



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:29 am GMT

PDB ID : 2GK0
Title : Structure of Catalytic Elimination Antibody 13G5 from a twinned crystal in space group C2
Authors : Debler, E.W.; Wilson, I.A.
Deposited on : 2006-03-31
Resolution : 2.45 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

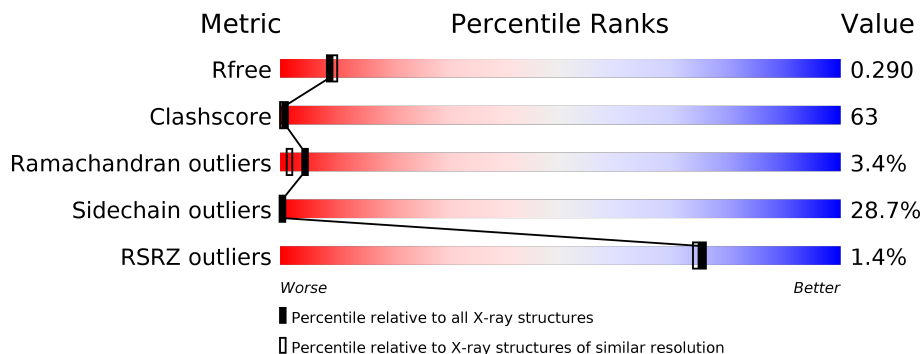
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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

Mol	Chain	Length	Quality of chain
1	A	217	<div> <div>18%</div> <div>62%</div> <div>20%</div> </div>
1	L	217	<div> <div>26%</div> <div>51%</div> <div>23%</div> </div>
2	B	221	<div> <div>19%</div> <div>57%</div> <div>21%</div> </div>
2	H	221	<div> <div>2%</div> <div>25%</div> <div>56%</div> <div>19%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6692 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 Catalytic elimination antibody 13G5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1683	1053	286	338	6			
1	A	217	Total	C	N	O	S	0	0	0
			1683	1053	286	338	6			

- Molecule 2 is a protein called Catalytic elimination antibody 13G5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1649	1043	270	327	9			
2	B	216	Total	C	N	O	S	0	0	0
			1606	1012	265	320	9			

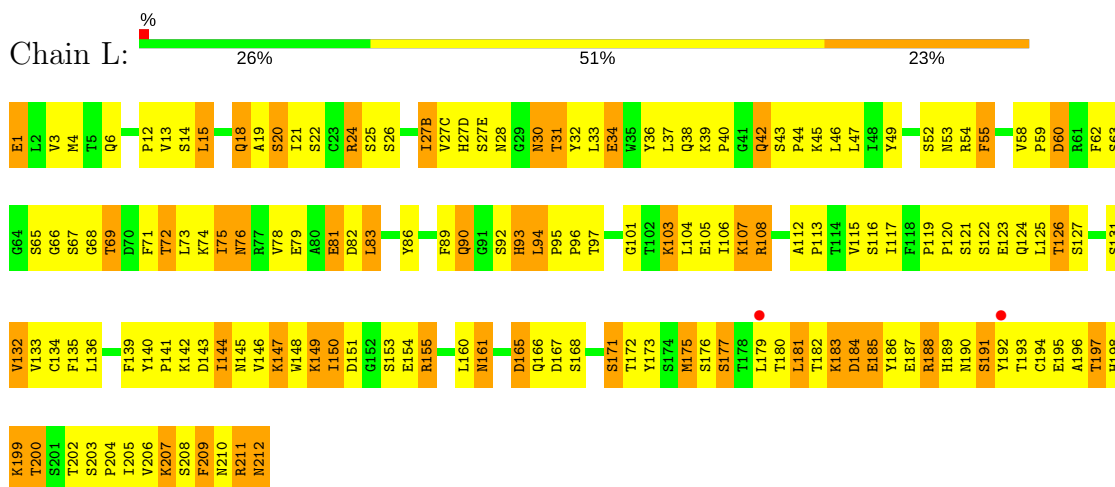
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	17	Total	O	0	0
			17	17		
3	H	24	Total	O	0	0
			24	24		
3	L	18	Total	O	0	0
			18	18		

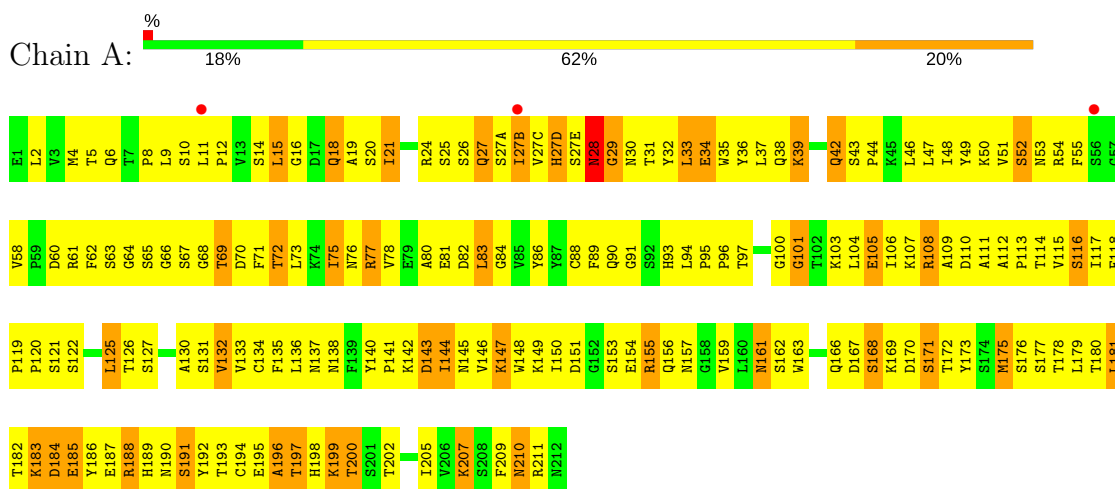
3 Residue-property plots

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

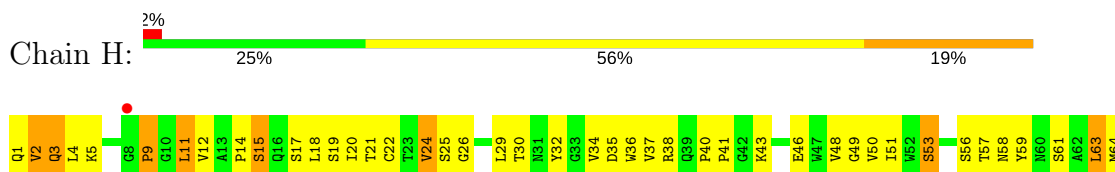
• Molecule 1: Catalytic elimination antibody 13G5 light chain

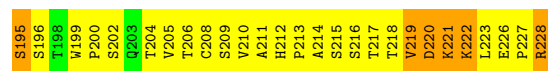
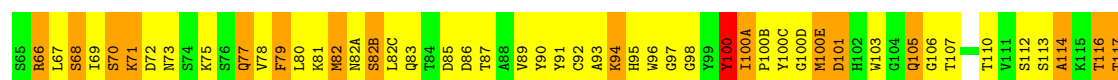


• Molecule 1: Catalytic elimination antibody 13G5 light chain

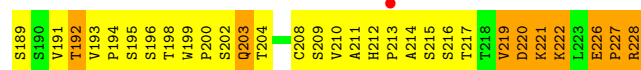
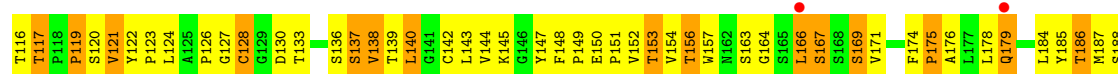
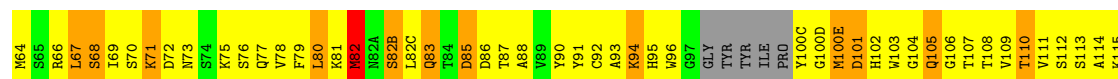
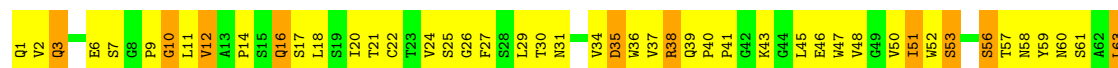


• Molecule 2: Catalytic elimination antibody 13G5 heavy chain





• Molecule 2: Catalytic elimination antibody 13G5 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.88Å 84.62Å 150.07Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 49.92 – 2.44	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.45) 97.5 (49.92-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.45Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.191 , 0.255 0.227 , 0.290	Depositor DCC
R_{free} test set	1557 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6692	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.39	0/1722	0.82	1/2337 (0.0%)
1	L	0.40	1/1722 (0.1%)	0.80	0/2337
2	B	0.35	0/1649	0.86	1/2257 (0.0%)
2	H	0.41	2/1696 (0.1%)	0.84	2/2324 (0.1%)
All	All	0.39	3/6789 (0.0%)	0.83	4/9255 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	VAL	CB-CG1	5.33	1.64	1.52
1	L	212	ASN	CG-OD1	5.32	1.35	1.24
2	H	9	PRO	N-CD	5.18	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100(E)	MET	C-N-CA	7.25	139.83	121.70
2	H	100(E)	MET	C-N-CA	6.79	138.69	121.70
1	A	28	ASN	C-N-CA	5.10	133.00	122.30
2	H	100	TYR	C-N-CA	5.00	134.20	121.70

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	1683	0	1628	242	0
1	L	1683	0	1628	196	0
2	B	1606	0	1564	225	1
2	H	1649	0	1604	191	0
3	A	12	0	0	0	0
3	B	17	0	0	0	0
3	H	24	0	0	0	0
3	L	18	0	0	0	0
All	All	6692	0	6424	819	1

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 63.

