (79%)	49 (21%)	1	5
1	G	233/234 (100%)	187 (80%)	46 (20%)	1	6
1	H	233/234 (100%)	185 (79%)	48 (21%)	1	5
1	I	233/234 (100%)	187 (80%)	46 (20%)	1	6
1	J	233/234 (100%)	187 (80%)	46 (20%)	1	6
2	K	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	L	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	M	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	N	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	O	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	P	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	Q	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	R	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	S	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	T	5/5 (100%)	3 (60%)	2 (40%)	0	0
All	All	2380/2390 (100%)	1884 (79%)	496 (21%)	1	5

All (496) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	GLU
1	A	7	LEU
1	A	10	SER
1	A	16	GLU
1	A	17	LYS
1	A	41	ASP
1	A	55	LEU
1	A	58	VAL
1	A	60	VAL
1	A	67	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	68	VAL
1	A	69	LYS
1	A	73	ARG
1	A	78	LEU
1	A	81	LEU
1	A	82	ARG
1	A	84	THR
1	A	89	LEU
1	A	96	GLU
1	A	104	LEU
1	A	124	ARG
1	A	129	SER
1	A	131	VAL
1	A	139	GLU
1	A	140	ARG
1	A	143	GLU
1	A	147	THR
1	A	153	GLU
1	A	156	VAL
1	A	159	LEU
1	A	172	THR
1	A	173	LEU
1	A	175	ILE
1	A	179	ARG
1	A	184	LEU
1	A	190	HIS
1	A	196	ARG
1	A	207	ILE
1	A	229	LEU
1	A	234	SER
1	A	240	ARG
1	A	243	ASP
1	A	252	THR
1	A	261	GLU
1	A	265	LEU
1	A	267	LYS
1	B	4	MET
1	B	5	GLU
1	B	7	LEU
1	B	10	SER
1	B	16	GLU
1	B	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	25	ARG
1	B	41	ASP
1	B	55	LEU
1	B	58	VAL
1	B	60	VAL
1	B	67	VAL
1	B	68	VAL
1	B	69	LYS
1	B	73	ARG
1	B	78	LEU
1	B	81	LEU
1	B	82	ARG
1	B	84	THR
1	B	89	LEU
1	B	96	GLU
1	B	104	LEU
1	B	113	LYS
1	B	124	ARG
1	B	131	VAL
1	B	139	GLU
1	B	140	ARG
1	B	143	GLU
1	B	147	THR
1	B	153	GLU
1	B	156	VAL
1	B	159	LEU
1	B	172	THR
1	B	173	LEU
1	B	175	ILE
1	B	179	ARG
1	B	184	LEU
1	B	190	HIS
1	B	196	ARG
1	B	219	SER
1	B	229	LEU
1	B	234	SER
1	B	240	ARG
1	B	243	ASP
1	B	252	THR
1	B	261	GLU
1	B	265	LEU
1	B	267	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4	MET
1	C	5	GLU
1	C	7	LEU
1	C	10	SER
1	C	16	GLU
1	C	17	LYS
1	C	41	ASP
1	C	55	LEU
1	C	58	VAL
1	C	60	VAL
1	C	67	VAL
1	C	68	VAL
1	C	69	LYS
1	C	73	ARG
1	C	78	LEU
1	C	81	LEU
1	C	82	ARG
1	C	84	THR
1	C	89	LEU
1	C	96	GLU
1	C	104	LEU
1	C	106	SER
1	C	113	LYS
1	C	124	ARG
1	C	126	CYS
1	C	129	SER
1	C	131	VAL
1	C	139	GLU
1	C	140	ARG
1	C	143	GLU
1	C	147	THR
1	C	153	GLU
1	C	159	LEU
1	C	172	THR
1	C	173	LEU
1	C	175	ILE
1	C	179	ARG
1	C	184	LEU
1	C	190	HIS
1	C	196	ARG
1	C	229	LEU
1	C	234	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	243	ASP
1	C	252	THR
1	C	261	GLU
1	C	265	LEU
1	C	267	LYS
