Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:18 PM GMT

PDB ID	:	4OFS
Title	:	Crystal structure of a truncated catalytic core of the 2-oxoacid dehydrogenase multienzyme complex from Thermoplasma acidophilum
Authors	:	Marrot, N.L.; Marshall, J.J.T.; Svergun, D.I.; Crennell, S.J.; Hough, D.W.; van den Elsen, J.M.H.; Danson, M.J.
Deposited on	:	2014-01-15
Resolution	:	4.10 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
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:

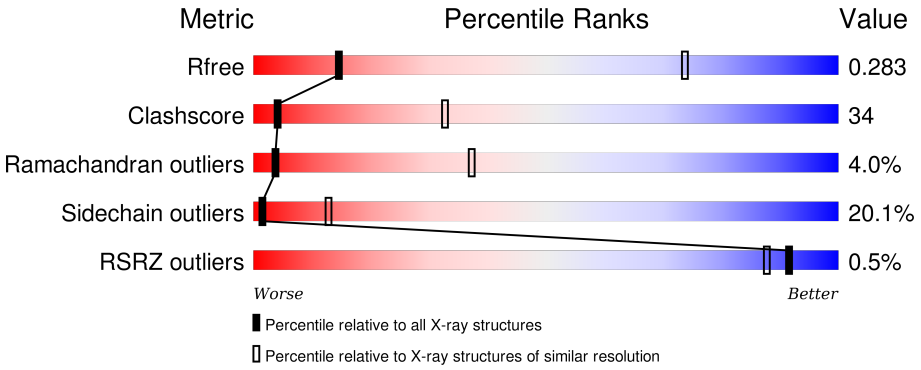
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.10 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.



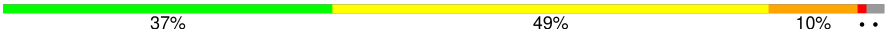
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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	219	38% 44% 13%
1	B	219	% 43% 40% 13%
1	C	219	40% 47% 9%
1	D	219	34% 49% 14%
1	E	219	% 41% 46% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	219	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10241 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 Probable lipoamide acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1705	1084	294	318	9			
1	B	214	Total	C	N	O	S	0	0	0
			1705	1084	294	318	9			
1	C	214	Total	C	N	O	S	0	0	0
			1705	1084	294	318	9			
1	D	214	Total	C	N	O	S	0	0	0
			1705	1084	294	318	9			
1	E	214	Total	C	N	O	S	0	0	0
			1705	1084	294	318	9			
1	F	215	Total	C	N	O	S	0	0	0
			1716	1090	298	319	9			

There are 6 discrepancies between the modelled and reference sequences:

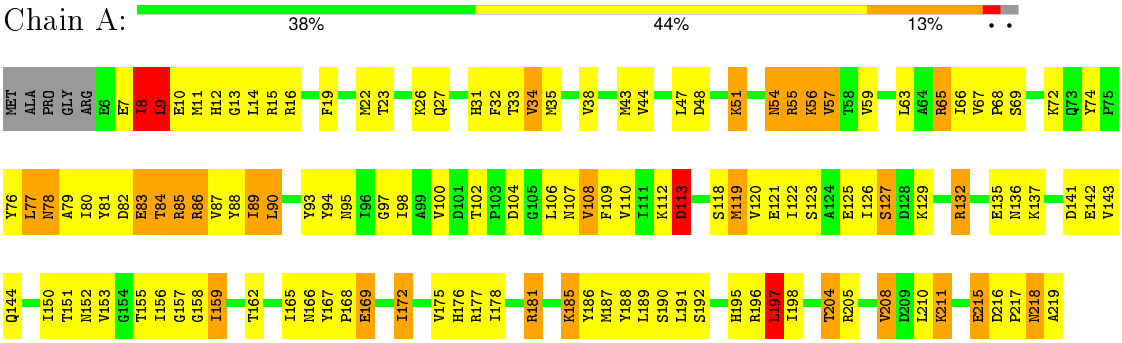
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9HIA5
B	1	MET	-	EXPRESSION TAG	UNP Q9HIA5
C	1	MET	-	EXPRESSION TAG	UNP Q9HIA5
D	1	MET	-	EXPRESSION TAG	UNP Q9HIA5
E	1	MET	-	EXPRESSION TAG	UNP Q9HIA5
F	1	MET	-	EXPRESSION TAG	UNP Q9HIA5

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.

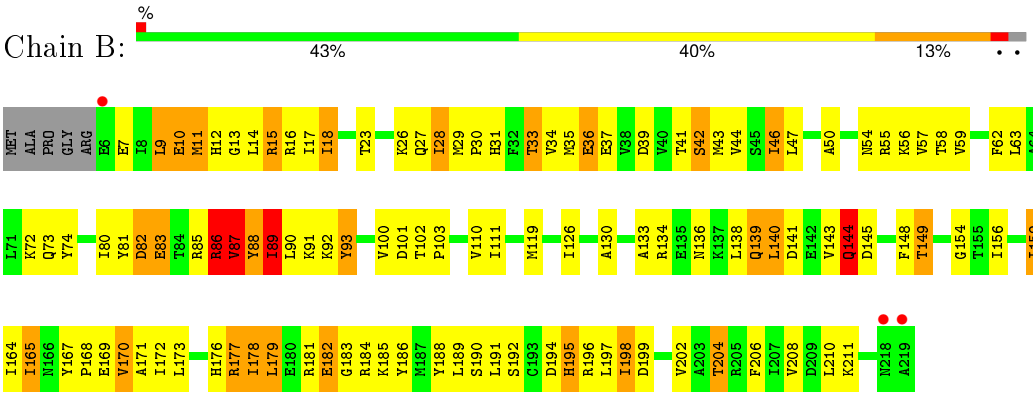
- Molecule 1: Probable lipoamide acyltransferase

Chain A:



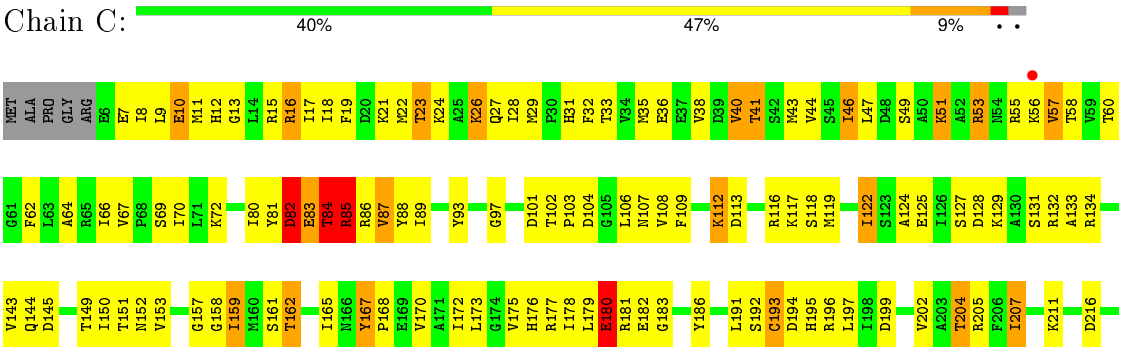
- Molecule 1: Probable lipoamide acyltransferase

Chain B:



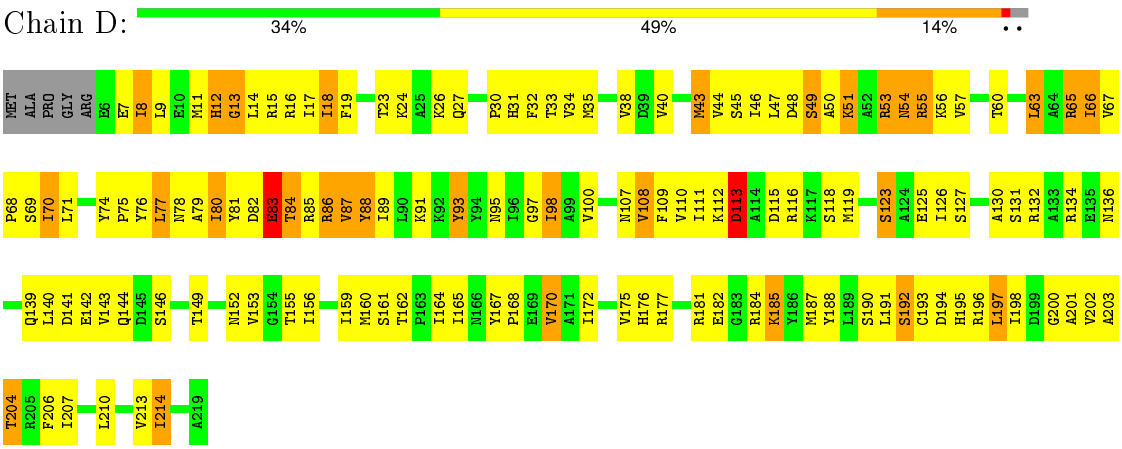
- Molecule 1: Probable lipoamide acyltransferase

Chain C:



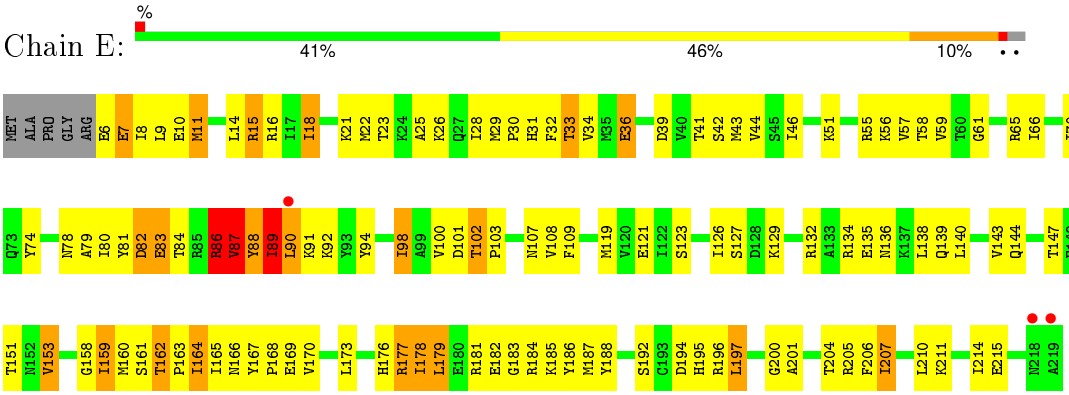
• Molecule 1: Probable lipoamide acyltransferase

