Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JKT
Title	:	TETRAGONAL CRYSTAL FORM OF A CATALYTIC DOMAIN OF DEATH-ASSOCIATED PROTEIN KINASE
Authors	:	Tereshko, V.; Teplova, M.; Brunzelle, J.; Watterson, D.M.; Egli, M.
Deposited on	:	2001-07-13
Resolution	:	3.50 Å(reported)

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

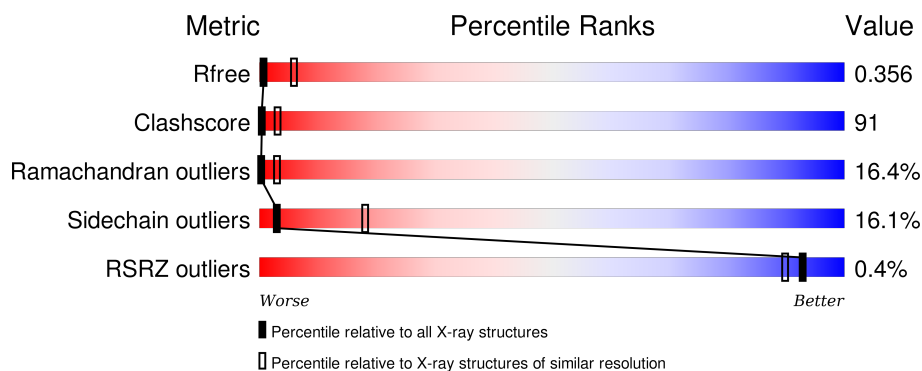|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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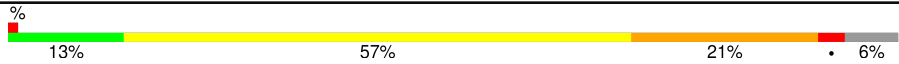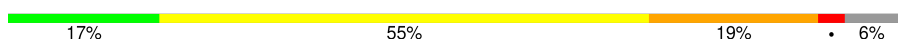*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.356
Clashscore		91
Ramachandran outliers		16.4%
Sidechain outliers		16.1%
RSRZ outliers		0.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	294	13% 57% 21% • 6%
1	B	294	17% 55% 19% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4468 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 DEATH-ASSOCIATED PROTEIN KINASE.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2234	1436	372	422	4			
1	B	276	Total	C	N	O	S	0	0	0
			2234	1436	372	422	4			

There are 20 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	286	SER	-	SEE REMARK 999	UNP P53355
A	287	ALA	-	SEE REMARK 999	UNP P53355
A	288	TRP	-	SEE REMARK 999	UNP P53355
A	289	SER	-	SEE REMARK 999	UNP P53355
A	290	HIS	-	SEE REMARK 999	UNP P53355
A	291	PRO	-	SEE REMARK 999	UNP P53355
A	292	GLN	-	SEE REMARK 999	UNP P53355
A	293	PHE	-	SEE REMARK 999	UNP P53355
A	294	GLU	-	SEE REMARK 999	UNP P53355
A	295	LYS	-	SEE REMARK 999	UNP P53355
B	286	SER	-	SEE REMARK 999	UNP P53355
B	287	ALA	-	SEE REMARK 999	UNP P53355
B	288	TRP	-	SEE REMARK 999	UNP P53355
B	289	SER	-	SEE REMARK 999	UNP P53355
B	290	HIS	-	SEE REMARK 999	UNP P53355
B	291	PRO	-	SEE REMARK 999	UNP P53355
B	292	GLN	-	SEE REMARK 999	UNP P53355
B	293	PHE	-	SEE REMARK 999	UNP P53355
B	294	GLU	-	SEE REMARK 999	UNP P53355
B	295	LYS	-	SEE REMARK 999	UNP P53355

3 Residue-property plots ⓘ

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

- Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE
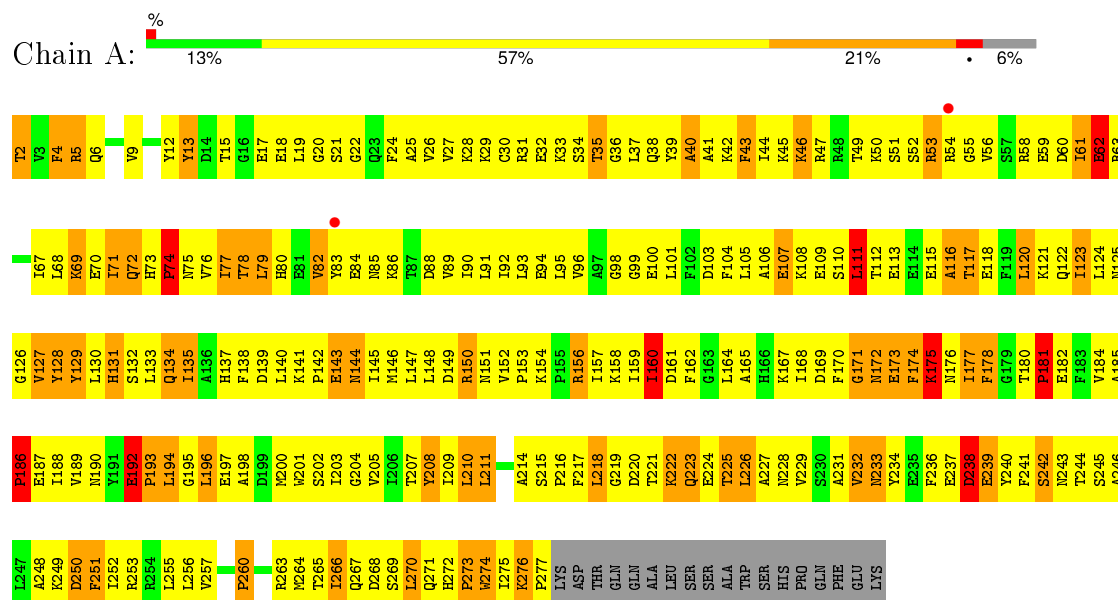
- Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE
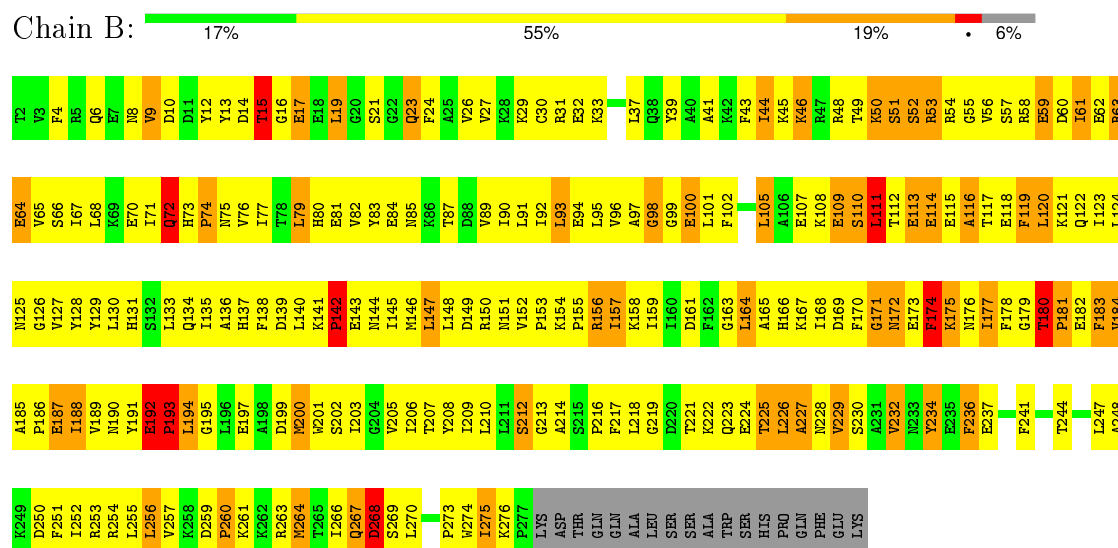
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	58.37Å 58.37Å 212.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.72 – 3.50 19.81 – 3.49	Depositor EDS
% Data completeness (in resolution range)	95.5 (58.72-3.50) 94.7 (19.81-3.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.272 , 0.297 0.284 , 0.356	Depositor DCC
R_{free} test set	903 reflections (11.89%)	DCC
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 14.1	EDS
Estimated twinning fraction	0.299 for h,-k,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.41, < L^2 > = 0.23$	Xtriage
Outliers	0 of 8549 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 (i)

5.1 Standard geometry (i)

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	0.51	0/2280	0.79	4/3080 (0.1%)
1	B	0.46	0/2280	0.78	3/3080 (0.1%)
All	All	0.49	0/4560	0.78	7/6160 (0.1%)

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	A	192	GLU	N-CA-C	6.72	129.15	111.00
1	B	192	GLU	N-CA-C	6.67	129.00	111.00
1	B	180	THR	N-CA-C	6.57	128.75	111.00
1	A	172	ASN	N-CA-C	-5.82	95.29	111.00
1	A	178	PHE	N-CA-C	5.60	126.12	111.00
1	B	183	PHE	N-CA-C	5.49	125.82	111.00
1	A	175	LYS	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2234	0	2236	458	0
1	B	2234	0	2236	370	0
All	All	4468	0	4472	817	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 91.