1	D	4	MET
1	D	5	GLU
1	D	7	LEU
1	D	10	SER
1	D	16	GLU
1	D	17	LYS
1	D	41	ASP
1	D	55	LEU
1	D	58	VAL
1	D	60	VAL
1	D	63	ASP
1	D	67	VAL
1	D	68	VAL
1	D	69	LYS
1	D	73	ARG
1	D	78	LEU
1	D	81	LEU
1	D	82	ARG
1	D	84	THR
1	D	89	LEU
1	D	96	GLU
1	D	104	LEU
1	D	124	ARG
1	D	129	SER
1	D	131	VAL
1	D	139	GLU
1	D	140	ARG
1	D	143	GLU
1	D	147	THR
1	D	153	GLU
1	D	156	VAL
1	D	159	LEU
1	D	172	THR
1	D	173	LEU
1	D	175	ILE
1	D	179	ARG
1	D	184	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	190	HIS
1	D	196	ARG
1	D	229	LEU
1	D	234	SER
1	D	243	ASP
1	D	252	THR
1	D	261	GLU
1	D	265	LEU
1	D	267	LYS
1	E	4	MET
1	E	5	GLU
1	E	7	LEU
1	E	10	SER
1	E	16	GLU
1	E	17	LYS
1	E	41	ASP
1	E	55	LEU
1	E	58	VAL
1	E	60	VAL
1	E	67	VAL
1	E	68	VAL
1	E	69	LYS
1	E	73	ARG
1	E	78	LEU
1	E	81	LEU
1	E	82	ARG
1	E	84	THR
1	E	89	LEU
1	E	96	GLU
1	E	104	LEU
1	E	124	ARG
1	E	126	CYS
1	E	129	SER
1	E	131	VAL
1	E	139	GLU
1	E	140	ARG
1	E	143	GLU
1	E	147	THR
1	E	153	GLU
1	E	156	VAL
1	E	159	LEU
1	E	172	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	173	LEU
1	E	175	ILE
1	E	179	ARG
1	E	184	LEU
1	E	190	HIS
1	E	196	ARG
1	E	200	CYS
1	E	219	SER
1	E	229	LEU
1	E	234	SER
1	E	237	TYR
1	E	240	ARG
1	E	243	ASP
1	E	252	THR
1	E	261	GLU
1	E	265	LEU
1	E	267	LYS
1	F	4	MET
1	F	5	GLU
1	F	7	LEU
1	F	10	SER
1	F	16	GLU
1	F	17	LYS
1	F	41	ASP
1	F	55	LEU
1	F	58	VAL
1	F	60	VAL
1	F	63	ASP
1	F	67	VAL
1	F	68	VAL
1	F	69	LYS
1	F	73	ARG
1	F	78	LEU
1	F	81	LEU
1	F	82	ARG
1	F	84	THR
1	F	89	LEU
1	F	96	GLU
1	F	104	LEU
1	F	105	SER
1	F	106	SER
1	F	113	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	124	ARG
1	F	126	CYS
1	F	131	VAL
1	F	139	GLU
1	F	140	ARG
1	F	143	GLU
1	F	147	THR
1	F	153	GLU
1	F	156	VAL
1	F	159	LEU
1	F	172	THR
1	F	173	LEU
1	F	175	ILE
1	F	179	ARG
1	F	184	LEU
1	F	190	HIS
1	F	196	ARG
1	F	229	LEU
1	F	234	SER
1	F	243	ASP
1	F	252	THR
1	F	261	GLU
1	F	265	LEU
1	F	267	LYS
1	G	4	MET
1	G	5	GLU
1	G	7	LEU
1	G	10	SER
1	G	16	GLU
1	G	17	LYS
1	G	41	ASP
1	G	55	LEU
1	G	58	VAL
1	G	60	VAL
1	G	67	VAL
1	G	68	VAL
1	G	69	LYS
1	G	73	ARG
1	G	78	LEU
1	G	81	LEU
1	G	82	ARG
1	G	84	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	89	LEU
1	G	96	GLU
1	G	104	LEU
1	G	113	LYS
1	G	124	ARG
1	G	126	CYS
1	G	129	SER
1	G	131	VAL
1	G	139	GLU
1	G	140	ARG
1	G	143	GLU
1	G	147	THR
1	G	153	GLU
1	G	156	VAL
1	G	159	LEU
1	G	172	THR
1	G	173	LEU
1	G	175	ILE
1	G	184	LEU
1	G	190	HIS
1	G	196	ARG
1	G	229	LEU
1	G	234	SER
1	G	243	ASP
1	G	252	THR
1	G	261	GLU
1	G	265	LEU
1	G	267	LYS
1	H	4	MET
1	H	5	GLU
1	H	7	LEU
1	H	10	SER
1	H	16	GLU
1	H	17	LYS
1	H	41	ASP
1	H	55	LEU
1	H	58	VAL
1	H	60	VAL
1	H	67	VAL
1	H	68	VAL
1	H	69	LYS
1	H	73	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	78	LEU
1	H	81	LEU
1	H	82	ARG
1	H	84	THR