Chain D:



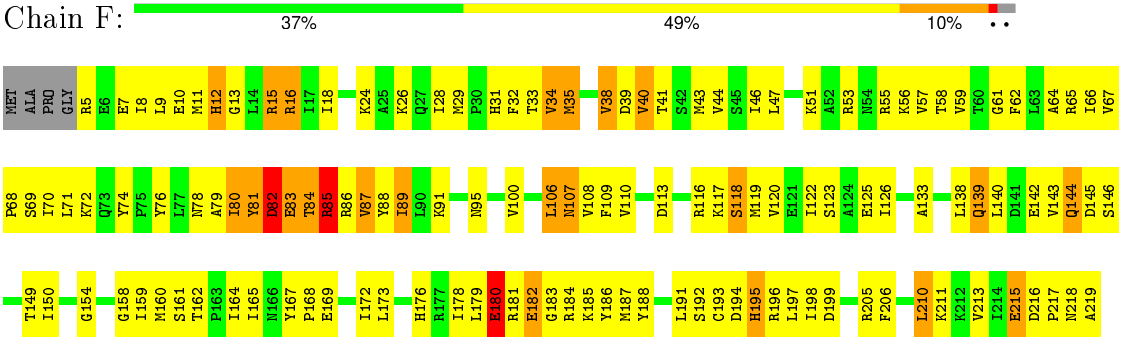
• Molecule 1: Probable lipoamide acyltransferase

Chain E:



• Molecule 1: Probable lipoamide acyltransferase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.15Å 107.15Å 238.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 4.10 48.87 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.87-4.10) 99.3 (48.87-4.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.212 , 0.284 0.206 , 0.283	Depositor DCC
R_{free} test set	628 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	154.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.8	EDS
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 12902 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10241	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	0.53	0/1730	0.79	1/2335 (0.0%)
1	B	0.53	0/1730	0.80	2/2335 (0.1%)
1	C	0.55	0/1730	0.80	2/2335 (0.1%)
1	D	0.52	0/1730	0.76	0/2335
1	E	0.54	0/1730	0.75	0/2335
1	F	0.52	0/1741	0.77	2/2349 (0.1%)
All	All	0.53	0/10391	0.78	7/14024 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	197	LEU	CA-CB-CG	5.85	128.75	115.30
1	F	106	LEU	CA-CB-CG	5.73	128.48	115.30
1	C	82	ASP	N-CA-C	5.18	124.99	111.00
1	B	140	LEU	CA-CB-CG	5.10	127.04	115.30
1	C	197	LEU	CA-CB-CG	5.06	126.93	115.30
1	F	82	ASP	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	81	TYR	Peptide
1	F	81	TYR	Peptide

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	1705	0	1764	129	0
1	B	1705	0	1764	131	0
1	C	1705	0	1764	138	0
1	D	1705	0	1764	136	0
1	E	1705	0	1764	130	0
1	F	1716	0	1777	157	0
All	All	10241	0	10597	703	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 34.