All (819) 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:94:LEU:HD23	1:A:96:PRO:HD3	1.40	1.01
1:L:115:VAL:HG22	1:L:136:LEU:HG	1.46	0.98
1:A:19:ALA:HB3	1:A:75:ILE:HD12	1.45	0.97
1:A:190:ASN:HA	1:A:211:ARG:HB2	1.47	0.96
2:B:12:VAL:HG23	2:B:111:VAL:HG22	1.46	0.96
2:H:171:VAL:HG22	2:H:191:VAL:HG23	1.46	0.96
2:H:152:VAL:HG12	2:H:212:HIS:HB2	1.47	0.95
1:A:117:ILE:HD12	1:A:194:CYS:HB2	1.49	0.94
2:H:40:PRO:HB2	2:H:43:LYS:HD2	1.49	0.94
1:A:83:LEU:HD13	1:A:106:ILE:HD12	1.48	0.93
2:B:87:THR:HG23	2:B:111:VAL:H	1.33	0.93
2:B:20:ILE:HG21	2:B:107:THR:HG21	1.51	0.93
2:H:97:GLY:HA3	2:H:100(C):TYR:H	1.35	0.92
1:A:52:SER:HA	1:A:64:GLY:HA3	1.52	0.92
2:H:100:TYR:O	2:H:100(A):ILE:HG23	1.68	0.92
1:L:39:LYS:HB2	1:L:42:GLN:HG3	1.54	0.90
2:B:138:VAL:HG21	2:B:199:TRP:HB3	1.54	0.89
2:B:20:ILE:HD11	2:B:109:VAL:HG21	1.54	0.88
2:B:144:VAL:HB	2:B:187:MET:HG3	1.56	0.88
1:L:94:LEU:HD23	1:L:95:PRO:HA	1.57	0.86
1:L:190:ASN:HA	1:L:211:ARG:HH11	1.40	0.85
2:B:40:PRO:HB2	2:B:43:LYS:HD3	1.58	0.83
2:H:20:ILE:HG21	2:H:107:THR:HG21	1.60	0.83
2:H:213:PRO:HA	2:H:216:SER:HA	1.60	0.83
2:B:171:VAL:HG22	2:B:191:VAL:HG23	1.61	0.83
2:B:137:SER:HA	2:B:194:PRO:HA	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLY:HA2	1:A:71:PHE:HA	1.62	0.81
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.62	0.81
1:L:182:THR:HG23	1:L:185:GLU:OE2	1.81	0.81
1:A:54:ARG:HH21	1:A:63:SER:HA	1.47	0.80
2:H:178:LEU:HD21	2:H:183:GLY:HA2	1.63	0.80
1:A:33:LEU:HD23	1:A:51:VAL:HA	1.63	0.80
2:B:29:LEU:HD13	2:B:71:LYS:HG3	1.64	0.80
2:H:63:LEU:HB2	2:H:67:LEU:HD21	1.64	0.80
1:A:189:HIS:HB2	1:A:192:TYR:OH	1.81	0.79
2:H:49:GLY:HA3	2:H:69:ILE:HD11	1.63	0.79
2:B:114:ALA:HB3	2:B:148:PHE:CE2	2.18	0.79
1:L:113:PRO:HG2	1:L:205:ILE:HD12	1.65	0.79
1:A:120:PRO:HD3	1:A:132:VAL:HG13	1.65	0.78
1:A:147:LYS:HG3	1:A:154:GLU:OE1	1.83	0.78
2:B:123:PRO:HD3	2:B:221:LYS:HZ3	1.48	0.78
2:B:116:THR:HG22	2:B:215:SER:HB3	1.64	0.78
1:A:18:GLN:HB2	1:A:76:ASN:HA	1.65	0.77
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.66	0.77
2:H:22:CYS:HB3	2:H:78:VAL:HB	1.64	0.77
2:B:50:VAL:HG12	2:B:58:ASN:HB2	1.65	0.77
2:B:128:CYS:HB2	2:B:228:ARG:HA	1.67	0.76
1:A:46:LEU:HD21	1:A:49:TYR:HB3	1.67	0.76
2:B:166:LEU:HG	2:B:191:VAL:HG21	1.64	0.76
1:A:49:TYR:HB2	2:B:100(C):TYR:O	1.86	0.76
2:H:41:PRO:HD3	2:H:87:THR:O	1.85	0.76
2:B:222:LYS:HE3	2:B:226:GLU:OE1	1.86	0.76
1:A:189:HIS:O	1:A:211:ARG:HD3	1.86	0.76
2:B:29:LEU:O	2:B:53:SER:HB3	1.87	0.75
2:B:67:LEU:HD22	2:B:82:MET:HG2	1.69	0.75
2:H:41:PRO:O	2:H:43:LYS:HE3	1.87	0.75
1:A:185:GLU:HA	1:A:188:ARG:HD2	1.69	0.75
1:A:55:PHE:O	1:A:58:VAL:HB	1.87	0.75
2:H:11:LEU:O	2:H:12:VAL:HG13	1.87	0.75
1:L:73:LEU:HD23	1:L:75:ILE:HD11	1.67	0.75
2:H:19:SER:HA	2:H:80:LEU:O	1.87	0.74
2:B:72:ASP:OD1	2:B:75:LYS:HB2	1.88	0.74
1:L:27(D):HIS:HB3	1:L:28:ASN:OD1	1.88	0.74
2:H:153:THR:HG23	2:H:211:ALA:HB3	1.67	0.74
1:L:147:LYS:HG3	1:L:154:GLU:HG2	1.69	0.74
1:L:150:ILE:HG13	1:L:155:ARG:HG2	1.69	0.73
2:B:38:ARG:HD2	2:B:88:ALA:HB3	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG12	1:A:197:THR:O	1.89	0.73
1:A:159:VAL:HG22	1:A:179:LEU:HB2	1.69	0.73
1:L:1:GLU:N	1:L:95:PRO:HD2	2.04	0.73
1:A:12:PRO:HA	1:A:105:GLU:O	1.88	0.73
2:H:150:GLU:OE2	2:H:176:ALA:HB3	1.89	0.73
2:B:122:TYR:HA	2:B:221:LYS:HZ2	1.54	0.73
1:A:117:ILE:HG21	1:A:207:LYS:O	1.89	0.72
2:B:29:LEU:HD13	2:B:71:LYS:HE2	1.72	0.72
1:A:54:ARG:NH2	1:A:63:SER:HA	2.04	0.72
1:A:33:LEU:HA	1:A:89:PHE:O	1.89	0.72
1:A:50:LYS:HB2	1:A:53:ASN:HD22	1.54	0.72
2:B:228:ARG:HG3	2:B:228:ARG:O	1.89	0.72
2:B:11:LEU:HD12	2:B:110:THR:HG22	1.72	0.71
2:H:124:LEU:HD21	2:H:143:LEU:HB2	1.72	0.71
2:H:19:SER:HB3	2:H:81:LYS:HD3	1.72	0.71
2:H:66:ARG:O	2:H:82:MET:HG3	1.89	0.71
1:L:115:VAL:HA	1:L:135:PHE:O	1.91	0.71
2:H:63:LEU:HD12	2:H:67:LEU:HD11	1.72	0.71
1:A:83:LEU:HD23	1:A:167:ASP:O	1.89	0.71
2:H:121:VAL:HG21	2:H:219:VAL:HB	1.72	0.71
1:A:80:ALA:O	1:A:83:LEU:HB2	1.91	0.71
1:A:125:LEU:O	1:A:183:LYS:HD2	1.91	0.70
1:A:48:ILE:HA	1:A:53:ASN:O	1.92	0.70
1:A:27(B):ILE:HG12	1:A:90:GLN:HG3	1.72	0.70
2:H:100(A):ILE:HD12	2:H:100(A):ILE:O	1.92	0.70
1:A:147:LYS:HD2	1:A:195:GLU:HG3	1.74	0.70
1:A:33:LEU:HD21	1:A:35:TRP:HE1	1.57	0.70
1:L:13:VAL:HG12	1:L:105:GLU:O	1.92	0.70
1:A:52:SER:HB3	1:A:64:GLY:O	1.91	0.69
2:H:94:LYS:HG2	2:H:101:ASP:HB3	1.74	0.69
1:A:187:GLU:HG3	1:A:211:ARG:NH2	2.06	0.69
2:B:59:TYR:HE1	2:B:69:ILE:H	1.39	0.69
2:H:149:PRO:HD2	2:H:214:ALA:HB1	1.74	0.69
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.06	0.69
2:H:162:ASN:ND2	2:H:166:LEU:HD23	2.08	0.69
2:H:37:VAL:HG21	2:H:100(E):MET:HE1	1.75	0.69
1:L:143:ASP:HB2	1:L:199:LYS:HE3	1.75	0.69
1:L:206:VAL:O	1:L:207:LYS:HD3	1.93	0.69
1:A:116:SER:OG	2:B:139:THR:HG21	1.92	0.69
2:H:208:CYS:O	2:H:220:ASP:HA	1.93	0.69
2:H:66:ARG:O	2:H:82:MET:HA	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27(D):HIS:HB3	1:A:28:ASN:OD1	1.94	0.68
2:H:210:VAL:O	2:H:218:THR:HG23	1.93	0.68
2:B:154:VAL:HG21	2:B:189:SER:HB2	1.75	0.68
1:A:119:PRO:HA	1:A:132:VAL:HG13	1.74	0.68
1:L:12:PRO:HA	1:L:105:GLU:HG2	1.75	0.68
2:B:37:VAL:HG13	2:B:46:GLU:O	1.94	0.68
1:A:184:ASP:O	1:A:188:ARG:HG2	1.94	0.68
2:H:4:LEU:HG	2:H:24:VAL:HG22	1.75	0.68
2:B:93:ALA:HB1	2:B:100(E):MET:HB3	1.75	0.67
2:B:36:TRP:O	2:B:48:VAL:HB	1.94	0.67
1:L:32:TYR:OH	2:H:100(A):ILE:HD13	1.93	0.67
1:A:161:ASN:HA	1:A:176:SER:O	1.94	0.67
1:A:138:ASN:HA	1:A:172:THR:HB	1.77	0.67
1:A:108:ARG:HG2	1:A:171:SER:HB2	1.74	0.67
2:B:122:TYR:HA	2:B:221:LYS:NZ	2.09	0.67
2:B:18:LEU:HD21	2:B:109:VAL:HG11	1.75	0.67
1:L:147:LYS:HD2	1:L:149:LYS:HD2	1.77	0.67
1:L:150:ILE:HG22	1:L:189:HIS:CD2	2.30	0.67
1:A:130:ALA:O	1:A:180:THR:HG23	1.95	0.67
2:B:90:TYR:O	2:B:107:THR:HG22	1.95	0.67
1:L:133:VAL:HG21	2:H:143:LEU:HD13	1.75	0.67
1:A:80:ALA:HA	1:A:106:ILE:HD13	1.76	0.66
2:B:138:VAL:HG23	2:B:193:VAL:O	1.94	0.66
1:A:108:ARG:HD3	1:A:140:TYR:CD2	2.30	0.66
1:A:141:PRO:HG2	1:A:199:LYS:HE3	1.76	0.66
1:A:147:LYS:HD3	1:A:149:LYS:HE3	1.77	0.66
1:L:190:ASN:HA	1:L:211:ARG:NH1	2.11	0.66
1:L:189:HIS:HB2	1:L:192:TYR:OH	1.96	0.66
1:A:191:SER:HA	1:A:210:ASN:HA	1.77	0.66
2:B:22:CYS:HB3	2:B:78:VAL:HB	1.78	0.65
1:L:184:ASP:O	1:L:187:GLU:HB3	1.96	0.65
2:H:176:ALA:HB2	2:H:187:MET:HB3	1.77	0.65
2:B:11:LEU:O	2:B:12:VAL:HG13	1.95	0.65
2:H:171:VAL:HG22	2:H:191:VAL:CG2	2.23	0.65
1:L:4:MET:HA	1:L:24:ARG:O	1.96	0.65
1:L:21:ILE:O	1:L:72:THR:HA	1.96	0.65
1:L:15:LEU:HD11	1:L:108:ARG:HB3	1.79	0.65
1:L:1:GLU:H1	1:L:95:PRO:HD2	1.60	0.65
2:B:6:GLU:OE2	2:B:91:TYR:HA	1.96	0.65
2:B:7:SER:O	2:B:20:ILE:HG23	1.96	0.65
2:H:63:LEU:HD13	2:H:67:LEU:HD21	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:TYR:O	2:B:185:TYR:HB2	1.98	0.64
2:H:34:VAL:HG22	2:H:94:LYS:HA	1.78	0.64
2:H:145:LYS:HD2	2:H:186:THR:OG1	1.96	0.64
1:A:21:ILE:O	1:A:72:THR:HA	1.98	0.64
2:B:108:THR:HG21	2:B:151:PRO:HD3	1.78	0.64
2:B:96:TRP:HA	2:B:101:ASP:OD2	1.97	0.64
1:L:193:THR:HA	1:L:208:SER:HA	1.78	0.64
1:L:193:THR:HG23	1:L:208:SER:HB2	1.79	0.64
1:A:2:LEU:HG	1:A:27:GLN:HG2	1.80	0.64
2:B:157:TRP:CZ3	2:B:208:CYS:HB3	2.33	0.64
1:L:37:LEU:HD12	1:L:38:GLN:H	1.63	0.64
1:A:117:ILE:HD13	1:A:207:LYS:O	1.98	0.63
