Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:03 AM GMT

PDB ID	:	3D5N
Title	:	Crystal structure of the Q97W15_SULSO protein from Sulfolobus solfataricus. NESG target SsR125.
Authors	:	Vorobiev, S.M.; Chen, Y.; Seetharaman, J.; Lee, D.; Foote, R.E.; Maglaqui, M.; Janjua, H.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-05-16
Resolution	:	2.80 Å(reported)

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

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

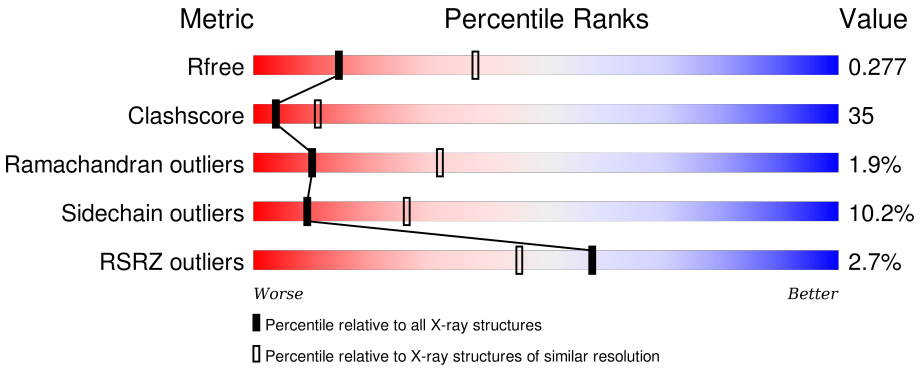
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	197	3% 44% 39% 8% 10%
1	B	197	3% 47% 31% 6% • 15%
1	D	197	2% 44% 40% 6% 10%
1	E	197	2% 38% 41% 8% • 13%
1	F	197	2% 44% 40% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	197	2% 36% 45% 16%
1	H	197	2% 34% 44% 10% 12%
1	I	197	4% 42% 38% 8% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10496 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 Q97W15_SULSO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	Se	0	0	0
			1356	882	223	243	3	5			
1	B	167	Total	C	N	O	S	Se	0	0	0
			1268	831	201	229	3	4			
1	D	178	Total	C	N	O	S	Se	0	0	0
			1373	894	226	245	3	5			
1	E	172	Total	C	N	O	S	Se	0	0	0
			1300	848	208	236	3	5			
1	F	172	Total	C	N	O	S	Se	0	0	0
			1292	847	214	223	3	5			
1	G	166	Total	C	N	O	S	Se	0	0	0
			1269	829	207	225	3	5			
1	H	173	Total	C	N	O	S	Se	0	0	0
			1315	855	212	241	3	4			
1	I	171	Total	C	N	O	S	Se	0	0	0
			1290	842	206	235	3	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	LEU	-	expression tag	UNP Q97W15
A	191	GLU	-	expression tag	UNP Q97W15
A	192	HIS	-	expression tag	UNP Q97W15
A	193	HIS	-	expression tag	UNP Q97W15
A	194	HIS	-	expression tag	UNP Q97W15
A	195	HIS	-	expression tag	UNP Q97W15
A	196	HIS	-	expression tag	UNP Q97W15
A	197	HIS	-	expression tag	UNP Q97W15
B	190	LEU	-	expression tag	UNP Q97W15
B	191	GLU	-	expression tag	UNP Q97W15
B	192	HIS	-	expression tag	UNP Q97W15
B	193	HIS	-	expression tag	UNP Q97W15
B	194	HIS	-	expression tag	UNP Q97W15

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	HIS	-	expression tag	UNP Q97W15
B	196	HIS	-	expression tag	UNP Q97W15
B	197	HIS	-	expression tag	UNP Q97W15
D	190	LEU	-	expression tag	UNP Q97W15
D	191	GLU	-	expression tag	UNP Q97W15
D	192	HIS	-	expression tag	UNP Q97W15
D	193	HIS	-	expression tag	UNP Q97W15
D	194	HIS	-	expression tag	UNP Q97W15
D	195	HIS	-	expression tag	UNP Q97W15
D	196	HIS	-	expression tag	UNP Q97W15
D	197	HIS	-	expression tag	UNP Q97W15
E	190	LEU	-	expression tag	UNP Q97W15
E	191	GLU	-	expression tag	UNP Q97W15
E	192	HIS	-	expression tag	UNP Q97W15
E	193	HIS	-	expression tag	UNP Q97W15
E	194	HIS	-	expression tag	UNP Q97W15
E	195	HIS	-	expression tag	UNP Q97W15
E	196	HIS	-	expression tag	UNP Q97W15
E	197	HIS	-	expression tag	UNP Q97W15
F	190	LEU	-	expression tag	UNP Q97W15
F	191	GLU	-	expression tag	UNP Q97W15
F	192	HIS	-	expression tag	UNP Q97W15
F	193	HIS	-	expression tag	UNP Q97W15
F	194	HIS	-	expression tag	UNP Q97W15
F	195	HIS	-	expression tag	UNP Q97W15
F	196	HIS	-	expression tag	UNP Q97W15
F	197	HIS	-	expression tag	UNP Q97W15
G	190	LEU	-	expression tag	UNP Q97W15
G	191	GLU	-	expression tag	UNP Q97W15
G	192	HIS	-	expression tag	UNP Q97W15
G	193	HIS	-	expression tag	UNP Q97W15
G	194	HIS	-	expression tag	UNP Q97W15
G	195	HIS	-	expression tag	UNP Q97W15
G	196	HIS	-	expression tag	UNP Q97W15
G	197	HIS	-	expression tag	UNP Q97W15
H	190	LEU	-	expression tag	UNP Q97W15
H	191	GLU	-	expression tag	UNP Q97W15
H	192	HIS	-	expression tag	UNP Q97W15
H	193	HIS	-	expression tag	UNP Q97W15
H	194	HIS	-	expression tag	UNP Q97W15
H	195	HIS	-	expression tag	UNP Q97W15
H	196	HIS	-	expression tag	UNP Q97W15

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	197	HIS	-	expression tag	UNP Q97W15
I	190	LEU	-	expression tag	UNP Q97W15
I	191	GLU	-	expression tag	UNP Q97W15
I	192	HIS	-	expression tag	UNP Q97W15
I	193	HIS	-	expression tag	UNP Q97W15
I	194	HIS	-	expression tag	UNP Q97W15
I	195	HIS	-	expression tag	UNP Q97W15
I	196	HIS	-	expression tag	UNP Q97W15
I	197	HIS	-	expression tag	UNP Q97W15

- Molecule 2 is water.

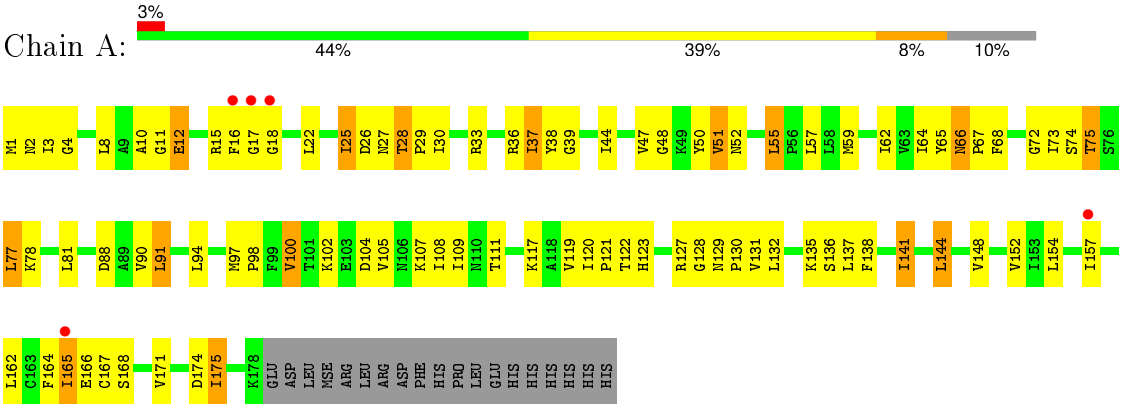
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	4	Total O 4 4	0	0
2	D	6	Total O 6 6	0	0
2	E	4	Total O 4 4	0	0
2	F	4	Total O 4 4	0	0
2	G	2	Total O 2 2	0	0
2	H	5	Total O 5 5	0	0
2	I	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

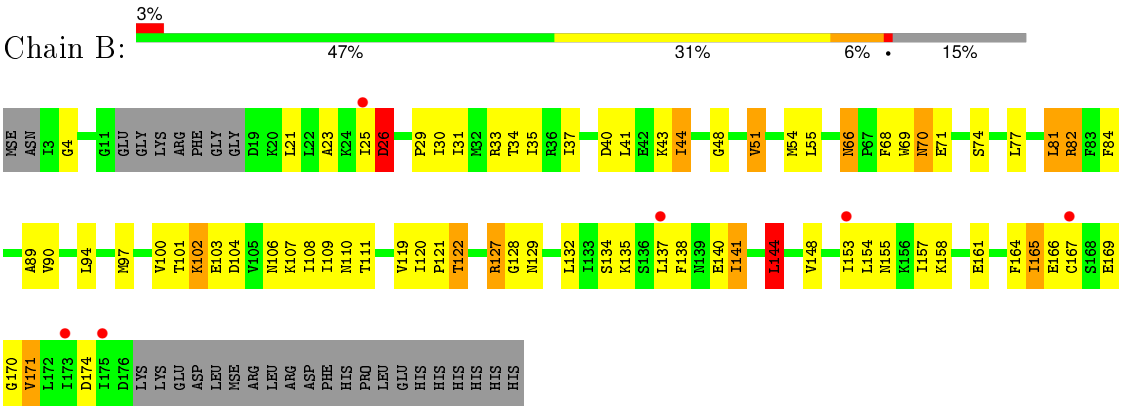
- Molecule 1: Q97W15_SULSO

Chain A:



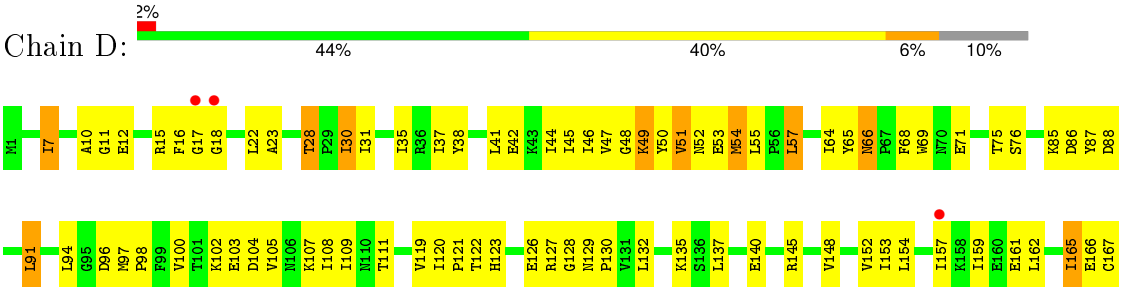
- Molecule 1: Q97W15_SULSO

Chain B:



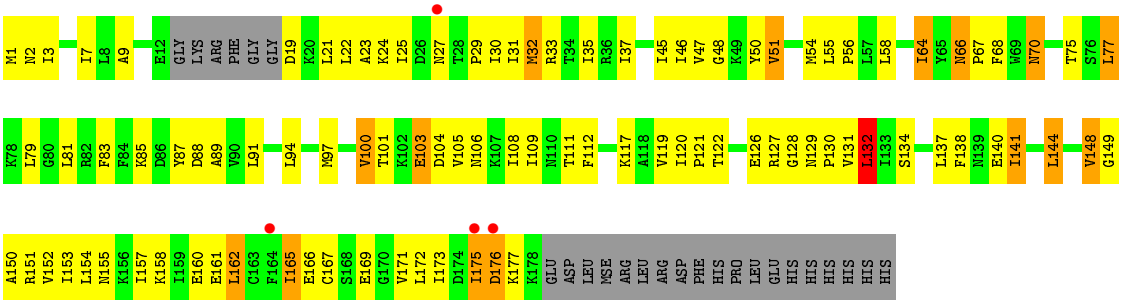
- Molecule 1: Q97W15_SULSO

Chain D:



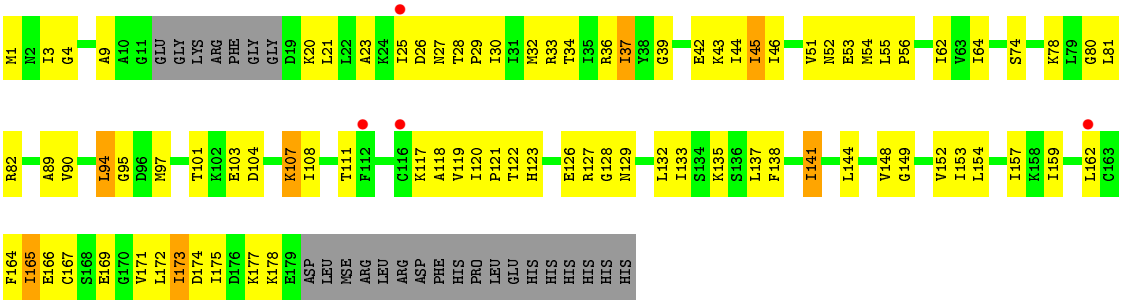
• Molecule 1: Q97W15_SULSO

Chain E:



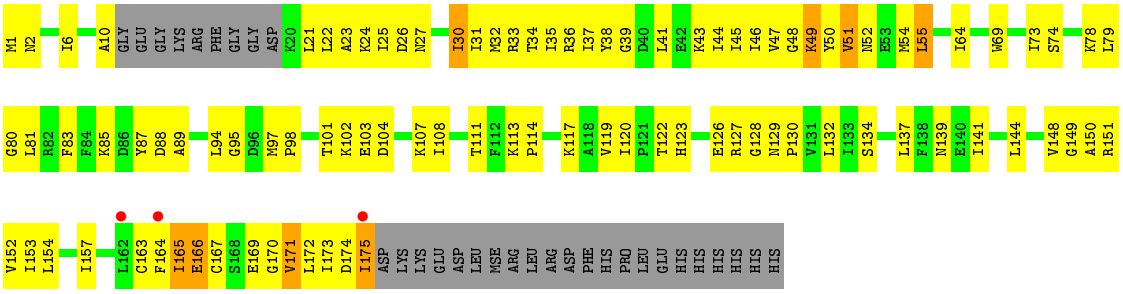
• Molecule 1: Q97W15_SULSO

Chain F:



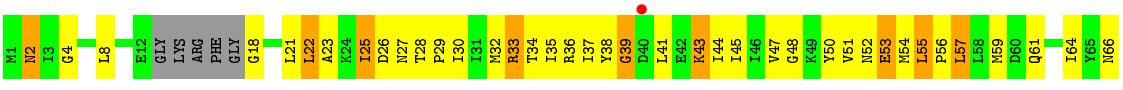
• Molecule 1: Q97W15_SULSO

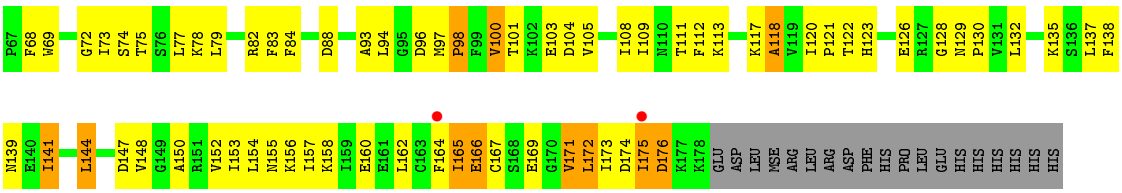
Chain G:



• Molecule 1: Q97W15_SULSO

Chain H:





- Molecule 1: Q97W15_SULSO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.96Å 169.23Å 173.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.80 48.47 – 2.77	Depositor EDS
% Data completeness (in resolution range)	86.2 (48.47-2.80) 96.7 (48.47-2.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.266 0.244 , 0.277	Depositor DCC
R_{free} test set	3140 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.8	EDS
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 126312 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10496	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/1373	0.70	0/1852
1	B	0.41	0/1283	0.71	1/1734 (0.1%)
1	D	0.40	0/1390	0.69	0/1870
1	E	0.45	0/1315	0.70	1/1778 (0.1%)
1	F	0.41	0/1307	0.68	0/1765
1	G	0.41	0/1284	0.71	0/1736
1	H	0.48	0/1330	0.70	0/1797
1	I	0.38	0/1305	0.68	0/1767
All	All	0.42	0/10587	0.70	2/14299 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	132	LEU	CA-CB-CG	5.60	128.19	115.30
1	B	144	LEU	CA-CB-CG	5.57	128.11	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1356	0	1391	78	0
1	B	1268	0	1300	76	0
1	D	1373	0	1430	91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1300	0	1324	105	0
1	F	1292	0	1335	96	0
1	G	1269	0	1309	98	0
1	H	1315	0	1339	122	0
1	I	1290	0	1305	110	0
2	A	3	0	0	0	0
2	B	4	0	0	1	0
2	D	6	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	2	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
All	All	10496	0	10733	740	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 35.