All (703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HZ1	1:B:26:LYS:NZ	1.34	1.21
1:E:33:THR:HG23	1:F:162:THR:CG2	1.73	1.18
1:C:84:THR:HG23	1:C:87:VAL:HG21	1.29	1.14
1:D:86:ARG:HH12	1:E:11:MET:HB2	1.12	1.13
1:E:33:THR:HG23	1:F:162:THR:HG22	1.33	1.11
1:F:82:ASP:HB2	1:F:87:VAL:HG23	1.28	1.10
1:A:26:LYS:NZ	1:B:26:LYS:NZ	1.99	1.09
1:F:84:THR:HG23	1:F:87:VAL:HG21	1.35	1.05
1:A:26:LYS:HE2	1:B:26:LYS:HE2	1.34	1.05
1:E:56:LYS:HB3	1:E:57:VAL:HA	1.39	1.02
1:B:86:ARG:HE	1:C:10:GLU:HG2	1.25	1.00
1:C:12:HIS:HB3	1:C:15:ARG:HB2	1.44	0.99
1:E:83:GLU:HG2	1:E:84:THR:H	1.24	0.99
1:E:182:GLU:N	1:E:183:GLY:HA2	1.76	0.99
1:D:15:ARG:NH1	1:F:196:ARG:O	1.97	0.98
1:B:89:ILE:HB	1:C:8:ILE:HG12	1.44	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASP:HB2	1:C:202:VAL:HG12	1.47	0.96
1:C:53:ARG:NH1	1:D:69:SER:HB3	1.85	0.91
1:E:30:PRO:HD2	1:E:196:ARG:HD2	1.54	0.90
1:F:80:ILE:HG13	1:F:168:PRO:O	1.72	0.89
1:A:108:VAL:O	1:A:143:VAL:HG13	1.73	0.89
1:A:26:LYS:CE	1:B:26:LYS:HE2	2.03	0.89
1:C:179:LEU:O	1:C:180:GLU:HB2	1.72	0.88
1:A:102:THR:HG21	1:A:107:ASN:HD22	1.39	0.88
1:B:86:ARG:O	1:B:87:VAL:HG22	1.73	0.87
1:A:26:LYS:NZ	1:B:26:LYS:CE	2.38	0.87
1:F:11:MET:HG2	1:F:16:ARG:HG3	1.54	0.87
1:D:43:MET:O	1:D:46:ILE:HG22	1.72	0.87
1:E:90:LEU:HG	1:F:9:LEU:HD13	1.57	0.86
1:C:53:ARG:CZ	1:D:69:SER:HB3	2.05	0.86
1:F:43:MET:O	1:F:46:ILE:HG22	1.76	0.86
1:E:33:THR:CG2	1:F:162:THR:CG2	2.55	0.85
1:B:172:ILE:O	1:B:191:LEU:HD12	1.77	0.84
1:E:178:ILE:HD12	1:E:178:ILE:H	1.41	0.84
1:E:26:LYS:HE3	1:F:26:LYS:NZ	1.93	0.84
1:E:78:ASN:HD21	1:E:147:THR:HB	1.43	0.83
1:A:44:VAL:HG21	1:A:185:LYS:HE2	1.60	0.83
1:F:179:LEU:N	1:F:186:TYR:O	2.12	0.83
1:A:26:LYS:HZ1	1:B:26:LYS:HZ3	0.84	0.83
1:D:86:ARG:NH1	1:E:11:MET:HB2	1.92	0.83
1:C:38:VAL:HG12	1:C:211:LYS:HG3	1.61	0.83
1:E:33:THR:HG23	1:F:162:THR:HG21	1.58	0.82
1:A:95:ASN:HB3	1:A:112:LYS:HA	1.60	0.82
1:F:82:ASP:HB2	1:F:87:VAL:CG2	2.08	0.82
1:D:88:TYR:CZ	1:D:197:LEU:HD23	2.14	0.82
1:B:86:ARG:NE	1:C:10:GLU:HG2	1.93	0.82
1:E:44:VAL:HG11	1:E:185:LYS:HD2	1.58	0.82
1:E:83:GLU:HG2	1:E:84:THR:N	1.93	0.81
1:C:53:ARG:HB3	1:C:53:ARG:CZ	2.10	0.81
1:B:15:ARG:HA	1:B:15:ARG:HH11	1.46	0.80
1:A:166:ASN:H	1:A:172:ILE:HD12	1.46	0.80
1:D:86:ARG:HH21	1:E:16:ARG:NE	1.80	0.80
1:D:26:LYS:HE2	1:F:26:LYS:NZ	1.97	0.80
1:B:31:HIS:NE2	1:B:165:ILE:HG12	1.97	0.79
1:E:86:ARG:O	1:E:87:VAL:HG22	1.83	0.79
1:A:54:ASN:O	1:A:55:ARG:HB2	1.82	0.79
1:A:122:ILE:O	1:A:126:ILE:HG23	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:HB3	1:C:159:ILE:HD11	1.63	0.79
1:F:82:ASP:CB	1:F:87:VAL:HG23	2.13	0.79
1:F:70:ILE:CD1	1:F:210:LEU:HD12	2.12	0.79
1:A:26:LYS:NZ	1:B:26:LYS:HZ3	1.71	0.78
1:B:93:TYR:H	1:B:93:TYR:HD1	1.29	0.78
1:F:12:HIS:CD2	1:F:13:GLY:H	2.01	0.78
1:B:182:GLU:N	1:B:183:GLY:HA2	1.99	0.78
1:A:82:ASP:OD2	1:A:87:VAL:HB	1.84	0.77
1:F:38:VAL:HG12	1:F:211:LYS:HG3	1.66	0.77
1:F:70:ILE:HD12	1:F:210:LEU:HD12	1.67	0.77
1:D:210:LEU:O	1:D:213:VAL:HG22	1.83	0.77
1:E:26:LYS:HE3	1:F:26:LYS:HZ1	1.50	0.76
1:A:95:ASN:CB	1:A:112:LYS:HA	2.16	0.76
1:B:176:HIS:HD2	1:B:188:TYR:O	1.67	0.76
1:A:65:ARG:HG2	1:A:122:ILE:HD12	1.68	0.75
1:C:32:PHE:HB2	1:C:195:HIS:CD2	2.21	0.75
1:F:181:ARG:HB2	1:F:186:TYR:HD2	1.52	0.75
1:C:33:THR:HA	1:C:191:LEU:O	1.87	0.75
1:A:158:GLY:HA2	1:C:36:GLU:HG2	1.68	0.75
1:B:83:GLU:CD	1:B:83:GLU:H	1.89	0.75
1:C:84:THR:CG2	1:C:87:VAL:HG21	2.12	0.74
1:A:196:ARG:HD3	1:B:23:THR:OG1	1.87	0.74
1:F:110:VAL:HG12	1:F:146:SER:HB3	1.69	0.74
1:D:13:GLY:O	1:D:17:ILE:HG12	1.88	0.74
1:B:23:THR:O	1:B:27:GLN:HB2	1.88	0.74
1:D:54:ASN:O	1:D:55:ARG:HB2	1.88	0.73
1:D:40:VAL:O	1:D:43:MET:HB3	1.87	0.73
1:B:82:ASP:OD2	1:B:88:TYR:HA	1.86	0.73
1:F:144:GLN:HG2	1:F:145:ASP:N	2.03	0.73
1:C:57:VAL:HG11	1:C:119:MET:HE1	1.71	0.73
1:C:83:GLU:OE1	1:C:83:GLU:HA	1.86	0.73
1:A:155:THR:HG23	1:A:156:ILE:HD12	1.71	0.72
1:C:131:SER:HA	1:C:134:ARG:HD2	1.71	0.72
1:A:33:THR:OG1	1:A:192:SER:HB3	1.88	0.72
1:B:36:GLU:HG2	1:C:158:GLY:HA2	1.72	0.72
1:E:181:ARG:C	1:E:183:GLY:HA2	2.10	0.71
1:A:26:LYS:NZ	1:B:26:LYS:HZ1	1.87	0.71
1:B:182:GLU:HG2	1:B:184:ARG:HG2	1.72	0.71
1:B:29:MET:HE2	1:B:170:VAL:HG23	1.71	0.71
1:A:102:THR:CG2	1:A:107:ASN:HD22	2.02	0.71
1:A:23:THR:O	1:A:27:GLN:HB3	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LYS:HE2	1:F:7:GLU:CD	2.10	0.71
1:E:29:MET:SD	1:E:165:ILE:HD11	2.30	0.71
1:F:154:GLY:HA3	1:F:176:HIS:C	2.11	0.71
1:E:11:MET:HG2	1:E:15:ARG:HB3	1.73	0.70
1:E:30:PRO:CD	1:E:196:ARG:HD2	2.20	0.70
1:F:79:ALA:HB1	1:F:89:ILE:O	1.91	0.70
1:F:176:HIS:HD2	1:F:188:TYR:O	1.74	0.70
1:C:129:LYS:HA	1:C:132:ARG:NH1	2.07	0.70
1:A:23:THR:O	1:A:27:GLN:CB	2.40	0.70
1:E:26:LYS:HZ1	1:F:26:LYS:HZ3	1.40	0.69
1:D:195:HIS:HB3	1:E:164:ILE:HD11	1.74	0.69
1:F:32:PHE:HB2	1:F:195:HIS:CD2	2.27	0.69
1:D:45:SER:O	1:D:49:SER:HB2	1.91	0.69
1:B:26:LYS:NZ	1:C:26:LYS:HE2	2.08	0.69
1:F:180:GLU:HA	1:F:184:ARG:O	1.92	0.69
1:C:179:LEU:N	1:C:186:TYR:O	2.25	0.68
1:C:108:VAL:O	1:C:143:VAL:HG13	1.94	0.68
1:D:77:LEU:HG	1:D:198:ILE:HD12	1.76	0.68
1:C:53:ARG:NH1	1:C:53:ARG:HB3	2.09	0.67
1:E:31:HIS:O	1:F:164:ILE:HD11	1.95	0.67
1:D:80:ILE:O	1:D:88:TYR:O	2.13	0.67
1:A:197:LEU:HD12	1:A:198:ILE:HG12	1.76	0.67
1:B:154:GLY:HA3	1:B:176:HIS:C	2.14	0.67
1:E:26:LYS:NZ	1:F:26:LYS:HZ3	1.92	0.67
1:B:63:LEU:O	1:B:66:ILE:HG13	1.94	0.67
1:F:28:ILE:HD11	1:F:167:TYR:OH	1.95	0.67
1:D:86:ARG:HA	1:D:86:ARG:HH11	1.59	0.67
1:F:149:THR:HG23	1:F:172:ILE:HG13	1.77	0.67
1:B:26:LYS:HZ1	1:C:26:LYS:HE2	1.59	0.66
1:F:133:ALA:HB2	1:F:138:LEU:HD22	1.75	0.66
1:C:62:PHE:CE2	1:C:66:ILE:HD11	2.29	0.66
1:B:33:THR:HG23	1:C:162:THR:CG2	2.25	0.66
1:E:33:THR:CG2	1:F:162:THR:HG21	2.22	0.66
1:D:34:VAL:HG11	1:D:204:THR:HG23	1.77	0.66
1:C:62:PHE:HD1	1:C:119:MET:SD	2.18	0.66
1:F:139:GLN:HG2	1:F:142:GLU:HG3	1.78	0.66
1:C:23:THR:O	1:C:27:GLN:HB2	1.95	0.66
1:B:188:TYR:CE1	1:C:159:ILE:HD12	2.31	0.66
1:F:29:MET:HE1	1:F:169:GLU:O	1.96	0.66
1:B:29:MET:CE	1:B:170:VAL:HG23	2.25	0.66
1:E:43:MET:O	1:E:46:ILE:HG22	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:VAL:HG23	1:C:43:MET:HB3	1.76	0.66
1:B:89:ILE:HA	1:C:8:ILE:HA	1.76	0.65
1:E:160:MET:HA	1:E:176:HIS:CD2	2.32	0.65
1:D:86:ARG:HH22	1:E:11:MET:HB3	1.62	0.65
1:D:38:VAL:HG11	1:D:214:ILE:HD12	1.78	0.65
1:C:83:GLU:C	1:C:85:ARG:H	1.99	0.65
1:E:56:LYS:HB3	1:E:57:VAL:CA	2.22	0.65
1:F:159:ILE:HG22	1:F:160:MET:HG2	1.77	0.65
1:B:188:TYR:HE1	1:C:159:ILE:HD12	1.61	0.65
1:E:32:PHE:HB2	1:E:195:HIS:CD2	2.31	0.65
1:F:83:GLU:HA	1:F:83:GLU:OE1	1.95	0.65
1:E:109:PHE:CE1	1:E:129:LYS:HB2	2.32	0.65
1:A:44:VAL:O	1:A:47:LEU:HB2	1.96	0.65
1:E:32:PHE:HB2	1:E:195:HIS:HD2	1.61	0.65
1:C:49:SER:O	1:C:53:ARG:HD2	1.97	0.64
1:D:95:ASN:HB3	1:D:113:ASP:N	2.12	0.64
1:D:181:ARG:HD3	1:F:181:ARG:NH1	2.12	0.64
1:D:65:ARG:HH12	1:D:118:SER:HA	1.62	0.64
1:D:123:SER:HA	1:D:126:ILE:CG1	2.27	0.64
1:E:74:TYR:OH	1:E:205:ARG:HG2	1.98	0.64
1:B:208:VAL:HG21	1:C:157:GLY:HA3	1.80	0.64
1:C:12:HIS:O	1:C:16:ARG:HG3	1.97	0.64
1:E:78:ASN:HD21	1:E:147:THR:CB	2.10	0.64
1:A:181:ARG:HD3	1:C:181:ARG:HD2	1.79	0.64
1:E:82:ASP:OD2	1:E:88:TYR:HA	1.97	0.64
1:D:9:LEU:HB2	1:F:88:TYR:CE1	2.33	0.64
1:E:90:LEU:HD21	1:F:9:LEU:HD22	1.79	0.63
1:D:33:THR:OG1	1:D:192:SER:HB3	1.98	0.63
1:C:47:LEU:O	1:C:51:LYS:N	2.30	0.63
1:B:81:TYR:HD1	1:B:88:TYR:CE1	2.16	0.63
1:A:211:LYS:HE2	1:B:177:ARG:HH12	1.64	0.63
1:A:26:LYS:CE	1:B:26:LYS:CE	2.74	0.63
1:D:130:ALA:O	1:D:134:ARG:HG3	1.98	0.63
1:D:26:LYS:HE2	1:F:26:LYS:HZ2	1.64	0.63
1:A:65:ARG:HG3	1:A:119:MET:HG3	1.81	0.63
1:C:24:LYS:HE3	1:C:167:TYR:HE2	1.64	0.63
1:B:12:HIS:ND1	1:B:15:ARG:HB2	2.14	0.63
1:F:167:TYR:CD1	1:F:168:PRO:HA	2.34	0.62