2:H:9:PRO:HG2	2:H:18:LEU:HD13	1.78	0.63
1:A:66:GLY:HA3	1:A:71:PHE:HD2	1.62	0.63
1:L:13:VAL:HG11	1:L:104:LEU:HD11	1.81	0.63
1:L:22:SER:HA	1:L:71:PHE:O	1.98	0.63
1:A:33:LEU:HD11	1:A:35:TRP:NE1	2.14	0.63
1:L:13:VAL:O	1:L:106:ILE:HA	1.99	0.63
1:A:113:PRO:HG2	1:A:205:ILE:HD12	1.81	0.63
2:H:72:ASP:OD2	2:H:75:LYS:HD3	1.98	0.63
1:L:182:THR:OG1	1:L:185:GLU:HG3	1.99	0.63
2:H:206:THR:HG23	2:H:221:LYS:O	1.99	0.63
1:L:108:ARG:HD3	1:L:171:SER:O	1.98	0.63
2:H:157:TRP:HZ3	2:H:223:LEU:HD11	1.64	0.63
2:B:178:LEU:HG	2:B:179:GLN:H	1.62	0.63
1:L:191:SER:HA	1:L:210:ASN:HA	1.79	0.63
1:A:106:ILE:O	1:A:140:TYR:OH	2.13	0.62
1:L:107:LYS:HA	1:L:140:TYR:OH	1.99	0.62
1:L:46:LEU:HD23	1:L:55:PHE:CD2	2.33	0.62
1:A:34:GLU:OE2	2:B:100(D):GLY:HA2	1.99	0.62
1:L:25:SER:HB3	1:L:27(B):ILE:HD12	1.81	0.62
1:A:38:GLN:HG3	1:A:42:GLN:O	1.99	0.62
1:A:49:TYR:HE2	2:B:100(C):TYR:HD2	1.44	0.62
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.34	0.62
2:B:179:GLN:O	2:B:179:GLN:HG2	1.98	0.62
2:H:30:THR:O	2:H:53:SER:HB2	2.00	0.62
1:L:181:LEU:HD13	1:L:185:GLU:HB2	1.81	0.62
1:A:117:ILE:HD12	1:A:194:CYS:CB	2.28	0.62
1:A:187:GLU:HA	1:A:211:ARG:NH2	2.15	0.62
2:B:213:PRO:HA	2:B:216:SER:HA	1.81	0.62
1:L:62:PHE:CD2	1:L:75:ILE:HG12	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:CE1	1:A:75:ILE:HG12	2.35	0.62
1:A:16:GLY:O	1:A:77:ARG:HD3	2.00	0.62
1:L:46:LEU:HD21	1:L:49:TYR:HB3	1.82	0.62
2:H:120:SER:HB2	2:H:145:LYS:O	1.98	0.61
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.35	0.61
1:A:190:ASN:HD21	1:A:210:ASN:HB3	1.65	0.61
1:L:33:LEU:HD22	1:L:71:PHE:CD2	2.35	0.61
1:L:149:LYS:HA	1:L:153:SER:O	2.00	0.61
1:A:182:THR:HG23	1:A:185:GLU:OE2	1.99	0.61
1:A:186:TYR:CZ	1:A:211:ARG:HD2	2.35	0.61
1:A:83:LEU:HD21	1:A:166:GLN:NE2	2.15	0.61
1:L:108:ARG:HD2	1:L:171:SER:HB2	1.83	0.61
2:B:152:VAL:HG21	2:B:187:MET:HG2	1.83	0.61
1:A:188:ARG:N	1:A:211:ARG:HH12	1.98	0.61
1:A:146:VAL:HG22	1:A:196:ALA:HB2	1.81	0.61
1:L:120:PRO:HD3	1:L:132:VAL:HG13	1.82	0.61
2:B:123:PRO:HD3	2:B:221:LYS:NZ	2.16	0.60
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.82	0.60
2:B:209:SER:HA	2:B:220:ASP:HA	1.83	0.60
1:L:133:VAL:HG11	2:H:143:LEU:HD13	1.83	0.60
1:L:146:VAL:HG22	1:L:196:ALA:HB2	1.83	0.60
1:L:83:LEU:HD12	1:L:106:ILE:HD12	1.82	0.60
1:L:146:VAL:HG22	1:L:196:ALA:CB	2.31	0.60
1:L:167:ASP:O	1:L:171:SER:HA	2.02	0.60
1:A:190:ASN:ND2	1:A:210:ASN:HB3	2.16	0.60
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.37	0.60
2:H:66:ARG:HB3	2:H:66:ARG:HH11	1.65	0.60
2:H:96:TRP:HB2	2:H:101:ASP:HB2	1.82	0.60
1:L:19:ALA:O	1:L:74:LYS:HA	2.01	0.60
2:H:50:VAL:HG12	2:H:58:ASN:O	2.01	0.60
2:B:68:SER:OG	2:B:81:LYS:HB2	2.02	0.60
2:B:35:ASP:HB2	2:B:93:ALA:HB3	1.83	0.60
1:A:115:VAL:HG22	1:A:136:LEU:HG	1.84	0.59
1:A:142:LYS:HD2	1:A:173:TYR:CZ	2.37	0.59
2:B:53:SER:HA	2:B:71:LYS:NZ	2.17	0.59
1:A:33:LEU:HG	1:A:33:LEU:O	2.02	0.59
2:B:2:VAL:HG22	2:B:27:PHE:HD1	1.66	0.59
1:A:2:LEU:HA	1:A:26:SER:OG	2.02	0.59
2:B:51:ILE:HD11	2:B:71:LYS:HD2	1.84	0.59
1:A:159:VAL:HG23	1:A:179:LEU:HD13	1.85	0.59
2:B:156:THR:O	2:B:208:CYS:HA	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:LYS:HE2	1:L:81:GLU:O	2.03	0.59
1:A:150:ILE:HG23	1:A:192:TYR:CE1	2.38	0.59
1:A:18:GLN:CB	1:A:76:ASN:HA	2.31	0.59
2:B:122:TYR:O	2:B:142:CYS:HA	2.03	0.58
2:H:80:LEU:O	2:H:80:LEU:HD23	2.02	0.58
1:L:54:ARG:CZ	1:L:60:ASP:HA	2.33	0.58
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.38	0.58
2:B:194:PRO:HB2	2:B:196:SER:OG	2.03	0.58
1:A:190:ASN:HA	1:A:211:ARG:CB	2.30	0.58
1:A:39:LYS:HB2	1:A:42:GLN:HG3	1.85	0.58
1:L:139:PHE:HE1	1:L:142:LYS:HA	1.68	0.58
1:A:147:LYS:HD3	1:A:149:LYS:HG3	1.86	0.58
2:B:90:TYR:HE1	2:B:109:VAL:HB	1.67	0.58
2:B:138:VAL:HG12	2:B:139:THR:H	1.68	0.58
2:H:4:LEU:HD22	2:H:92:CYS:O	2.04	0.58
1:L:147:LYS:CD	1:L:154:GLU:HG2	2.33	0.58
1:L:147:LYS:CG	1:L:154:GLU:HG2	2.33	0.58
1:A:37:LEU:HD12	1:A:38:GLN:N	2.19	0.58
1:A:44:PRO:HG2	2:B:103:TRP:CZ3	2.39	0.58
1:L:192:TYR:HB2	1:L:209:PHE:CE1	2.38	0.58
1:L:78:VAL:HA	1:L:82:ASP:OD2	2.03	0.58
2:H:124:LEU:HD21	2:H:143:LEU:CB	2.34	0.58
1:L:40:PRO:O	1:L:42:GLN:HG2	2.03	0.58
1:A:145:ASN:O	1:A:196:ALA:HA	2.04	0.58
2:B:11:LEU:HA	2:B:110:THR:O	2.02	0.58
2:B:144:VAL:HG22	2:B:210:VAL:HG21	1.85	0.58
2:H:63:LEU:O	2:H:67:LEU:HG	2.03	0.58
1:L:119:PRO:HB3	1:L:209:PHE:CE2	2.38	0.58
1:L:37:LEU:HD22	1:L:86:TYR:CZ	2.39	0.57
1:A:37:LEU:HD11	1:A:84:GLY:HA3	1.87	0.57
2:B:20:ILE:HB	2:B:80:LEU:HD22	1.85	0.57
1:A:120:PRO:CG	1:A:132:VAL:HG22	2.34	0.57
1:A:27(B):ILE:HD11	1:A:90:GLN:OE1	2.04	0.57
1:A:46:LEU:HD23	1:A:55:PHE:CG	2.40	0.57
2:B:91:TYR:HE1	2:B:105:GLN:O	1.87	0.57
1:A:181:LEU:HB2	1:A:185:GLU:OE2	2.05	0.57
1:A:37:LEU:HD12	1:A:38:GLN:H	1.69	0.57
2:B:34:VAL:HG13	2:B:93:ALA:O	2.04	0.57
2:B:83:GLN:HB2	2:B:86:ASP:OD1	2.05	0.57
1:A:117:ILE:CG2	1:A:207:LYS:HB3	2.34	0.56
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:THR:CB	2:B:69:ILE:HB	2.34	0.56
2:B:66:ARG:HD2	2:B:82(B):SER:HB3	1.87	0.56
2:H:71:LYS:HE2	2:H:73:ASN:OD1	2.05	0.56
2:B:178:LEU:HA	2:B:184:LEU:O	2.04	0.56
1:L:147:LYS:HD3	1:L:154:GLU:HG2	1.87	0.56
1:L:34:GLU:HG3	1:L:89:PHE:HD2	1.69	0.56
1:A:182:THR:OG1	1:A:185:GLU:HG3	2.05	0.56
1:L:37:LEU:HD12	1:L:38:GLN:N	2.20	0.56
2:B:36:TRP:HZ3	2:B:90:TYR:O	1.88	0.56
1:L:27(B):ILE:HD11	1:L:90:GLN:HB2	1.86	0.56
1:A:120:PRO:HG3	1:A:132:VAL:HG22	1.88	0.56
1:A:46:LEU:HD11	1:A:49:TYR:HB3	1.86	0.56
1:A:118:PHE:HE1	2:B:126:PRO:HG3	1.70	0.56
2:H:36:TRP:O	2:H:48:VAL:HB	2.05	0.56
1:L:95:PRO:HG2	2:H:61:SER:OG	2.06	0.56
1:A:188:ARG:HG3	1:A:189:HIS:CD2	2.41	0.56
1:A:118:PHE:CZ	2:B:140:LEU:HA	2.41	0.56
1:A:21:ILE:HG13	1:A:73:LEU:HD23	1.88	0.56
1:A:115:VAL:HA	1:A:135:PHE:O	2.06	0.56
1:A:15:LEU:HA	1:A:78:VAL:O	2.06	0.56
2:H:20:ILE:HD13	2:H:107:THR:CG2	2.36	0.56
1:L:120:PRO:HD2	1:L:186:TYR:OH	2.05	0.56
1:A:146:VAL:HG22	1:A:196:ALA:CB	2.35	0.56
2:B:200:PRO:HB3	2:B:227:PRO:HG3	1.87	0.56
2:B:51:ILE:HD12	2:B:57:THR:CG2	2.36	0.56
2:B:87:THR:HG23	2:B:111:VAL:N	2.12	0.56
2:H:11:LEU:HG	2:H:12:VAL:N	2.20	0.56
2:H:19:SER:HB3	2:H:81:LYS:HA	1.88	0.56
1:L:112:ALA:HA	1:L:200:THR:HG21	1.85	0.56
2:B:153:THR:HG23	2:B:211:ALA:HB3	1.88	0.55
2:B:156:THR:HG22	2:B:164:GLY:N	2.21	0.55
2:B:174:PHE:HD1	2:B:188:SER:O	1.90	0.55
2:B:29:LEU:HB3	2:B:71:LYS:HE2	1.88	0.55
1:A:50:LYS:HE2	1:A:53:ASN:ND2	2.22	0.55
2:B:124:LEU:O	2:B:140:LEU:HB3	2.06	0.55
1:L:27(C):VAL:HA	1:L:31:THR:HB	1.88	0.55
1:A:96:PRO:HG2	2:B:47:TRP:CG	2.42	0.55
2:B:119:PRO:CB	2:B:147:TYR:HB3	2.35	0.55
1:L:112:ALA:CA	1:L:200:THR:HG21	2.36	0.55
1:A:21:ILE:HB	1:A:73:LEU:HB3	1.87	0.55
2:B:157:TRP:HB2	2:B:166:LEU:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:GLN:HB2	2:H:122:TYR:CE1	2.41	0.55
2:H:93:ALA:HB1	2:H:100(E):MET:HB3	1.89	0.55
1:A:4:MET:HA	1:A:24:ARG:O	2.07	0.55
2:B:40:PRO:HA	2:B:88:ALA:HB2	1.89	0.55
1:A:120:PRO:CD	1:A:132:VAL:HG22	2.37	0.55
1:A:150:ILE:HG13	1:A:155:ARG:HG2	1.88	0.55
1:A:117:ILE:HB	1:A:134:CYS:SG	2.47	0.55
2:B:145:LYS:HA	2:B:186:THR:OG1	2.07	0.55
1:L:32:TYR:CE1	2:H:100(A):ILE:HD13	2.41	0.55
1:A:149:LYS:H	1:A:193:THR:HB	1.71	0.54
2:B:147:TYR:OH	2:B:150:GLU:OE2	2.25	0.54