All (817) 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:276:LYS:HZ2	1:A:276:LYS:HA	0.98	1.13
1:A:252:ILE:HA	1:A:255:LEU:HD12	1.30	1.09
1:B:172:ASN:HB3	1:B:194:LEU:HD12	1.37	1.06
1:B:19:LEU:HD21	1:B:29:LYS:HE3	1.33	1.05
1:B:218:LEU:HD12	1:B:219:GLY:H	1.21	1.04
1:A:174:PHE:HB3	1:A:175:LYS:HD2	1.39	1.04
1:A:237:GLU:HB2	1:A:240:TYR:HB2	1.40	1.04
1:A:276:LYS:HA	1:A:276:LYS:NZ	1.75	1.00
1:A:141:LYS:HE3	1:A:144:ASN:HD21	1.23	0.99
1:B:61:ILE:HD13	1:B:89:VAL:HG21	1.43	0.99
1:B:102:PHE:HA	1:B:105:LEU:HD21	1.42	0.97
1:A:127:VAL:HG21	1:A:203:ILE:HD11	1.45	0.97
1:A:175:LYS:O	1:A:177:ILE:HG13	1.65	0.97
1:A:193:PRO:HB3	1:B:191:TYR:CE1	1.99	0.96
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.49	0.94
1:A:170:PHE:HB3	1:B:175:LYS:HE3	1.49	0.94
1:A:144:ASN:O	1:A:160:ILE:HD11	1.68	0.93
1:B:174:PHE:CE2	1:B:192:GLU:HB2	2.03	0.93
1:B:63:ARG:HB3	1:B:63:ARG:NH1	1.84	0.92
1:A:120:LEU:HD12	1:A:124:LEU:HD11	1.51	0.92
1:B:168:ILE:HD12	1:B:172:ASN:HA	1.52	0.92
1:B:127:VAL:HG21	1:B:203:ILE:HD11	1.51	0.91
1:A:31:ARG:HG2	1:A:32:GLU:H	1.33	0.91
1:A:225:THR:O	1:A:228:ASN:N	2.03	0.91
1:B:63:ARG:HE	1:B:166:HIS:CD2	1.87	0.91
1:A:201:TRP:O	1:A:205:VAL:HG23	1.71	0.91
1:A:173:GLU:HG3	1:A:194:LEU:HD11	1.52	0.91
1:A:266:ILE:HG23	1:A:267:GLN:H	1.36	0.90
1:B:61:ILE:HG21	1:B:89:VAL:HG11	1.53	0.89
1:B:166:HIS:HB3	1:B:173:GLU:HG3	1.52	0.89
1:B:70:GLU:O	1:B:70:GLU:HG2	1.73	0.89
1:B:218:LEU:HD12	1:B:219:GLY:N	1.88	0.88
1:A:193:PRO:HB3	1:B:191:TYR:HE1	1.37	0.88
1:A:187:GLU:O	1:A:193:PRO:HD2	1.74	0.87
1:A:31:ARG:CG	1:A:36:GLY:HA2	2.04	0.87
1:A:77:ILE:HG13	1:A:94:GLU:HB3	1.55	0.87
1:A:19:LEU:HD11	1:A:29:LYS:HG3	1.57	0.86