1:D:167:TYR:CG	1:D:168:PRO:HA	2.34	0.62
1:F:86:ARG:O	1:F:86:ARG:HG3	1.98	0.62
1:D:108:VAL:O	1:D:143:VAL:HG13	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:HIS:CG	1:F:13:GLY:N	2.68	0.62
1:C:41:THR:HA	1:C:44:VAL:HG12	1.81	0.62
1:C:69:SER:HA	1:C:72:LYS:HD2	1.82	0.62
1:C:26:LYS:HB3	1:C:31:HIS:CE1	2.34	0.62
1:F:179:LEU:O	1:F:180:GLU:HB2	1.99	0.62
1:C:18:ILE:O	1:C:22:MET:HG2	1.99	0.62
1:D:159:ILE:O	1:D:188:TYR:HB2	1.99	0.62
1:E:26:LYS:CE	1:F:26:LYS:HZ3	2.13	0.61
1:B:86:ARG:C	1:B:87:VAL:HG22	2.19	0.61
1:D:71:LEU:HD13	1:D:78:ASN:HB3	1.82	0.61
1:D:93:TYR:HD1	1:D:93:TYR:H	1.48	0.61
1:D:88:TYR:CE1	1:D:197:LEU:HD23	2.35	0.61
1:D:181:ARG:NH2	1:D:188:TYR:OH	2.29	0.61
1:D:76:TYR:CD1	1:D:197:LEU:HD13	2.36	0.61
1:A:26:LYS:HZ3	1:B:26:LYS:CE	2.14	0.61
1:E:81:TYR:CD2	1:E:82:ASP:N	2.68	0.61
1:C:205:ARG:HB2	1:C:205:ARG:NH1	2.15	0.61
1:F:12:HIS:ND1	1:F:15:ARG:HB2	2.16	0.61
1:C:43:MET:HG3	1:C:62:PHE:CE2	2.36	0.61
1:D:12:HIS:O	1:D:16:ARG:CB	2.48	0.61
1:D:23:THR:O	1:D:27:GLN:HB2	2.01	0.61
1:C:82:ASP:OD1	1:C:87:VAL:HG23	1.99	0.60
1:E:182:GLU:N	1:E:183:GLY:CA	2.60	0.60
1:D:26:LYS:CE	1:F:26:LYS:NZ	2.64	0.60
1:D:111:ILE:HD12	1:D:111:ILE:O	2.02	0.60
1:A:211:LYS:CE	1:B:177:ARG:HH12	2.15	0.60
1:A:153:VAL:HG11	1:C:204:THR:HG21	1.84	0.60
1:A:78:ASN:O	1:A:78:ASN:OD1	2.19	0.60
1:D:65:ARG:NH1	1:D:118:SER:HA	2.17	0.60
1:A:32:PHE:O	1:A:192:SER:HA	2.00	0.59
1:F:61:GLY:HA3	1:F:123:SER:OG	2.02	0.59
1:D:167:TYR:CD1	1:D:168:PRO:HA	2.36	0.59
1:A:35:MET:O	1:B:159:ILE:HG12	2.01	0.59
1:E:194:ASP:OD1	1:E:196:ARG:HD3	2.02	0.59
1:D:82:ASP:OD2	1:D:87:VAL:HG23	2.02	0.59
1:A:204:THR:O	1:A:208:VAL:HB	2.02	0.59
1:A:26:LYS:HZ3	1:B:26:LYS:NZ	1.99	0.59
1:B:74:TYR:HD2	1:B:206:PHE:HD1	1.50	0.59
1:E:26:LYS:HE3	1:F:26:LYS:HZ3	1.68	0.59
1:E:194:ASP:OD2	1:E:196:ARG:NH1	2.34	0.59
1:E:41:THR:HA	1:E:44:VAL:HG12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:HA	1:A:191:LEU:O	2.03	0.58
1:A:35:MET:HG3	1:A:190:SER:HB3	1.84	0.58
1:B:196:ARG:O	1:C:15:ARG:NH2	2.35	0.58
1:C:62:PHE:CZ	1:C:66:ILE:HD11	2.38	0.58
1:D:123:SER:HA	1:D:126:ILE:HG13	1.85	0.58
1:C:150:ILE:HG22	1:C:173:LEU:HB3	1.85	0.58
1:F:44:VAL:HA	1:F:47:LEU:HD12	1.85	0.58
1:F:81:TYR:CD1	1:F:197:LEU:HD11	2.36	0.58
1:F:181:ARG:O	1:F:182:GLU:HB2	2.03	0.58
1:F:31:HIS:NE2	1:F:165:ILE:HG13	2.19	0.58
1:D:14:LEU:O	1:D:18:ILE:HG23	2.04	0.58
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.36	0.58
1:D:140:LEU:HD12	1:D:144:GLN:HE22	1.67	0.58
1:A:8:ILE:O	1:A:9:LEU:HB2	2.03	0.58
1:C:57:VAL:HG11	1:C:119:MET:CE	2.34	0.58
1:C:53:ARG:CZ	1:D:69:SER:CB	2.81	0.58
1:B:198:ILE:HG22	1:B:202:VAL:HG13	1.85	0.58
1:E:6:GLU:O	1:E:7:GLU:HB2	2.04	0.58
1:F:70:ILE:HD13	1:F:210:LEU:HD12	1.84	0.57
1:D:79:ALA:O	1:D:170:VAL:HB	2.04	0.57
1:D:67:VAL:HG23	1:D:68:PRO:HD3	1.86	0.57
1:E:39:ASP:HA	1:E:186:TYR:HD1	1.69	0.57
1:D:7:GLU:HG2	1:D:8:ILE:H	1.69	0.57
1:E:158:GLY:O	1:E:176:HIS:HB3	2.05	0.57
1:D:86:ARG:HH22	1:E:11:MET:CB	2.16	0.57
1:E:182:GLU:HG3	1:E:184:ARG:H	1.69	0.57
1:D:152:ASN:HA	1:D:175:VAL:HB	1.86	0.57
1:B:176:HIS:CD2	1:B:188:TYR:O	2.54	0.57
1:A:19:PHE:HA	1:C:196:ARG:HB3	1.87	0.57
1:B:41:THR:HG22	1:B:185:LYS:HB2	1.85	0.57
1:B:28:ILE:O	1:B:30:PRO:HD3	2.05	0.57
1:B:37:GLU:CB	1:C:159:ILE:HD11	2.31	0.57
1:D:16:ARG:HH12	1:F:86:ARG:HD2	1.70	0.57
1:F:81:TYR:HA	1:F:82:ASP:OD2	2.04	0.56
1:B:89:ILE:H	1:C:8:ILE:HG23	1.69	0.56
1:C:32:PHE:O	1:C:192:SER:HA	2.05	0.56
1:E:72:LYS:HA	1:E:94:TYR:OH	2.05	0.56
1:F:194:ASP:OD2	1:F:197:LEU:HD12	2.04	0.56
1:C:29:MET:SD	1:C:194:ASP:HB2	2.45	0.56
1:C:143:VAL:O	1:C:143:VAL:HG12	2.05	0.56
1:B:56:LYS:HB3	1:B:57:VAL:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ARG:HG3	1:E:15:ARG:HH11	1.71	0.56
1:A:102:THR:HG21	1:A:107:ASN:ND2	2.17	0.56
1:C:38:VAL:CG1	1:C:211:LYS:HG3	2.35	0.56
1:E:86:ARG:C	1:E:87:VAL:HG22	2.25	0.56
1:B:30:PRO:HA	1:C:26:LYS:HE3	1.87	0.56
1:D:50:ALA:HA	1:D:53:ARG:HG2	1.87	0.56
1:A:162:THR:HG22	1:C:33:THR:HB	1.87	0.56
1:E:83:GLU:CG	1:E:84:THR:H	2.02	0.56
1:C:53:ARG:HH21	1:D:66:ILE:HA	1.71	0.56
1:A:152:ASN:OD1	1:A:155:THR:HG22	2.04	0.56
1:E:100:VAL:HG22	1:E:101:ASP:N	2.20	0.56
1:B:181:ARG:C	1:B:183:GLY:HA2	2.26	0.56
1:A:33:THR:H	1:B:162:THR:HG23	1.71	0.56
1:C:8:ILE:O	1:C:9:LEU:HD12	2.06	0.55
1:B:33:THR:HB	1:B:192:SER:HA	1.88	0.55
1:D:162:THR:HG22	1:F:33:THR:HB	1.88	0.55
1:D:204:THR:HG21	1:E:153:VAL:HG12	1.88	0.55
1:B:189:LEU:HD13	1:B:210:LEU:HD21	1.88	0.55
1:B:143:VAL:HG12	1:B:143:VAL:O	2.07	0.55
1:F:43:MET:O	1:F:46:ILE:N	2.39	0.55
1:D:140:LEU:CD1	1:D:144:GLN:HE22	2.19	0.55
1:C:149:THR:HG23	1:C:172:ILE:HG13	1.89	0.55
1:F:12:HIS:CD2	1:F:13:GLY:N	2.72	0.55
1:F:38:VAL:CG1	1:F:211:LYS:HG3	2.35	0.55
1:C:17:ILE:HG23	1:C:21:LYS:HE3	1.89	0.55
1:C:16:ARG:HB3	1:C:16:ARG:HH11	1.71	0.55
1:C:26:LYS:HB3	1:C:31:HIS:HE1	1.72	0.55
1:D:197:LEU:O	1:E:15:ARG:NH2	2.40	0.55
1:D:16:ARG:NH1	1:F:86:ARG:HD2	2.22	0.55
1:E:210:LEU:HG	1:E:214:ILE:HD11	1.89	0.55
1:B:50:ALA:O	1:B:54:ASN:HB2	2.07	0.55
1:D:7:GLU:HG2	1:D:8:ILE:N	2.21	0.55
1:F:194:ASP:O	1:F:198:ILE:HB	2.07	0.55
1:A:56:LYS:O	1:A:57:VAL:HG22	2.07	0.55
1:F:70:ILE:HD13	1:F:210:LEU:HA	1.88	0.55
1:E:98:ILE:O	1:E:98:ILE:HG13	2.07	0.54
1:D:33:THR:HA	1:D:191:LEU:O	2.07	0.54
1:F:74:TYR:CE2	1:F:206:PHE:HA	2.43	0.54
1:F:61:GLY:O	1:F:122:ILE:HD11	2.06	0.54
1:A:211:LYS:O	1:A:215:GLU:HB2	2.07	0.54
1:D:156:ILE:O	1:D:156:ILE:HG22	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:THR:CG2	1:B:185:LYS:H	2.21	0.54
1:D:181:ARG:HD3	1:F:181:ARG:HH11	1.71	0.54
1:D:123:SER:HA	1:D:126:ILE:HG12	1.89	0.54
1:D:161:SER:HB2	1:F:33:THR:O	2.08	0.54
1:B:12:HIS:CE1	1:B:15:ARG:H	2.26	0.54
1:B:42:SER:O	1:B:46:ILE:HB	2.07	0.54
1:B:12:HIS:O	1:B:16:ARG:HB2	2.08	0.54
1:C:83:GLU:C	1:C:85:ARG:N	2.60	0.54
1:B:27:GLN:HE21	1:B:28:ILE:HD11	1.73	0.54
1:B:41:THR:HA	1:B:44:VAL:HG12	1.90	0.54
1:C:64:ALA:HA	1:C:67:VAL:HG12	1.89	0.54
1:B:178:ILE:HD12	1:B:178:ILE:H	1.73	0.53
1:C:102:THR:O	1:C:104:ASP:N	2.42	0.53
1:D:35:MET:O	1:E:159:ILE:N	2.38	0.53
1:B:30:PRO:HD2	1:B:196:ARG:HD2	1.91	0.53
1:A:23:THR:O	1:A:27:GLN:HB2	2.09	0.53
1:F:193:CYS:HB2	1:F:198:ILE:CD1	2.38	0.53
1:E:98:ILE:HD11	1:E:109:PHE:CZ	2.44	0.53
1:D:9:LEU:H	1:F:88:TYR:HB2	1.73	0.53
1:B:39:ASP:OD2	1:B:186:TYR:HE1	1.91	0.53
1:D:91:LYS:HD3	1:D:93:TYR:HE1	1.74	0.53
1:B:80:ILE:HG21	1:B:91:LYS:HE3	1.90	0.53
1:C:12:HIS:O	1:C:16:ARG:HB2	2.09	0.53
1:F:12:HIS:CG	1:F:13:GLY:H	2.24	0.53
1:A:176:HIS:HE1	1:A:190:SER:OG	1.92	0.53
1:A:196:ARG:HD3	1:B:23:THR:HG1	1.73	0.53
1:E:177:ARG:HG2	1:E:178:ILE:N	2.24	0.53
1:A:126:ILE:HG13	1:A:127:SER:N	2.24	0.53
1:D:9:LEU:HB2	1:F:88:TYR:CD1	2.44	0.53
1:E:34:VAL:HG13	1:E:207:ILE:HD11	1.91	0.53
1:B:102:THR:HB	1:B:103:PRO:HD2	1.91	0.53
1:F:84:THR:HG23	1:F:87:VAL:CG2	2.24	0.52
1:A:44:VAL:HG11	1:A:185:LYS:NZ	2.24	0.52
1:B:14:LEU:O	1:B:18:ILE:HG22	2.10	0.52
1:E:126:ILE:HD12	1:E:127:SER:N	2.23	0.52
1:D:12:HIS:O	1:D:16:ARG:HB2	2.10	0.52
1:B:92:LYS:HE2	1:C:7:GLU:HG2	1.90	0.52
1:B:27:GLN:HE21	1:B:28:ILE:CD1	2.22	0.52
1:D:195:HIS:CB	1:E:164:ILE:HD11	2.39	0.52
1:B:100:VAL:HG22	1:B:101:ASP:H	1.74	0.52
1:E:15:ARG:HG3	1:E:15:ARG:NH1	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:MET:SD	1:F:194:ASP:HB2	2.49	0.52
1:C:179:LEU:O	1:C:180:GLU:CB	2.51	0.52
1:D:65:ARG:HG3	1:D:119:MET:HG3	1.92	0.52
1:A:74:TYR:OH	1:A:205:ARG:HG2	2.10	0.52
1:A:31:HIS:CE1	1:A:165:ILE:HD12	2.45	0.52
1:D:176:HIS:HE1	1:D:190:SER:OG	1.93	0.52
1:C:129:LYS:HA	1:C:132:ARG:HH11	1.75	0.52
1:E:102:THR:HB	1:E:103:PRO:HD2	1.92	0.52
1:A:48:ASP:O	1:A:51:LYS:HD3	2.09	0.52
1:D:32:PHE:O	1:D:192:SER:HA	2.10	0.51
1:D:78:ASN:OD1	1:D:78:ASN:O	2.27	0.51