2:B:29:LEU:CD1	2:B:71:LYS:HG3	2.35	0.54
1:L:125:LEU:HD22	1:L:183:LYS:HD3	1.88	0.54
1:L:150:ILE:O	1:L:151:ASP:HB2	2.05	0.54
2:B:50:VAL:CG1	2:B:58:ASN:HB2	2.34	0.54
1:L:3:VAL:HB	1:L:26:SER:HB3	1.89	0.54
1:A:150:ILE:HG23	1:A:192:TYR:CD1	2.42	0.54
1:A:183:LYS:O	1:A:187:GLU:HB2	2.07	0.54
1:A:50:LYS:CB	1:A:53:ASN:HD22	2.20	0.54
2:B:96:TRP:N	2:B:101:ASP:HB2	2.22	0.54
2:B:3:GLN:HG3	2:B:25:SER:OG	2.07	0.54
2:H:117:THR:OG1	2:H:184:LEU:HD21	2.08	0.54
1:L:12:PRO:HA	1:L:105:GLU:HB3	1.90	0.54
2:H:215:SER:O	2:H:217:THR:HG23	2.06	0.54
2:H:228:ARG:HG3	2:H:228:ARG:O	2.08	0.54
1:A:136:LEU:HD21	1:A:146:VAL:HG22	1.89	0.54
1:L:39:LYS:HB2	1:L:42:GLN:CG	2.34	0.54
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.89	0.54
2:H:36:TRP:HZ2	2:H:78:VAL:O	1.91	0.54
1:A:141:PRO:HD2	1:A:199:LYS:HG3	1.88	0.54
2:H:210:VAL:O	2:H:218:THR:HA	2.06	0.54
2:H:34:VAL:HG13	2:H:93:ALA:O	2.07	0.54
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.43	0.54
2:H:77:GLN:HB3	2:H:79:PHE:CE1	2.43	0.53
1:L:148:TRP:HB3	1:L:179:LEU:HD22	1.89	0.53
1:A:2:LEU:HD23	1:A:26:SER:OG	2.08	0.53
1:A:66:GLY:HA3	1:A:71:PHE:CD2	2.42	0.53
1:A:46:LEU:HD23	1:A:55:PHE:CD1	2.43	0.53
2:B:79:PHE:HB3	2:B:81:LYS:NZ	2.22	0.53
2:H:157:TRP:CH2	2:H:208:CYS:HB3	2.43	0.53
1:A:168:SER:O	1:A:169:LYS:HD3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:HD12	2:B:110:THR:CG2	2.39	0.53
2:H:59:TYR:CD2	2:H:67:LEU:HB2	2.44	0.53
1:L:139:PHE:CE1	1:L:142:LYS:HA	2.43	0.53
1:L:184:ASP:O	1:L:188:ARG:HG2	2.09	0.53
2:H:143:LEU:HD12	2:H:188:SER:HB3	1.91	0.53
2:H:154:VAL:HG22	2:H:210:VAL:HG22	1.91	0.53
1:A:27:GLN:O	1:A:69:THR:HG23	2.09	0.53
1:A:27(D):HIS:HB2	1:A:30:ASN:H	1.73	0.53
1:L:32:TYR:CZ	2:H:100(A):ILE:HD13	2.44	0.53
1:L:36:TYR:CZ	1:L:46:LEU:HD13	2.44	0.53
1:A:138:ASN:OD1	1:A:170:ASP:OD2	2.26	0.52
1:A:49:TYR:CE2	2:B:100(C):TYR:HD2	2.25	0.52
2:B:80:LEU:HD23	2:B:80:LEU:O	2.09	0.52
1:L:27(B):ILE:HG13	1:L:90:GLN:HG3	1.91	0.52
2:H:83:GLN:O	2:H:86:ASP:HB2	2.09	0.52
1:A:55:PHE:HB3	1:A:58:VAL:CG2	2.40	0.52
1:A:187:GLU:HA	1:A:211:ARG:CZ	2.40	0.52
2:B:40:PRO:CB	2:B:43:LYS:HD3	2.33	0.52
1:A:142:LYS:HD2	1:A:173:TYR:CE1	2.45	0.52
2:B:94:LYS:O	2:B:100(E):MET:HA	2.10	0.52
2:B:18:LEU:CD2	2:B:109:VAL:HG11	2.40	0.52
1:A:163:TRP:O	2:B:175:PRO:HG2	2.09	0.52
2:B:150:GLU:OE2	2:B:176:ALA:HB2	2.10	0.52
2:H:4:LEU:HG	2:H:24:VAL:CG2	2.38	0.52
1:A:117:ILE:HG22	1:A:207:LYS:HB3	1.91	0.52
2:H:61:SER:HA	2:H:64:MET:CE	2.40	0.52
1:L:144:ILE:HG13	1:L:198:HIS:CD2	2.44	0.52
1:A:162:SER:O	1:A:175:MET:HA	2.10	0.51
1:A:95:PRO:HG2	2:B:61:SER:OG	2.10	0.51
1:L:190:ASN:O	1:L:211:ARG:HB2	2.11	0.51
2:B:179:GLN:O	2:B:184:LEU:HB2	2.10	0.51
1:L:4:MET:SD	1:L:27(B):ILE:HD11	2.49	0.51
1:A:166:GLN:HE21	1:A:171:SER:HB3	1.76	0.51
2:B:82:MET:O	2:B:82(C):LEU:HD21	2.10	0.51
1:A:49:TYR:CE1	1:A:53:ASN:HB3	2.45	0.51
2:H:149:PRO:HD2	2:H:214:ALA:CB	2.40	0.51
1:L:147:LYS:HD3	1:L:154:GLU:CG	2.41	0.51
2:B:116:THR:HA	2:B:148:PHE:O	2.09	0.51
2:B:60:ASN:HB3	2:B:63:LEU:CD1	2.40	0.51
2:H:67:LEU:O	2:H:68:SER:HB3	2.10	0.51
1:A:141:PRO:HB2	1:A:143:ASP:OD2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:CD2	1:A:49:TYR:HB3	2.37	0.51
2:B:66:ARG:NH1	2:B:82(B):SER:O	2.44	0.51
2:B:117:THR:OG1	2:B:148:PHE:HB3	2.10	0.51
2:H:162:ASN:OD1	2:H:205:VAL:HA	2.10	0.51
1:L:190:ASN:HD21	1:L:212:ASN:ND2	2.09	0.51
2:H:105:GLN:HG2	2:H:106:GLY:N	2.25	0.51
2:H:19:SER:CB	2:H:81:LYS:HD3	2.41	0.51
1:L:94:LEU:HD13	2:H:58:ASN:HD22	1.76	0.51
1:L:15:LEU:CD2	1:L:106:ILE:HG21	2.41	0.51
1:L:32:TYR:HD2	1:L:92:SER:HA	1.76	0.51
1:L:37:LEU:HD22	1:L:86:TYR:CE2	2.46	0.51
1:L:36:TYR:CE2	1:L:46:LEU:HD13	2.46	0.51
1:L:139:PHE:HD1	1:L:141:PRO:O	1.94	0.50
2:H:211:ALA:HA	2:H:218:THR:OG1	2.11	0.50
1:L:150:ILE:HG13	1:L:155:ARG:CG	2.41	0.50
1:A:108:ARG:HD3	1:A:140:TYR:CG	2.46	0.50
1:A:55:PHE:HB3	1:A:58:VAL:HG21	1.93	0.50
2:B:204:THR:HG23	2:B:204:THR:O	2.11	0.50
2:H:116:THR:O	2:H:116:THR:HG22	2.09	0.50
1:L:142:LYS:HG2	1:L:142:LYS:O	2.12	0.50
1:L:49:TYR:CZ	1:L:53:ASN:HB3	2.47	0.50
2:B:90:TYR:CE1	2:B:109:VAL:HB	2.45	0.50
1:L:20:SER:HA	1:L:73:LEU:O	2.12	0.50
1:L:20:SER:OG	1:L:74:LYS:HG2	2.12	0.50
1:A:159:VAL:CG2	1:A:179:LEU:HD13	2.42	0.50
2:B:10:GLY:O	2:B:109:VAL:HA	2.12	0.50
2:H:14:PRO:O	2:H:15:SER:CB	2.59	0.50
2:H:168:SER:O	2:H:168:SER:OG	2.29	0.50
2:H:138:VAL:CG2	2:H:195:SER:HA	2.42	0.50
2:H:66:ARG:NH1	2:H:66:ARG:HB3	2.26	0.50
1:A:34:GLU:OE1	1:A:49:TYR:HB2	2.11	0.50
2:B:36:TRP:NE1	2:B:80:LEU:HB2	2.26	0.50
2:H:138:VAL:HG12	2:H:139:THR:H	1.76	0.50
1:L:54:ARG:HD3	1:L:58:VAL:HG12	1.94	0.50
2:B:60:ASN:HB3	2:B:63:LEU:HD12	1.94	0.50
2:B:94:LYS:HB3	2:B:102:HIS:O	2.12	0.50
1:L:212:ASN:OD1	1:A:156:GLN:O	2.30	0.50
2:H:204:THR:OG1	2:H:222:LYS:HE3	2.12	0.50
1:L:123:GLU:O	1:L:126:THR:OG1	2.25	0.50
1:L:90:GLN:OE1	1:L:93:HIS:O	2.30	0.50
1:A:100:GLY:O	1:A:101:GLY:O	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:O	1:A:155:ARG:HD3	2.11	0.49
2:H:209:SER:HA	2:H:220:ASP:HA	1.94	0.49
2:H:72:ASP:HB2	2:H:79:PHE:HZ	1.77	0.49
1:A:34:GLU:OE1	2:B:100(C):TYR:O	2.29	0.49
1:A:151:ASP:OD1	1:A:191:SER:O	2.30	0.49
2:B:157:TRP:HB2	2:B:166:LEU:CB	2.42	0.49
2:H:154:VAL:HA	2:H:209:SER:O	2.12	0.49
1:L:124:GLN:HB2	2:H:122:TYR:CD1	2.47	0.49
1:L:83:LEU:CD1	1:L:106:ILE:HD12	2.41	0.49
2:H:2:VAL:CG2	2:H:26:GLY:HA3	2.42	0.49
1:A:150:ILE:O	1:A:151:ASP:HB2	2.11	0.49
1:L:133:VAL:CG2	2:H:143:LEU:HD13	2.40	0.49
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.47	0.49
1:A:149:LYS:HB2	1:A:193:THR:CB	2.43	0.49
2:H:199:TRP:CH2	2:H:227:PRO:HG3	2.47	0.49
1:L:34:GLU:OE1	2:H:100(C):TYR:O	2.30	0.49
2:B:105:GLN:OE1	2:B:106:GLY:O	2.30	0.49
2:H:162:ASN:HB2	2:H:166:LEU:HB2	1.95	0.49
2:B:94:LYS:CG	2:B:101:ASP:HB3	2.42	0.49
2:B:30:THR:OG1	2:B:31:ASN:OD1	2.30	0.49
2:H:72:ASP:CG	2:H:75:LYS:HB2	2.33	0.49
2:H:90:TYR:O	2:H:107:THR:HG22	2.13	0.49
1:L:182:THR:OG1	1:L:184:ASP:HB2	2.13	0.49
2:B:51:ILE:HB	2:B:57:THR:HG22	1.94	0.49
1:L:125:LEU:HD22	1:L:183:LYS:CD	2.42	0.49
2:H:34:VAL:HG22	2:H:93:ALA:O	2.13	0.49
2:H:63:LEU:CD1	2:H:67:LEU:HD21	2.43	0.49
1:A:120:PRO:HA	1:A:131:SER:O	2.13	0.48
2:B:20:ILE:HD13	2:B:90:TYR:HB2	1.94	0.48
2:B:209:SER:HB2	2:B:220:ASP:OD2	2.13	0.48
2:B:40:PRO:HB2	2:B:43:LYS:HB2	1.95	0.48
2:H:20:ILE:CG2	2:H:107:THR:HG21	2.38	0.48
2:H:36:TRP:CD1	2:H:69:ILE:HG12	2.48	0.48
1:A:146:VAL:HG21	1:A:175:MET:SD	2.53	0.48
2:B:213:PRO:C	2:B:216:SER:H	2.17	0.48
2:H:63:LEU:HB2	2:H:67:LEU:CD2	2.38	0.48
1:L:83:LEU:HD22	1:L:166:GLN:O	2.13	0.48
1:L:12:PRO:HA	1:L:105:GLU:CG	2.43	0.48
1:L:175:MET:HG2	1:L:176:SER:N	2.28	0.48
1:L:24:ARG:HA	1:L:69:THR:O	2.13	0.48
1:A:147:LYS:CD	1:A:149:LYS:HE3	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:CD1	1:A:97:THR:O	2.67	0.48
2:B:108:THR:CG2	2:B:151:PRO:HD3	2.43	0.48
2:B:87:THR:CG2	2:B:111:VAL:H	2.18	0.48
2:H:87:THR:HG23	2:H:110:THR:HA	1.94	0.48
2:B:16:GLN:HB3	2:B:17:SER:H	1.49	0.48
2:B:72:ASP:CG	2:B:75:LYS:HB2	2.33	0.48
1:L:27(D):HIS:HB2	1:L:30:ASN:O	2.13	0.48
2:B:36:TRP:CD2	2:B:80:LEU:HD13	2.48	0.48
1:L:192:TYR:O	1:L:209:PHE:N	2.46	0.48
1:A:190:ASN:CG	1:A:211:ARG:H	2.17	0.48
1:A:120:PRO:HD3	1:A:132:VAL:CG1	2.40	0.48
1:L:145:ASN:O	1:L:196:ALA:HA	2.13	0.48