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:O	1:A:55:GLY:HA3	1.77	0.85
1:A:5:ARG:CZ	1:A:5:ARG:HA	2.08	0.84
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.06	0.84
1:B:59:GLU:HG2	1:B:175:LYS:NZ	1.93	0.83
1:B:179:GLY:O	1:B:180:THR:HG22	1.79	0.83
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.44	0.82
1:B:191:TYR:O	1:B:193:PRO:HD3	1.79	0.82
1:B:68:LEU:HB2	1:B:79:LEU:HD23	1.61	0.82
1:B:121:LYS:HE2	1:B:275:ILE:HG22	1.61	0.82
1:A:276:LYS:HZ2	1:A:276:LYS:CA	1.88	0.81
1:A:237:GLU:CB	1:A:240:TYR:HB2	2.10	0.81
1:A:20:GLY:O	1:A:27:VAL:N	2.14	0.80
1:B:63:ARG:HB3	1:B:63:ARG:HH11	1.45	0.80
1:A:204:GLY:HA3	1:A:255:LEU:HB3	1.64	0.80
1:A:176:ASN:OD1	1:A:192:GLU:HG2	1.83	0.79
1:A:189:VAL:HG12	1:A:190:ASN:ND2	1.97	0.79
1:A:68:LEU:O	1:A:71:ILE:HG13	1.82	0.79
1:B:49:THR:HB	1:B:52:SER:HB2	1.63	0.79
1:B:163:GLY:C	1:B:164:LEU:HD23	2.03	0.79
1:B:168:ILE:CD1	1:B:173:GLU:HG2	2.13	0.79
1:B:96:VAL:HG12	1:B:96:VAL:O	1.81	0.79
1:A:245:SER:OG	1:A:248:ALA:HB2	1.83	0.78
1:A:123:ILE:O	1:A:127:VAL:HG23	1.83	0.78
1:A:141:LYS:HE3	1:A:144:ASN:ND2	1.97	0.78
1:A:35:THR:HB	1:A:37:LEU:HD12	1.66	0.78
1:A:42:LYS:O	1:A:90:ILE:HG23	1.83	0.78
1:B:76:VAL:HG12	1:B:159:ILE:HB	1.66	0.78
1:B:59:GLU:HG2	1:B:175:LYS:HZ2	1.47	0.77
1:A:144:ASN:HD22	1:A:144:ASN:N	1.82	0.77
1:B:67:ILE:HG23	1:B:135:ILE:HD13	1.65	0.77
1:B:209:ILE:HG12	1:B:214:ALA:O	1.85	0.77
1:B:123:ILE:HG13	1:B:157:ILE:HD11	1.65	0.77
1:B:152:VAL:HG13	1:B:153:PRO:HD2	1.67	0.77
1:A:139:ASP:O	1:A:141:LYS:HG2	1.84	0.77
1:A:77:ILE:HG22	1:A:159:ILE:O	1.84	0.77
1:A:187:GLU:C	1:A:193:PRO:HD2	2.06	0.76
1:A:76:VAL:HG12	1:A:159:ILE:HD12	1.67	0.76
1:A:204:GLY:HA2	1:A:255:LEU:HD13	1.66	0.76
1:A:43:PHE:CD2	1:A:90:ILE:HG12	2.20	0.76
1:A:91:LEU:HB3	1:A:93:LEU:HD21	1.68	0.76
1:A:113:GLU:OE2	1:A:274:TRP:NE1	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:HG22	1:A:178:PHE:H	1.51	0.76
1:A:19:LEU:H	1:A:19:LEU:HD12	1.51	0.75
1:B:248:ALA:HB2	1:B:274:TRP:HE1	1.52	0.75
1:B:194:LEU:HD23	1:B:194:LEU:O	1.86	0.75
1:B:254:ARG:O	1:B:255:LEU:HD23	1.85	0.75
1:B:188:ILE:HG23	1:B:192:GLU:HG2	1.68	0.75
1:A:236:PHE:HE1	1:A:252:ILE:HD11	1.53	0.74
1:A:5:ARG:HA	1:A:5:ARG:NE	2.01	0.74
1:B:174:PHE:CZ	1:B:192:GLU:HB2	2.22	0.74
1:B:61:ILE:CG2	1:B:89:VAL:HG11	2.16	0.74
1:B:172:ASN:HB3	1:B:194:LEU:CD1	2.15	0.74
1:B:254:ARG:O	1:B:264:MET:HG3	1.88	0.74
1:B:102:PHE:HA	1:B:105:LEU:CD2	2.17	0.74
1:B:96:VAL:HG12	1:B:146:MET:HE2	1.70	0.74
1:A:276:LYS:HZ2	1:A:277:PRO:HD2	1.53	0.73
1:B:73:HIS:CD2	1:B:126:GLY:HA2	2.22	0.73
1:A:198:ALA:HA	1:A:263:ARG:NH1	2.03	0.73
1:B:248:ALA:HB2	1:B:274:TRP:NE1	2.03	0.73
1:B:230:SER:O	1:B:232:VAL:HG23	1.88	0.73
1:B:14:ASP:O	1:B:15:THR:HG23	1.88	0.73
1:A:160:ILE:HD12	1:A:160:ILE:H	1.53	0.73
1:A:196:LEU:H	1:A:196:LEU:HD23	1.53	0.73
1:A:131:HIS:CD2	1:A:266:ILE:HB	2.24	0.72
1:B:194:LEU:HD22	1:B:194:LEU:H	1.52	0.72
1:A:31:ARG:NE	1:A:36:GLY:HA2	2.04	0.72
1:A:198:ALA:HA	1:A:263:ARG:HH12	1.55	0.72
1:A:187:GLU:HB2	1:A:193:PRO:HB2	1.72	0.72
1:A:19:LEU:N	1:A:27:VAL:O	2.22	0.72
1:A:127:VAL:HG21	1:A:203:ILE:CD1	2.18	0.72
1:A:68:LEU:O	1:A:70:GLU:N	2.23	0.71
1:A:120:LEU:HD21	1:A:207:THR:OG1	1.90	0.71
1:A:248:ALA:HA	1:A:274:TRP:NE1	2.06	0.71
1:A:170:PHE:HB3	1:B:175:LYS:CE	2.20	0.71
1:A:4:PHE:CB	1:A:82:VAL:HB	2.19	0.71
1:A:4:PHE:HB3	1:A:82:VAL:HB	1.71	0.71
1:A:137:HIS:O	1:A:138:PHE:HB2	1.90	0.71
1:A:95:LEU:HD12	1:A:96:VAL:N	2.05	0.71
1:A:210:LEU:O	1:A:210:LEU:HD23	1.91	0.70
1:A:173:GLU:HG3	1:A:194:LEU:CD1	2.21	0.70
1:A:237:GLU:HB2	1:A:240:TYR:CB	2.20	0.70
1:A:223:GLN:HG2	1:A:224:GLU:N	2.05	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:CYS:O	1:A:39:TYR:N	2.23	0.70
1:B:92:ILE:C	1:B:93:LEU:HD23	2.10	0.70
1:B:209:ILE:O	1:B:213:GLY:N	2.23	0.70
1:A:59:GLU:O	1:A:63:ARG:HB2	1.92	0.70
1:B:257:VAL:O	1:B:263:ARG:NH2	2.21	0.69
1:A:134:GLN:NE2	1:A:168:ILE:HB	2.07	0.69
1:A:252:ILE:CA	1:A:255:LEU:HD12	2.16	0.69
1:A:39:TYR:HA	1:A:95:LEU:HB2	1.72	0.69
1:B:217:PHE:CE1	1:B:234:TYR:HB3	2.28	0.69
1:A:103:ASP:HA	1:A:106:ALA:HB2	1.74	0.69
1:A:135:ILE:HD11	1:A:167:LYS:HE3	1.75	0.69
1:A:105:LEU:HD21	1:A:110:SER:O	1.93	0.68
1:A:160:ILE:HA	1:A:162:PHE:HE1	1.59	0.68
1:B:63:ARG:NE	1:B:166:HIS:CD2	2.61	0.68
1:A:173:GLU:CG	1:A:194:LEU:HD11	2.22	0.68
1:B:212:SER:HB3	1:B:241:PHE:CZ	2.28	0.68
1:B:168:ILE:HD11	1:B:173:GLU:HG2	1.75	0.68
1:B:184:VAL:HG23	1:B:185:ALA:O	1.94	0.68
1:A:250:ASP:CA	1:A:253:ARG:HH11	2.06	0.68
1:B:44:ILE:HD12	1:B:89:VAL:O	1.93	0.68
1:B:99:GLY:O	1:B:147:LEU:HD13	1.93	0.68
1:B:119:PHE:HA	1:B:122:GLN:NE2	2.09	0.68
1:A:248:ALA:HA	1:A:274:TRP:CD1	2.29	0.67
1:A:174:PHE:CB	1:A:175:LYS:HD2	2.19	0.67
1:A:47:ARG:HB3	1:A:52:SER:HB3	1.77	0.67
1:B:53:ARG:H	1:B:53:ARG:HD2	1.57	0.67
1:A:12:TYR:C	1:A:13:TYR:HD2	1.97	0.67
1:B:119:PHE:HA	1:B:122:GLN:HE21	1.59	0.67
1:B:64:GLU:O	1:B:68:LEU:HG	1.94	0.67
1:B:49:THR:CB	1:B:52:SER:HB2	2.25	0.67
1:A:276:LYS:NZ	1:A:277:PRO:HD2	2.09	0.67
1:A:111:LEU:HD22	1:A:112:THR:N	2.10	0.67
1:A:68:LEU:C	1:A:70:GLU:H	1.99	0.67
1:B:136:ALA:O	1:B:165:ALA:HA	1.94	0.67
1:B:6:GLN:HE22	1:B:84:GLU:HG3	1.60	0.66
1:A:160:ILE:HD12	1:A:160:ILE:N	2.11	0.66
1:A:185:ALA:N	1:A:188:ILE:HD13	2.10	0.66
1:A:238:ASP:O	1:A:240:TYR:N	2.29	0.66
1:A:250:ASP:HA	1:A:253:ARG:HH11	1.59	0.66
1:B:67:ILE:HG23	1:B:135:ILE:CD1	2.25	0.66
1:B:141:LYS:NZ	1:B:181:PRO:HG2	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HA	1:A:201:TRP:CD1	2.31	0.66
1:B:49:THR:HB	1:B:52:SER:CB	2.24	0.66
1:A:130:LEU:O	1:A:133:LEU:N	2.28	0.66
1:A:105:LEU:O	1:A:105:LEU:HD23	1.96	0.66
1:B:134:GLN:O	1:B:167:LYS:HD3	1.95	0.66
1:B:119:PHE:CE2	1:B:155:PRO:HD2	2.30	0.66
1:B:48:ARG:HB3	1:B:48:ARG:NH1	2.11	0.66
1:B:135:ILE:HG12	1:B:167:LYS:HG2	1.77	0.66
1:A:195:GLY:O	1:A:198:ALA:HB3	1.96	0.66
1:B:73:HIS:HD2	1:B:126:GLY:HA2	1.60	0.66
1:B:109:GLU:O	1:B:110:SER:O	2.12	0.66
1:A:201:TRP:CZ3	1:A:256:LEU:HA	2.31	0.66
1:B:58:ARG:NH2	1:B:84:GLU:OE1	2.29	0.66
1:B:166:HIS:CB	1:B:173:GLU:HG3	2.25	0.66
1:A:73:HIS:CD2	1:A:74:PRO:HD2	2.31	0.65
1:B:226:LEU:O	1:B:227:ALA:C	2.33	0.65
1:B:187:GLU:OE1	1:B:260:PRO:HG3	1.96	0.65
1:A:147:LEU:HD12	1:A:157:ILE:HG22	1.79	0.65
1:B:68:LEU:HD12	1:B:79:LEU:CD2	2.27	0.65
1:B:79:LEU:HD12	1:B:80:HIS:N	2.12	0.65
1:A:35:THR:CB	1:A:37:LEU:HD12	2.27	0.65
1:B:76:VAL:O	1:B:158:LYS:HE2	1.97	0.65
1:B:21:SER:OG	1:B:26:VAL:HG23	1.96	0.65
1:A:120:LEU:HD21	1:A:207:THR:CB	2.27	0.65
1:B:68:LEU:CB	1:B:79:LEU:HD23	2.27	0.65
1:B:97:ALA:O	1:B:99:GLY:N	2.29	0.65
1:B:46:LYS:NZ	1:B:58:ARG:HH12	1.95	0.64
1:A:19:LEU:HD12	1:A:19:LEU:N	2.11	0.64
1:A:249:LYS:O	1:A:250:ASP:C	2.34	0.64
1:B:236:PHE:HZ	1:B:252:ILE:HD12	1.63	0.64
1:A:188:ILE:H	1:A:188:ILE:HD12	1.61	0.64
1:A:31:ARG:HG3	1:A:36:GLY:HA2	1.79	0.64
1:A:45:LYS:HA	1:A:88:ASP:OD1	1.96	0.64
1:A:112:THR:HG1	1:A:115:GLU:HB2	1.63	0.64
1:A:58:ARG:O	1:A:62:GLU:HG3	1.96	0.64
1:B:26:VAL:O	1:B:26:VAL:HG13	1.98	0.64
1:A:171:GLY:HA3	1:A:173:GLU:OE1	1.97	0.64
1:A:208:TYR:HE1	1:A:214:ALA:O	1.80	0.64
1:B:113:GLU:OE1	1:B:244:THR:HG23	1.98	0.64
1:A:49:THR:C	1:A:51:SER:H	2.01	0.64
1:A:78:THR:HG23	1:A:94:GLU:OE2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLN:O	1:B:269:SER:N	2.31	0.64
1:B:236:PHE:CZ	1:B:252:ILE:HD12	2.33	0.63
1:A:124:LEU:O	1:A:266:ILE:HD11	1.97	0.63
1:A:18:GLU:OE1	1:A:28:LYS:NZ	2.30	0.63
1:B:128:TYR:HD1	1:B:266:ILE:HG21	1.63	0.63
1:A:237:GLU:O	1:A:241:PHE:N	2.31	0.63
1:B:207:THR:O	1:B:210:LEU:N	2.31	0.63
1:A:172:ASN:O	1:A:174:PHE:N	2.31	0.63
1:A:266:ILE:HG23	1:A:267:GLN:N	2.11	0.63
1:B:168:ILE:HD13	1:B:173:GLU:HG2	1.78	0.63
1:A:24:PHE:O	1:A:44:ILE:HA	1.98	0.63
1:A:2:THR:O	1:A:4:PHE:CE1	2.51	0.63
1:A:43:PHE:CD1	1:A:43:PHE:N	2.66	0.63
1:B:194:LEU:CD2	1:B:194:LEU:H	2.12	0.63
1:B:94:GLU:OE1	1:B:158:LYS:NZ	2.31	0.63
1:B:183:PHE:HE2	1:B:209:ILE:HD11	1.64	0.63
1:B:71:ILE:CG2	1:B:72:GLN:N	2.62	0.63
1:A:185:ALA:H	1:A:188:ILE:HD13	1.63	0.63
1:A:61:ILE:O	1:A:63:ARG:N	2.31	0.63
1:B:110:SER:O	1:B:111:LEU:HB2	1.98	0.63
1:B:255:LEU:O	1:B:257:VAL:HG23	1.99	0.62
1:B:200:MET:HE2	1:B:266:ILE:HA	1.81	0.62
1:A:77:ILE:HG21	1:A:160:ILE:CG2	2.30	0.62
1:B:112:THR:O	1:B:114:GLU:N	2.32	0.62
1:A:160:ILE:HA	1:A:162:PHE:CE1	2.34	0.62
1:A:31:ARG:HE	1:A:36:GLY:HA2	1.62	0.62
1:B:19:LEU:HD21	1:B:29:LYS:CE	2.20	0.62
1:B:44:ILE:HD13	1:B:89:VAL:HB	1.80	0.62
1:B:19:LEU:HD11	1:B:95:LEU:HD11	1.81	0.62
1:A:73:HIS:CG	1:A:74:PRO:HD2	2.35	0.62
1:B:101:LEU:CD1	1:B:147:LEU:HD11	2.29	0.62
1:A:175:LYS:HB2	1:A:177:ILE:HD11	1.80	0.62
1:A:18:GLU:HG3	1:A:26:VAL:CG2	2.30	0.62
1:B:179:GLY:O	1:B:181:PRO:HD3	2.00	0.62
1:A:225:THR:O	1:A:226:LEU:C	2.38	0.61
1:B:12:TYR:C	1:B:33:LYS:HG3	2.20	0.61
1:B:230:SER:C	1:B:232:VAL:H	2.03	0.61
1:A:123:ILE:HG12	1:A:157:ILE:CD1	2.30	0.61
1:A:175:LYS:HB2	1:A:177:ILE:CD1	2.31	0.61
1:A:91:LEU:HB3	1:A:93:LEU:CD2	2.30	0.61
1:A:225:THR:O	1:A:227:ALA:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:HA	1:B:53:ARG:CZ	2.30	0.61
1:B:127:VAL:HG21	1:B:203:ILE:CD1	2.29	0.61
1:B:148:LEU:HD12	1:B:156:ARG:HB2	1.82	0.61
1:A:149:ASP:OD1	1:A:151:ASN:HB2	2.00	0.61
1:B:166:HIS:HB3	1:B:173:GLU:CG	2.28	0.61
1:B:250:ASP:O	1:B:253:ARG:N	2.34	0.61
1:A:248:ALA:HB2	1:A:274:TRP:HE1	1.65	0.60
1:A:144:ASN:HB3	1:A:160:ILE:CD1	2.31	0.60
1:A:187:GLU:HG2	1:A:188:ILE:HD12	1.83	0.60
1:A:42:LYS:O	1:A:90:ILE:CG2	2.48	0.60
1:A:20:GLY:H	1:A:27:VAL:HB	1.66	0.60
1:A:117:THR:HB	1:A:121:LYS:HE3	1.82	0.60
1:B:125:ASN:O	1:B:128:TYR:HB3	2.01	0.60
1:B:212:SER:HB3	1:B:241:PHE:HZ	1.66	0.60
1:A:21:SER:HB2	1:A:26:VAL:HG23	1.83	0.60
1:B:45:LYS:NZ	1:B:87:THR:HB	2.16	0.60
1:B:19:LEU:HB2	1:B:27:VAL:O	2.02	0.60
1:B:73:HIS:HB2	1:B:129:TYR:CD2	2.36	0.60
1:A:39:TYR:O	1:A:40:ALA:HB2	2.02	0.59
1:A:94:GLU:OE1	1:A:158:LYS:NZ	2.33	0.59
1:A:112:THR:O	1:A:116:ALA:N	2.28	0.59
1:A:208:TYR:CD1	1:A:208:TYR:C	2.76	0.59
1:A:264:MET:HG2	1:A:265:THR:H	1.66	0.59
1:A:61:ILE:HG21	1:A:89:VAL:HG21	1.84	0.59
1:A:120:LEU:O	1:A:124:LEU:HG	2.02	0.59
1:B:149:ASP:OD1	1:B:150:ARG:N	2.35	0.59
1:A:69:LYS:HA	1:A:79:LEU:HD22	1.84	0.59
1:A:252:ILE:O	1:A:255:LEU:HB2	2.02	0.59
1:B:4:PHE:HB2	1:B:84:GLU:HG2	1.83	0.59
1:B:100:GLU:HG3	1:B:146:MET:HG2	1.83	0.59
1:B:187:GLU:HG2	1:B:188:ILE:H	1.67	0.59
1:B:164:LEU:N	1:B:164:LEU:HD23	2.17	0.59
1:A:154:LYS:O	1:A:154:LYS:HG3	2.03	0.59
1:B:6:GLN:HE22	1:B:84:GLU:CG	2.16	0.59
1:A:224:GLU:O	1:A:227:ALA:HB3	2.03	0.59
1:A:103:ASP:O	1:A:106:ALA:N	2.35	0.59
1:A:112:THR:OG1	1:A:115:GLU:HG3	2.03	0.59
1:B:149:ASP:OD1	1:B:151:ASN:N	2.36	0.59
1:B:92:ILE:O	1:B:93:LEU:HD23	2.03	0.59
1:B:127:VAL:O	1:B:131:HIS:HB2	2.03	0.59
1:A:245:SER:OG	1:A:248:ALA:CB	2.52	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:GLU:N	2.18	0.58
1:B:6:GLN:NE2	1:B:84:GLU:HG3	2.19	0.58
1:A:38:GLN:O	1:A:95:LEU:HD23	2.03	0.58
1:B:266:ILE:CG2	1:B:267:GLN:N	2.66	0.58
1:A:168:ILE:HG22	1:A:168:ILE:O	2.04	0.58
1:B:123:ILE:HD11	1:B:145:ILE:HG21	1.84	0.58
1:B:254:ARG:HB3	1:B:264:MET:CG	2.34	0.58
1:A:49:THR:O	1:A:51:SER:N	2.36	0.58
1:A:201:TRP:HB2	1:A:263:ARG:CZ	2.34	0.58
1:B:172:ASN:HD22	1:B:194:LEU:CD1	2.16	0.58
1:B:82:VAL:HG13	1:B:91:LEU:HD23	1.86	0.58
1:A:117:THR:O	1:A:121:LYS:HG3	2.03	0.58
1:A:127:VAL:O	1:A:130:LEU:HB2	2.04	0.58
1:A:128:TYR:O	1:A:129:TYR:C	2.42	0.58
1:A:19:LEU:HD11	1:A:29:LYS:CG	2.31	0.58
1:B:187:GLU:CG	1:B:188:ILE:H	2.16	0.58
1:A:35:THR:OG1	1:A:37:LEU:HB2	2.03	0.58
1:B:73:HIS:ND1	1:B:74:PRO:HD2	2.19	0.58
1:A:71:ILE:HG22	1:A:72:GLN:H	1.69	0.58
1:A:74:PRO:O	1:A:76:VAL:N	2.36	0.58
1:A:209:ILE:O	1:A:211:LEU:N	2.37	0.57
1:A:180:THR:O	1:A:182:GLU:N	2.37	0.57
1:A:174:PHE:HB3	1:A:175:LYS:CD	2.26	0.57
1:A:120:LEU:HD21	1:A:207:THR:HG23	1.86	0.57
1:A:221:THR:HG22	1:A:222:LYS:N	2.20	0.57
1:B:63:ARG:HG2	1:B:64:GLU:N	2.19	0.57
1:A:59:GLU:HA	1:A:62:GLU:OE1	2.05	0.57
1:A:76:VAL:HG23	1:A:76:VAL:O	2.03	0.57
1:B:182:GLU:HG3	1:B:225:THR:HG21	1.87	0.57
1:A:238:ASP:C	1:A:240:TYR:N	2.57	0.57
1:B:168:ILE:HD12	1:B:172:ASN:CA	2.31	0.57
1:B:81:GLU:HB2	1:B:92:ILE:HB	1.86	0.57
1:A:193:PRO:O	1:A:194:LEU:HG	2.05	0.57
1:B:96:VAL:HG13	1:B:147:LEU:O	2.04	0.57
1:A:234:TYR:C	1:A:234:TYR:CD2	2.78	0.57
1:B:67:ILE:CD1	1:B:165:ALA:O	2.53	0.57
1:B:145:ILE:HG22	1:B:157:ILE:HD12	1.87	0.57
1:B:83:TYR:HB2	1:B:90:ILE:HB	1.87	0.57
1:B:251:PHE:CE2	1:B:275:ILE:HD11	2.40	0.57
1:A:104:PHE:HA	1:A:150:ARG:HH22	1.70	0.56
1:B:60:ASP:OD1	1:B:175:LYS:HE2	2.05	0.56