1:B:34:VAL:HG21	1:B:204:THR:HG23	1.92	0.51
1:C:117:LYS:HE2	1:C:125:GLU:OE2	2.09	0.51
1:E:88:TYR:OH	1:E:194:ASP:OD2	2.28	0.51
1:E:205:ARG:HH11	1:E:205:ARG:HB2	1.76	0.51
1:A:120:VAL:HG13	1:A:121:GLU:N	2.25	0.51
1:F:213:VAL:O	1:F:213:VAL:HG12	2.11	0.51
1:B:31:HIS:H	1:C:26:LYS:HE3	1.75	0.51
1:F:167:TYR:CG	1:F:168:PRO:HA	2.45	0.51
1:C:205:ARG:HB2	1:C:205:ARG:HH11	1.74	0.51
1:D:74:TYR:CE2	1:D:206:PHE:HA	2.45	0.51
1:E:41:THR:HG22	1:E:185:LYS:HG3	1.93	0.51
1:A:84:THR:C	1:A:85:ARG:O	2.47	0.51
1:D:156:ILE:CG2	1:F:205:ARG:HA	2.41	0.51
1:A:125:GLU:O	1:A:129:LYS:HD2	2.11	0.51
1:B:165:ILE:HG22	1:B:171:ALA:C	2.31	0.51
1:E:167:TYR:CG	1:E:168:PRO:HA	2.46	0.51
1:E:90:LEU:CG	1:F:9:LEU:HD13	2.36	0.50
1:B:12:HIS:CD2	1:B:13:GLY:H	2.28	0.50
1:D:98:ILE:CD1	1:D:126:ILE:HG22	2.40	0.50
1:F:107:ASN:ND2	1:F:108:VAL:H	2.10	0.50
1:D:194:ASP:OD2	1:D:196:ARG:NH1	2.44	0.50
1:C:47:LEU:HD12	1:C:47:LEU:H	1.75	0.50
1:C:64:ALA:HB3	1:C:122:ILE:CD1	2.41	0.50
1:A:216:ASP:OD1	1:A:218:ASN:HB3	2.11	0.50
1:E:150:ILE:HG22	1:E:173:LEU:HD22	1.94	0.50
1:A:153:VAL:HG23	1:A:157:GLY:O	2.11	0.50
1:E:10:GLU:HG3	1:E:11:MET:N	2.26	0.50
1:F:51:LYS:HD2	1:F:55:ARG:HG2	1.92	0.50
1:E:74:TYR:CD2	1:E:206:PHE:HD1	2.29	0.50
1:F:178:ILE:HD13	1:F:185:LYS:HE3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:HIS:CE1	1:F:15:ARG:H	2.30	0.50
1:B:195:HIS:O	1:C:22:MET:HG3	2.12	0.50
1:A:95:ASN:HB3	1:A:113:ASP:N	2.26	0.50
1:B:83:GLU:CD	1:B:83:GLU:N	2.62	0.50
1:A:67:VAL:HG21	1:A:150:ILE:HD11	1.93	0.50
1:C:12:HIS:CG	1:C:13:GLY:H	2.30	0.50
1:C:12:HIS:O	1:C:16:ARG:CG	2.60	0.50
1:D:71:LEU:O	1:D:75:PRO:HA	2.12	0.50
1:F:40:VAL:HG11	1:F:187:MET:HB3	1.94	0.50
1:A:26:LYS:HE2	1:A:31:HIS:HB2	1.94	0.49
1:F:29:MET:CE	1:F:169:GLU:O	2.60	0.49
1:F:10:GLU:HG2	1:F:11:MET:H	1.76	0.49
1:A:77:LEU:HD12	1:A:198:ILE:HD12	1.94	0.49
1:C:47:LEU:O	1:C:51:LYS:HB2	2.12	0.49
1:F:81:TYR:HD1	1:F:197:LEU:HD11	1.76	0.49
1:A:95:ASN:HB3	1:A:112:LYS:CA	2.38	0.49
1:B:13:GLY:O	1:B:17:ILE:HG12	2.11	0.49
1:F:154:GLY:HA3	1:F:176:HIS:HA	1.94	0.49
1:B:10:GLU:HG3	1:B:11:MET:H	1.77	0.49
1:C:93:TYR:OH	1:C:145:ASP:OD1	2.22	0.49
1:A:217:PRO:C	1:A:219:ALA:H	2.16	0.49
1:D:81:TYR:HB2	1:D:88:TYR:HE2	1.77	0.49
1:A:79:ALA:HB1	1:A:89:ILE:O	2.12	0.49
1:E:88:TYR:CE2	1:E:197:LEU:HG	2.47	0.49
1:A:57:VAL:HA	1:A:123:SER:CB	2.42	0.49
1:E:88:TYR:HB2	1:F:9:LEU:O	2.12	0.49
1:F:28:ILE:HD11	1:F:167:TYR:CZ	2.47	0.49
1:A:69:SER:O	1:A:72:LYS:HB3	2.12	0.49
1:C:56:LYS:CE	1:C:124:ALA:HA	2.43	0.49
1:C:56:LYS:HE2	1:C:124:ALA:HA	1.95	0.49
1:F:211:LYS:O	1:F:215:GLU:HB2	2.13	0.49
1:B:12:HIS:CD2	1:B:13:GLY:N	2.81	0.49
1:F:158:GLY:O	1:F:176:HIS:HB3	2.13	0.49
1:D:204:THR:HG21	1:E:153:VAL:CG1	2.42	0.49
1:D:95:ASN:HB3	1:D:113:ASP:H	1.78	0.49
1:C:40:VAL:O	1:C:40:VAL:CG2	2.61	0.48
1:B:149:THR:HG23	1:B:169:GLU:OE1	2.13	0.48
1:C:87:VAL:C	1:C:88:TYR:HD2	2.17	0.48
1:D:8:ILE:HG23	1:F:89:ILE:H	1.79	0.48
1:D:126:ILE:HD12	1:D:127:SER:N	2.28	0.48
1:F:143:VAL:HG12	1:F:143:VAL:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:MET:HB2	1:C:196:ARG:HG2	1.95	0.48
1:B:199:ASP:O	1:B:202:VAL:HG12	2.13	0.48
1:B:139:GLN:HB3	1:B:141:ASP:HB3	1.95	0.48
1:C:12:HIS:CG	1:C:13:GLY:N	2.81	0.48
1:D:26:LYS:HE3	1:E:26:LYS:HE2	1.96	0.48
1:C:97:GLY:HA2	1:C:109:PHE:O	2.13	0.48
1:A:195:HIS:HB3	1:B:164:ILE:HD11	1.95	0.48
1:C:112:LYS:HD2	1:C:112:LYS:H	1.77	0.48
1:C:7:GLU:O	1:C:7:GLU:HG3	2.13	0.48
1:E:14:LEU:O	1:E:18:ILE:HG22	2.12	0.48
1:E:21:LYS:HE2	1:E:166:ASN:HD21	1.78	0.48
1:E:81:TYR:HD1	1:E:88:TYR:CZ	2.32	0.48
1:F:172:ILE:HG12	1:F:173:LEU:N	2.29	0.48
1:A:118:SER:O	1:A:120:VAL:N	2.46	0.48
1:B:111:ILE:HG13	1:B:126:ILE:HG22	1.95	0.48
1:E:108:VAL:O	1:E:143:VAL:HG13	2.13	0.48
1:E:88:TYR:CZ	1:E:197:LEU:HG	2.49	0.48
1:E:89:ILE:HA	1:F:8:ILE:HA	1.96	0.48
1:A:143:VAL:O	1:A:143:VAL:HG12	2.14	0.48
1:D:12:HIS:CG	1:D:13:GLY:N	2.82	0.48
1:D:7:GLU:C	1:D:8:ILE:HG13	2.34	0.48
1:D:26:LYS:NZ	1:F:26:LYS:NZ	2.62	0.48
1:D:11:MET:HB2	1:D:16:ARG:HH11	1.78	0.48
1:E:143:VAL:O	1:E:143:VAL:HG12	2.14	0.48
1:A:132:ARG:NH2	1:A:142:GLU:OE1	2.34	0.48
1:A:112:LYS:O	1:A:113:ASP:C	2.52	0.48
1:A:81:TYR:CD2	1:A:82:ASP:N	2.82	0.48
1:A:78:ASN:ND2	1:A:94:TYR:CD1	2.82	0.48
1:D:31:HIS:CE1	1:D:165:ILE:HD12	2.49	0.47
1:F:62:PHE:HZ	1:F:217:PRO:HB3	1.79	0.47
1:D:197:LEU:C	1:D:197:LEU:HD12	2.34	0.47
1:A:57:VAL:O	1:A:57:VAL:HG23	2.14	0.47
1:A:152:ASN:HD22	1:A:175:VAL:HG11	1.79	0.47
1:F:216:ASP:OD2	1:F:219:ALA:HB3	2.13	0.47
1:B:133:ALA:HB2	1:B:138:LEU:HD22	1.95	0.47
1:C:216:ASP:OD2	1:C:219:ALA:HB2	2.13	0.47
1:A:153:VAL:CG1	1:C:204:THR:HG21	2.44	0.47
1:B:56:LYS:CB	1:B:57:VAL:HA	2.45	0.47
1:B:86:ARG:O	1:B:87:VAL:CG2	2.55	0.47
1:E:30:PRO:CG	1:E:196:ARG:HD2	2.45	0.47
1:A:152:ASN:HD22	1:A:175:VAL:CG1	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLU:HG2	1:F:158:GLY:HA2	1.95	0.47
1:F:80:ILE:HG22	1:F:89:ILE:HG21	1.96	0.47
1:D:26:LYS:HD2	1:D:164:ILE:HD12	1.97	0.47
1:A:76:TYR:HD1	1:A:197:LEU:HD13	1.80	0.47
1:D:97:GLY:HA2	1:D:109:PHE:O	2.15	0.47
1:A:84:THR:HB	1:A:87:VAL:HG23	1.97	0.47
1:F:62:PHE:HD1	1:F:119:MET:CE	2.27	0.47
1:A:95:ASN:HB2	1:A:110:VAL:HG12	1.97	0.47
1:C:128:ASP:O	1:C:132:ARG:HD3	2.15	0.47
1:F:123:SER:O	1:F:126:ILE:HG13	2.15	0.47
1:D:47:LEU:O	1:D:51:LYS:N	2.47	0.47
1:F:193:CYS:HB2	1:F:198:ILE:HD13	1.94	0.47
1:B:189:LEU:CD1	1:B:210:LEU:HD21	2.44	0.47
1:C:152:ASN:HA	1:C:175:VAL:HB	1.96	0.47
1:E:134:ARG:C	1:E:136:ASN:H	2.16	0.47
1:A:11:MET:HB2	1:A:16:ARG:NH1	2.29	0.47
1:B:11:MET:HG3	1:B:15:ARG:HB3	1.97	0.47
1:B:12:HIS:CG	1:B:13:GLY:N	2.81	0.47
1:D:195:HIS:O	1:D:195:HIS:ND1	2.46	0.47
1:E:61:GLY:HA3	1:E:123:SER:OG	2.15	0.47
1:D:196:ARG:HD3	1:E:23:THR:OG1	2.15	0.47
1:A:217:PRO:C	1:A:219:ALA:N	2.69	0.47
1:F:159:ILE:HG23	1:F:188:TYR:CD2	2.50	0.46
1:C:129:LYS:CG	1:C:132:ARG:HH12	2.28	0.46
1:E:132:ARG:O	1:E:135:GLU:N	2.47	0.46
1:F:108:VAL:O	1:F:143:VAL:HG13	2.15	0.46
1:A:79:ALA:HB2	1:A:90:LEU:HA	1.97	0.46
1:D:200:GLY:O	1:D:203:ALA:HB3	2.15	0.46
1:F:154:GLY:HA3	1:F:176:HIS:CA	2.45	0.46
1:B:86:ARG:CZ	1:B:86:ARG:HA	2.45	0.46
1:A:95:ASN:HB2	1:A:112:LYS:HA	1.95	0.46
1:A:85:ARG:O	1:A:86:ARG:CB	2.62	0.46
1:D:11:MET:HB2	1:D:16:ARG:NH1	2.30	0.46
1:E:109:PHE:HB3	1:E:138:LEU:HD21	1.96	0.46
1:D:201:ALA:C	1:D:203:ALA:N	2.69	0.46
1:C:80:ILE:HA	1:C:168:PRO:O	2.16	0.46
1:F:39:ASP:HA	1:F:186:TYR:CE1	2.50	0.46
1:C:66:ILE:HG22	1:C:70:ILE:HD11	1.97	0.46
1:C:55:ARG:HA	1:C:56:LYS:HA	1.71	0.46
1:C:80:ILE:O	1:C:88:TYR:O	2.34	0.46
1:E:83:GLU:CG	1:E:84:THR:N	2.66	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:O	1:A:65:ARG:HD3	2.14	0.46
1:D:161:SER:HB3	1:F:34:VAL:HA	1.98	0.46
1:F:55:ARG:HA	1:F:56:LYS:HA	1.61	0.46
1:E:169:GLU:H	1:E:169:GLU:HG3	1.59	0.46
1:F:83:GLU:C	1:F:85:ARG:H	2.19	0.46
1:E:201:ALA:H	1:F:106:LEU:HD13	1.81	0.46
1:E:22:MET:SD	1:E:164:ILE:HD12	2.56	0.46
1:E:211:LYS:HG2	1:E:215:GLU:OE2	2.15	0.46
1:A:120:VAL:HG13	1:A:121:GLU:H	1.81	0.46
1:D:40:VAL:O	1:D:44:VAL:HG23	2.16	0.46
1:A:162:THR:CG2	1:C:33:THR:HB	2.45	0.46
1:D:111:ILE:H	1:D:111:ILE:HG13	1.49	0.46
1:A:67:VAL:N	1:A:68:PRO:HD2	2.31	0.46
1:A:135:GLU:C	1:A:137:LYS:H	2.19	0.46
1:C:82:ASP:HB2	1:C:87:VAL:HG23	1.96	0.45
1:A:54:ASN:O	1:A:55:ARG:CB	2.60	0.45
1:D:204:THR:O	1:D:207:ILE:N	2.49	0.45
1:D:98:ILE:HD12	1:D:126:ILE:HG22	1.97	0.45
1:D:33:THR:HB	1:E:162:THR:HG22	1.98	0.45
1:A:54:ASN:HD22	1:A:55:ARG:N	2.13	0.45
1:E:195:HIS:CE1	1:E:200:GLY:H	2.34	0.45
1:A:7:GLU:HG2	1:A:8:ILE:H	1.82	0.45
1:F:67:VAL:HG13	1:F:68:PRO:HD3	1.98	0.45
1:F:29:MET:HE2	1:F:167:TYR:CD1	2.51	0.45
1:D:210:LEU:O	1:D:214:ILE:HG13	2.17	0.45
1:B:208:VAL:CG2	1:C:157:GLY:HA3	2.44	0.45