All (740) 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:G:111:THR:HG21	1:G:165:ILE:HG21	1.20	1.10
1:A:18:GLY:HA3	1:A:50:TYR:HB2	1.31	1.09
1:H:66:ASN:HD21	1:H:75:THR:HG23	1.17	1.09
1:E:68:PHE:HB2	1:E:75:THR:HG21	1.34	1.08
1:G:81:LEU:HD22	1:G:141:ILE:HD11	1.37	1.06
1:E:157:ILE:HD11	1:E:161:GLU:HB2	1.37	1.06
1:I:97:MSE:HE1	1:I:129:ASN:HB2	1.41	1.01
1:E:66:ASN:ND2	1:E:68:PHE:H	1.61	0.97
1:E:70:ASN:HD22	1:E:70:ASN:H	1.03	0.96
1:A:157:ILE:HG13	1:A:162:LEU:HD11	1.48	0.95
1:D:157:ILE:HD11	1:D:162:LEU:HD22	1.50	0.93
1:H:74:SER:HB2	1:H:144:LEU:HD23	1.52	0.92
1:B:70:ASN:HD22	1:B:70:ASN:H	1.18	0.92
1:I:21:LEU:HD23	1:I:30:ILE:HD11	1.51	0.91
1:I:24:LYS:H	1:I:24:LYS:HD3	1.37	0.89
1:H:66:ASN:ND2	1:H:75:THR:HG23	1.88	0.89
1:H:56:PRO:HA	1:H:59:MSE:CE	2.03	0.88
1:D:66:ASN:ND2	1:D:68:PHE:H	1.71	0.88
1:H:56:PRO:HA	1:H:59:MSE:HE2	1.53	0.87
1:I:66:ASN:ND2	1:I:68:PHE:H	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:PRO:HB2	1:F:32:MSE:HB2	1.57	0.85
1:G:101:THR:HG22	1:G:103:GLU:H	1.41	0.85
1:A:66:ASN:OD1	1:A:75:THR:HG23	1.75	0.85
1:H:111:THR:OG1	1:H:165:ILE:HG21	1.76	0.85
1:E:117:LYS:HB3	1:E:137:LEU:HD11	1.60	0.84
1:E:131:VAL:HG11	1:E:154:LEU:HD11	1.60	0.84
1:F:97:MSE:HE1	1:F:129:ASN:HB2	1.59	0.83
1:G:2:ASN:HB2	1:G:88:ASP:H	1.44	0.83
1:I:97:MSE:HE1	1:I:129:ASN:CB	2.08	0.82
1:H:21:LEU:HB2	1:H:54:MSE:HE1	1.61	0.82
1:A:33:ARG:HD3	1:A:98:PRO:HB2	1.60	0.82
1:B:111:THR:HG21	1:B:165:ILE:HD11	1.59	0.82
1:G:141:ILE:HG22	1:G:153:ILE:HG21	1.60	0.82
1:B:127:ARG:H	1:B:127:ARG:HD2	1.43	0.82
1:I:148:VAL:HG23	1:I:149:GLY:H	1.45	0.82
1:F:94:LEU:HB2	1:F:97:MSE:HE2	1.62	0.81
1:F:101:THR:OG1	1:F:103:GLU:HG2	1.81	0.80
1:D:22:LEU:HD11	1:D:53:GLU:HB3	1.61	0.80
1:E:30:ILE:HG13	1:E:175:ILE:HD13	1.63	0.80
1:E:70:ASN:H	1:E:70:ASN:ND2	1.79	0.80
1:D:128:GLY:HA3	1:D:171:VAL:HG12	1.62	0.80
1:G:144:LEU:HD21	1:G:149:GLY:HA2	1.63	0.79
1:E:31:ILE:O	1:E:35:ILE:HG12	1.82	0.79
1:D:49:LYS:HG2	1:D:69:TRP:CH2	2.16	0.79
1:E:103:GLU:H	1:E:103:GLU:CD	1.83	0.78
1:B:70:ASN:HD22	1:B:70:ASN:N	1.78	0.78
1:D:45:ILE:HG22	1:D:47:VAL:HG13	1.66	0.78
1:B:66:ASN:ND2	1:B:68:PHE:H	1.81	0.77
1:I:101:THR:HB	1:I:104:ASP:OD1	1.85	0.77
1:I:24:LYS:N	1:I:24:LYS:HD3	1.99	0.77
1:F:157:ILE:HD11	1:F:162:LEU:HD13	1.65	0.76
1:G:24:LYS:HD3	1:G:27:ASN:HA	1.65	0.76
1:D:102:LYS:HE3	1:I:126:GLU:OE2	1.85	0.76
1:D:11:GLY:HA3	1:D:17:GLY:HA2	1.68	0.76
1:G:111:THR:HG21	1:G:165:ILE:CG2	2.11	0.75
1:H:174:ASP:OD1	1:H:176:ASP:HB3	1.86	0.75
1:F:97:MSE:HE1	1:F:129:ASN:CB	2.16	0.74
1:D:85:LYS:C	1:D:85:LYS:HE2	2.08	0.74
1:G:81:LEU:HD22	1:G:141:ILE:CD1	2.15	0.74
1:F:148:VAL:HG23	1:F:149:GLY:H	1.51	0.74
1:I:3:ILE:O	1:I:3:ILE:HD12	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:ILE:HD11	1:I:173:ILE:HD12	1.71	0.73
1:B:70:ASN:H	1:B:70:ASN:ND2	1.86	0.73
1:B:141:ILE:HG22	1:B:153:ILE:HG13	1.70	0.73
1:G:101:THR:HG22	1:G:103:GLU:N	2.03	0.72
1:F:107:LYS:HB3	1:F:165:ILE:HD12	1.70	0.72
1:A:55:LEU:HD13	1:B:55:LEU:HD11	1.72	0.72
1:D:7:ILE:HG12	1:D:45:ILE:HG13	1.71	0.72
1:H:33:ARG:HG3	1:H:33:ARG:HH11	1.54	0.72
1:H:44:ILE:HD11	1:H:64:ILE:CD1	2.20	0.71
1:B:97:MSE:HE1	1:B:129:ASN:CB	2.20	0.71
1:A:25:ILE:O	1:A:26:ASP:HB2	1.91	0.71
1:B:34:THR:O	1:B:37:ILE:HG12	1.90	0.71
1:H:94:LEU:HD22	1:H:97:MSE:HE3	1.73	0.71
1:B:138:PHE:O	1:B:141:ILE:HD13	1.90	0.70
1:H:45:ILE:HD13	1:H:61:GLN:HG2	1.72	0.70
1:A:167:CYS:HB2	1:A:171:VAL:HG21	1.73	0.70
1:B:158:LYS:HB2	1:B:161:GLU:HG3	1.73	0.70
1:A:18:GLY:HA3	1:A:50:TYR:CB	2.16	0.70
1:H:144:LEU:HD12	1:H:153:ILE:HD11	1.74	0.69
1:I:141:ILE:O	1:I:144:LEU:HD22	1.92	0.69
1:D:45:ILE:HG22	1:D:47:VAL:CG1	2.22	0.69
1:G:45:ILE:HG22	1:G:47:VAL:HG13	1.73	0.69
1:D:104:ASP:OD1	1:D:167:CYS:HB3	1.94	0.68
1:D:175:ILE:O	1:D:175:ILE:HD13	1.93	0.68
1:H:94:LEU:HD22	1:H:97:MSE:CE	2.23	0.68
1:E:165:ILE:H	1:E:165:ILE:HD13	1.59	0.68
1:I:101:THR:HG22	1:I:103:GLU:H	1.59	0.68
1:A:131:VAL:HG11	1:A:154:LEU:HD11	1.75	0.68
1:B:122:THR:HG23	1:B:166:GLU:OE2	1.94	0.68
1:I:47:VAL:HG23	1:I:51:VAL:HG13	1.76	0.68
1:D:104:ASP:O	1:D:108:ILE:HG13	1.93	0.67
1:G:22:LEU:HD11	1:G:54:MSE:HB3	1.76	0.67
1:I:28:THR:HB	1:I:33:ARG:HE	1.59	0.67
1:I:22:LEU:HD23	1:I:22:LEU:H	1.60	0.67
1:E:104:ASP:O	1:E:108:ILE:HG13	1.93	0.67
1:E:94:LEU:HD12	1:E:97:MSE:HE3	1.77	0.67
1:I:34:THR:O	1:I:37:ILE:HG23	1.94	0.67
1:A:37:ILE:HD13	1:A:100:VAL:HG13	1.77	0.67
1:A:66:ASN:ND2	1:A:68:PHE:H	1.93	0.66
1:E:35:ILE:HD12	1:E:45:ILE:HD11	1.78	0.66
1:A:47:VAL:HG11	1:A:51:VAL:HA	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:THR:OG1	1:A:165:ILE:HG21	1.94	0.66
1:E:111:THR:OG1	1:E:165:ILE:HG21	1.94	0.66
1:F:34:THR:O	1:F:37:ILE:HG23	1.95	0.66
1:D:7:ILE:CD1	1:D:45:ILE:HG13	2.25	0.66
1:E:129:ASN:O	1:E:171:VAL:HG13	1.94	0.66
1:F:25:ILE:HD11	1:F:175:ILE:HD12	1.76	0.66
1:A:104:ASP:OD1	1:A:167:CYS:HB3	1.94	0.66
1:G:94:LEU:HB2	1:G:97:MSE:HE2	1.78	0.66
1:B:97:MSE:HE1	1:B:129:ASN:HB2	1.78	0.66
1:D:16:PHE:CE1	1:D:175:ILE:HG21	2.31	0.66
1:G:150:ALA:HA	1:G:153:ILE:HD11	1.78	0.65
1:I:94:LEU:HB2	1:I:97:MSE:HE2	1.78	0.65
1:E:169:GLU:HG2	1:E:173:ILE:HD11	1.79	0.65
1:D:48:GLY:O	1:D:51:VAL:HG22	1.97	0.65
1:B:97:MSE:HE3	2:B:302:HOH:O	1.95	0.65
1:E:121:PRO:HB2	1:E:171:VAL:HG11	1.79	0.65
1:G:123:HIS:HA	1:G:166:GLU:OE2	1.97	0.65
1:G:34:THR:HG21	1:G:95:GLY:HA2	1.78	0.65
1:F:174:ASP:HB3	1:I:178:LYS:HE2	1.78	0.65
1:I:74:SER:HB2	1:I:144:LEU:HD23	1.79	0.65
1:I:22:LEU:CD2	1:I:22:LEU:H	2.09	0.65
1:G:120:ILE:HD11	1:G:154:LEU:HD13	1.77	0.65
1:B:25:ILE:O	1:B:26:ASP:HB2	1.96	0.64
1:D:44:ILE:HD12	1:D:64:ILE:HD12	1.80	0.64
1:E:148:VAL:HG12	1:E:149:GLY:N	2.13	0.64
1:I:175:ILE:HG22	1:I:176:ASP:N	2.13	0.64
1:H:33:ARG:HG3	1:H:33:ARG:NH1	2.11	0.64
1:H:157:ILE:HD11	1:H:162:LEU:HG	1.80	0.64
1:A:17:GLY:O	1:A:50:TYR:HD2	1.81	0.64
1:F:122:THR:O	1:F:166:GLU:HA	1.96	0.64
1:D:30:ILE:HD11	1:D:96:ASP:HA	1.79	0.63
1:B:141:ILE:O	1:B:144:LEU:HD22	1.98	0.63
1:D:64:ILE:HD13	1:E:83:PHE:HZ	1.63	0.63
1:H:77:LEU:HB3	1:H:141:ILE:HD11	1.81	0.63
1:D:7:ILE:CG1	1:D:45:ILE:HG13	2.29	0.63
1:H:28:THR:HG23	1:H:33:ARG:HD2	1.80	0.63
1:I:7:ILE:HD11	1:I:45:ILE:HG23	1.80	0.62
1:H:93:ALA:HA	1:H:130:PRO:HB3	1.80	0.62
1:D:10:ALA:HA	1:D:48:GLY:H	1.64	0.62
1:H:68:PHE:O	1:H:75:THR:HG21	1.99	0.62
1:G:51:VAL:HG13	1:G:52:ASN:N	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ILE:HD11	1:F:80:GLY:HA3	1.82	0.62
1:F:81:LEU:HD22	1:F:141:ILE:HD12	1.81	0.62
1:E:70:ASN:HD22	1:E:70:ASN:N	1.86	0.62
1:B:82:ARG:HB3	1:B:82:ARG:HH11	1.65	0.62
1:B:82:ARG:HB3	1:B:82:ARG:NH1	2.14	0.62
1:H:117:LYS:HB3	1:H:137:LEU:HD21	1.82	0.62
1:A:91:LEU:HD22	1:A:130:PRO:HB2	1.82	0.62
1:E:37:ILE:HD13	1:E:100:VAL:HG13	1.82	0.61
1:E:9:ALA:HB1	1:E:21:LEU:CD1	2.30	0.61