1	H	89	LEU
1	H	96	GLU
1	H	104	LEU
1	H	106	SER
1	H	124	ARG
1	H	126	CYS
1	H	129	SER
1	H	131	VAL
1	H	139	GLU
1	H	140	ARG
1	H	143	GLU
1	H	147	THR
1	H	153	GLU
1	H	156	VAL
1	H	159	LEU
1	H	172	THR
1	H	173	LEU
1	H	175	ILE
1	H	179	ARG
1	H	184	LEU
1	H	190	HIS
1	H	196	ARG
1	H	219	SER
1	H	229	LEU
1	H	234	SER
1	H	243	ASP
1	H	252	THR
1	H	261	GLU
1	H	265	LEU
1	H	267	LYS
1	I	4	MET
1	I	5	GLU
1	I	7	LEU
1	I	10	SER
1	I	16	GLU
1	I	17	LYS
1	I	41	ASP
1	I	55	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	58	VAL
1	I	60	VAL
1	I	67	VAL
1	I	68	VAL
1	I	69	LYS
1	I	73	ARG
1	I	78	LEU
1	I	81	LEU
1	I	82	ARG
1	I	84	THR
1	I	89	LEU
1	I	96	GLU
1	I	104	LEU
1	I	106	SER
1	I	124	ARG
1	I	126	CYS
1	I	129	SER
1	I	131	VAL
1	I	139	GLU
1	I	140	ARG
1	I	143	GLU
1	I	147	THR
1	I	153	GLU
1	I	156	VAL
1	I	159	LEU
1	I	172	THR
1	I	173	LEU
1	I	175	ILE
1	I	184	LEU
1	I	190	HIS
1	I	196	ARG
1	I	229	LEU
1	I	234	SER
1	I	243	ASP
1	I	252	THR
1	I	261	GLU
1	I	265	LEU
1	I	267	LYS
1	J	4	MET
1	J	5	GLU
1	J	7	LEU
1	J	10	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	16	GLU
1	J	17	LYS
1	J	41	ASP
1	J	55	LEU
1	J	58	VAL
1	J	60	VAL
1	J	67	VAL
1	J	68	VAL
1	J	69	LYS
1	J	73	ARG
1	J	78	LEU
1	J	81	LEU
1	J	82	ARG
1	J	84	THR
1	J	89	LEU
1	J	96	GLU
1	J	104	LEU
1	J	124	ARG
1	J	126	CYS
1	J	129	SER
1	J	131	VAL
1	J	139	GLU
1	J	140	ARG
1	J	143	GLU
1	J	147	THR
1	J	153	GLU
1	J	156	VAL
1	J	159	LEU
1	J	172	THR
1	J	173	LEU
1	J	175	ILE
1	J	179	ARG
1	J	184	LEU
1	J	190	HIS
1	J	196	ARG
1	J	229	LEU
1	J	234	SER
1	J	243	ASP
1	J	252	THR
1	J	261	GLU
1	J	265	LEU
1	J	267	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	109	LEU
2	K	111	ILE
2	L	109	LEU
2	L	111	ILE
2	M	109	LEU
2	M	111	ILE
2	M	112	ARG
2	N	109	LEU
2	N	111	ILE
2	O	109	LEU
2	O	111	ILE
2	O	112	ARG
2	P	109	LEU
2	P	111	ILE
2	Q	109	LEU
2	Q	111	ILE
2	Q	112	ARG
2	R	109	LEU
2	R	111	ILE
2	S	109	LEU
2	S	111	ILE
2	T	109	LEU
2	T	111	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	B	176	ASN
1	C	176	ASN
1	D	176	ASN
1	E	176	ASN
1	F	176	ASN
1	G	176	ASN
1	H	176	ASN
1	I	176	ASN
1	J	176	ASN

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	264/265 (99%)	0.33	9 (3%) 48 28	99, 128, 173, 221	0
1	B	264/265 (99%)	0.41	10 (3%) 44 25	94, 128, 173, 228	0
1	C	264/265 (99%)	0.17	8 (3%) 52 31	89, 123, 172, 232	0
1	D	264/265 (99%)	0.29	14 (5%) 32 17	95, 126, 173, 232	0
1	E	264/265 (99%)	0.41	9 (3%) 48 28	97, 128, 175, 230	0
1	F	264/265 (99%)	0.13	8 (3%) 52 31	76, 108, 161, 226	0
1	G	264/265 (99%)	0.24	10 (3%) 44 25	89, 119, 166, 226	0
1	H	264/265 (99%)	0.30	9 (3%) 48 28	94, 123, 166, 209	0
1	I	264/265 (99%)	0.14	4 (1%) 72 52	86, 117, 166, 219	0
1	J	264/265 (99%)	0.28	8 (3%) 52 31	82, 115, 166, 222	0
2	K	8/8 (100%)	1.48	3 (37%) 1 0	133, 150, 185, 199	0