1:E:25:ALA:HB2	1:E:167:TYR:HB2	1.98	0.45
1:D:12:HIS:O	1:D:16:ARG:HB3	2.15	0.45
1:E:31:HIS:NE2	1:E:165:ILE:HG12	2.31	0.45
1:F:8:ILE:HG22	1:F:9:LEU:N	2.32	0.45
1:F:38:VAL:O	1:F:186:TYR:HD1	1.99	0.45
1:B:36:GLU:OE2	1:B:211:LYS:HD3	2.16	0.45
1:B:7:GLU:OE1	1:B:9:LEU:HD22	2.16	0.45
1:B:182:GLU:N	1:B:183:GLY:CA	2.75	0.45
1:F:107:ASN:HD22	1:F:108:VAL:H	1.64	0.45
1:F:70:ILE:HG22	1:F:206:PHE:CE1	2.51	0.45
1:E:195:HIS:ND1	1:E:195:HIS:O	2.50	0.45
1:C:144:GLN:O	1:C:145:ASP:HB3	2.15	0.45
1:D:139:GLN:HB2	1:D:142:GLU:HG3	1.98	0.45
1:C:161:SER:H	1:C:176:HIS:CE1	2.33	0.45
1:F:182:GLU:HA	1:F:183:GLY:HA2	1.69	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HA	1:B:189:LEU:HD23	1.74	0.45
1:A:112:LYS:HE2	1:A:144:GLN:O	2.17	0.44
1:C:40:VAL:O	1:C:44:VAL:N	2.40	0.44
1:C:69:SER:HA	1:C:72:LYS:CD	2.47	0.44
1:D:81:TYR:HB2	1:D:88:TYR:CE2	2.51	0.44
1:B:89:ILE:CB	1:C:8:ILE:HG12	2.31	0.44
1:D:40:VAL:HG23	1:D:185:LYS:HB3	1.98	0.44
1:A:22:MET:HG3	1:C:195:HIS:O	2.18	0.44
1:E:179:LEU:HD23	1:E:187:MET:HA	1.98	0.44
1:E:182:GLU:HG3	1:E:184:ARG:N	2.33	0.44
1:A:208:VAL:HG21	1:B:156:ILE:O	2.17	0.44
1:B:199:ASP:HB3	1:C:106:LEU:HD13	1.99	0.44
1:B:35:MET:SD	1:B:190:SER:HB3	2.57	0.44
1:C:113:ASP:HB3	1:C:116:ARG:CG	2.47	0.44
1:E:194:ASP:CG	1:E:196:ARG:HH11	2.21	0.44
1:F:181:ARG:HB2	1:F:186:TYR:CD2	2.42	0.44
1:C:84:THR:HG23	1:C:87:VAL:CG2	2.20	0.44
1:F:12:HIS:O	1:F:16:ARG:HB2	2.18	0.44
1:F:144:GLN:O	1:F:145:ASP:HB3	2.17	0.44
1:A:135:GLU:C	1:A:137:LYS:N	2.71	0.44
1:A:80:ILE:HG22	1:A:169:GLU:HA	2.00	0.44
1:E:178:ILE:CD1	1:E:178:ILE:H	2.13	0.44
1:C:43:MET:O	1:C:46:ILE:N	2.49	0.44
1:D:30:PRO:CG	1:D:196:ARG:HG3	2.48	0.44
1:F:62:PHE:CZ	1:F:66:ILE:HD11	2.53	0.44
1:A:135:GLU:O	1:A:137:LYS:N	2.51	0.44
1:C:165:ILE:HD11	1:C:193:CYS:CA	2.48	0.44
1:B:88:TYR:CE2	1:B:197:LEU:HG	2.53	0.43
1:D:111:ILE:HG22	1:D:125:GLU:OE2	2.18	0.43
1:F:69:SER:O	1:F:72:LYS:HB2	2.18	0.43
1:A:12:HIS:CE1	1:A:14:LEU:HB3	2.53	0.43
1:B:177:ARG:HE	1:B:179:LEU:HD23	1.83	0.43
1:E:121:GLU:HG3	1:E:121:GLU:H	1.61	0.43
1:F:29:MET:HE2	1:F:167:TYR:CE1	2.54	0.43
1:E:32:PHE:CB	1:E:195:HIS:CD2	3.01	0.43
1:B:86:ARG:NH2	1:C:11:MET:HB2	2.33	0.43
1:F:31:HIS:HE1	1:F:164:ILE:HG23	1.83	0.43
1:F:32:PHE:O	1:F:192:SER:HA	2.18	0.43
1:A:159:ILE:O	1:A:188:TYR:HB2	2.18	0.43
1:D:11:MET:CB	1:D:16:ARG:HH11	2.31	0.43
1:F:160:MET:HA	1:F:176:HIS:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:THR:HA	1:F:191:LEU:O	2.18	0.43
1:D:160:MET:HB3	1:F:35:MET:HG2	1.99	0.43
1:D:70:ILE:HG13	1:D:70:ILE:H	1.70	0.43
1:A:47:LEU:HD22	1:A:57:VAL:O	2.19	0.43
1:C:57:VAL:HG21	1:C:119:MET:HE3	2.01	0.43
1:E:159:ILE:O	1:E:188:TYR:HB2	2.18	0.43
1:F:100:VAL:HG11	1:F:109:PHE:CE2	2.54	0.43
1:D:26:LYS:HD2	1:D:164:ILE:CD1	2.49	0.43
1:B:198:ILE:CG2	1:B:202:VAL:HG13	2.47	0.43
1:F:162:THR:O	1:F:162:THR:HG23	2.19	0.42
1:A:97:GLY:HA2	1:A:109:PHE:O	2.19	0.42
1:A:57:VAL:HA	1:A:123:SER:HB2	2.00	0.42
1:F:61:GLY:O	1:F:64:ALA:HB3	2.19	0.42
1:B:70:ILE:H	1:B:70:ILE:HG13	1.62	0.42
1:D:68:PRO:HB2	1:D:115:ASP:HB3	2.01	0.42
1:A:167:TYR:CG	1:A:168:PRO:HA	2.54	0.42
1:A:81:TYR:HD2	1:A:82:ASP:H	1.66	0.42
1:F:117:LYS:HE2	1:F:125:GLU:OE2	2.18	0.42
1:B:165:ILE:H	1:B:165:ILE:HG12	1.63	0.42
1:D:26:LYS:NZ	1:F:26:LYS:HZ3	2.17	0.42
1:B:74:TYR:CE2	1:B:206:PHE:HA	2.53	0.42
1:E:211:LYS:HA	1:E:214:ILE:HD12	2.01	0.42
1:E:21:LYS:HE2	1:E:166:ASN:ND2	2.34	0.42
1:D:63:LEU:O	1:D:66:ILE:HG13	2.19	0.42
1:F:64:ALA:HB3	1:F:122:ILE:CD1	2.50	0.42
1:A:93:TYR:O	1:A:93:TYR:CD2	2.73	0.42
1:A:44:VAL:HG11	1:A:185:LYS:HZ1	1.84	0.42
1:B:181:ARG:HG3	1:B:186:TYR:HD2	1.85	0.42
1:D:112:LYS:O	1:D:113:ASP:C	2.58	0.42
1:A:34:VAL:HG12	1:B:161:SER:HB3	2.00	0.42
1:E:28:ILE:HG21	1:E:167:TYR:OH	2.19	0.42
1:F:62:PHE:CE2	1:F:66:ILE:HD11	2.54	0.42
1:A:38:VAL:O	1:A:186:TYR:HA	2.19	0.42
1:B:165:ILE:HA	1:B:172:ILE:HB	2.01	0.42
1:A:100:VAL:HG21	1:A:109:PHE:CE2	2.54	0.42
1:E:33:THR:HB	1:E:192:SER:HA	2.01	0.42
1:F:76:TYR:HD1	1:F:197:LEU:O	2.02	0.42
1:D:26:LYS:CE	1:F:26:LYS:HZ2	2.29	0.42
1:B:181:ARG:HG3	1:B:186:TYR:CD2	2.55	0.42
1:C:158:GLY:O	1:C:177:ARG:HG2	2.20	0.42
1:C:129:LYS:O	1:C:133:ALA:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:HD2	1:C:112:LYS:N	2.34	0.42
1:D:100:VAL:HG21	1:D:109:PHE:CE2	2.55	0.42
1:B:43:MET:SD	1:B:62:PHE:CD2	3.13	0.42
1:C:167:TYR:HA	1:C:168:PRO:HA	1.78	0.42
1:E:79:ALA:HB2	1:E:90:LEU:HD22	2.02	0.42
1:C:109:PHE:CE1	1:C:129:LYS:HB2	2.55	0.42
1:E:205:ARG:NH1	1:E:205:ARG:HB2	2.34	0.42
1:F:44:VAL:HG11	1:F:185:LYS:HG3	2.02	0.42
1:E:66:ILE:O	1:E:70:ILE:HG13	2.20	0.42
1:F:18:ILE:HD13	1:F:18:ILE:HA	1.91	0.42
1:D:149:THR:O	1:D:172:ILE:HA	2.19	0.42
1:E:196:ARG:O	1:F:15:ARG:NH2	2.52	0.42
1:E:26:LYS:HZ1	1:F:26:LYS:NZ	2.15	0.42
1:B:144:GLN:HB3	1:B:145:ASP:H	1.76	0.42
1:A:26:LYS:HZ1	1:B:26:LYS:CE	2.12	0.41
1:C:82:ASP:CG	1:C:87:VAL:HG23	2.40	0.41
1:D:159:ILE:HA	1:D:176:HIS:HB3	2.02	0.41
1:C:85:ARG:HB3	1:C:86:ARG:H	1.77	0.41
1:A:89:ILE:O	1:A:89:ILE:HG13	2.19	0.41
1:C:24:LYS:HE3	1:C:167:TYR:CE2	2.51	0.41
1:D:88:TYR:CE1	1:D:197:LEU:CD2	3.03	0.41
1:D:214:ILE:H	1:D:214:ILE:HG13	1.64	0.41
1:C:40:VAL:O	1:C:40:VAL:HG22	2.20	0.41
1:A:26:LYS:HZ3	1:B:26:LYS:HZ1	1.63	0.41
1:B:86:ARG:C	1:B:87:VAL:CG2	2.89	0.41
1:C:64:ALA:HB3	1:C:122:ILE:HD11	2.01	0.41
1:F:71:LEU:HD13	1:F:78:ASN:OD1	2.20	0.41
1:A:59:VAL:O	1:A:63:LEU:HD13	2.20	0.41
1:E:161:SER:O	1:E:163:PRO:HD3	2.20	0.41
1:A:166:ASN:N	1:A:172:ILE:HD12	2.25	0.41
1:C:113:ASP:HB3	1:C:116:ARG:HG3	2.01	0.41
1:D:83:GLU:HB3	1:D:84:THR:H	1.71	0.41
1:D:19:PHE:CE2	1:F:196:ARG:HD2	2.55	0.41
1:A:15:ARG:NH1	1:C:196:ARG:O	2.44	0.41
1:B:70:ILE:HB	1:B:206:PHE:CE1	2.56	0.41
1:E:100:VAL:CG2	1:E:101:ASP:N	2.82	0.41
1:C:165:ILE:HD11	1:C:193:CYS:C	2.41	0.41
1:B:167:TYR:CD1	1:B:168:PRO:HA	2.56	0.41
1:A:26:LYS:CE	1:A:31:HIS:HB2	2.50	0.41
1:F:83:GLU:C	1:F:85:ARG:N	2.73	0.41
1:C:19:PHE:C	1:C:19:PHE:CD2	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:VAL:HG23	1:F:161:SER:HB3	2.02	0.41
1:F:100:VAL:HG11	1:F:109:PHE:HE2	1.86	0.41
1:F:193:CYS:HB2	1:F:198:ILE:HD12	2.02	0.41
1:D:31:HIS:CD2	1:D:164:ILE:HD13	2.55	0.41
1:A:126:ILE:HG13	1:A:127:SER:H	1.85	0.41
1:B:88:TYR:OH	1:B:194:ASP:OD2	2.38	0.41
1:D:193:CYS:HB2	1:D:198:ILE:HG13	2.01	0.41
1:C:205:ARG:CB	1:C:205:ARG:HH11	2.34	0.41
1:C:204:THR:HA	1:C:207:ILE:HG22	2.03	0.41
1:A:34:VAL:O	1:A:190:SER:HA	2.20	0.41
1:E:29:MET:SD	1:E:165:ILE:CD1	3.05	0.41
1:F:65:ARG:NE	1:F:118:SER:HA	2.36	0.41
1:E:56:LYS:CB	1:E:57:VAL:HA	2.21	0.40
1:F:181:ARG:CB	1:F:186:TYR:HD2	2.27	0.40
1:B:148:PHE:CE1	1:B:171:ALA:HB3	2.56	0.40
1:E:26:LYS:CE	1:F:26:LYS:NZ	2.67	0.40
1:F:65:ARG:HG2	1:F:119:MET:HG2	2.03	0.40
1:D:201:ALA:C	1:D:203:ALA:H	2.23	0.40
1:E:15:ARG:HH11	1:E:15:ARG:CG	2.33	0.40
1:A:109:PHE:HB3	1:A:143:VAL:HG22	2.03	0.40
1:B:33:THR:HB	1:B:192:SER:OG	2.22	0.40
1:D:67:VAL:HG23	1:D:68:PRO:CD	2.51	0.40
1:B:44:VAL:HA	1:B:47:LEU:HD12	2.04	0.40
1:E:123:SER:O	1:E:126:ILE:HG13	2.21	0.40
1:A:66:ILE:C	1:A:68:PRO:HD2	2.41	0.40
1:A:79:ALA:CB	1:A:90:LEU:HA	2.51	0.40
1:B:173:LEU:HD21	1:B:189:LEU:HD22	2.04	0.40
1:D:110:VAL:CG2	1:D:146:SER:HB3	2.51	0.40
1:E:80:ILE:HG21	1:E:91:LYS:HE3	2.02	0.40
1:C:182:GLU:HA	1:C:183:GLY:HA2	1.67	0.40
1:B:130:ALA:O	1:B:134:ARG:HG2	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	212/219 (97%)	173 (82%)	27 (13%)	12 (6%)	2	29
1	B	212/219 (97%)	182 (86%)	23 (11%)	7 (3%)	5	43
1	C	212/219 (97%)	171 (81%)	34 (16%)	7 (3%)	5	43
1	D	212/219 (97%)	177 (84%)	25 (12%)	10 (5%)	3	33
1	E	212/219 (97%)	177 (84%)	27 (13%)	8 (4%)	4	39
1	F	213/219 (97%)	172 (81%)	34 (16%)	7 (3%)	5	43
All	All	1273/1314 (97%)	1052 (83%)	170 (13%)	51 (4%)	4	37