1:A:83:LEU:HD21	1:A:166:GLN:CD	2.35	0.47
1:A:186:TYR:O	1:A:211:ARG:NH1	2.46	0.47
2:B:20:ILE:HB	2:B:80:LEU:CD2	2.44	0.47
2:H:81:LYS:O	2:H:82:MET:HB2	2.14	0.47
1:A:81:GLU:HG2	1:A:169:LYS:HE2	1.96	0.47
2:B:222:LYS:HD2	2:B:226:GLU:OE2	2.14	0.47
1:L:79:GLU:CB	1:L:81:GLU:HG3	2.44	0.47
2:B:57:THR:HG21	2:B:69:ILE:HB	1.95	0.47
2:H:166:LEU:HD11	2:H:193:VAL:HG12	1.97	0.47
1:L:148:TRP:CD1	1:L:179:LEU:HD13	2.49	0.47
1:L:73:LEU:CD2	1:L:75:ILE:HD11	2.41	0.47
1:A:8:PRO:HG2	1:A:11:LEU:HB2	1.95	0.47
1:A:69:THR:HB	1:A:70:ASP:OD1	2.13	0.47
2:B:91:TYR:CE1	2:B:106:GLY:HA3	2.49	0.47
2:H:116:THR:HA	2:H:148:PHE:O	2.14	0.47
2:H:94:LYS:HG3	2:H:95:HIS:N	2.28	0.47
1:L:108:ARG:CD	1:L:171:SER:HB2	2.44	0.47
2:B:38:ARG:HG3	2:B:39:GLN:N	2.28	0.47
1:L:181:LEU:HB2	1:L:185:GLU:OE1	2.14	0.47
2:H:20:ILE:HD13	2:H:107:THR:HG21	1.97	0.47
2:H:162:ASN:HB2	2:H:166:LEU:HD23	1.96	0.47
2:H:38:ARG:HA	2:H:89:VAL:O	2.13	0.47
1:L:25:SER:CB	1:L:27(B):ILE:HD12	2.43	0.47
1:A:16:GLY:C	1:A:77:ARG:HA	2.35	0.47
1:A:83:LEU:HD12	1:A:104:LEU:O	2.15	0.47
2:B:86:ASP:O	2:B:90:TYR:OH	2.30	0.47
1:L:54:ARG:HD3	1:L:59:PRO:O	2.14	0.47
1:A:38:GLN:NE2	1:A:42:GLN:O	2.44	0.47
2:B:53:SER:HA	2:B:71:LYS:HZ2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:CYS:HB3	2:B:78:VAL:O	2.14	0.47
2:H:19:SER:HB3	2:H:81:LYS:CD	2.43	0.47
2:H:157:TRP:CZ3	2:H:208:CYS:HB3	2.49	0.47
2:H:64:MET:HA	2:H:67:LEU:HG	1.95	0.47
1:A:170:ASP:OD1	1:A:172:THR:OG1	2.30	0.47
1:A:187:GLU:HG3	1:A:211:ARG:HH22	1.79	0.47
2:B:94:LYS:HG2	2:B:101:ASP:HB3	1.97	0.47
1:L:44:PRO:HG2	2:H:103:TRP:CZ3	2.50	0.47
1:A:147:LYS:HG2	1:A:148:TRP:N	2.29	0.47
2:H:97:GLY:CA	2:H:100(C):TYR:H	2.17	0.47
2:B:88:ALA:O	2:B:109:VAL:O	2.33	0.47
2:B:95:HIS:C	2:B:101:ASP:HB2	2.35	0.47
2:H:38:ARG:HG2	2:H:46:GLU:HB2	1.97	0.47
1:A:117:ILE:HA	1:A:134:CYS:HA	1.97	0.46
2:H:97:GLY:HA3	2:H:100(B):PRO:HA	1.97	0.46
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.49	0.46
2:H:71:LYS:HE2	2:H:73:ASN:CG	2.36	0.46
2:H:9:PRO:HG2	2:H:18:LEU:CD1	2.44	0.46
1:A:83:LEU:HD22	1:A:106:ILE:CD1	2.45	0.46
1:A:141:PRO:HD2	1:A:198:HIS:NE2	2.31	0.46
1:A:147:LYS:HG3	1:A:154:GLU:CD	2.34	0.46
1:A:52:SER:HA	1:A:64:GLY:CA	2.34	0.46
2:H:206:THR:HA	2:H:221:LYS:O	2.15	0.46
1:L:192:TYR:O	1:L:208:SER:HA	2.16	0.46
1:A:120:PRO:CB	1:A:125:LEU:HD21	2.45	0.46
1:A:35:TRP:CZ2	1:A:88:CYS:HB3	2.51	0.46
1:A:32:TYR:HD2	1:A:91:GLY:O	1.98	0.46
2:B:169:SER:O	2:B:191:VAL:HA	2.15	0.46
2:H:186:THR:HG22	2:H:186:THR:O	2.14	0.46
1:A:51:VAL:CG1	1:A:66:GLY:HA3	2.46	0.46
2:B:2:VAL:HG22	2:B:27:PHE:CD1	2.48	0.46
2:B:51:ILE:CB	2:B:57:THR:HG22	2.45	0.46
1:L:131:SER:HA	1:L:180:THR:HA	1.97	0.46
1:L:42:GLN:H	1:L:42:GLN:HG2	1.47	0.46
1:A:34:GLU:HB2	1:A:36:TYR:CE1	2.51	0.46
1:A:36:TYR:CZ	2:B:100(E):MET:HE3	2.50	0.46
2:B:121:VAL:HG21	2:B:210:VAL:HB	1.97	0.46
2:H:63:LEU:CD1	2:H:67:LEU:HD11	2.43	0.46
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.98	0.46
1:A:149:LYS:HB2	1:A:193:THR:HB	1.96	0.46
1:A:54:ARG:NE	1:A:62:PHE:O	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:TYR:OH	2:B:150:GLU:HG2	2.15	0.46
2:B:154:VAL:HG23	2:B:187:MET:HE3	1.97	0.46
2:H:71:LYS:HG2	2:H:72:ASP:N	2.29	0.46
1:L:119:PRO:HA	1:L:132:VAL:HG13	1.98	0.46
1:L:12:PRO:HA	1:L:105:GLU:CB	2.46	0.46
1:A:149:LYS:HA	1:A:153:SER:O	2.16	0.46
1:A:130:ALA:C	1:A:180:THR:HG23	2.36	0.46
1:A:25:SER:CB	1:A:27(B):ILE:HD12	2.45	0.46
2:B:96:TRP:HB2	2:B:101:ASP:HA	1.97	0.46
2:B:66:ARG:NH2	2:B:83:GLN:OE1	2.49	0.46
2:H:66:ARG:NH1	2:H:82(A):ASN:O	2.48	0.46
1:L:135:PHE:HE1	1:L:176:SER:HG	1.63	0.46
1:L:182:THR:CG2	1:L:185:GLU:OE2	2.60	0.46
1:L:193:THR:HA	1:L:208:SER:CA	2.46	0.46
1:L:89:PHE:CZ	1:L:96:PRO:HB2	2.51	0.46
2:B:35:ASP:OD1	2:B:95:HIS:NE2	2.49	0.46
2:H:204:THR:HG23	2:H:204:THR:O	2.16	0.46
1:L:113:PRO:HG2	1:L:205:ILE:CD1	2.42	0.46
1:L:147:LYS:HB3	1:L:147:LYS:HE2	1.33	0.46
2:H:169:SER:HB3	2:H:192:THR:HB	1.98	0.45
1:L:203:SER:OG	1:L:204:PRO:HD2	2.16	0.45
1:A:83:LEU:CD1	1:A:106:ILE:HD12	2.34	0.45
1:A:130:ALA:O	1:A:180:THR:HA	2.17	0.45
2:B:94:LYS:O	2:B:101:ASP:N	2.50	0.45
2:B:22:CYS:HB2	2:B:36:TRP:CZ2	2.51	0.45
2:B:50:VAL:O	2:B:58:ASN:N	2.47	0.45
1:A:10:SER:HB2	1:A:103:LYS:HB3	1.98	0.45
1:A:184:ASP:HB3	1:A:188:ARG:NH1	2.31	0.45
1:A:207:LYS:HD3	1:A:207:LYS:HA	1.65	0.45
1:A:47:LEU:HD11	1:A:86:TYR:CD2	2.51	0.45
2:H:157:TRP:CZ3	2:H:223:LEU:HD11	2.49	0.45
1:L:189:HIS:O	1:L:211:ARG:NH1	2.50	0.45
1:A:38:GLN:OE1	2:B:39:GLN:NE2	2.50	0.45
2:H:91:TYR:HE1	2:H:105:GLN:O	2.00	0.45
2:H:169:SER:O	2:H:191:VAL:HA	2.15	0.45
2:H:35:ASP:OD2	2:H:95:HIS:NE2	2.49	0.45
2:H:59:TYR:CB	2:H:64:MET:HB3	2.47	0.45
1:L:125:LEU:O	1:L:183:LYS:HG3	2.15	0.45
1:A:143:ASP:HB2	1:A:199:LYS:NZ	2.31	0.45
2:B:208:CYS:O	2:B:221:LYS:N	2.50	0.45
2:H:20:ILE:HD13	2:H:107:THR:HG23	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:SER:HB2	2:H:79:PHE:HD2	1.82	0.45
2:H:83:GLN:N	2:H:86:ASP:OD2	2.50	0.45
1:L:153:SER:OG	1:L:154:GLU:N	2.50	0.45
2:B:117:THR:N	2:B:148:PHE:O	2.50	0.45
2:B:35:ASP:OD2	2:B:47:TRP:NE1	2.49	0.45
2:B:46:GLU:O	2:B:48:VAL:HG23	2.17	0.45
1:L:133:VAL:CG1	2:H:143:LEU:HD13	2.46	0.45
2:H:40:PRO:HG2	2:H:43:LYS:CB	2.46	0.45
1:L:38:GLN:OE1	1:L:44:PRO:HG3	2.16	0.45
1:A:108:ARG:NE	1:A:109:ALA:O	2.50	0.45
2:B:45:LEU:N	2:B:45:LEU:HD23	2.32	0.45
2:B:51:ILE:HA	2:B:57:THR:HG22	1.97	0.45
1:A:166:GLN:NE2	1:A:171:SER:HB3	2.32	0.45
1:A:27(C):VAL:HG12	1:A:29:GLY:HA2	1.99	0.45
1:L:13:VAL:N	1:L:105:GLU:O	2.50	0.45
2:B:221:LYS:HA	2:B:221:LYS:HD2	1.91	0.44
2:B:24:VAL:HG22	2:B:27:PHE:CZ	2.52	0.44
2:H:141:GLY:HA3	2:H:189:SER:O	2.18	0.44
2:H:199:TRP:CG	2:H:200:PRO:HA	2.52	0.44
1:A:189:HIS:HB2	1:A:192:TYR:CZ	2.50	0.44
2:H:120:SER:N	2:H:145:LYS:O	2.50	0.44
2:H:12:VAL:CG2	2:H:82(C):LEU:HD13	2.46	0.44
2:H:21:THR:HA	2:H:79:PHE:HA	2.00	0.44
1:A:34:GLU:HB2	1:A:36:TYR:HE1	1.81	0.44
2:B:72:ASP:O	2:B:76:SER:N	2.50	0.44
2:H:72:ASP:HB2	2:H:79:PHE:CZ	2.51	0.44
1:L:161:ASN:HA	1:L:176:SER:O	2.17	0.44
2:B:120:SER:N	2:B:145:LYS:O	2.50	0.44
1:L:34:GLU:OE2	2:H:100(D):GLY:HA2	2.17	0.44
2:H:212:HIS:CE1	2:H:214:ALA:HB3	2.52	0.44
2:B:212:HIS:N	2:B:213:PRO:HD3	2.33	0.44
2:B:220:ASP:N	2:B:220:ASP:OD1	2.49	0.44
2:H:117:THR:N	2:H:148:PHE:O	2.50	0.44
1:L:13:VAL:CG1	1:L:104:LEU:HD11	2.45	0.44
1:L:148:TRP:CE2	1:L:179:LEU:HB2	2.53	0.44
2:B:209:SER:HB2	2:B:220:ASP:HB3	1.99	0.44
2:B:7:SER:OG	2:B:21:THR:OG1	2.35	0.44
2:H:206:THR:OG1	2:H:222:LYS:HG2	2.17	0.44
1:L:143:ASP:HB2	1:L:199:LYS:CE	2.47	0.44
1:L:90:GLN:NE2	1:L:97:THR:OG1	2.50	0.44
1:A:162:SER:OG	2:B:175:PRO:HD2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ILE:HD12	2:B:80:LEU:CD2	2.47	0.44
2:H:100(A):ILE:CD1	2:H:100(A):ILE:O	2.65	0.44
2:H:17:SER:OG	2:H:82(A):ASN:HA	2.17	0.44
2:B:147:TYR:CE2	2:B:152:VAL:HG13	2.52	0.44
2:H:124:LEU:HD21	2:H:143:LEU:N	2.33	0.44
2:H:67:LEU:N	2:H:67:LEU:HD23	2.32	0.43
1:L:143:ASP:O	1:L:198:HIS:HD2	2.01	0.43
2:B:47:TRP:HZ2	2:B:50:VAL:HB	1.82	0.43
2:B:50:VAL:HG11	2:B:52:TRP:CZ2	2.53	0.43
2:B:35:ASP:N	2:B:93:ALA:O	2.50	0.43
1:L:123:GLU:HG2	1:L:124:GLN:H	1.83	0.43
1:L:195:GLU:OE1	1:L:206:VAL:HG22	2.17	0.43
1:A:147:LYS:CD	1:A:149:LYS:HG3	2.46	0.43