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HG2	1:A:36:GLY:HA2	1.86	0.56
1:A:219:GLY:N	1:A:225:THR:OG1	2.38	0.56
1:B:200:MET:CE	1:B:266:ILE:HA	2.34	0.56
1:A:186:PRO:HD3	1:A:201:TRP:CE2	2.39	0.56
1:A:260:PRO:O	1:A:263:ARG:HB3	2.05	0.56
1:B:173:GLU:O	1:B:174:PHE:HB2	2.05	0.56
1:B:189:VAL:HG11	1:B:230:SER:HB2	1.88	0.56
1:A:223:GLN:HE21	1:A:223:GLN:H	1.51	0.56
1:A:276:LYS:NZ	1:A:276:LYS:CA	2.61	0.56
1:A:264:MET:HG2	1:A:268:ASP:HB2	1.88	0.56
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.68	0.56
1:A:121:LYS:O	1:A:125:ASN:OD1	2.24	0.56
1:A:187:GLU:O	1:A:193:PRO:CD	2.50	0.56
1:B:254:ARG:NH1	1:B:254:ARG:HG2	2.17	0.56
1:A:46:LYS:HA	1:A:56:VAL:O	2.05	0.56
1:A:58:ARG:HG3	1:A:62:GLU:HG2	1.88	0.56
1:B:174:PHE:O	1:B:175:LYS:HB3	2.04	0.56
1:B:254:ARG:HB3	1:B:264:MET:HG3	1.88	0.56
1:B:79:LEU:HD13	1:B:93:LEU:HD22	1.88	0.56
1:B:101:LEU:O	1:B:105:LEU:HG	2.05	0.56
1:A:31:ARG:HG2	1:A:32:GLU:N	2.11	0.56
1:A:105:LEU:C	1:A:105:LEU:HD23	2.26	0.56
1:A:41:ALA:HB1	1:A:90:ILE:CG2	2.35	0.56
1:A:103:ASP:O	1:A:106:ALA:HB3	2.05	0.56
1:A:175:LYS:O	1:A:177:ILE:N	2.39	0.56
1:A:135:ILE:HG12	1:A:167:LYS:HD3	1.87	0.56
1:A:225:THR:HG22	1:A:226:LEU:N	2.20	0.55
1:B:141:LYS:HZ3	1:B:181:PRO:HG2	1.70	0.55
1:B:221:THR:C	1:B:223:GLN:H	2.08	0.55
1:A:42:LYS:C	1:A:90:ILE:HG23	2.27	0.55
1:B:90:ILE:N	1:B:90:ILE:HD12	2.21	0.55
1:B:274:TRP:CE3	1:B:275:ILE:HD13	2.42	0.55
1:B:53:ARG:CD	1:B:53:ARG:H	2.20	0.55
1:B:203:ILE:O	1:B:203:ILE:CG2	2.54	0.55
1:B:112:THR:C	1:B:114:GLU:H	2.09	0.55
1:A:204:GLY:HA3	1:A:255:LEU:CB	2.35	0.55
1:A:241:PHE:O	1:A:242:SER:C	2.44	0.55
1:A:171:GLY:O	1:B:175:LYS:HD2	2.07	0.55
1:B:255:LEU:O	1:B:257:VAL:N	2.39	0.55
1:B:100:GLU:HA	1:B:146:MET:HG2	1.87	0.55
1:A:181:PRO:HG2	1:A:222:LYS:HE2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:HIS:CG	1:A:273:PRO:HD2	2.42	0.55
1:A:138:PHE:CZ	1:A:194:LEU:HD23	2.41	0.55
1:A:250:ASP:O	1:A:253:ARG:HB3	2.06	0.55
1:A:103:ASP:O	1:A:106:ALA:CB	2.55	0.55
1:A:105:LEU:O	1:A:108:LYS:HB2	2.07	0.55
1:B:60:ASP:O	1:B:62:GLU:N	2.40	0.55
1:A:19:LEU:H	1:A:19:LEU:CD1	2.19	0.55
1:B:116:ALA:O	1:B:119:PHE:HB2	2.06	0.55
1:B:110:SER:O	1:B:111:LEU:CB	2.54	0.55
1:B:107:GLU:C	1:B:108:LYS:HD3	2.27	0.55
1:A:233:ASN:C	1:A:233:ASN:HD22	2.10	0.55
1:B:91:LEU:O	1:B:93:LEU:HD23	2.07	0.55
1:B:274:TRP:HE3	1:B:275:ILE:CD1	2.20	0.55
1:B:217:PHE:CZ	1:B:234:TYR:HB3	2.42	0.55
1:A:31:ARG:HE	1:A:36:GLY:CA	2.20	0.54
1:A:29:LYS:HA	1:A:40:ALA:HB2	1.88	0.54
1:B:52:SER:HA	1:B:53:ARG:NH1	2.22	0.54
1:A:105:LEU:HD11	1:A:111:LEU:HB2	1.88	0.54
1:A:113:GLU:O	1:A:116:ALA:HB3	2.08	0.54
1:B:46:LYS:O	1:B:55:GLY:HA3	2.06	0.54
1:B:156:ARG:N	1:B:156:ARG:CD	2.69	0.54
1:A:77:ILE:HG21	1:A:160:ILE:HG22	1.88	0.54
1:A:174:PHE:O	1:A:176:ASN:N	2.39	0.54
1:A:186:PRO:O	1:A:189:VAL:N	2.40	0.54
1:B:4:PHE:HB2	1:B:84:GLU:CG	2.37	0.54
1:A:225:THR:HA	1:A:228:ASN:HD22	1.72	0.54
1:B:60:ASP:O	1:B:61:ILE:C	2.46	0.54
1:B:79:LEU:CD1	1:B:80:HIS:N	2.70	0.54
1:B:53:ARG:CD	1:B:53:ARG:N	2.70	0.54
1:B:13:TYR:CE1	1:B:92:ILE:HD12	2.43	0.54
1:B:226:LEU:O	1:B:229:VAL:N	2.41	0.54
1:B:13:TYR:OH	1:B:92:ILE:HG21	2.07	0.54
1:A:112:THR:OG1	1:A:115:GLU:HB2	2.08	0.54
1:A:176:ASN:O	1:A:177:ILE:HB	2.08	0.54
1:A:68:LEU:C	1:A:70:GLU:N	2.61	0.54
1:A:99:GLY:O	1:A:146:MET:HA	2.08	0.54
1:A:95:LEU:HD12	1:A:96:VAL:H	1.70	0.54
1:A:120:LEU:HD12	1:A:124:LEU:CD1	2.32	0.54
1:B:71:ILE:HG23	1:B:72:GLN:N	2.23	0.54
1:A:170:PHE:CE1	1:B:57:SER:HB3	2.43	0.53
1:A:20:GLY:O	1:A:27:VAL:HG23	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:N	1:A:144:ASN:ND2	2.52	0.53
1:A:175:LYS:O	1:A:176:ASN:C	2.46	0.53
1:A:131:HIS:C	1:A:133:LEU:H	2.11	0.53
1:B:119:PHE:HE2	1:B:155:PRO:HD2	1.72	0.53
1:A:130:LEU:O	1:A:131:HIS:C	2.47	0.53
1:A:43:PHE:HD1	1:A:43:PHE:N	2.05	0.53
1:A:131:HIS:HD2	1:A:266:ILE:CB	2.22	0.53
1:A:112:THR:OG1	1:A:115:GLU:CG	2.56	0.53
1:A:113:GLU:OE2	1:A:248:ALA:HB2	2.09	0.53
1:B:230:SER:C	1:B:232:VAL:N	2.60	0.53
1:A:76:VAL:CG1	1:A:159:ILE:HD12	2.38	0.53
1:A:208:TYR:HD2	1:A:252:ILE:HD12	1.73	0.53
1:B:79:LEU:CD1	1:B:80:HIS:H	2.21	0.53
1:A:31:ARG:CG	1:A:32:GLU:H	2.16	0.53
1:B:182:GLU:HG3	1:B:225:THR:CG2	2.39	0.53
1:A:131:HIS:CD2	1:A:266:ILE:CB	2.92	0.53
1:A:115:GLU:O	1:A:118:GLU:HB2	2.08	0.52
1:B:187:GLU:O	1:B:189:VAL:N	2.41	0.52
1:A:223:GLN:HG2	1:A:224:GLU:H	1.73	0.52
1:A:130:LEU:O	1:A:133:LEU:HB2	2.08	0.52
1:A:187:GLU:OE1	1:A:187:GLU:N	2.31	0.52
1:A:187:GLU:CB	1:A:193:PRO:HB2	2.38	0.52
1:A:144:ASN:C	1:A:160:ILE:HD11	2.27	0.52
1:B:171:GLY:O	1:B:194:LEU:HD12	2.09	0.52
1:B:185:ALA:O	1:B:189:VAL:HG23	2.09	0.52
1:B:8:ASN:O	1:B:10:ASP:N	2.43	0.52
1:A:202:SER:OG	1:A:203:ILE:N	2.43	0.52
1:A:248:ALA:CA	1:A:274:TRP:NE1	2.73	0.52
1:B:60:ASP:C	1:B:62:GLU:N	2.62	0.52
1:A:79:LEU:O	1:A:79:LEU:HD23	2.09	0.52
1:B:83:TYR:O	1:B:90:ILE:N	2.39	0.52
1:A:21:SER:HA	1:A:26:VAL:HA	1.91	0.52
1:A:266:ILE:HA	1:A:269:SER:OG	2.10	0.52
1:B:134:GLN:HE21	1:B:134:GLN:HA	1.74	0.52
1:B:230:SER:O	1:B:232:VAL:N	2.43	0.52
1:B:100:GLU:HG3	1:B:146:MET:SD	2.50	0.52
1:B:146:MET:C	1:B:147:LEU:HD12	2.30	0.52
1:B:31:ARG:HG2	1:B:31:ARG:NH1	2.25	0.52
1:A:144:ASN:O	1:A:146:MET:HG3	2.09	0.52
1:B:101:LEU:HD12	1:B:147:LEU:HD11	1.91	0.52
1:B:194:LEU:HD23	1:B:194:LEU:C	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:C	1:A:54:ARG:HD2	2.31	0.51
1:A:146:MET:O	1:A:158:LYS:N	2.43	0.51
1:A:31:ARG:CD	1:A:36:GLY:HA2	2.40	0.51
1:A:5:ARG:HB2	1:A:83:TYR:HA	1.91	0.51
1:B:16:GLY:O	1:B:17:GLU:C	2.49	0.51
1:B:96:VAL:CG1	1:B:96:VAL:O	2.53	0.51
1:A:113:GLU:HA	1:A:116:ALA:HB3	1.93	0.51
1:A:238:ASP:C	1:A:240:TYR:H	2.13	0.51
1:A:90:ILE:N	1:A:90:ILE:HD12	2.25	0.51
1:B:46:LYS:NZ	1:B:58:ARG:NH1	2.58	0.51
1:A:117:THR:HG22	1:A:274:TRP:CZ3	2.45	0.51
1:A:123:ILE:O	1:A:126:GLY:N	2.44	0.51
1:A:120:LEU:CD2	1:A:207:THR:HG23	2.41	0.51
1:B:45:LYS:O	1:B:56:VAL:N	2.44	0.51
1:B:221:THR:C	1:B:223:GLN:N	2.64	0.51
1:B:97:ALA:O	1:B:98:GLY:C	2.49	0.51
1:A:147:LEU:CD1	1:A:157:ILE:HG22	2.40	0.51
1:A:186:PRO:O	1:A:187:GLU:C	2.47	0.51
1:A:217:PHE:O	1:A:218:LEU:C	2.48	0.51
1:A:108:LYS:O	1:A:110:SER:N	2.43	0.51
1:A:245:SER:O	1:A:248:ALA:N	2.44	0.51
1:B:189:VAL:O	1:B:189:VAL:HG12	2.11	0.51
1:B:101:LEU:HD13	1:B:147:LEU:HD11	1.92	0.51
1:B:145:ILE:HD11	1:B:206:ILE:CD1	2.40	0.51
1:B:119:PHE:CZ	1:B:155:PRO:HD2	2.45	0.51
1:B:153:PRO:O	1:B:155:PRO:HD3	2.11	0.51
1:A:207:THR:HG22	1:A:207:THR:O	2.11	0.51
1:A:76:VAL:HG12	1:A:159:ILE:HB	1.92	0.50
1:A:63:ARG:NH2	1:A:175:LYS:HG3	2.26	0.50
1:A:198:ALA:O	1:A:201:TRP:HB3	2.11	0.50
1:B:6:GLN:NE2	1:B:84:GLU:OE2	2.43	0.50
1:A:85:ASN:OD1	1:A:90:ILE:HD11	2.11	0.50
1:B:183:PHE:CE2	1:B:209:ILE:HD11	2.45	0.50
1:A:236:PHE:CE1	1:A:252:ILE:HD11	2.39	0.50
1:A:74:PRO:C	1:A:76:VAL:H	2.14	0.50
1:A:128:TYR:HB2	1:A:266:ILE:HD11	1.94	0.50
1:A:164:LEU:O	1:A:165:ALA:C	2.49	0.50
1:A:207:THR:HG21	1:A:251:PHE:CD1	2.47	0.50
1:B:254:ARG:HB3	1:B:264:MET:SD	2.51	0.50
1:A:9:VAL:HG22	1:A:13:TYR:HB2	1.93	0.50
1:A:172:ASN:O	1:A:174:PHE:HB2	2.11	0.50