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	55	ARG
1	A	136	ASN
1	B	87	VAL
1	B	89	ILE
1	C	82	ASP
1	C	180	GLU
1	D	55	ARG
1	D	85	ARG
1	E	9	LEU
1	E	83	GLU
1	E	87	VAL
1	F	82	ASP
1	F	85	ARG
1	A	113	ASP
1	A	119	MET
1	A	218	ASN
1	B	9	LEU
1	B	86	ARG
1	D	13	GLY
1	D	83	GLU
1	D	113	ASP
1	E	7	GLU
1	E	86	ARG
1	E	89	ILE
1	F	180	GLU
1	F	182	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	83	GLU
1	A	85	ARG
1	A	89	ILE
1	B	83	GLU
1	B	144	GLN
1	C	85	ARG
1	C	103	PRO
1	E	144	GLN
1	E	162	THR
1	C	84	THR
1	C	89	ILE
1	D	89	ILE
1	D	136	ASN
1	F	113	ASP
1	C	57	VAL
1	D	57	VAL
1	D	182	GLU
1	B	10	GLU
1	D	202	VAL
1	F	57	VAL
1	A	13	GLY
1	A	8	ILE
1	F	89	ILE
1	A	57	VAL

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	190/193 (98%)	150 (79%)	40 (21%)	1 11
1	B	190/193 (98%)	150 (79%)	40 (21%)	1 11
1	C	190/193 (98%)	155 (82%)	35 (18%)	2 16
1	D	190/193 (98%)	146 (77%)	44 (23%)	1 8
1	E	190/193 (98%)	154 (81%)	36 (19%)	2 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	191/193 (99%)	157 (82%)	34 (18%)	2 17
All	All	1141/1158 (98%)	912 (80%)	229 (20%)	1 13