1:A:188:ARG:HG3	1:A:189:HIS:HD2	1.80	0.43
2:B:29:LEU:HD11	2:B:77:GLN:O	2.18	0.43
2:H:162:ASN:CG	2:H:166:LEU:HD23	2.38	0.43
1:L:125:LEU:HD11	1:L:186:TYR:HE2	1.82	0.43
2:B:20:ILE:CG2	2:B:107:THR:HG21	2.36	0.43
2:B:178:LEU:HG	2:B:179:GLN:N	2.32	0.43
2:B:79:PHE:HB3	2:B:81:LYS:HZ3	1.83	0.43
2:H:162:ASN:CB	2:H:166:LEU:HD23	2.48	0.43
2:B:147:TYR:CE2	2:B:150:GLU:HG2	2.54	0.43
2:B:52:TRP:NE1	2:B:58:ASN:OD1	2.43	0.43
2:B:57:THR:OG1	2:B:69:ILE:HB	2.16	0.43
2:H:11:LEU:HD11	2:H:114:ALA:O	2.19	0.43
1:A:125:LEU:O	1:A:183:LYS:CD	2.63	0.43
2:H:32:TYR:O	2:H:53:SER:HB3	2.18	0.43
2:H:40:PRO:CB	2:H:43:LYS:HD2	2.33	0.43
2:H:29:LEU:HB2	2:H:73:ASN:OD1	2.19	0.43
1:L:27(B):ILE:O	1:L:31:THR:HB	2.19	0.43
2:B:213:PRO:O	2:B:216:SER:N	2.51	0.43
2:H:121:VAL:O	2:H:122:TYR:CD1	2.71	0.43
2:H:140:LEU:HD21	2:H:199:TRP:CE3	2.53	0.43
2:H:121:VAL:HG13	2:H:144:VAL:HG22	2.01	0.43
1:L:155:ARG:HD2	1:L:155:ARG:HA	1.68	0.43
1:L:34:GLU:HB2	1:L:36:TYR:CE1	2.54	0.43
1:A:8:PRO:HG3	1:A:11:LEU:HD13	2.00	0.43
1:L:188:ARG:HA	1:A:163:TRP:CZ3	2.53	0.43
2:B:53:SER:HA	2:B:71:LYS:HZ1	1.82	0.43
2:H:4:LEU:HD23	2:H:92:CYS:SG	2.59	0.43
1:L:6:GLN:OE1	1:L:101:GLY:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD21	1:A:196:ALA:HB1	2.00	0.43
1:A:141:PRO:CD	1:A:198:HIS:HE2	2.32	0.43
1:A:61:ARG:HH22	1:A:82:ASP:CG	2.21	0.43
2:H:96:TRP:HB2	2:H:101:ASP:CB	2.46	0.43
1:A:108:ARG:NH2	1:A:109:ALA:O	2.50	0.42
2:B:157:TRP:HB3	2:B:166:LEU:HD23	2.01	0.42
2:H:122:TYR:O	2:H:143:LEU:N	2.52	0.42
2:H:220:ASP:OD1	2:H:220:ASP:N	2.52	0.42
2:H:9:PRO:O	2:H:11:LEU:N	2.50	0.42
1:L:131:SER:CB	1:L:180:THR:HG1	2.31	0.42
1:A:141:PRO:HD2	1:A:198:HIS:HE2	1.83	0.42
2:B:154:VAL:HG23	2:B:187:MET:CE	2.49	0.42
2:B:59:TYR:CE1	2:B:69:ILE:HD12	2.54	0.42
1:L:145:ASN:O	1:L:197:THR:N	2.51	0.42
1:L:81:GLU:H	1:L:81:GLU:HG3	1.61	0.42
1:A:6:GLN:HG3	1:A:88:CYS:SG	2.60	0.42
2:H:147:TYR:O	2:H:185:TYR:HB2	2.19	0.42
2:H:213:PRO:C	2:H:216:SER:H	2.23	0.42
1:L:142:LYS:HB2	1:L:173:TYR:CE2	2.54	0.42
1:A:136:LEU:HD21	1:A:196:ALA:CB	2.49	0.42
2:H:162:ASN:ND2	2:H:166:LEU:CD2	2.81	0.42
1:L:79:GLU:HB3	1:L:81:GLU:HG3	2.01	0.42
1:A:118:PHE:HD1	2:B:126:PRO:HA	1.85	0.42
2:B:66:ARG:HD2	2:B:82(B):SER:CB	2.49	0.42
2:B:73:ASN:C	2:B:76:SER:H	2.22	0.42
2:B:9:PRO:O	2:B:11:LEU:N	2.50	0.42
1:A:159:VAL:HA	1:A:178:THR:O	2.19	0.42
1:L:124:GLN:HG3	2:H:122:TYR:CE2	2.54	0.42
1:A:108:ARG:HH22	1:A:111:ALA:HB2	1.80	0.42
2:B:198:THR:C	2:B:203:GLN:H	2.23	0.42
2:B:29:LEU:HD21	2:B:78:VAL:CG2	2.50	0.42
1:L:27(B):ILE:O	1:L:27(B):ILE:HG23	2.20	0.42
1:L:63:SER:O	1:L:73:LEU:HA	2.20	0.42
1:A:136:LEU:HD13	1:A:175:MET:CG	2.49	0.42
2:B:116:THR:HG21	2:B:215:SER:N	2.35	0.42
1:L:13:VAL:O	1:L:107:LYS:N	2.50	0.42
1:L:147:LYS:HD3	1:L:154:GLU:CD	2.40	0.42
1:A:147:LYS:HD2	1:A:195:GLU:HB2	2.02	0.42
1:A:195:GLU:O	1:A:196:ALA:HB2	2.20	0.42
1:A:21:ILE:HG13	1:A:73:LEU:HB3	2.01	0.42
1:A:27(D):HIS:O	1:A:29:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:HE1	1:A:75:ILE:HG12	1.84	0.42
2:B:186:THR:O	2:B:186:THR:HG22	2.20	0.42
2:B:139:THR:OG1	2:B:192:THR:OG1	2.30	0.42
2:B:215:SER:O	2:B:217:THR:HG23	2.20	0.42
1:L:37:LEU:O	1:L:45:LYS:N	2.52	0.42
1:A:136:LEU:HD13	1:A:175:MET:HG2	2.02	0.42
1:A:106:ILE:HB	1:A:166:GLN:HE22	1.85	0.42
2:B:121:VAL:HG21	2:B:219:VAL:O	2.20	0.42
2:H:18:LEU:HB3	2:H:82(C):LEU:HD21	2.02	0.42
1:L:141:PRO:HB2	1:L:143:ASP:OD2	2.20	0.42
1:L:103:LYS:NZ	1:L:165:ASP:OD2	2.53	0.42
2:B:12:VAL:O	2:B:111:VAL:HA	2.19	0.41
2:B:6:GLU:OE2	2:B:92:CYS:N	2.50	0.41
1:L:194:CYS:HB3	1:L:207:LYS:O	2.20	0.41
2:B:24:VAL:HG21	2:B:29:LEU:HD21	2.01	0.41
2:B:30:THR:OG1	2:B:31:ASN:N	2.53	0.41
2:B:51:ILE:HD13	2:B:71:LYS:HB3	2.01	0.41
2:H:36:TRP:HE1	2:H:69:ILE:HG23	1.86	0.41
1:L:18:GLN:HB2	1:L:76:ASN:OD1	2.20	0.41
1:A:169:LYS:HA	1:A:169:LYS:HD3	1.86	0.41
1:A:54:ARG:NH2	1:A:62:PHE:O	2.50	0.41
2:B:83:GLN:HB3	2:B:85:ASP:OD1	2.20	0.41
2:H:94:LYS:NZ	2:H:101:ASP:OD2	2.50	0.41
1:L:47:LEU:HA	1:L:58:VAL:HG21	2.03	0.41
1:A:48:ILE:HD13	1:A:54:ARG:HA	2.02	0.41
1:A:81:GLU:HG2	1:A:169:LYS:CE	2.50	0.41
1:L:161:ASN:OD1	1:L:177:SER:OG	2.34	0.41
1:L:189:HIS:O	1:L:211:ARG:HD3	2.20	0.41
1:L:27(B):ILE:CG1	1:L:90:GLN:HG3	2.50	0.41
1:A:83:LEU:HD22	1:A:106:ILE:HD13	2.02	0.41
2:B:148:PHE:HA	2:B:149:PRO:HA	1.63	0.41
1:A:96:PRO:HG2	2:B:47:TRP:CD2	2.55	0.41
2:B:14:PRO:O	2:B:82(C):LEU:HB2	2.20	0.41
1:L:108:ARG:CZ	1:L:108:ARG:HB2	2.46	0.41
1:L:185:GLU:H	1:L:185:GLU:HG3	1.39	0.41
1:L:34:GLU:HG3	1:L:89:PHE:CD2	2.54	0.41
1:A:141:PRO:CD	1:A:199:LYS:HG3	2.50	0.41
2:B:149:PRO:HA	2:B:185:TYR:CE2	2.56	0.41
2:B:116:THR:CG2	2:B:215:SER:HB3	2.44	0.41
2:B:83:GLN:HB3	2:B:85:ASP:H	1.85	0.41
2:H:18:LEU:HD12	2:H:19:SER:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.55	0.41
1:A:144:ILE:HG23	1:A:145:ASN:N	2.35	0.41
1:A:133:VAL:HG13	1:A:178:THR:OG1	2.21	0.41
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.50	0.41
1:A:2:LEU:HD13	1:A:90:GLN:OE1	2.21	0.41
2:H:116:THR:CG2	2:H:215:SER:HB3	2.51	0.41
2:H:61:SER:HA	2:H:64:MET:HE1	2.02	0.41
1:L:37:LEU:HB2	1:L:47:LEU:HD11	2.02	0.41
1:A:185:GLU:O	1:A:189:HIS:HD2	2.04	0.41
2:B:116:THR:HG21	2:B:214:ALA:C	2.42	0.41
2:H:86:ASP:O	2:H:90:TYR:OH	2.34	0.41
1:L:27(B):ILE:O	1:L:92:SER:OG	2.29	0.41
1:A:135:PHE:CD1	1:A:176:SER:HA	2.56	0.41
2:B:154:VAL:HG21	2:B:189:SER:CB	2.47	0.41
2:B:149:PRO:HA	2:B:185:TYR:CD2	2.56	0.41
2:B:169:SER:HB2	2:B:192:THR:O	2.21	0.41
2:B:36:TRP:NE1	2:B:79:PHE:O	2.49	0.41
1:L:192:TYR:HB2	1:L:209:PHE:CD1	2.56	0.41
1:A:120:PRO:HB2	1:A:125:LEU:HD21	2.02	0.41
1:A:47:LEU:O	1:A:58:VAL:HG11	2.21	0.41
1:A:86:TYR:O	1:A:101:GLY:HA2	2.21	0.41
2:H:141:GLY:HA2	2:H:157:TRP:CZ2	2.55	0.41
2:H:63:LEU:C	2:H:67:LEU:HG	2.42	0.41
1:L:167:ASP:N	1:L:172:THR:O	2.47	0.41
1:L:190:ASN:ND2	1:L:212:ASN:ND2	2.69	0.41
1:L:199:LYS:H	1:L:199:LYS:HG2	1.32	0.41
1:L:66:GLY:HA3	1:L:71:PHE:CD2	2.56	0.41
1:A:181:LEU:HB2	1:A:182:THR:H	1.47	0.40
2:B:67:LEU:HD23	2:B:67:LEU:N	2.36	0.40
2:B:11:LEU:HG	2:B:12:VAL:N	2.37	0.40
2:B:37:VAL:HG12	2:B:38:ARG:N	2.36	0.40
1:L:153:SER:HB2	2:B:41:PRO:HB2	2.03	0.40
2:H:59:TYR:HB3	2:H:64:MET:HB3	2.03	0.40
1:A:114:THR:HB	1:A:137:ASN:HB2	2.03	0.40
1:A:198:HIS:CD2	1:A:199:LYS:HG2	2.56	0.40
1:A:27(D):HIS:HB2	1:A:30:ASN:N	2.36	0.40
2:B:6:GLU:OE1	2:B:106:GLY:N	2.50	0.40
2:H:162:ASN:HD22	2:H:166:LEU:HD23	1.83	0.40
2:H:3:GLN:HG3	2:H:25:SER:OG	2.21	0.40
1:L:117:ILE:HG21	1:L:207:LYS:O	2.21	0.40
1:L:143:ASP:O	1:L:199:LYS:HE3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:HA	1:A:140:TYR:O	2.22	0.40
1:A:185:GLU:H	1:A:185:GLU:HG3	1.46	0.40
2:B:11:LEU:HD11	2:B:112:SER:OG	2.21	0.40
2:H:11:LEU:O	2:H:12:VAL:CG1	2.65	0.40
2:H:57:THR:HG21	2:H:69:ILE:O	2.22	0.40
1:L:135:PHE:HE1	1:L:176:SER:OG	2.04	0.40
1:L:47:LEU:HD23	1:L:58:VAL:HG21	2.03	0.40
1:A:112:ALA:HA	1:A:200:THR:HG21	2.03	0.40
1:A:187:GLU:HA	1:A:211:ARG:HH22	1.86	0.40
1:A:190:ASN:ND2	1:A:191:SER:N	2.70	0.40
2:B:100(E):MET:HB2	2:B:103:TRP:NE1	2.37	0.40
2:B:178:LEU:HG	2:B:184:LEU:O	2.21	0.40
2:H:59:TYR:HD2	2:H:67:LEU:HB2	1.85	0.40
2:H:72:ASP:HB3	2:H:75:LYS:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:SER:O	2:B:56:SER:OG[2_556]	2.05	0.15