1:H:56:PRO:HA	1:H:59:MSE:HE3	1.83	0.61
1:H:44:ILE:HD11	1:H:64:ILE:HD12	1.80	0.61
1:E:24:LYS:HE3	1:E:27:ASN:HA	1.82	0.61
1:F:23:ALA:O	1:F:30:ILE:HG13	1.99	0.61
1:E:48:GLY:O	1:E:51:VAL:HG22	2.00	0.61
1:B:97:MSE:HE1	1:B:129:ASN:HB3	1.82	0.61
1:G:144:LEU:HG	1:G:148:VAL:HG23	1.83	0.61
1:I:66:ASN:HD22	1:I:66:ASN:C	2.03	0.61
1:F:103:GLU:O	1:F:107:LYS:HD3	2.00	0.61
1:I:33:ARG:O	1:I:37:ILE:HG22	2.00	0.61
1:E:103:GLU:N	1:E:103:GLU:CD	2.54	0.60
1:E:2:ASN:ND2	1:E:87:TYR:HA	2.16	0.60
1:I:128:GLY:HA3	1:I:171:VAL:HG12	1.83	0.60
1:I:175:ILE:HG22	1:I:176:ASP:H	1.67	0.60
1:A:121:PRO:HB2	1:A:171:VAL:HG11	1.83	0.60
1:F:119:VAL:HB	1:F:132:LEU:HB3	1.84	0.60
1:E:141:ILE:HG12	1:E:144:LEU:HD22	1.83	0.60
1:G:97:MSE:HE1	1:G:129:ASN:HB2	1.84	0.60
1:A:104:ASP:O	1:A:108:ILE:HG13	2.02	0.59
1:F:169:GLU:CB	1:I:24:LYS:HE2	2.32	0.59
1:G:25:ILE:HB	1:G:33:ARG:HD2	1.85	0.59
1:B:48:GLY:O	1:B:51:VAL:HG22	2.02	0.59
1:D:161:GLU:O	1:D:161:GLU:HG2	2.02	0.59
1:E:46:ILE:HD13	1:E:64:ILE:HG23	1.84	0.59
1:G:165:ILE:N	1:G:165:ILE:HD13	2.18	0.59
1:F:148:VAL:HG23	1:F:149:GLY:N	2.16	0.59
1:F:82:ARG:HH21	1:G:83:PHE:HD2	1.49	0.59
1:E:66:ASN:ND2	1:E:68:PHE:N	2.43	0.59
1:E:1:MSE:HB3	1:E:88:ASP:OD2	2.02	0.59
1:I:48:GLY:O	1:I:51:VAL:HG22	2.03	0.59
1:A:74:SER:O	1:A:78:LYS:HG3	2.02	0.59
1:D:154:LEU:O	1:D:157:ILE:HG13	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:O	1:B:81:LEU:HB2	2.02	0.58
1:B:121:PRO:HB2	1:B:171:VAL:HG11	1.84	0.58
1:I:26:ASP:HB2	1:I:33:ARG:NH2	2.19	0.58
1:B:31:ILE:O	1:B:35:ILE:HG13	2.03	0.58
1:E:66:ASN:HD22	1:E:68:PHE:H	1.46	0.58
1:H:129:ASN:HB3	1:H:130:PRO:HA	1.86	0.58
1:I:3:ILE:HD11	1:I:41:LEU:HD22	1.85	0.58
1:H:141:ILE:HA	1:H:144:LEU:CD1	2.32	0.58
1:A:164:PHE:O	1:A:165:ILE:HG23	2.04	0.58
1:E:47:VAL:CG2	1:E:51:VAL:HG13	2.34	0.58
1:D:111:THR:OG1	1:D:165:ILE:HG21	2.04	0.58
1:A:55:LEU:CD1	1:B:55:LEU:HD11	2.34	0.58
1:B:109:ILE:HD12	1:B:110:ASN:N	2.18	0.58
1:B:129:ASN:O	1:B:171:VAL:HG13	2.04	0.58
1:H:34:THR:O	1:H:37:ILE:HG12	2.03	0.58
1:G:37:ILE:HD11	1:G:38:TYR:CZ	2.39	0.57
1:H:103:GLU:H	1:H:103:GLU:CD	2.06	0.57
1:G:148:VAL:HB	1:G:152:VAL:HG21	1.86	0.57
1:H:122:THR:HG22	1:H:166:GLU:HG2	1.86	0.57
1:G:33:ARG:O	1:G:37:ILE:HG23	2.05	0.57
1:H:104:ASP:OD1	1:H:167:CYS:HB3	2.04	0.57
1:B:23:ALA:O	1:B:29:PRO:HA	2.05	0.57
1:I:29:PRO:HB2	1:I:32:MSE:HG3	1.87	0.57
1:H:51:VAL:HG13	1:H:52:ASN:N	2.19	0.57
1:I:81:LEU:HD12	1:I:141:ILE:HD11	1.85	0.57
1:H:120:ILE:HD12	1:H:162:LEU:HD21	1.85	0.57
1:A:28:THR:HB	1:I:53:GLU:OE1	2.04	0.57
1:I:129:ASN:O	1:I:171:VAL:HG13	2.04	0.57
1:F:52:ASN:HD21	1:G:55:LEU:HB3	1.70	0.57
1:H:154:LEU:C	1:H:156:LYS:H	2.08	0.57
1:E:141:ILE:HA	1:E:144:LEU:HD13	1.87	0.57
1:A:11:GLY:HA2	1:A:16:PHE:O	2.05	0.56
1:D:49:LYS:HD2	1:D:50:TYR:CE2	2.41	0.56
1:I:97:MSE:CE	1:I:129:ASN:HB2	2.24	0.56
1:F:46:ILE:HD11	1:F:80:GLY:CA	2.35	0.56
1:D:100:VAL:HG21	1:D:130:PRO:HD3	1.86	0.56
1:B:140:GLU:HG3	1:B:153:ILE:HD12	1.86	0.56
1:H:64:ILE:HD11	1:H:83:PHE:CE2	2.40	0.56
1:I:111:THR:OG1	1:I:165:ILE:HG13	2.05	0.56
1:D:107:LYS:HG2	1:I:159:ILE:HG12	1.86	0.56
1:G:108:ILE:HA	1:G:165:ILE:HD11	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:LYS:H	1:I:24:LYS:CD	2.09	0.56
1:F:30:ILE:HD13	1:F:175:ILE:HD13	1.88	0.56
1:G:117:LYS:HB3	1:G:137:LEU:HD21	1.86	0.56
1:A:171:VAL:HG12	1:A:171:VAL:O	2.06	0.56
1:A:47:VAL:O	1:A:65:TYR:HA	2.06	0.56
1:A:81:LEU:HD22	1:A:141:ILE:HD12	1.87	0.56
1:F:29:PRO:O	1:F:32:MSE:HB3	2.05	0.56
1:F:122:THR:HG23	1:F:166:GLU:HA	1.87	0.56
1:E:66:ASN:C	1:E:66:ASN:HD22	2.09	0.56
1:F:23:ALA:HA	1:I:169:GLU:OE1	2.06	0.56
1:F:51:VAL:HG13	1:F:52:ASN:N	2.21	0.56
1:F:121:PRO:HB2	1:F:171:VAL:HG11	1.88	0.55
1:H:66:ASN:O	1:H:69:TRP:HD1	1.89	0.55
1:I:26:ASP:HB2	1:I:33:ARG:HH21	1.71	0.55
1:D:121:PRO:HB2	1:D:171:VAL:HG11	1.88	0.55
1:I:47:VAL:CG2	1:I:51:VAL:HG13	2.36	0.55
1:F:141:ILE:HA	1:F:153:ILE:HD11	1.89	0.55
1:A:122:THR:O	1:A:166:GLU:HA	2.07	0.55
1:A:136:SER:OG	1:A:137:LEU:HD22	2.07	0.55
1:G:51:VAL:HG13	1:G:52:ASN:H	1.71	0.55
1:G:1:MSE:HG3	1:G:88:ASP:OD2	2.07	0.55
1:A:141:ILE:O	1:A:144:LEU:HB2	2.07	0.55
1:D:145:ARG:O	1:D:148:VAL:HG23	2.05	0.55
1:F:94:LEU:HD22	1:F:97:MSE:HE2	1.87	0.55
1:E:47:VAL:HG23	1:E:51:VAL:HG13	1.87	0.55
1:H:94:LEU:CB	1:H:97:MSE:HE3	2.36	0.55
1:I:144:LEU:HD23	1:I:144:LEU:O	2.07	0.55
1:H:18:GLY:HA2	1:H:50:TYR:CD2	2.40	0.55
1:B:69:TRP:HZ2	1:I:71:GLU:HG2	1.72	0.55
1:H:135:LYS:HA	1:H:138:PHE:CE2	2.42	0.55
1:E:50:TYR:O	1:E:54:MSE:HG3	2.06	0.55
1:E:101:THR:OG1	1:E:103:GLU:HG2	2.07	0.55
1:F:135:LYS:HA	1:F:138:PHE:CD1	2.42	0.55
1:B:97:MSE:HG2	1:B:174:ASP:HB3	1.89	0.54
1:H:148:VAL:HG13	1:H:152:VAL:HG21	1.87	0.54
1:D:7:ILE:CD1	1:D:35:ILE:HG12	2.38	0.54
1:I:127:ARG:HD2	1:I:164:PHE:HE1	1.72	0.54
1:F:1:MSE:HA	1:F:1:MSE:HE2	1.89	0.54
1:H:98:PRO:HG3	1:H:175:ILE:HD11	1.89	0.54
1:A:37:ILE:HG12	1:A:38:TYR:CD1	2.42	0.54
1:F:141:ILE:HD13	1:F:141:ILE:C	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:GLY:HA3	1:H:171:VAL:CG1	2.37	0.54
1:G:89:ALA:HB2	1:G:134:SER:HA	1.87	0.54
1:A:47:VAL:CG1	1:A:51:VAL:HA	2.38	0.54
1:A:148:VAL:HG13	1:A:152:VAL:HG21	1.87	0.54
1:I:66:ASN:ND2	1:I:66:ASN:C	2.61	0.54
1:D:18:GLY:HA3	1:D:50:TYR:HB2	1.88	0.54
1:H:44:ILE:HD11	1:H:64:ILE:HD11	1.90	0.54
1:I:66:ASN:HD22	1:I:67:PRO:N	2.05	0.54
1:A:128:GLY:HA3	1:A:171:VAL:HG12	1.90	0.54
1:D:122:THR:O	1:D:166:GLU:HA	2.08	0.54
1:I:122:THR:O	1:I:166:GLU:HA	2.07	0.54
1:F:45:ILE:HG13	1:F:45:ILE:O	2.08	0.54
1:H:126:GLU:HB2	1:H:172:LEU:HD21	1.90	0.54
1:E:157:ILE:CG1	1:E:162:LEU:HD13	2.38	0.53
1:I:66:ASN:ND2	1:I:68:PHE:N	2.52	0.53
1:I:141:ILE:HA	1:I:153:ILE:HD11	1.90	0.53
1:A:77:LEU:HD13	1:A:141:ILE:CG1	2.39	0.53
1:H:162:LEU:HD22	1:H:164:PHE:CZ	2.43	0.53
1:G:10:ALA:HB1	1:G:49:LYS:H	1.73	0.53
1:E:157:ILE:HG13	1:E:162:LEU:HD13	1.91	0.53
1:B:164:PHE:C	1:B:165:ILE:HD13	2.29	0.53
1:F:81:LEU:CD2	1:F:141:ILE:HD12	2.37	0.53
1:G:44:ILE:O	1:G:44:ILE:HG13	2.08	0.53
1:A:37:ILE:HG12	1:A:38:TYR:CE1	2.44	0.53
1:D:165:ILE:HD13	1:D:165:ILE:N	2.24	0.53
1:F:127:ARG:HD2	1:F:164:PHE:CE1	2.44	0.53
1:G:119:VAL:HB	1:G:132:LEU:HB3	1.89	0.53
1:A:72:GLY:O	1:A:75:THR:HG22	2.09	0.53
1:F:104:ASP:OD1	1:F:167:CYS:HB3	2.08	0.53
1:G:89:ALA:CB	1:G:134:SER:HA	2.38	0.53
1:E:29:PRO:HD2	1:E:32:MSE:HG3	1.90	0.53
1:I:148:VAL:HG23	1:I:149:GLY:N	2.20	0.53
1:B:81:LEU:HD11	1:B:141:ILE:HD11	1.91	0.53
1:G:45:ILE:HG22	1:G:47:VAL:CG1	2.37	0.53
1:G:97:MSE:HG2	1:G:174:ASP:HA	1.90	0.53
1:E:66:ASN:HD21	1:E:68:PHE:HB2	1.73	0.53
1:F:126:GLU:HB3	1:F:172:LEU:HD11	1.90	0.53
1:I:73:ILE:HG23	1:I:74:SER:N	2.23	0.53
1:A:117:LYS:HB3	1:A:137:LEU:HD21	1.90	0.53
1:H:39:GLY:O	1:H:43:LYS:NZ	2.34	0.52