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	LEU
1	A	10	GLU
1	A	34	VAL
1	A	43	MET
1	A	51	LYS
1	A	54	ASN
1	A	56	LYS
1	A	65	ARG
1	A	77	LEU
1	A	78	ASN
1	A	83	GLU
1	A	84	THR
1	A	86	ARG
1	A	88	TYR
1	A	90	LEU
1	A	98	ILE
1	A	104	ASP
1	A	106	LEU
1	A	108	VAL
1	A	113	ASP
1	A	127	SER
1	A	132	ARG
1	A	141	ASP
1	A	151	THR
1	A	159	ILE
1	A	169	GLU
1	A	172	ILE
1	A	177	ARG
1	A	178	ILE
1	A	181	ARG
1	A	185	LYS
1	A	187	MET
1	A	189	LEU
1	A	197	LEU
1	A	204	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	208	VAL
1	A	210	LEU
1	A	211	LYS
1	A	215	GLU
1	B	11	MET
1	B	15	ARG
1	B	18	ILE
1	B	28	ILE
1	B	33	THR
1	B	36	GLU
1	B	42	SER
1	B	46	ILE
1	B	55	ARG
1	B	58	THR
1	B	59	VAL
1	B	65	ARG
1	B	70	ILE
1	B	72	LYS
1	B	73	GLN
1	B	82	ASP
1	B	85	ARG
1	B	86	ARG
1	B	87	VAL
1	B	88	TYR
1	B	89	ILE
1	B	90	LEU
1	B	93	TYR
1	B	110	VAL
1	B	119	MET
1	B	136	ASN
1	B	139	GLN
1	B	140	LEU
1	B	144	GLN
1	B	149	THR
1	B	159	ILE
1	B	162	THR
1	B	165	ILE
1	B	170	VAL
1	B	177	ARG
1	B	178	ILE
1	B	182	GLU
1	B	195	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	198	ILE
1	B	204	THR
1	C	10	GLU
1	C	16	ARG
1	C	23	THR
1	C	26	LYS
1	C	28	ILE
1	C	35	MET
1	C	40	VAL
1	C	41	THR
1	C	46	ILE
1	C	51	LYS
1	C	53	ARG
1	C	58	THR
1	C	60	THR
1	C	82	ASP
1	C	83	GLU
1	C	84	THR
1	C	85	ARG
1	C	87	VAL
1	C	101	ASP
1	C	107	ASN
1	C	112	LYS
1	C	118	SER
1	C	122	ILE
1	C	127	SER
1	C	151	THR
1	C	153	VAL
1	C	159	ILE
1	C	162	THR
1	C	167	TYR
1	C	170	VAL
1	C	178	ILE
1	C	180	GLU
1	C	193	CYS
1	C	204	THR
1	C	207	ILE
1	D	8	ILE
1	D	12	HIS
1	D	18	ILE
1	D	24	LYS
1	D	43	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	48	ASP
1	D	49	SER
1	D	51	LYS
1	D	53	ARG
1	D	54	ASN
1	D	56	LYS
1	D	60	THR
1	D	63	LEU
1	D	65	ARG
1	D	66	ILE
1	D	70	ILE
1	D	77	LEU
1	D	80	ILE
1	D	83	GLU
1	D	84	THR
1	D	86	ARG
1	D	87	VAL
1	D	88	TYR
1	D	93	TYR
1	D	98	ILE
1	D	107	ASN
1	D	108	VAL
1	D	113	ASP
1	D	116	ARG
1	D	123	SER
1	D	131	SER
1	D	132	ARG
1	D	141	ASP
1	D	153	VAL
1	D	155	THR
1	D	170	VAL
1	D	177	ARG
1	D	184	ARG
1	D	185	LYS
1	D	187	MET
1	D	192	SER
1	D	197	LEU
1	D	204	THR
1	D	214	ILE
1	E	8	ILE
1	E	11	MET
1	E	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	18	ILE
1	E	33	THR
1	E	36	GLU
1	E	42	SER
1	E	51	LYS
1	E	55	ARG
1	E	58	THR
1	E	59	VAL
1	E	65	ARG
1	E	82	ASP
1	E	86	ARG
1	E	87	VAL
1	E	88	TYR
1	E	89	ILE
1	E	90	LEU
1	E	98	ILE
1	E	102	THR
1	E	107	ASN
1	E	119	MET
1	E	139	GLN
1	E	140	LEU
1	E	149	THR
1	E	151	THR
1	E	153	VAL
1	E	159	ILE
1	E	164	ILE
1	E	170	VAL
1	E	177	ARG
1	E	178	ILE
1	E	179	LEU
1	E	197	LEU
1	E	204	THR
1	E	207	ILE
1	F	5	ARG
1	F	12	HIS
1	F	15	ARG
1	F	16	ARG
1	F	24	LYS
1	F	34	VAL
1	F	35	MET
1	F	38	VAL
1	F	40	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	41	THR
1	F	53	ARG
1	F	58	THR
1	F	59	VAL
1	F	80	ILE
1	F	83	GLU
1	F	84	THR
1	F	85	ARG
1	F	87	VAL
1	F	91	LYS
1	F	95	ASN
1	F	107	ASN
1	F	116	ARG
1	F	118	SER
1	F	120	VAL
1	F	139	GLN
1	F	140	LEU
1	F	144	GLN
1	F	150	ILE
1	F	180	GLU
1	F	195	HIS
1	F	199	ASP
1	F	210	LEU
1	F	215	GLU
1	F	218	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	54	ASN
1	A	78	ASN
1	A	107	ASN
1	A	176	HIS
1	B	27	GLN
1	B	54	ASN
1	B	78	ASN
1	B	144	GLN
1	B	195	HIS
1	B	218	ASN
1	C	31	HIS
1	C	139	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	195	HIS
1	C	218	ASN
1	D	78	ASN
1	D	144	GLN
1	E	78	ASN
1	E	166	ASN
1	E	218	ASN
1	F	107	ASN
1	F	139	GLN
1	F	176	HIS
1	F	195	HIS
1	F	218	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	214/219 (97%)	-0.17	0 100 100	43, 63, 103, 127	0
1	B	214/219 (97%)	-0.28	3 (1%) 78 69	40, 67, 98, 126	0
1	C	214/219 (97%)	-0.46	1 (0%) 91 88	47, 68, 94, 109	0
1	D	214/219 (97%)	-0.27	0 100 100	42, 65, 119, 137	0
1	E	214/219 (97%)	-0.24	3 (1%) 78 69	50, 78, 118, 139	0
1	F	215/219 (98%)	-0.19	0 100 100	61, 86, 120, 151	0
All	All	1285/1314 (97%)	-0.27	7 (0%) 91 88	40, 72, 112, 151	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	ALA	4.8
1	B	219	ALA	4.5
1	B	6	GLU	3.0
1	C	56	LYS	2.2
1	E	218	ASN	2.2
1	B	218	ASN	2.2
1	E	90	LEU	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.