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ARG:O	1:A:84:GLU:N	2.39	0.50
1:B:259:ASP:OD1	1:B:261:LYS:HG3	2.12	0.50
1:A:120:LEU:HD21	1:A:207:THR:CG2	2.42	0.50
1:B:59:GLU:HG2	1:B:175:LYS:HZ1	1.72	0.50
1:A:226:LEU:C	1:A:228:ASN:N	2.64	0.50
1:B:119:PHE:HZ	1:B:155:PRO:HG2	1.76	0.50
1:A:47:ARG:CB	1:A:52:SER:HB3	2.41	0.50
1:B:63:ARG:CZ	1:B:63:ARG:HB3	2.42	0.50
1:B:259:ASP:OD2	1:B:261:LYS:HE2	2.12	0.50
1:B:107:GLU:HB3	1:B:108:LYS:NZ	2.27	0.50
1:A:105:LEU:HD11	1:A:110:SER:O	2.12	0.49
1:A:159:ILE:HG22	1:A:162:PHE:CZ	2.46	0.49
1:A:100:GLU:O	1:A:103:ASP:N	2.35	0.49
1:B:67:ILE:CG2	1:B:135:ILE:HD13	2.38	0.49
1:B:50:LYS:O	1:B:51:SER:HB2	2.13	0.49
1:A:9:VAL:O	1:A:12:TYR:N	2.36	0.49
1:A:214:ALA:HB2	1:A:240:TYR:CE1	2.47	0.49
1:B:225:THR:O	1:B:228:ASN:HB2	2.12	0.49
1:B:176:ASN:O	1:B:177:ILE:O	2.29	0.49
1:B:61:ILE:O	1:B:65:VAL:HG23	2.13	0.49
1:A:19:LEU:HD11	1:A:29:LYS:H	1.78	0.49
1:B:247:LEU:O	1:B:251:PHE:N	2.32	0.49
1:B:51:SER:O	1:B:52:SER:O	2.31	0.49
1:A:252:ILE:HG13	1:A:253:ARG:N	2.28	0.49
1:B:175:LYS:O	1:B:177:ILE:HG13	2.13	0.49
1:B:152:VAL:CG1	1:B:153:PRO:HD2	2.40	0.49
1:A:104:PHE:HB2	1:A:150:ARG:NH2	2.27	0.49
1:A:145:ILE:O	1:A:146:MET:HG2	2.12	0.49
1:A:214:ALA:HB2	1:A:240:TYR:CD1	2.48	0.49
1:B:9:VAL:O	1:B:13:TYR:HB2	2.12	0.49
1:B:117:THR:O	1:B:119:PHE:N	2.46	0.49
1:B:112:THR:C	1:B:114:GLU:N	2.63	0.49
1:B:137:HIS:O	1:B:139:ASP:N	2.40	0.49
1:A:6:GLN:HG3	1:A:84:GLU:HG3	1.93	0.49
1:A:13:TYR:HD2	1:A:13:TYR:N	2.11	0.49
1:A:172:ASN:HB3	1:B:63:ARG:HH22	1.77	0.49
1:A:173:GLU:CB	1:A:194:LEU:HD11	2.43	0.49
1:B:39:TYR:HB3	1:B:93:LEU:O	2.13	0.49
1:A:25:ALA:HB2	1:A:44:ILE:HA	1.95	0.49
1:A:41:ALA:HB1	1:A:90:ILE:HG22	1.94	0.49
1:A:185:ALA:O	1:A:186:PRO:C	2.51	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:O	1:A:251:PHE:N	2.46	0.49
1:A:113:GLU:HG2	1:A:274:TRP:CZ2	2.47	0.48
1:B:8:ASN:C	1:B:10:ASP:N	2.66	0.48
1:A:139:ASP:OD1	1:A:141:LYS:HE2	2.14	0.48
1:A:123:ILE:HD13	1:A:145:ILE:HD11	1.95	0.48
1:A:98:GLY:HA2	1:A:150:ARG:HG2	1.94	0.48
1:A:171:GLY:C	1:A:173:GLU:N	2.67	0.48
1:A:19:LEU:HD11	1:A:29:LYS:N	2.28	0.48
1:B:186:PRO:HA	1:B:189:VAL:HB	1.96	0.48
1:B:67:ILE:HD11	1:B:165:ALA:O	2.13	0.48
1:A:4:PHE:CG	1:A:82:VAL:HB	2.47	0.48
1:B:153:PRO:HG2	1:B:154:LYS:H	1.77	0.48
1:B:259:ASP:OD1	1:B:259:ASP:C	2.52	0.48
1:A:143:GLU:C	1:A:144:ASN:HD22	2.16	0.48
1:A:92:ILE:HG22	1:A:92:ILE:O	2.13	0.48
1:A:135:ILE:HD11	1:A:167:LYS:CE	2.42	0.48
1:A:80:HIS:HB3	1:A:92:ILE:HG22	1.95	0.48
1:B:120:LEU:O	1:B:120:LEU:HD13	2.13	0.48
1:A:111:LEU:HD13	1:A:116:ALA:N	2.29	0.48
1:A:71:ILE:HG23	1:A:129:TYR:HE2	1.78	0.48
1:A:266:ILE:O	1:A:267:GLN:C	2.51	0.48
1:B:134:GLN:NE2	1:B:134:GLN:HA	2.29	0.48
1:B:174:PHE:O	1:B:175:LYS:CB	2.61	0.48
1:A:223:GLN:H	1:A:223:GLN:NE2	2.11	0.48
1:A:4:PHE:CD1	1:A:4:PHE:N	2.82	0.48
1:A:266:ILE:CG2	1:A:267:GLN:H	2.17	0.48
1:A:63:ARG:O	1:A:67:ILE:HG13	2.13	0.48
1:B:100:GLU:HG3	1:B:146:MET:CG	2.43	0.48
1:B:208:TYR:CE2	1:B:216:PRO:HB3	2.49	0.48
1:A:177:ILE:HG22	1:A:178:PHE:N	2.25	0.48
1:A:131:HIS:HD2	1:A:266:ILE:HB	1.75	0.48
1:B:79:LEU:HD11	1:B:81:GLU:O	2.14	0.48
1:A:5:ARG:CA	1:A:5:ARG:CZ	2.88	0.48
1:A:221:THR:HG22	1:A:222:LYS:H	1.77	0.48
1:B:273:PRO:HA	1:B:276:LYS:O	2.14	0.48
1:A:176:ASN:HB3	1:B:170:PHE:CE2	2.48	0.48
1:A:42:LYS:HB3	1:A:91:LEU:HB2	1.96	0.48
1:B:197:GLU:HB2	1:B:260:PRO:HB3	1.96	0.47
1:B:4:PHE:HD2	1:B:84:GLU:CD	2.18	0.47
1:A:24:PHE:O	1:A:45:LYS:N	2.45	0.47
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:O	1:A:192:GLU:OE2	2.32	0.47
1:A:238:ASP:O	1:A:239:GLU:C	2.53	0.47
1:B:19:LEU:HG	1:B:29:LYS:HG3	1.95	0.47
1:B:274:TRP:HE3	1:B:275:ILE:HD13	1.78	0.47
1:A:128:TYR:CD2	1:A:128:TYR:C	2.87	0.47
1:B:68:LEU:HD12	1:B:79:LEU:HD23	1.97	0.47
1:A:31:ARG:HD3	1:A:32:GLU:O	2.14	0.47
1:B:156:ARG:HD2	1:B:156:ARG:N	2.29	0.47
1:B:221:THR:O	1:B:223:GLN:N	2.47	0.47
1:A:101:LEU:HB3	1:A:145:ILE:CG2	2.44	0.47
1:B:141:LYS:O	1:B:142:PRO:C	2.53	0.47
1:A:49:THR:C	1:A:51:SER:N	2.68	0.47
1:A:105:LEU:O	1:A:108:LYS:N	2.44	0.47
1:B:70:GLU:OE2	1:B:167:LYS:NZ	2.39	0.47
1:A:13:TYR:CD2	1:A:13:TYR:N	2.83	0.47
1:B:43:PHE:CD2	1:B:90:ILE:HG13	2.50	0.47
1:A:117:THR:CB	1:A:121:LYS:HE3	2.45	0.47
1:A:241:PHE:HD2	1:A:244:THR:OG1	1.97	0.47
1:A:244:THR:O	1:A:249:LYS:NZ	2.46	0.47
1:A:18:GLU:HB2	1:A:28:LYS:HZ2	1.79	0.47
1:B:250:ASP:O	1:B:253:ARG:HB2	2.15	0.47
1:A:141:LYS:O	1:A:142:PRO:C	2.53	0.47
1:A:106:ALA:C	1:A:108:LYS:N	2.67	0.47
1:A:42:LYS:O	1:A:90:ILE:HA	2.14	0.47
1:A:61:ILE:C	1:A:63:ARG:N	2.68	0.47
1:A:111:LEU:CD2	1:A:112:THR:N	2.78	0.46
1:B:186:PRO:O	1:B:189:VAL:HB	2.15	0.46
1:B:61:ILE:CD1	1:B:89:VAL:HG21	2.29	0.46
1:B:142:PRO:O	1:B:144:ASN:N	2.48	0.46
1:A:253:ARG:C	1:A:255:LEU:H	2.17	0.46
1:A:77:ILE:HD11	1:A:93:LEU:HB3	1.98	0.46
1:A:39:TYR:CA	1:A:95:LEU:HB2	2.45	0.46
1:B:63:ARG:CB	1:B:63:ARG:CZ	2.93	0.46
1:A:128:TYR:O	1:A:130:LEU:N	2.49	0.46
1:A:207:THR:HG21	1:A:251:PHE:CE1	2.49	0.46
1:A:236:PHE:HE1	1:A:252:ILE:CD1	2.26	0.46
1:B:187:GLU:OE1	1:B:260:PRO:CG	2.63	0.46
1:B:226:LEU:O	1:B:228:ASN:N	2.49	0.46
1:B:199:ASP:O	1:B:200:MET:C	2.52	0.46
1:B:201:TRP:O	1:B:202:SER:C	2.54	0.46
1:B:82:VAL:HA	1:B:90:ILE:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HE2	1:B:95:LEU:HD11	1.98	0.46
1:B:96:VAL:O	1:B:146:MET:HE2	2.15	0.46
1:B:166:HIS:ND1	1:B:173:GLU:HB3	2.31	0.46
1:B:194:LEU:N	1:B:194:LEU:CD2	2.75	0.46
1:B:17:GLU:OE1	1:B:29:LYS:HE3	2.16	0.46
1:A:229:VAL:O	1:A:232:VAL:N	2.48	0.46
1:B:274:TRP:CE3	1:B:275:ILE:CD1	2.99	0.46
1:A:196:LEU:HD21	1:A:197:GLU:OE2	2.15	0.46
1:A:77:ILE:HG21	1:A:160:ILE:HG23	1.96	0.45
1:A:225:THR:CA	1:A:228:ASN:HD22	2.29	0.45
1:B:117:THR:C	1:B:119:PHE:N	2.69	0.45
1:B:10:ASP:O	1:B:33:LYS:HE2	2.16	0.45
1:A:131:HIS:O	1:A:133:LEU:N	2.49	0.45
1:A:61:ILE:O	1:A:62:GLU:C	2.54	0.45
1:A:19:LEU:HB2	1:A:27:VAL:HB	1.98	0.45
1:A:168:ILE:CD1	1:A:173:GLU:OE2	2.64	0.45
1:A:250:ASP:HA	1:A:253:ARG:HE	1.79	0.45
1:B:134:GLN:CA	1:B:134:GLN:HE21	2.27	0.45
1:A:182:GLU:OE1	1:A:215:SER:OG	2.21	0.45
1:A:194:LEU:HB3	1:A:195:GLY:H	1.34	0.45
1:B:170:PHE:CD1	1:B:170:PHE:O	2.70	0.45
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.96	0.45
1:A:272:HIS:O	1:A:275:ILE:N	2.41	0.45
1:A:120:LEU:CD1	1:A:124:LEU:HD21	2.47	0.45
1:A:128:TYR:HD2	1:A:129:TYR:N	2.14	0.45
1:A:267:GLN:O	1:A:271:GLN:HG2	2.16	0.45
1:B:267:GLN:C	1:B:269:SER:N	2.70	0.45
1:B:229:VAL:O	1:B:232:VAL:N	2.49	0.45
1:B:37:LEU:HD12	1:B:39:TYR:OH	2.17	0.45
1:A:19:LEU:CD1	1:A:29:LYS:H	2.30	0.45
1:A:4:PHE:HB2	1:A:5:ARG:H	1.57	0.45
1:B:141:LYS:HZ1	1:B:181:PRO:HG2	1.79	0.45
1:B:44:ILE:N	1:B:44:ILE:HD12	2.32	0.45
1:A:147:LEU:HA	1:A:157:ILE:HA	1.98	0.45
1:A:189:VAL:HG12	1:A:190:ASN:HD21	1.77	0.45
1:B:102:PHE:O	1:B:105:LEU:HD11	2.16	0.45
1:B:117:THR:C	1:B:119:PHE:H	2.20	0.45
1:A:12:TYR:C	1:A:13:TYR:CD2	2.85	0.45
1:A:120:LEU:HD21	1:A:207:THR:HA	1.98	0.45
1:A:170:PHE:CE1	1:B:57:SER:CB	3.00	0.45
1:A:6:GLN:NE2	1:A:84:GLU:OE1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:O	1:B:32:GLU:C	2.54	0.45
1:B:154:LYS:O	1:B:156:ARG:NH1	2.49	0.45
1:B:31:ARG:HG2	1:B:31:ARG:O	2.17	0.45