1:H:141:ILE:HG12	1:H:144:LEU:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ILE:HG13	1:E:175:ILE:CD1	2.36	0.52
1:D:7:ILE:HD11	1:D:45:ILE:HG13	1.91	0.52
1:G:26:ASP:O	1:G:27:ASN:HB2	2.10	0.52
1:B:94:LEU:HB2	1:B:97:MSE:HE2	1.90	0.52
1:H:38:TYR:O	1:H:41:LEU:HB2	2.08	0.52
1:H:121:PRO:HB2	1:H:171:VAL:HG21	1.92	0.52
1:I:109:ILE:HG13	1:I:110:ASN:N	2.25	0.52
1:B:167:CYS:HB2	1:B:171:VAL:HG21	1.90	0.52
1:A:117:LYS:O	1:A:137:LEU:HD23	2.09	0.52
1:E:112:PHE:HE1	1:E:134:SER:HG	1.56	0.52
1:I:149:GLY:O	1:I:152:VAL:HG22	2.10	0.52
1:G:128:GLY:HA3	1:G:171:VAL:O	2.10	0.52
1:B:111:THR:HG21	1:B:165:ILE:CD1	2.34	0.52
1:A:26:ASP:O	1:A:27:ASN:HB2	2.09	0.52
1:H:138:PHE:HA	1:H:141:ILE:HG22	1.91	0.52
1:E:94:LEU:HD12	1:E:97:MSE:CE	2.39	0.52
1:H:37:ILE:HD12	1:H:100:VAL:HG22	1.92	0.52
1:A:77:LEU:HD13	1:A:141:ILE:HG13	1.91	0.52
1:F:117:LYS:HB3	1:F:137:LEU:HD11	1.92	0.52
1:D:23:ALA:O	1:D:30:ILE:HG23	2.09	0.52
1:H:32:MSE:HE2	1:H:36:ARG:HH21	1.74	0.52
1:A:18:GLY:O	1:A:22:LEU:HG	2.10	0.52
1:H:111:THR:HG21	1:H:165:ILE:HG23	1.92	0.52
1:G:97:MSE:HE1	1:G:129:ASN:CB	2.39	0.52
1:F:122:THR:HG22	1:F:165:ILE:C	2.30	0.51
1:E:165:ILE:N	1:E:165:ILE:HD13	2.24	0.51
1:H:55:LEU:HD13	1:I:51:VAL:HB	1.91	0.51
1:D:111:THR:HG22	1:D:111:THR:O	2.09	0.51
1:I:106:ASN:HA	1:I:109:ILE:HG12	1.91	0.51
1:D:66:ASN:C	1:D:66:ASN:HD22	2.14	0.51
1:E:119:VAL:HB	1:E:132:LEU:HB3	1.92	0.51
1:E:171:VAL:O	1:E:171:VAL:HG12	2.10	0.51
1:G:120:ILE:HD11	1:G:154:LEU:CD1	2.40	0.51
1:F:178:LYS:HE3	1:I:94:LEU:CD1	2.40	0.51
1:I:23:ALA:O	1:I:29:PRO:HA	2.11	0.51
1:G:107:LYS:O	1:G:111:THR:HG23	2.11	0.51
1:A:67:PRO:HG2	1:A:68:PHE:CD2	2.46	0.51
1:H:21:LEU:HD23	1:H:30:ILE:HD11	1.92	0.51
1:D:47:VAL:HG23	1:D:47:VAL:O	2.11	0.51
1:E:64:ILE:HD11	1:E:79:LEU:HD21	1.93	0.51
1:F:51:VAL:HG22	1:G:55:LEU:CD1	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ILE:CG1	1:E:175:ILE:HD13	2.38	0.51
1:H:148:VAL:HG13	1:H:152:VAL:CG2	2.41	0.51
1:D:51:VAL:HG12	1:D:55:LEU:HD23	1.92	0.51
1:D:176:ASP:O	1:D:178:LYS:N	2.42	0.51
1:A:129:ASN:HB3	1:A:130:PRO:HA	1.92	0.51
1:F:51:VAL:HG22	1:G:55:LEU:HD11	1.92	0.51
1:F:127:ARG:HD2	1:F:164:PHE:HE1	1.75	0.51
1:F:36:ARG:HH11	1:F:36:ARG:HG3	1.75	0.51
1:D:38:TYR:O	1:D:41:LEU:HB2	2.10	0.51
1:I:171:VAL:O	1:I:171:VAL:HG12	2.10	0.51
1:B:128:GLY:HA3	1:B:171:VAL:HG12	1.93	0.51
1:A:44:ILE:HG13	1:A:64:ILE:HD11	1.91	0.51
1:D:30:ILE:CD1	1:D:96:ASP:HA	2.40	0.51
1:H:47:VAL:HG12	1:H:48:GLY:N	2.26	0.51
1:B:4:GLY:HA3	1:B:84:PHE:CE1	2.46	0.51
1:E:23:ALA:O	1:E:30:ILE:HG12	2.11	0.51
1:H:94:LEU:HB2	1:H:97:MSE:HE3	1.92	0.51
1:A:94:LEU:HD12	1:A:97:MSE:SE	2.61	0.51
1:F:127:ARG:HB2	1:I:180:ASP:HB3	1.92	0.51
1:E:66:ASN:C	1:E:66:ASN:ND2	2.64	0.50
1:G:94:LEU:HD12	1:G:97:MSE:SE	2.60	0.50
1:F:141:ILE:HG12	1:F:144:LEU:HD22	1.93	0.50
1:B:33:ARG:HH11	1:B:33:ARG:HG2	1.75	0.50
1:D:148:VAL:HG13	1:D:152:VAL:HG21	1.94	0.50
1:H:112:PHE:O	1:H:113:LYS:HE2	2.11	0.50
1:F:169:GLU:O	1:F:173:ILE:HG12	2.10	0.50
1:D:12:GLU:HB3	1:D:69:TRP:O	2.11	0.50
1:A:120:ILE:HD11	1:A:154:LEU:HD13	1.93	0.50
1:F:44:ILE:HD12	1:F:64:ILE:HD12	1.92	0.50
1:G:74:SER:O	1:G:78:LYS:HG3	2.12	0.50
1:G:41:LEU:O	1:G:43:LYS:HE2	2.11	0.50
1:G:21:LEU:O	1:G:30:ILE:HG23	2.12	0.50
1:D:71:GLU:HB3	1:D:75:THR:HG21	1.94	0.50
1:I:117:LYS:O	1:I:137:LEU:HD22	2.11	0.50
1:E:3:ILE:HD12	1:E:109:ILE:HG23	1.92	0.50
1:H:56:PRO:CA	1:H:59:MSE:HE2	2.35	0.50
1:B:122:THR:O	1:B:166:GLU:HA	2.12	0.50
1:E:104:ASP:CG	1:E:167:CYS:HB3	2.32	0.50
1:E:129:ASN:HB3	1:E:130:PRO:HA	1.92	0.50
1:H:120:ILE:HD11	1:H:154:LEU:HD13	1.93	0.50
1:H:144:LEU:CD1	1:H:153:ILE:HD11	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:CG2	1:E:33:ARG:HD2	2.42	0.50
1:G:101:THR:CG2	1:G:103:GLU:H	2.20	0.50
1:I:7:ILE:HG13	1:I:45:ILE:HA	1.93	0.50
1:B:100:VAL:HG12	1:B:101:THR:N	2.27	0.50
1:H:72:GLY:O	1:H:75:THR:HG22	2.12	0.49
1:E:157:ILE:HD12	1:E:158:LYS:H	1.77	0.49
1:D:171:VAL:O	1:D:171:VAL:HG12	2.11	0.49
1:D:129:ASN:O	1:D:171:VAL:HG13	2.12	0.49
1:F:177:LYS:HG2	1:I:173:ILE:HG22	1.93	0.49
1:B:106:ASN:O	1:B:109:ILE:HG13	2.12	0.49
1:H:165:ILE:N	1:H:165:ILE:HD13	2.27	0.49
1:F:33:ARG:HH11	1:F:33:ARG:HG3	1.78	0.49
1:I:127:ARG:HD2	1:I:164:PHE:CE1	2.46	0.49
1:H:25:ILE:O	1:H:26:ASP:HB3	2.12	0.49
1:F:74:SER:O	1:F:78:LYS:HG3	2.12	0.49
1:G:44:ILE:HD11	1:G:80:GLY:HA2	1.94	0.49
1:E:3:ILE:CD1	1:E:109:ILE:HG23	2.42	0.49
1:D:88:ASP:O	1:D:135:LYS:N	2.41	0.49
1:H:94:LEU:HD13	1:H:97:MSE:HE1	1.93	0.49
1:I:7:ILE:HG12	1:I:45:ILE:HG13	1.94	0.49
1:B:4:GLY:O	1:B:90:VAL:HA	2.13	0.49
1:H:113:LYS:HA	1:H:113:LYS:HE2	1.95	0.49
1:I:101:THR:O	1:I:104:ASP:HB2	2.12	0.49
1:I:73:ILE:CG2	1:I:74:SER:N	2.76	0.49
1:A:37:ILE:O	1:A:102:LYS:HG2	2.12	0.49
1:E:137:LEU:HD12	1:E:137:LEU:N	2.27	0.49
1:D:22:LEU:CD1	1:D:53:GLU:HB3	2.39	0.49
1:F:121:PRO:HB2	1:F:171:VAL:CG1	2.43	0.49
1:D:37:ILE:HD11	1:D:98:PRO:O	2.13	0.49
1:G:23:ALA:O	1:G:30:ILE:HG22	2.13	0.48
1:G:64:ILE:HD11	1:G:83:PHE:CE1	2.48	0.48
1:B:70:ASN:N	1:B:70:ASN:ND2	2.49	0.48
1:I:120:ILE:HG21	1:I:127:ARG:HB3	1.94	0.48
1:I:129:ASN:HB3	1:I:130:PRO:HA	1.96	0.48
1:B:66:ASN:HD22	1:B:68:PHE:H	1.59	0.48
1:G:123:HIS:HB3	1:G:172:LEU:CD1	2.44	0.48
1:D:126:GLU:HB2	1:D:172:LEU:HD21	1.95	0.48
1:F:81:LEU:HD11	1:F:138:PHE:CD2	2.49	0.48
1:F:52:ASN:ND2	1:G:55:LEU:HB3	2.29	0.48
1:F:20:LYS:HA	1:F:177:LYS:HE3	1.96	0.48
1:G:21:LEU:HD12	1:G:54:MSE:HE1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:THR:HB	1:I:33:ARG:NE	2.26	0.48
1:H:158:LYS:C	1:H:160:GLU:H	2.17	0.48
1:B:43:LYS:O	1:B:44:ILE:HD12	2.13	0.48
1:D:46:ILE:HD13	1:D:64:ILE:HB	1.93	0.48
1:F:128:GLY:HA3	1:F:171:VAL:HG12	1.96	0.48
1:B:41:LEU:O	1:B:43:LYS:HG3	2.14	0.48
1:D:94:LEU:HD12	1:D:97:MSE:SE	2.64	0.48
1:F:173:ILE:HG22	1:I:176:ASP:O	2.14	0.48
1:G:2:ASN:HB3	1:G:87:TYR:HA	1.95	0.48
1:E:140:GLU:HB3	1:E:153:ILE:HD13	1.96	0.48
1:H:21:LEU:CD2	1:H:30:ILE:HD11	2.43	0.48
1:H:157:ILE:HD11	1:H:162:LEU:CG	2.43	0.48
1:E:2:ASN:HD22	1:E:87:TYR:HA	1.79	0.48
1:H:137:LEU:HD12	1:H:153:ILE:CG2	2.44	0.47
1:I:66:ASN:HD21	1:I:68:PHE:H	1.57	0.47
1:G:25:ILE:O	1:G:26:ASP:HB2	2.14	0.47
1:D:85:LYS:HD3	1:E:85:LYS:HE2	1.96	0.47
1:A:164:PHE:C	1:A:165:ILE:HD13	2.35	0.47
1:I:99:PHE:CE2	1:I:175:ILE:HD11	2.49	0.47
1:I:22:LEU:N	1:I:22:LEU:CD2	2.77	0.47
1:B:25:ILE:HB	1:B:33:ARG:HD3	1.96	0.47
1:E:176:ASP:OD1	1:E:177:LYS:N	2.47	0.47
1:F:165:ILE:O	1:F:165:ILE:HG23	2.14	0.47
1:E:22:LEU:HD11	1:E:54:MSE:HG2	1.95	0.47
1:B:94:LEU:HG	1:B:97:MSE:HE2	1.96	0.47
1:E:148:VAL:HG13	1:E:152:VAL:CG2	2.45	0.47
1:F:144:LEU:CD1	1:F:153:ILE:HD11	2.45	0.47
1:E:141:ILE:C	1:E:141:ILE:HD13	2.35	0.47
1:D:140:GLU:HB3	1:D:153:ILE:HD13	1.95	0.47
1:D:22:LEU:HD21	1:D:57:LEU:HD21	1.96	0.47
1:D:85:LYS:O	1:D:85:LYS:HE2	2.14	0.47