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	215/217 (99%)	182 (85%)	27 (13%)	6 (3%)	6	3
1	L	215/217 (99%)	186 (86%)	27 (13%)	2 (1%)	20	23
2	B	212/221 (96%)	178 (84%)	24 (11%)	10 (5%)	3	1
2	H	219/221 (99%)	180 (82%)	28 (13%)	11 (5%)	2	1
All	All	861/876 (98%)	726 (84%)	106 (12%)	29 (3%)	4	2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	68	SER
1	A	101	GLY
2	B	167	SER
1	L	184	ASP
2	H	82	MET
2	H	98	GLY
2	H	100(A)	ILE
2	H	167	SER
1	A	29	GLY
1	A	184	ASP
2	B	82	MET
2	B	127	GLY
2	H	101	ASP
2	H	114	ALA
2	H	136	SER
1	A	196	ALA
2	B	101	ASP
2	B	175	PRO
1	L	68	GLY
2	H	175	PRO
1	A	27	GLN
2	H	82(B)	SER
2	H	116	THR
2	B	68	SER
2	B	119	PRO
1	A	68	GLY
2	B	227	PRO
2	B	10	GLY
2	B	104	GLY

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	194/194 (100%)	135 (70%)	59 (30%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	194/194 (100%)	134 (69%)	60 (31%)	0	0
2	B	187/191 (98%)	135 (72%)	52 (28%)	0	0
2	H	191/191 (100%)	142 (74%)	49 (26%)	0	0
All	All	766/770 (100%)	546 (71%)	220 (29%)	0	0