1:A:112:THR:OG1	1:A:115:GLU:CB	2.65	0.44
1:A:116:ALA:O	1:A:118:GLU:N	2.50	0.44
1:A:200:MET:HG3	1:A:265:THR:HA	1.99	0.44
1:A:31:ARG:NE	1:A:36:GLY:CA	2.76	0.44
1:A:226:LEU:O	1:A:228:ASN:N	2.50	0.44
1:A:19:LEU:CD1	1:A:29:LYS:N	2.80	0.44
1:B:266:ILE:HG23	1:B:267:GLN:N	2.32	0.44
1:B:267:GLN:O	1:B:268:ASP:C	2.55	0.44
1:B:44:ILE:CD1	1:B:89:VAL:HB	2.47	0.44
1:B:205:VAL:O	1:B:206:ILE:C	2.56	0.44
1:A:226:LEU:C	1:A:228:ASN:H	2.20	0.44
1:A:28:LYS:O	1:A:40:ALA:HA	2.17	0.44
1:A:134:GLN:HE22	1:A:168:ILE:HB	1.80	0.44
1:A:192:GLU:O	1:A:193:PRO:O	2.35	0.44
1:B:225:THR:O	1:B:226:LEU:C	2.56	0.44
1:A:6:GLN:HA	1:A:84:GLU:O	2.17	0.44
1:A:264:MET:CG	1:A:268:ASP:HB2	2.47	0.44
1:B:112:THR:O	1:B:115:GLU:N	2.51	0.44
1:A:162:PHE:N	1:A:162:PHE:CD1	2.85	0.44
1:A:248:ALA:CB	1:A:274:TRP:NE1	2.80	0.44
1:B:186:PRO:HD3	1:B:201:TRP:CZ3	2.53	0.44
1:B:189:VAL:O	1:B:190:ASN:HB2	2.18	0.44
1:B:79:LEU:HD12	1:B:80:HIS:H	1.82	0.44
1:B:23:GLN:NE2	1:B:24:PHE:CE2	2.80	0.44
1:B:172:ASN:CB	1:B:194:LEU:HB3	2.47	0.44
1:B:121:LYS:HE2	1:B:275:ILE:CG2	2.40	0.44
1:B:113:GLU:CD	1:B:244:THR:HG23	2.37	0.44
1:B:130:LEU:O	1:B:133:LEU:N	2.33	0.44
1:A:202:SER:O	1:A:205:VAL:N	2.46	0.44
1:B:172:ASN:HD22	1:B:194:LEU:HD12	1.83	0.44
1:B:75:ASN:ND2	1:B:122:GLN:HB3	2.33	0.44
1:A:150:ARG:HB3	1:A:150:ARG:CZ	2.47	0.44
1:A:168:ILE:O	1:A:169:ASP:C	2.56	0.44
1:A:187:GLU:HB2	1:A:193:PRO:CB	2.46	0.44
1:A:42:LYS:O	1:A:91:LEU:N	2.50	0.44
1:B:187:GLU:CG	1:B:188:ILE:N	2.81	0.44
1:A:152:VAL:CG1	1:A:153:PRO:CD	2.89	0.44
1:A:210:LEU:C	1:A:211:LEU:HD23	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:HG2	1:A:69:LYS:O	2.18	0.44
1:A:201:TRP:HZ3	1:A:257:VAL:N	2.16	0.43
1:B:183:PHE:O	1:B:201:TRP:HD1	2.01	0.43
1:B:52:SER:OG	1:B:53:ARG:NH2	2.51	0.43
1:B:73:HIS:ND1	1:B:74:PRO:CD	2.81	0.43
1:A:264:MET:HG2	1:A:265:THR:N	2.32	0.43
1:B:172:ASN:HB2	1:B:194:LEU:HB3	2.00	0.43
1:B:255:LEU:C	1:B:257:VAL:HG23	2.37	0.43
1:A:29:LYS:O	1:A:30:CYS:HB3	2.17	0.43
1:B:208:TYR:CD2	1:B:216:PRO:HB3	2.53	0.43
1:A:43:PHE:CD2	1:A:90:ILE:CG1	2.99	0.43
1:B:127:VAL:CG2	1:B:203:ILE:HD11	2.34	0.43
1:B:116:ALA:O	1:B:119:PHE:N	2.38	0.43
1:A:63:ARG:HH22	1:A:175:LYS:HG3	1.83	0.43
1:A:202:SER:O	1:A:205:VAL:HG23	2.18	0.43
1:A:252:ILE:HG13	1:A:253:ARG:H	1.83	0.43
1:B:30:CYS:SG	1:B:41:ALA:HB2	2.58	0.43
1:A:172:ASN:HB3	1:B:63:ARG:NH2	2.33	0.43
1:A:185:ALA:HB3	1:A:188:ILE:CD1	2.49	0.43
1:A:71:ILE:HG13	1:A:71:ILE:H	1.53	0.43
1:B:63:ARG:CG	1:B:64:GLU:N	2.81	0.43
1:A:127:VAL:HG12	1:A:131:HIS:CE1	2.54	0.43
1:A:233:ASN:ND2	1:A:233:ASN:O	2.51	0.43
1:A:131:HIS:C	1:A:133:LEU:N	2.72	0.43
1:B:149:ASP:OD1	1:B:151:ASN:OD1	2.36	0.43
1:A:60:ASP:OD1	1:A:63:ARG:NH2	2.51	0.43
1:B:195:GLY:C	1:B:197:GLU:H	2.16	0.43
1:B:197:GLU:O	1:B:263:ARG:NH1	2.52	0.43
1:A:18:GLU:HG3	1:A:26:VAL:HG22	1.98	0.43
1:B:259:ASP:OD1	1:B:261:LYS:N	2.51	0.43
1:B:120:LEU:HD12	1:B:124:LEU:CD1	2.48	0.43
1:A:248:ALA:CB	1:A:274:TRP:HE1	2.30	0.43
1:B:187:GLU:C	1:B:189:VAL:N	2.70	0.43
1:B:96:VAL:O	1:B:146:MET:CE	2.67	0.43
1:A:17:GLU:HG2	1:A:18:GLU:N	2.33	0.43
1:A:39:TYR:O	1:A:95:LEU:HD22	2.18	0.43
1:A:24:PHE:CD1	1:A:55:GLY:HA2	2.54	0.43
1:A:100:GLU:O	1:A:101:LEU:C	2.58	0.43
1:B:145:ILE:HD11	1:B:206:ILE:HD13	2.00	0.43
1:A:34:SER:O	1:A:35:THR:HG22	2.18	0.43
1:B:167:LYS:O	1:B:168:ILE:HD13	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PHE:HD2	1:B:175:LYS:N	2.17	0.42
1:B:93:LEU:N	1:B:93:LEU:HD23	2.33	0.42
1:A:17:GLU:O	1:A:28:LYS:HA	2.18	0.42
1:B:45:LYS:HB3	1:B:55:GLY:HA2	2.01	0.42
1:B:248:ALA:C	1:B:250:ASP:N	2.72	0.42
1:A:233:ASN:ND2	1:A:233:ASN:C	2.73	0.42
1:A:107:GLU:HG2	1:A:108:LYS:HG3	2.02	0.42
1:A:116:ALA:O	1:A:117:THR:C	2.57	0.42
1:B:63:ARG:HA	1:B:66:SER:HB3	2.01	0.42
1:B:79:LEU:HD13	1:B:80:HIS:H	1.84	0.42
1:A:164:LEU:HD11	1:A:178:PHE:O	2.19	0.42
1:A:41:ALA:HB1	1:A:90:ILE:HG21	2.02	0.42
1:B:17:GLU:OE1	1:B:19:LEU:CD2	2.67	0.42
1:A:91:LEU:HD13	1:A:93:LEU:HD21	2.02	0.42
1:A:209:ILE:C	1:A:211:LEU:N	2.71	0.42
1:A:185:ALA:HA	1:A:201:TRP:NE1	2.35	0.42
1:B:184:VAL:HG23	1:B:185:ALA:N	2.33	0.42
1:B:80:HIS:ND1	1:B:81:GLU:HG3	2.34	0.42
1:B:145:ILE:CG2	1:B:157:ILE:HD12	2.48	0.42
1:A:4:PHE:CD2	1:A:84:GLU:HB3	2.55	0.42
1:A:120:LEU:HD21	1:A:207:THR:CA	2.49	0.42
1:A:138:PHE:HZ	1:A:194:LEU:HD23	1.84	0.42
1:B:60:ASP:OD1	1:B:175:LYS:CE	2.67	0.42
1:B:45:LYS:HZ2	1:B:87:THR:HB	1.83	0.42
1:B:247:LEU:HB2	1:B:274:TRP:HD1	1.84	0.42
1:A:12:TYR:HA	1:A:33:LYS:HG3	2.00	0.42
1:A:122:GLN:HE22	1:A:156:ARG:HA	1.84	0.42
1:A:123:ILE:HG12	1:A:157:ILE:HD11	2.02	0.42
1:A:171:GLY:C	1:A:173:GLU:H	2.23	0.42
1:A:195:GLY:O	1:A:198:ALA:CB	2.65	0.42
1:A:245:SER:O	1:A:246:ALA:C	2.57	0.42
1:B:200:MET:HE2	1:B:266:ILE:CA	2.50	0.42
1:A:193:PRO:CB	1:B:191:TYR:HE1	2.20	0.42
1:B:195:GLY:C	1:B:197:GLU:N	2.69	0.42
1:B:207:THR:O	1:B:210:LEU:HB2	2.20	0.42
1:B:203:ILE:HG22	1:B:203:ILE:O	2.19	0.42
1:B:217:PHE:CZ	1:B:256:LEU:HD13	2.54	0.42
1:A:134:GLN:HE21	1:A:168:ILE:HB	1.82	0.41
1:A:266:ILE:O	1:A:270:LEU:N	2.48	0.41
1:B:46:LYS:HZ1	1:B:58:ARG:HH12	1.62	0.41
1:A:172:ASN:O	1:A:173:GLU:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:OG	1:B:53:ARG:HD2	2.21	0.41
1:B:187:GLU:C	1:B:193:PRO:HD2	2.41	0.41
1:A:276:LYS:HZ2	1:A:277:PRO:CD	2.29	0.41
1:B:113:GLU:O	1:B:117:THR:HG23	2.20	0.41
1:B:167:LYS:C	1:B:168:ILE:HG12	2.41	0.41
1:B:224:GLU:O	1:B:225:THR:C	2.58	0.41
1:A:134:GLN:CA	1:A:134:GLN:HE21	2.34	0.41
1:A:187:GLU:CA	1:A:193:PRO:HD2	2.50	0.41
1:A:76:VAL:O	1:A:77:ILE:O	2.39	0.41
1:B:56:VAL:HG12	1:B:57:SER:N	2.36	0.41
1:B:269:SER:OG	1:B:270:LEU:N	2.53	0.41
1:A:231:ALA:O	1:A:232:VAL:HB	2.20	0.41
1:B:209:ILE:O	1:B:210:LEU:C	2.59	0.41
1:A:184:VAL:HB	1:A:188:ILE:HB	2.02	0.41
1:A:263:ARG:HG2	1:A:264:MET:O	2.20	0.41
1:B:65:VAL:O	1:B:65:VAL:HG12	2.20	0.41
1:A:45:LYS:O	1:A:56:VAL:N	2.54	0.41
1:B:237:GLU:H	1:B:241:PHE:HD1	1.69	0.41
1:A:275:ILE:O	1:A:277:PRO:HD3	2.21	0.41
1:A:208:TYR:CE2	1:A:241:PHE:CE1	3.09	0.41
1:A:211:LEU:N	1:A:211:LEU:HD23	2.35	0.41
1:A:180:THR:HG22	1:A:182:GLU:H	1.85	0.41
1:B:107:GLU:HB3	1:B:108:LYS:HZ2	1.83	0.41
1:A:76:VAL:CG2	1:A:76:VAL:O	2.69	0.41
1:B:79:LEU:HD13	1:B:93:LEU:CD2	2.49	0.41
1:B:123:ILE:O	1:B:127:VAL:HG23	2.21	0.41
1:A:68:LEU:HA	1:A:71:ILE:HD11	2.03	0.40
1:A:113:GLU:O	1:A:117:THR:HG23	2.21	0.40
1:A:176:ASN:OD1	1:A:192:GLU:OE1	2.39	0.40
1:A:98:GLY:HA3	1:A:147:LEU:O	2.21	0.40
1:B:168:ILE:HG22	1:B:169:ASP:N	2.36	0.40
1:A:149:ASP:OD1	1:A:151:ASN:N	2.52	0.40
1:A:112:THR:O	1:A:113:GLU:C	2.59	0.40
1:A:176:ASN:HB3	1:A:177:ILE:H	1.68	0.40
1:B:176:ASN:C	1:B:177:ILE:HG13	2.39	0.40
1:B:188:ILE:HG22	1:B:188:ILE:O	2.21	0.40
1:B:247:LEU:O	1:B:250:ASP:N	2.55	0.40
1:B:48:ARG:HB3	1:B:48:ARG:HH11	1.82	0.40
1:A:112:THR:HG1	1:A:115:GLU:CB	2.33	0.40
1:B:224:GLU:O	1:B:227:ALA:HB3	2.22	0.40
1:B:77:ILE:HG22	1:B:159:ILE:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HG23	1:B:72:GLN:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/294 (93%)	156 (57%)	72 (26%)	46 (17%)	0 3
1	B	274/294 (93%)	179 (65%)	51 (19%)	44 (16%)	0 3
All	All	548/588 (93%)	335 (61%)	123 (22%)	90 (16%)	0 3