1:B:104:ASP:O	1:B:108:ILE:HG13	2.14	0.47
1:H:45:ILE:CD1	1:H:61:GLN:HG2	2.42	0.47
1:D:41:LEU:HD21	1:D:109:ILE:HD11	1.95	0.47
1:D:157:ILE:HD12	1:D:157:ILE:O	2.14	0.47
1:A:27:ASN:ND2	1:I:56:PRO:HG2	2.30	0.47
1:E:167:CYS:HB2	1:E:171:VAL:HG21	1.96	0.47
1:E:9:ALA:HB1	1:E:21:LEU:HD13	1.96	0.47
1:F:132:LEU:C	1:F:132:LEU:HD13	2.34	0.47
1:H:2:ASN:N	1:H:88:ASP:OD2	2.47	0.47
1:D:66:ASN:C	1:D:66:ASN:ND2	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:MSE:HE1	1:F:129:ASN:HB3	1.95	0.47
1:I:7:ILE:HG13	1:I:7:ILE:O	2.13	0.47
1:D:105:VAL:O	1:D:109:ILE:HG13	2.15	0.47
1:G:169:GLU:O	1:G:173:ILE:HG13	2.14	0.47
1:D:119:VAL:HB	1:D:132:LEU:HB3	1.97	0.47
1:A:157:ILE:CG1	1:A:162:LEU:HD11	2.34	0.47
1:D:157:ILE:CD1	1:D:162:LEU:HD22	2.36	0.47
1:A:57:LEU:HG	1:H:59:MSE:CE	2.45	0.47
1:F:149:GLY:O	1:F:152:VAL:HG23	2.15	0.47
1:B:137:LEU:O	1:B:140:GLU:HB3	2.14	0.47
1:A:48:GLY:O	1:A:51:VAL:HG22	2.15	0.47
1:A:122:THR:HG22	1:A:123:HIS:N	2.30	0.47
1:F:64:ILE:HD13	1:G:83:PHE:HZ	1.80	0.46
1:I:157:ILE:HB	1:I:162:LEU:HD11	1.98	0.46
1:A:107:LYS:HE3	1:F:159:ILE:HG12	1.97	0.46
1:I:171:VAL:O	1:I:171:VAL:CG1	2.63	0.46
1:F:123:HIS:HB3	1:F:172:LEU:HD23	1.96	0.46
1:H:45:ILE:HD12	1:H:45:ILE:N	2.29	0.46
1:H:38:TYR:CZ	1:H:93:ALA:HB2	2.50	0.46
1:H:128:GLY:HA3	1:H:171:VAL:HG12	1.97	0.46
1:H:135:LYS:HA	1:H:138:PHE:CD2	2.51	0.46
1:H:104:ASP:CG	1:H:167:CYS:HB3	2.36	0.46
1:E:122:THR:O	1:E:166:GLU:HA	2.16	0.46
1:I:135:LYS:HA	1:I:138:PHE:CG	2.51	0.46
1:E:117:LYS:HD2	1:E:157:ILE:HD13	1.97	0.46
1:E:158:LYS:C	1:E:160:GLU:N	2.69	0.46
1:I:41:LEU:O	1:I:43:LYS:HG3	2.15	0.46
1:B:138:PHE:HA	1:B:141:ILE:CD1	2.46	0.46
1:I:28:THR:HG22	1:I:33:ARG:HG3	1.97	0.46
1:F:157:ILE:HD11	1:F:162:LEU:HD22	1.97	0.46
1:H:23:ALA:O	1:H:29:PRO:HA	2.16	0.46
1:A:128:GLY:HA3	1:A:171:VAL:O	2.16	0.46
1:H:26:ASP:O	1:H:27:ASN:HB2	2.14	0.46
1:G:170:GLY:HA2	1:G:173:ILE:HD12	1.98	0.46
1:G:32:MSE:O	1:G:36:ARG:HG2	2.15	0.46
1:G:149:GLY:O	1:G:153:ILE:HG12	2.16	0.46
1:A:165:ILE:HD13	1:A:165:ILE:N	2.31	0.46
1:G:129:ASN:HB3	1:G:130:PRO:HA	1.97	0.46
1:G:123:HIS:CA	1:G:166:GLU:OE2	2.64	0.46
1:F:82:ARG:NH2	1:G:83:PHE:HD2	2.14	0.46
1:A:8:LEU:HD13	1:A:73:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:ILE:C	1:G:30:ILE:HD13	2.35	0.46
1:E:138:PHE:O	1:E:141:ILE:HG22	2.16	0.46
1:D:123:HIS:HB3	1:D:172:LEU:HD13	1.96	0.46
1:H:117:LYS:O	1:H:118:ALA:HB2	2.15	0.46
1:G:35:ILE:HD11	1:G:45:ILE:HG12	1.98	0.46
1:G:154:LEU:O	1:G:157:ILE:HG12	2.16	0.46
1:H:38:TYR:CZ	1:H:93:ALA:CB	2.99	0.46
1:H:51:VAL:HG13	1:H:52:ASN:H	1.81	0.46
1:F:39:GLY:O	1:F:43:LYS:NZ	2.48	0.46
1:D:28:THR:HB	1:F:53:GLU:OE2	2.16	0.45
1:B:101:THR:HG22	1:B:102:LYS:N	2.31	0.45
1:D:157:ILE:HD12	1:D:157:ILE:C	2.37	0.45
1:H:97:MSE:HG2	1:H:173:ILE:O	2.16	0.45
1:H:104:ASP:O	1:H:108:ILE:HG13	2.17	0.45
1:D:7:ILE:HD13	1:D:35:ILE:HG12	1.97	0.45
1:B:94:LEU:CB	1:B:97:MSE:HE2	2.47	0.45
1:G:129:ASN:O	1:G:171:VAL:HG22	2.15	0.45
1:E:25:ILE:O	1:E:25:ILE:HG23	2.17	0.45
1:A:12:GLU:HG3	1:A:73:ILE:HB	1.98	0.45
1:F:9:ALA:HB1	1:F:54:MSE:CE	2.47	0.45
1:A:33:ARG:O	1:A:36:ARG:HB3	2.17	0.45
1:F:118:ALA:HB3	1:F:162:LEU:HD13	1.97	0.45
1:B:135:LYS:HA	1:B:138:PHE:CE2	2.52	0.45
1:G:22:LEU:HD11	1:G:54:MSE:CB	2.45	0.45
1:I:4:GLY:O	1:I:90:VAL:HA	2.17	0.45
1:E:55:LEU:N	1:E:56:PRO:CD	2.80	0.45
1:G:48:GLY:O	1:G:49:LYS:C	2.54	0.45
1:D:85:LYS:HD3	1:E:85:LYS:HZ3	1.82	0.45
1:G:30:ILE:HD13	1:G:31:ILE:N	2.32	0.45
1:B:21:LEU:HA	1:B:30:ILE:HD11	1.99	0.45
1:E:77:LEU:HD13	1:E:141:ILE:HG13	1.98	0.45
1:H:122:THR:O	1:H:166:GLU:HA	2.15	0.45
1:E:126:GLU:HG3	1:E:172:LEU:HD21	1.98	0.45
1:F:97:MSE:CE	1:F:129:ASN:HB2	2.40	0.45
1:D:157:ILE:HD11	1:D:162:LEU:HD13	1.98	0.45
1:H:83:PHE:HZ	1:I:64:ILE:HD13	1.82	0.45
1:E:148:VAL:HG13	1:E:152:VAL:HG21	1.99	0.45
1:E:70:ASN:N	1:E:70:ASN:ND2	2.53	0.44
1:F:154:LEU:O	1:F:157:ILE:HG12	2.17	0.44
1:H:35:ILE:HG23	1:H:43:LYS:HD2	1.98	0.44
1:H:2:ASN:HA	1:H:2:ASN:HD22	1.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:O	1:A:109:ILE:HG13	2.17	0.44
1:G:81:LEU:HD22	1:G:141:ILE:CG1	2.47	0.44
1:D:85:LYS:HE2	1:D:86:ASP:N	2.32	0.44
1:H:158:LYS:C	1:H:160:GLU:N	2.69	0.44
1:G:113:LYS:CB	1:G:114:PRO:CD	2.95	0.44
1:D:157:ILE:HD11	1:D:162:LEU:CD2	2.34	0.44
1:D:51:VAL:HG21	1:D:65:TYR:CE1	2.53	0.44
1:G:50:TYR:HB2	1:G:54:MSE:HE3	2.00	0.44
1:F:44:ILE:HG22	1:F:62:ILE:HB	1.98	0.44
1:D:120:ILE:HD11	1:D:154:LEU:HD13	1.99	0.44
1:H:169:GLU:O	1:H:173:ILE:HG13	2.16	0.44
1:F:135:LYS:O	1:F:138:PHE:HB2	2.17	0.44
1:B:169:GLU:O	1:B:170:GLY:C	2.55	0.44
1:D:16:PHE:CE1	1:D:175:ILE:CG2	3.00	0.44
1:G:174:ASP:O	1:G:175:ILE:HG22	2.18	0.44
1:B:103:GLU:HG2	1:B:107:LYS:HE3	1.99	0.44
1:F:111:THR:O	1:F:111:THR:HG22	2.18	0.44
1:B:108:ILE:HD11	1:B:121:PRO:HB3	1.99	0.44
1:I:141:ILE:HA	1:I:153:ILE:CD1	2.47	0.44
1:I:45:ILE:HD12	1:I:45:ILE:N	2.33	0.44
1:I:90:VAL:HG22	1:I:138:PHE:CE1	2.52	0.44
1:B:74:SER:HB2	1:B:144:LEU:CD2	2.48	0.44
1:E:45:ILE:HD13	1:E:58:LEU:HD22	1.99	0.44
1:I:43:LYS:HE3	1:I:43:LYS:HB2	1.87	0.44
1:H:94:LEU:HD13	1:H:97:MSE:CE	2.47	0.44
1:D:46:ILE:HG21	1:D:76:SER:HB3	2.00	0.44
1:H:150:ALA:O	1:H:154:LEU:HG	2.18	0.44
1:F:178:LYS:HE3	1:I:94:LEU:HD13	2.00	0.44
1:A:171:VAL:O	1:A:171:VAL:CG1	2.65	0.44
1:A:28:THR:HA	1:A:29:PRO:HD3	1.87	0.44
1:F:122:THR:HA	1:F:126:GLU:O	2.18	0.43
1:E:19:ASP:HA	1:E:22:LEU:HD23	2.00	0.43
1:D:47:VAL:O	1:D:65:TYR:HA	2.18	0.43
1:I:7:ILE:CG1	1:I:45:ILE:HG13	2.48	0.43
1:H:50:TYR:O	1:H:53:GLU:HG2	2.18	0.43
1:A:119:VAL:HB	1:A:132:LEU:HB3	2.00	0.43
1:H:78:LYS:HE3	1:H:144:LEU:HD22	2.01	0.43
1:G:122:THR:O	1:G:166:GLU:HA	2.18	0.43
1:D:22:LEU:CD2	1:D:57:LEU:HD11	2.48	0.43
1:D:49:LYS:HG2	1:D:69:TRP:CZ2	2.53	0.43
1:G:51:VAL:CG1	1:G:52:ASN:N	2.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:HG23	1:E:33:ARG:HD2	1.99	0.43
1:E:122:THR:HG22	1:E:127:ARG:HB3	2.00	0.43
1:E:89:ALA:HB1	1:E:132:LEU:HD13	2.00	0.43
1:I:162:LEU:N	1:I:162:LEU:HD12	2.33	0.43
1:B:119:VAL:HB	1:B:132:LEU:HB3	1.99	0.43
1:I:91:LEU:HD13	1:I:132:LEU:HD23	2.00	0.43
1:I:175:ILE:CG2	1:I:176:ASP:N	2.82	0.43
1:D:174:ASP:OD2	1:D:176:ASP:HB2	2.18	0.43
1:F:108:ILE:CD1	1:F:121:PRO:HG3	2.49	0.43
1:E:137:LEU:N	1:E:137:LEU:CD1	2.81	0.43
1:H:21:LEU:CB	1:H:54:MSE:HE1	2.40	0.43
1:F:25:ILE:HG22	1:F:33:ARG:HH12	1.83	0.43
1:B:97:MSE:HG2	1:B:174:ASP:CB	2.49	0.43
1:G:120:ILE:CD1	1:G:154:LEU:HD13	2.47	0.43
1:D:91:LEU:HD22	1:D:130:PRO:HB2	2.01	0.43
1:E:122:THR:HA	1:E:127:ARG:HA	2.01	0.43
1:A:3:ILE:CD1	1:A:109:ILE:HG23	2.48	0.43
1:E:66:ASN:HD21	1:E:68:PHE:CB	2.32	0.43
1:H:77:LEU:HD13	1:H:141:ILE:HD11	2.01	0.43
1:G:2:ASN:HB2	1:G:88:ASP:N	2.23	0.43
1:D:174:ASP:OD1	1:D:175:ILE:N	2.51	0.43
1:E:111:THR:HG21	1:E:165:ILE:CG2	2.49	0.43