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLU
1	L	14	SER
1	L	15	LEU
1	L	18	GLN
1	L	20	SER
1	L	24	ARG
1	L	27(B)	ILE
1	L	27(E)	SER
1	L	30	ASN
1	L	31	THR
1	L	34	GLU
1	L	42	GLN
1	L	43	SER
1	L	52	SER
1	L	55	PHE
1	L	60	ASP
1	L	65	SER
1	L	67	SER
1	L	69	THR
1	L	72	THR
1	L	75	ILE
1	L	76	ASN
1	L	81	GLU
1	L	83	LEU
1	L	90	GLN
1	L	93	HIS
1	L	94	LEU
1	L	103	LYS
1	L	107	LYS
1	L	108	ARG
1	L	116	SER
1	L	121	SER
1	L	122	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	126	THR
1	L	127	SER
1	L	132	VAL
1	L	144	ILE
1	L	147	LYS
1	L	149	LYS
1	L	150	ILE
1	L	155	ARG
1	L	160	LEU
1	L	161	ASN
1	L	165	ASP
1	L	168	SER
1	L	171	SER
1	L	175	MET
1	L	177	SER
1	L	181	LEU
1	L	183	LYS
1	L	185	GLU
1	L	188	ARG
1	L	191	SER
1	L	197	THR
1	L	199	LYS
1	L	200	THR
1	L	202	THR
1	L	207	LYS
1	L	209	PHE
1	L	211	ARG
2	H	1	GLN
2	H	3	GLN
2	H	5	LYS
2	H	11	LEU
2	H	15	SER
2	H	24	VAL
2	H	51	ILE
2	H	53	SER
2	H	56	SER
2	H	63	LEU
2	H	66	ARG
2	H	70	SER
2	H	71	LYS
2	H	77	GLN
2	H	79	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	82(B)	SER
2	H	85	ASP
2	H	94	LYS
2	H	100	TYR
2	H	105	GLN
2	H	112	SER
2	H	113	SER
2	H	117	THR
2	H	121	VAL
2	H	128	CYS
2	H	133	THR
2	H	136	SER
2	H	137	SER
2	H	138	VAL
2	H	140	LEU
2	H	145	LYS
2	H	153	THR
2	H	163	SER
2	H	166	LEU
2	H	167	SER
2	H	177	LEU
2	H	178	LEU
2	H	179	GLN
2	H	186	THR
2	H	192	THR
2	H	195	SER
2	H	196	SER
2	H	202	SER
2	H	219	VAL
2	H	220	ASP
2	H	221	LYS
2	H	222	LYS
2	H	226	GLU
2	H	228	ARG
1	A	5	THR
1	A	9	LEU
1	A	14	SER
1	A	15	LEU
1	A	18	GLN
1	A	20	SER
1	A	21	ILE
1	A	27(A)	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	27(B)	ILE
1	A	27(D)	HIS
1	A	27(E)	SER
1	A	28	ASN
1	A	31	THR
1	A	33	LEU
1	A	34	GLU
1	A	39	LYS
1	A	42	GLN
1	A	43	SER
1	A	52	SER
1	A	60	ASP
1	A	65	SER
1	A	67	SER
1	A	69	THR
1	A	72	THR
1	A	75	ILE
1	A	77	ARG
1	A	83	LEU
1	A	93	HIS
1	A	105	GLU
1	A	107	LYS
1	A	108	ARG
1	A	116	SER
1	A	121	SER
1	A	122	SER
1	A	125	LEU
1	A	126	THR
1	A	127	SER
1	A	132	VAL
1	A	143	ASP
1	A	144	ILE
1	A	147	LYS
1	A	155	ARG
1	A	157	ASN
1	A	161	ASN
1	A	168	SER
1	A	171	SER
1	A	175	MET
1	A	177	SER
1	A	181	LEU
1	A	183	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	185	GLU
1	A	188	ARG
1	A	191	SER
1	A	197	THR
1	A	199	LYS
1	A	200	THR
1	A	202	THR
1	A	207	LYS
1	A	210	ASN
2	B	1	GLN
2	B	3	GLN
2	B	12	VAL
2	B	16	GLN
2	B	35	ASP
2	B	38	ARG
2	B	51	ILE
2	B	53	SER
2	B	56	SER
2	B	63	LEU
2	B	64	MET
2	B	67	LEU
2	B	70	SER
2	B	71	LYS
2	B	80	LEU
2	B	82	MET
2	B	82(B)	SER
2	B	83	GLN
2	B	85	ASP
2	B	94	LYS
2	B	105	GLN
2	B	110	THR
2	B	113	SER
2	B	115	LYS
2	B	117	THR
2	B	121	VAL
2	B	128	CYS
2	B	130	ASP
2	B	133	THR
2	B	136	SER
2	B	137	SER
2	B	138	VAL
2	B	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	143	LEU
2	B	153	THR
2	B	156	THR
2	B	163	SER
2	B	166	LEU
2	B	167	SER
2	B	169	SER
2	B	179	GLN
2	B	186	THR
2	B	192	THR
2	B	195	SER
2	B	202	SER
2	B	203	GLN
2	B	219	VAL
2	B	220	ASP
2	B	221	LYS
2	B	222	LYS
2	B	226	GLU
2	B	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	90	GLN
1	L	212	ASN
2	H	31	ASN
2	H	58	ASN
2	H	102	HIS
2	H	172	HIS
1	A	27	GLN
1	A	53	ASN
1	A	76	ASN
1	A	166	GLN
1	A	189	HIS
2	B	39	GLN
2	B	102	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	217/217 (100%)	-0.14	3 (1%) 75 74	21, 45, 62, 74	0
1	L	217/217 (100%)	-0.29	2 (0%) 84 85	20, 45, 62, 74	0
2	B	216/221 (97%)	-0.20	3 (1%) 75 74	17, 45, 72, 91	0
2	H	221/221 (100%)	-0.23	4 (1%) 69 65	17, 45, 71, 91	0
All	All	871/876 (99%)	-0.22	12 (1%) 75 74	17, 45, 66, 91	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	166	LEU	6.3
2	H	167	SER	5.6
2	H	166	LEU	4.1
2	H	163	SER	3.3
1	A	56	SER	3.0
1	A	11	LEU	2.9
1	A	27(B)	ILE	2.8
2	H	8	GLY	2.8
2	B	213	PRO	2.5
2	B	179	GLN	2.3
1	L	192	TYR	2.3
1	L	179	LEU	2.1

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.