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA
1	A	50	LYS
1	A	61	ILE
1	A	69	LYS
1	A	72	GLN
1	A	74	PRO
1	A	75	ASN
1	A	171	GLY
1	A	175	LYS
1	A	177	ILE
1	A	181	PRO
1	A	193	PRO
1	A	251	PHE
1	B	19	LEU
1	B	51	SER
1	B	52	SER
1	B	98	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	109	GLU
1	B	110	SER
1	B	175	LYS
1	B	180	THR
1	B	181	PRO
1	B	268	ASP
1	A	46	LYS
1	A	62	GLU
1	A	77	ILE
1	A	109	GLU
1	A	140	LEU
1	A	173	GLU
1	A	194	LEU
1	A	210	LEU
1	A	222	LYS
1	A	226	LEU
1	A	238	ASP
1	A	239	GLU
1	B	23	GLN
1	B	111	LEU
1	B	113	GLU
1	B	138	PHE
1	B	143	GLU
1	B	161	ASP
1	B	177	ILE
1	A	15	THR
1	A	128	TYR
1	A	132	SER
1	B	9	VAL
1	B	17	GLU
1	B	172	ASN
1	B	174	PHE
1	B	187	GLU
1	B	192	GLU
1	B	227	ALA
1	B	264	MET
1	A	86	LYS
1	A	116	ALA
1	A	117	THR
1	A	129	TYR
1	A	135	ILE
1	A	225	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	242	SER
1	A	250	ASP
1	A	266	ILE
1	B	15	THR
1	B	46	LYS
1	B	74	PRO
1	B	222	LYS
1	B	226	LEU
1	A	111	LEU
1	A	131	HIS
1	A	218	LEU
1	B	50	LYS
1	B	118	GLU
1	B	256	LEU
1	A	160	ILE
1	A	273	PRO
1	B	72	GLN
1	B	116	ALA
1	B	225	THR
1	A	232	VAL
1	B	61	ILE
1	B	188	ILE
1	A	22	GLY
1	A	260	PRO
1	B	232	VAL
1	A	186	PRO
1	B	142	PRO
1	B	171	GLY
1	B	193	PRO
1	B	260	PRO
1	B	229	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.