1:A:44:ILE:HD12	1:A:62:ILE:HB	1.99	0.43
1:H:154:LEU:C	1:H:156:LYS:N	2.72	0.43
1:F:144:LEU:HD11	1:F:153:ILE:HD11	2.01	0.43
1:H:101:THR:OG1	1:H:103:GLU:HG2	2.18	0.43
1:H:105:VAL:O	1:H:109:ILE:HG13	2.18	0.43
1:H:28:THR:HA	1:H:29:PRO:HD3	1.91	0.43
1:E:141:ILE:HA	1:E:153:ILE:HD11	2.01	0.43
1:B:120:ILE:HD11	1:B:154:LEU:HD13	2.00	0.43
1:G:6:ILE:HG23	1:G:46:ILE:HD13	2.01	0.43
1:H:141:ILE:HA	1:H:144:LEU:HD11	2.01	0.42
1:H:30:ILE:CD1	1:H:96:ASP:HA	2.49	0.42
1:E:31:ILE:HG21	1:E:54:MSE:HE2	2.01	0.42
1:B:66:ASN:HD22	1:B:66:ASN:C	2.22	0.42
1:G:50:TYR:O	1:G:51:VAL:C	2.56	0.42
1:G:30:ILE:HG12	1:G:98:PRO:HB3	2.01	0.42
1:I:28:THR:CG2	1:I:33:ARG:HG3	2.48	0.42
1:E:128:GLY:HA3	1:E:171:VAL:HG12	2.00	0.42
1:E:141:ILE:HD13	1:E:141:ILE:O	2.18	0.42
1:D:111:THR:CG2	1:D:111:THR:O	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:THR:O	1:F:104:ASP:HB2	2.19	0.42
1:D:129:ASN:N	1:D:171:VAL:HG13	2.35	0.42
1:H:33:ARG:CG	1:H:33:ARG:NH1	2.81	0.42
1:G:123:HIS:HB3	1:G:172:LEU:HD11	2.01	0.42
1:F:4:GLY:O	1:F:90:VAL:HA	2.19	0.42
1:H:44:ILE:O	1:H:44:ILE:HG23	2.19	0.42
1:G:49:LYS:HA	1:G:69:TRP:CZ2	2.55	0.42
1:F:3:ILE:HA	1:F:89:ALA:O	2.19	0.42
1:D:15:ARG:HH11	1:D:15:ARG:HG3	1.84	0.42
1:E:120:ILE:HD11	1:E:154:LEU:HD13	2.01	0.42
1:B:135:LYS:HA	1:B:138:PHE:CD2	2.55	0.42
1:E:77:LEU:HD13	1:E:141:ILE:CG1	2.50	0.42
1:A:4:GLY:O	1:A:90:VAL:HA	2.20	0.42
1:G:37:ILE:HG13	1:G:38:TYR:CD1	2.55	0.42
1:I:132:LEU:C	1:I:132:LEU:HD13	2.40	0.42
1:G:151:ARG:HG2	1:G:151:ARG:HH11	1.84	0.42
1:B:89:ALA:CB	1:B:134:SER:HA	2.50	0.42
1:G:164:PHE:O	1:G:165:ILE:HG23	2.20	0.42
1:H:78:LYS:O	1:H:82:ARG:HG3	2.19	0.42
1:B:164:PHE:CD2	1:B:164:PHE:N	2.87	0.42
1:F:123:HIS:HB3	1:F:172:LEU:CD2	2.50	0.42
1:B:81:LEU:CD1	1:B:141:ILE:HD11	2.49	0.42
1:A:104:ASP:OD2	1:A:168:SER:OG	2.36	0.42
1:F:108:ILE:HD13	1:F:121:PRO:HG3	2.01	0.42
1:H:32:MSE:SE	1:H:57:LEU:HG	2.70	0.42
1:A:44:ILE:HD11	1:A:62:ILE:HG21	2.00	0.42
1:A:12:GLU:O	1:A:15:ARG:HB2	2.20	0.42
1:H:132:LEU:HD23	1:H:132:LEU:C	2.40	0.42
1:H:4:GLY:HA3	1:H:84:PHE:CE1	2.54	0.42
1:E:66:ASN:HD22	1:E:67:PRO:N	2.18	0.42
1:I:154:LEU:HD23	1:I:157:ILE:CD1	2.50	0.42
1:D:42:GLU:OE2	1:D:87:TYR:OH	2.36	0.42
1:E:157:ILE:HD12	1:E:158:LYS:N	2.35	0.41
1:H:83:PHE:HD1	1:I:82:ARG:NH2	2.18	0.41
1:H:45:ILE:CD1	1:H:45:ILE:N	2.83	0.41
1:A:47:VAL:HG12	1:A:51:VAL:HG13	2.01	0.41
1:F:51:VAL:CG1	1:F:52:ASN:N	2.83	0.41
1:E:29:PRO:HB2	1:E:32:MSE:HG3	2.02	0.41
1:E:126:GLU:HG3	1:E:172:LEU:CD2	2.50	0.41
1:F:89:ALA:HB1	1:F:133:ILE:O	2.19	0.41
1:H:8:LEU:CD1	1:H:73:ILE:HD11	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:O	1:B:171:VAL:HG12	2.20	0.41
1:B:132:LEU:O	1:B:132:LEU:HD13	2.20	0.41
1:I:3:ILE:HA	1:I:89:ALA:O	2.20	0.41
1:B:158:LYS:HB2	1:B:161:GLU:OE2	2.20	0.41
1:H:55:LEU:CD1	1:I:55:LEU:HD12	2.50	0.41
1:F:141:ILE:HD13	1:F:141:ILE:O	2.20	0.41
1:H:123:HIS:HB3	1:H:172:LEU:HD22	2.02	0.41
1:E:158:LYS:O	1:E:160:GLU:N	2.53	0.41
1:G:101:THR:HB	1:G:104:ASP:CG	2.40	0.41
1:G:104:ASP:CG	1:G:167:CYS:HB3	2.40	0.41
1:H:22:LEU:HD23	1:H:54:MSE:HE2	2.01	0.41
1:I:104:ASP:OD2	1:I:167:CYS:HB3	2.19	0.41
1:G:171:VAL:CG1	1:G:171:VAL:O	2.69	0.41
1:I:31:ILE:HG23	1:I:32:MSE:N	2.36	0.41
1:D:169:GLU:HB3	1:D:173:ILE:HD11	2.03	0.41
1:G:101:THR:CG2	1:G:102:LYS:N	2.83	0.41
1:E:91:LEU:HD22	1:E:130:PRO:HB2	2.01	0.41
1:A:97:MSE:SE	1:A:129:ASN:HB2	2.71	0.41
1:F:120:ILE:HA	1:F:121:PRO:HD3	1.94	0.41
1:D:94:LEU:HB2	1:D:97:MSE:HG3	2.01	0.41
1:B:154:LEU:HA	1:B:157:ILE:HD12	2.02	0.41
1:F:34:THR:HG21	1:F:95:GLY:HA2	2.03	0.41
1:G:122:THR:HA	1:G:126:GLU:O	2.21	0.41
1:F:55:LEU:HD22	1:G:55:LEU:HD11	2.01	0.41
1:H:72:GLY:HA3	1:H:147:ASP:HA	2.01	0.41
1:I:129:ASN:N	1:I:171:VAL:HG13	2.35	0.41
1:G:37:ILE:O	1:G:37:ILE:HD12	2.21	0.41
1:E:97:MSE:HG2	1:E:173:ILE:O	2.20	0.41
1:A:30:ILE:HG23	1:A:98:PRO:HG3	2.02	0.41
1:F:56:PRO:HG3	1:G:52:ASN:HD21	1.85	0.41
1:E:91:LEU:HD11	1:E:105:VAL:HG13	2.03	0.41
1:G:119:VAL:HG22	1:G:163:CYS:HB2	2.03	0.41
1:E:158:LYS:C	1:E:160:GLU:H	2.23	0.41
1:I:104:ASP:O	1:I:108:ILE:HG13	2.20	0.41
1:H:169:GLU:HG2	1:H:173:ILE:HD11	2.01	0.41
1:I:55:LEU:HA	1:I:55:LEU:HD23	1.78	0.41
1:I:37:ILE:HG12	1:I:38:TYR:N	2.36	0.41
1:D:44:ILE:HD12	1:D:64:ILE:CD1	2.48	0.41
1:H:53:GLU:HG2	1:H:53:GLU:H	1.65	0.41
1:I:135:LYS:HA	1:I:138:PHE:CD2	2.56	0.41
1:F:26:ASP:O	1:F:27:ASN:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:LEU:HD13	1:H:144:LEU:H	1.86	0.41
1:D:31:ILE:O	1:D:35:ILE:HG13	2.21	0.41
1:I:119:VAL:HB	1:I:132:LEU:HB3	2.02	0.41
1:A:135:LYS:HA	1:A:138:PHE:CD2	2.56	0.41
1:E:7:ILE:CD1	1:E:35:ILE:HD13	2.51	0.40
1:D:31:ILE:HG21	1:D:54:MSE:HE1	2.03	0.40
1:B:66:ASN:ND2	1:B:68:PHE:N	2.60	0.40
1:B:94:LEU:CG	1:B:97:MSE:HE2	2.50	0.40
1:A:2:ASN:HB2	1:A:88:ASP:OD2	2.21	0.40
1:H:66:ASN:HD21	1:H:75:THR:CG2	2.08	0.40
1:H:138:PHE:O	1:H:139:ASN:C	2.59	0.40
1:I:74:SER:HB2	1:I:144:LEU:CD2	2.49	0.40
1:A:59:MSE:HB2	1:I:69:TRP:CZ2	2.56	0.40
1:A:10:ALA:HA	1:A:48:GLY:H	1.86	0.40
1:A:111:THR:HG21	1:A:165:ILE:HG23	2.02	0.40
1:B:30:ILE:O	1:B:33:ARG:N	2.54	0.40
1:H:154:LEU:O	1:H:156:LYS:N	2.55	0.40
1:A:174:ASP:O	1:A:175:ILE:C	2.59	0.40
1:I:112:PHE:CE1	1:I:134:SER:HB3	2.56	0.40
1:H:94:LEU:CD2	1:H:97:MSE:HE3	2.47	0.40
1:E:81:LEU:HD22	1:E:141:ILE:HD12	2.04	0.40
1:B:31:ILE:HG12	1:B:54:MSE:CE	2.51	0.40
1:I:165:ILE:HG22	1:I:165:ILE:O	2.21	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	176/197 (89%)	155 (88%)	18 (10%)	3 (2%)	11	36
1	B	163/197 (83%)	141 (86%)	19 (12%)	3 (2%)	11	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	176/197 (89%)	157 (89%)	18 (10%)	1 (1%)	30 65
1	E	168/197 (85%)	150 (89%)	14 (8%)	4 (2%)	7 25
1	F	168/197 (85%)	152 (90%)	16 (10%)	0	100 100
1	G	162/197 (82%)	142 (88%)	15 (9%)	5 (3%)	5 17
1	H	169/197 (86%)	149 (88%)	14 (8%)	6 (4%)	4 14
1	I	167/197 (85%)	147 (88%)	17 (10%)	3 (2%)	11 34
All	All	1349/1576 (86%)	1193 (88%)	131 (10%)	25 (2%)	10 32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	85	LYS
1	B	171	VAL
1	D	159	ILE
1	G	49	LYS
1	H	155	ASN
1	H	175	ILE
1	B	26	ASP
1	E	150	ALA
1	G	39	GLY
1	H	118	ALA
1	I	59	MSE
1	A	39	GLY
1	E	144	LEU
1	H	39	GLY
1	H	171	VAL
1	B	148	VAL
1	E	148	VAL
1	G	51	VAL
1	H	25	ILE
1	E	175	ILE
1	G	73	ILE
1	I	114	PRO
1	A	25	ILE
1	A	175	ILE
1	I	148	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/169 (85%)	128 (89%)	16 (11%)	8	23
1	B	136/169 (80%)	120 (88%)	16 (12%)	6	19
1	D	148/169 (88%)	132 (89%)	16 (11%)	8	23
1	E	139/169 (82%)	123 (88%)	16 (12%)	7	21
1	F	135/169 (80%)	125 (93%)	10 (7%)	17	43
1	G	137/169 (81%)	128 (93%)	9 (7%)	21	51
1	H	141/169 (83%)	125 (89%)	16 (11%)	7	22
1	I	137/169 (81%)	122 (89%)	15 (11%)	8	23
All	All	1117/1352 (83%)	1003 (90%)	114 (10%)	9	26