2	L	8/8 (100%)	1.30	2 (25%) 2 1	130, 150, 180, 193	0
2	M	8/8 (100%)	1.30	2 (25%) 2 1	125, 139, 185, 191	0
2	N	8/8 (100%)	1.34	4 (50%) 0 0	122, 146, 191, 200	0
2	O	8/8 (100%)	1.72	4 (50%) 0 0	132, 153, 185, 201	0
2	P	8/8 (100%)	1.16	2 (25%) 2 1	123, 135, 189, 211	0
2	Q	8/8 (100%)	1.96	5 (62%) 0 0	129, 148, 177, 187	0
2	R	8/8 (100%)	1.69	3 (37%) 1 0	129, 142, 172, 197	0
2	S	8/8 (100%)	1.27	3 (37%) 1 0	116, 139, 177, 190	0
2	T	8/8 (100%)	1.74	4 (50%) 0 0	119, 141, 183, 193	0
All	All	2720/2730 (99%)	0.31	121 (4%) 39 21	76, 123, 174, 232	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	TRP	7.4
1	D	90	TRP	7.2
1	A	90	TRP	7.0
1	G	90	TRP	6.6
1	E	90	TRP	6.4
1	H	90	TRP	6.3
1	J	90	TRP	6.2
1	I	90	TRP	6.0
1	C	90	TRP	5.8
1	F	90	TRP	5.6
2	M	106	GLY	4.3
1	I	242	LYS	4.1
2	T	106	GLY	4.0
2	O	107	GLY	3.9
1	C	189	GLY	3.7
1	J	186	GLU	3.7
1	G	238	GLU	3.6
2	Q	113	LYS	3.6
1	J	242	LYS	3.5
2	O	113	LYS	3.5
1	H	214	ASP	3.5
1	B	267	LYS	3.4
1	A	185	LYS	3.4
2	N	106	GLY	3.4
1	H	4	MET	3.4
2	Q	106	GLY	3.3
1	D	267	LYS	3.3
2	R	106	GLY	3.3
1	D	242	LYS	3.2
2	R	113	LYS	3.2
1	B	238	GLU	3.2
1	E	238	GLU	3.1
2	K	106	GLY	3.1
1	H	186	GLU	3.1
2	S	106	GLY	3.1
1	D	214	ASP	3.0
2	L	113	LYS	3.0
2	P	106	GLY	3.0
1	G	4	MET	3.0
1	A	238	GLU	2.9
2	R	107	GLY	2.9
1	B	93	ASP	2.9
1	J	4	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	242	LYS	2.9
1	G	243	ASP	2.9
1	H	189	GLY	2.9
1	J	93	ASP	2.8
1	J	189	GLY	2.8
1	B	242	LYS	2.8
1	E	241	GLU	2.8
1	B	149	LYS	2.8
1	D	185	LYS	2.7
1	D	238	GLU	2.7
1	B	82	ARG	2.7
1	A	128	LYS	2.7
2	Q	112	ARG	2.7
1	H	243	ASP	2.6
2	K	113	LYS	2.6
2	S	113	LYS	2.6
1	I	243	ASP	2.6
1	J	243	ASP	2.6
1	F	187	GLU	2.6
2	T	113	LYS	2.6
1	C	238	GLU	2.6
2	O	106	GLY	2.5
1	F	168	GLU	2.5
1	D	84	THR	2.5
1	J	146	SER	2.5
2	T	107	GLY	2.5
1	F	188	ALA	2.4
1	F	4	MET	2.4
1	G	187	GLU	2.4
2	L	108	ASP	2.4
2	T	108	ASP	2.4
1	C	242	LYS	2.4
1	E	20	GLN	2.4
1	F	186	GLU	2.4
2	Q	107	GLY	2.4
1	C	243	ASP	2.4
2	N	107	GLY	2.3
2	Q	108	ASP	2.3
1	H	215	ALA	2.3
1	C	267	LYS	2.3
1	E	267	LYS	2.3
1	D	4	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	113	LYS	2.3
2	M	107	GLY	2.3
1	E	243	ASP	2.3
2	K	108	ASP	2.3
1	B	4	MET	2.2
1	B	145	GLY	2.2
1	C	185	LYS	2.2
1	A	214	ASP	2.2
2	O	108	ASP	2.2
1	E	4	MET	2.2
1	E	189	GLY	2.2
2	S	107	GLY	2.2
1	A	242	LYS	2.2
1	B	84	THR	2.2
1	D	243	ASP	2.2
1	C	4	MET	2.1
1	F	190	HIS	2.1
1	D	187	GLU	2.1
1	G	186	GLU	2.1
1	H	58	VAL	2.1
2	N	108	ASP	2.1
1	E	168	GLU	2.1
1	I	214	ASP	2.1
2	P	108	ASP	2.1
1	A	168	GLU	2.1
1	A	4	MET	2.1
1	G	93	ASP	2.1
1	F	267	LYS	2.0
1	A	5	GLU	2.0
1	D	17	LYS	2.0
1	D	149	LYS	2.0
1	G	149	LYS	2.0
1	G	82	ARG	2.0
1	D	189	GLY	2.0
1	H	242	LYS	2.0
1	D	82	ARG	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.