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/262 (94%)	202 (82%)	43 (18%)	2	13
1	B	245/262 (94%)	209 (85%)	36 (15%)	4	22
All	All	490/524 (94%)	411 (84%)	79 (16%)	3	18

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	PHE
1	A	5	ARG
1	A	13	TYR
1	A	35	THR
1	A	43	PHE
1	A	53	ARG
1	A	62	GLU
1	A	71	ILE
1	A	74	PRO
1	A	78	THR
1	A	79	LEU
1	A	82	VAL
1	A	107	GLU
1	A	111	LEU
1	A	120	LEU
1	A	123	ILE
1	A	127	VAL
1	A	134	GLN
1	A	143	GLU
1	A	144	ASN
1	A	148	LEU
1	A	150	ARG
1	A	156	ARG
1	A	160	ILE
1	A	161	ASP
1	A	174	PHE
1	A	175	LYS
1	A	181	PRO
1	A	186	PRO
1	A	192	GLU
1	A	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	208	TYR
1	A	211	LEU
1	A	216	PRO
1	A	220	ASP
1	A	223	GLN
1	A	233	ASN
1	A	238	ASP
1	A	243	ASN
1	A	270	LEU
1	A	274	TRP
1	A	276	LYS
1	B	15	THR
1	B	44	ILE
1	B	53	ARG
1	B	54	ARG
1	B	59	GLU
1	B	63	ARG
1	B	64	GLU
1	B	72	GLN
1	B	79	LEU
1	B	85	ASN
1	B	93	LEU
1	B	100	GLU
1	B	105	LEU
1	B	111	LEU
1	B	114	GLU
1	B	119	PHE
1	B	120	LEU
1	B	140	LEU
1	B	142	PRO
1	B	147	LEU
1	B	156	ARG
1	B	157	ILE
1	B	164	LEU
1	B	174	PHE
1	B	178	PHE
1	B	180	THR
1	B	184	VAL
1	B	193	PRO
1	B	194	LEU
1	B	200	MET
1	B	212	SER

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	B	234	TYR
1	B	236	PHE
1	B	267	GLN
1	B	268	ASP
1	B	275	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	125	ASN
1	A	131	HIS
1	A	134	GLN
1	A	144	ASN
1	A	172	ASN
1	A	190	ASN
1	A	223	GLN
1	A	228	ASN
1	A	233	ASN
1	A	243	ASN
1	A	267	GLN
1	A	271	GLN
1	B	6	GLN
1	B	122	GLN
1	B	134	GLN
1	B	166	HIS
1	B	172	ASN
1	B	190	ASN
1	B	228	ASN
1	B	243	ASN
1	B	267	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	276/294 (93%)	-0.15	2 (0%)	89	82	0, 31, 51, 67	0
1	B	276/294 (93%)	-0.19	0	100	100	0, 32, 52, 67	0
All	All	552/588 (93%)	-0.17	2 (0%)	93	90	0, 32, 51, 67	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	ARG	2.1
1	A	83	TYR	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.