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	12	GLU
1	A	28	THR
1	A	37	ILE
1	A	51	VAL
1	A	52	ASN
1	A	55	LEU
1	A	66	ASN
1	A	75	THR
1	A	77	LEU
1	A	91	LEU
1	A	100	VAL
1	A	127	ARG
1	A	141	ILE
1	A	144	LEU
1	A	165	ILE
1	B	26	ASP
1	B	40	ASP
1	B	44	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	VAL
1	B	66	ASN
1	B	70	ASN
1	B	71	GLU
1	B	81	LEU
1	B	82	ARG
1	B	102	LYS
1	B	122	THR
1	B	127	ARG
1	B	141	ILE
1	B	144	LEU
1	B	155	ASN
1	B	165	ILE
1	D	7	ILE
1	D	28	THR
1	D	30	ILE
1	D	49	LYS
1	D	51	VAL
1	D	52	ASN
1	D	54	MSE
1	D	57	LEU
1	D	66	ASN
1	D	91	LEU
1	D	103	GLU
1	D	127	ARG
1	D	137	LEU
1	D	165	ILE
1	D	174	ASP
1	D	175	ILE
1	E	32	MSE
1	E	51	VAL
1	E	64	ILE
1	E	66	ASN
1	E	70	ASN
1	E	77	LEU
1	E	100	VAL
1	E	103	GLU
1	E	106	ASN
1	E	132	LEU
1	E	141	ILE
1	E	151	ARG
1	E	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	162	LEU
1	E	165	ILE
1	E	176	ASP
1	F	21	LEU
1	F	28	THR
1	F	37	ILE
1	F	42	GLU
1	F	45	ILE
1	F	94	LEU
1	F	107	LYS
1	F	141	ILE
1	F	165	ILE
1	F	173	ILE
1	G	30	ILE
1	G	55	LEU
1	G	79	LEU
1	G	127	ARG
1	G	139	ASN
1	G	165	ILE
1	G	166	GLU
1	G	171	VAL
1	G	175	ILE
1	H	2	ASN
1	H	22	LEU
1	H	33	ARG
1	H	43	LYS
1	H	53	GLU
1	H	55	LEU
1	H	57	LEU
1	H	79	LEU
1	H	98	PRO
1	H	100	VAL
1	H	141	ILE
1	H	144	LEU
1	H	165	ILE
1	H	166	GLU
1	H	172	LEU
1	H	176	ASP
1	I	7	ILE
1	I	22	LEU
1	I	24	LYS
1	I	32	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	37	ILE
1	I	51	VAL
1	I	66	ASN
1	I	81	LEU
1	I	103	GLU
1	I	104	ASP
1	I	141	ILE
1	I	144	LEU
1	I	165	ILE
1	I	179	GLU
1	I	180	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	123	HIS
1	A	129	ASN
1	A	155	ASN
1	B	27	ASN
1	B	52	ASN
1	B	66	ASN
1	B	70	ASN
1	B	106	ASN
1	D	2	ASN
1	D	66	ASN
1	D	106	ASN
1	D	155	ASN
1	E	2	ASN
1	E	66	ASN
1	E	70	ASN
1	E	155	ASN
1	F	52	ASN
1	G	52	ASN
1	G	110	ASN
1	H	2	ASN
1	H	106	ASN
1	H	110	ASN
1	I	66	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	173/197 (87%)	0.20	5 (2%)	55	43	42, 66, 92, 98	0
1	B	163/197 (82%)	0.36	6 (3%)	45	33	39, 70, 99, 100	0
1	D	173/197 (87%)	0.28	3 (1%)	73	63	45, 69, 94, 100	0
1	E	167/197 (84%)	0.30	4 (2%)	62	50	28, 69, 89, 93	0
1	F	167/197 (84%)	0.28	4 (2%)	62	50	34, 74, 99, 100	0
1	G	161/197 (81%)	0.24	3 (1%)	70	59	45, 70, 90, 96	0
1	H	168/197 (85%)	0.22	3 (1%)	71	61	33, 68, 93, 95	0
1	I	166/197 (84%)	0.41	8 (4%)	34	23	44, 77, 100, 100	0
All	All	1338/1576 (84%)	0.29	36 (2%)	58	45	28, 70, 96, 100	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ILE	5.3
1	A	18	GLY	4.8
1	A	17	GLY	4.7
1	I	108	ILE	4.2
1	H	175	ILE	3.6
1	E	175	ILE	3.6
1	E	27	ASN	3.2
1	I	116	CYS	3.2
1	F	116	CYS	3.1
1	D	17	GLY	3.1
1	G	175	ILE	3.0
1	A	165	ILE	3.0
1	B	25	ILE	3.0
1	I	107	LYS	2.8
1	G	164	PHE	2.8
1	I	159	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	173	ILE	2.6
1	B	153	ILE	2.6
1	F	162	LEU	2.5
1	D	18	GLY	2.5
1	I	163	CYS	2.5
1	B	167	CYS	2.4
1	F	25	ILE	2.4
1	H	40	ASP	2.4
1	I	105	VAL	2.4
1	E	164	PHE	2.4
1	D	157	ILE	2.3
1	A	157	ILE	2.3
1	G	162	LEU	2.3
1	H	164	PHE	2.3
1	E	176	ASP	2.3
1	I	114	PRO	2.2
1	A	16	PHE	2.1
1	B	137	LEU	2.1
1	F	112	PHE	2.0
1	I	109	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.