Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:59 PM GMT

PDB ID	:	4GTU
Title	:	LIGAND-FREE HOMODIMERIC HUMAN GLUTATHIONE S-TRANSFERASE M4-4
Authors	:	Patskovsky, Y.V.; Patskovska, L.N.; Listowsky, I.
Deposited on	:	1999-05-12
Resolution	:	3.30 Å(reported)

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

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

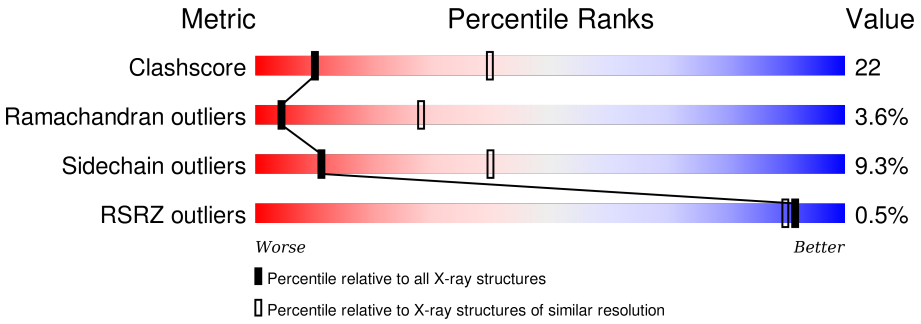
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	217	51% 44% 5%
1	B	217	54% 40% 6%
1	C	217	47% 46% 7%
1	D	217	% 50% 47% .
1	E	217	53% 41% 6%
1	F	217	% 39% 53% 8%
1	G	217	52% 41% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	217	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14352 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 GLUTATHIONE S-TRANSFERASE.

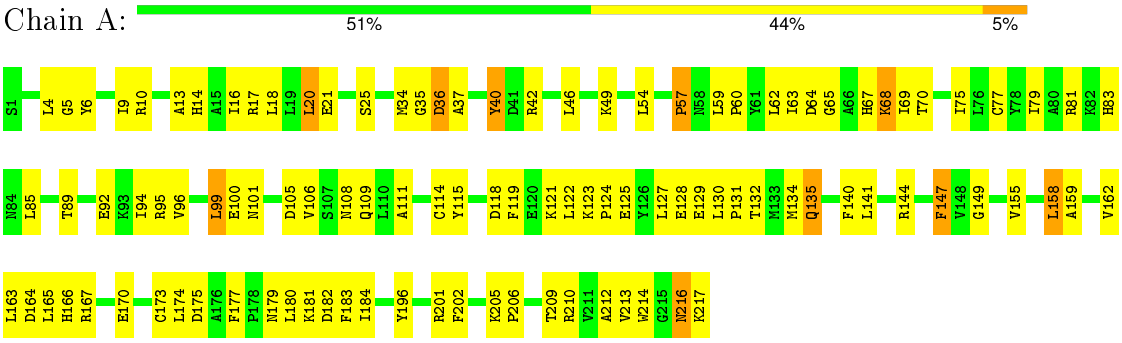
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	B	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	C	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	D	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	E	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	F	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	G	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			
1	H	217	Total	C	N	O	S	0	0	0
			1794	1160	295	329	10			

3 Residue-property plots (i)

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

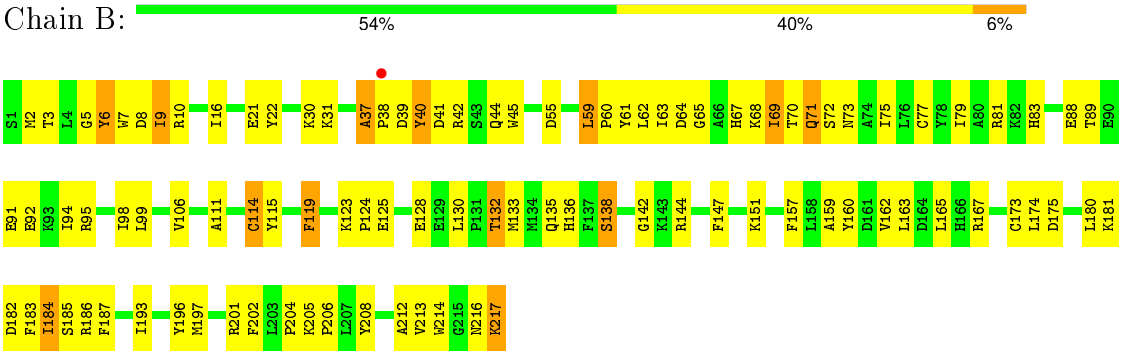
- Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain A:



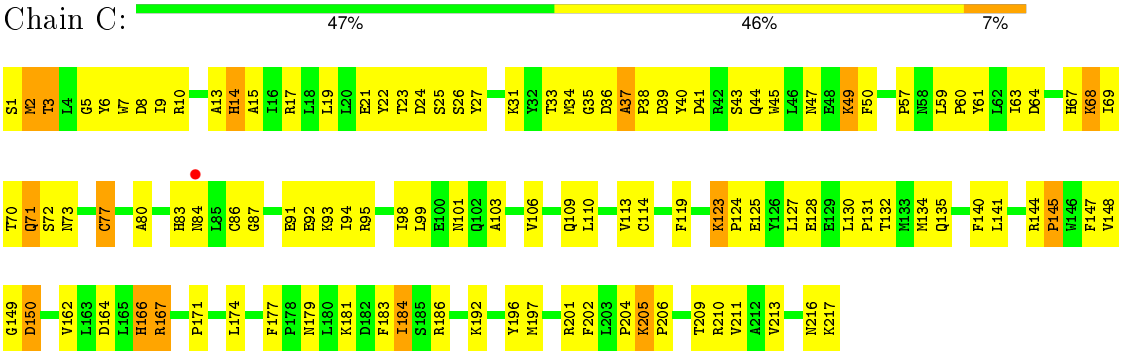
- Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain B:



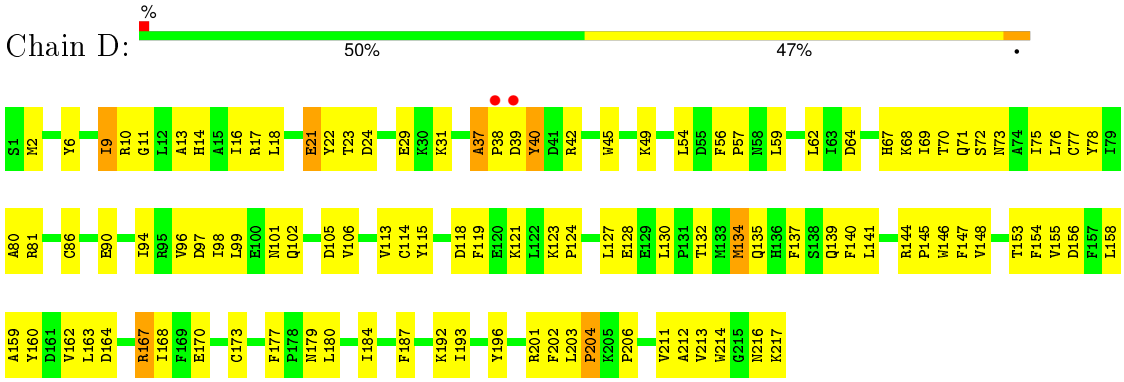
- Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain C:



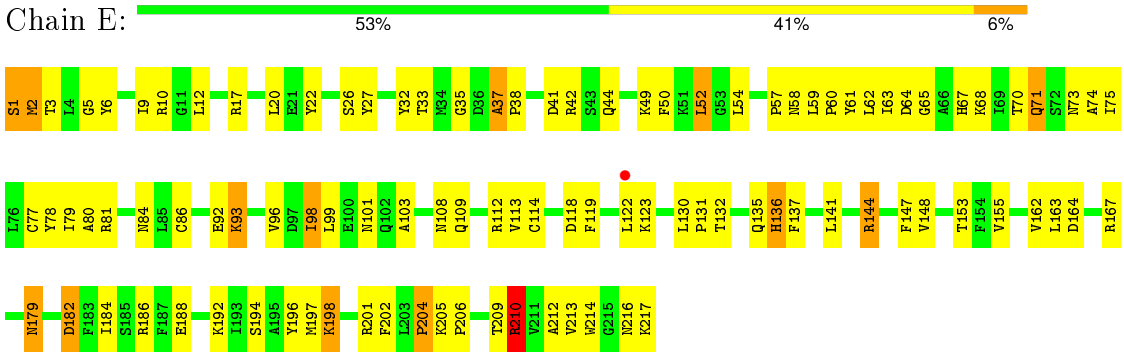
• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain D:



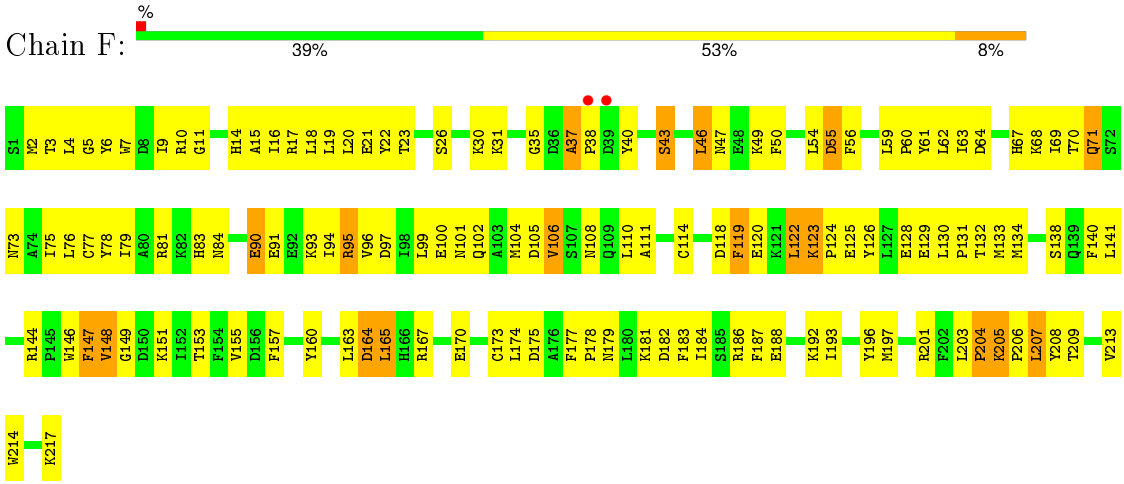
• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain E:



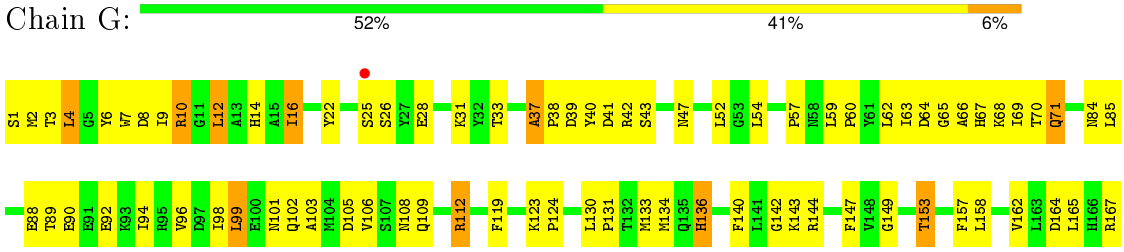
• Molecule 1: GLUTATHIONE S-TRANSFERASE

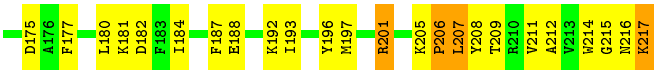
Chain F:



• Molecule 1: GLUTATHIONE S-TRANSFERASE

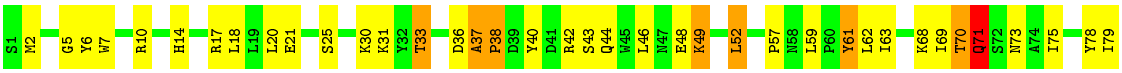
Chain G:





- Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.00Å 215.70Å 94.56Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30 39.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.5 (10.00-3.30) 63.5 (39.38-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.245 , 0.315 0.260 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 73.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	1 of 31560 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	14352	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/1842	0.61	0/2489
1	B	0.44	0/1842	0.62	0/2489
1	C	0.42	0/1842	0.61	0/2489
1	D	0.42	0/1842	0.57	0/2489
1	E	0.41	0/1842	0.60	0/2489
1	F	0.43	0/1842	0.58	0/2489
1	G	0.42	0/1842	0.63	0/2489
1	H	0.40	0/1842	0.59	0/2489
All	All	0.42	0/14736	0.60	0/19912

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1794	0	1762	83	0
1	B	1794	0	1762	83	0
1	C	1794	0	1762	84	0
1	D	1794	0	1762	74	0
1	E	1794	0	1762	75	0
1	F	1794	0	1762	107	0
1	G	1794	0	1762	75	0
1	H	1794	0	1762	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14352	0	14096	623	0

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

All (623) 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:C:206:PRO:HG3	1:C:217:LYS:HB3	1.50	0.94
1:A:144:ARG:HD3	1:A:149:GLY:HA2	1.50	0.92
1:C:37:ALA:HB1	1:C:38:PRO:HD2	1.55	0.89
1:E:80:ALA:HB1	1:E:86:CYS:SG	2.12	0.89
1:A:114:CYS:SG	1:A:214:TRP:HB3	2.14	0.87
1:G:4:LEU:HD13	1:G:16:ILE:HG21	1.60	0.83
1:B:114:CYS:HG	1:B:214:TRP:HE3	1.24	0.83
1:A:63:ILE:HG12	1:A:68:LYS:HG3	1.62	0.82
1:G:1:SER:HB2	1:G:26:SER:O	1.79	0.81
1:H:174:LEU:HG	1:H:181:LYS:HD2	1.62	0.81
1:H:5:GLY:HA3	1:H:61:TYR:CE1	2.16	0.81
1:F:62:LEU:HD22	1:F:75:ILE:HG23	1.62	0.81
1:H:37:ALA:HB1	1:H:38:PRO:HD2	1.61	0.80
1:E:6:TYR:HA	1:E:59:LEU:HD22	1.63	0.80
1:E:71:GLN:HG2	1:F:101:ASN:HB2	1.62	0.80
1:E:210:ARG:HA	1:E:216:ASN:HB2	1.63	0.80
1:D:37:ALA:HB1	1:D:38:PRO:HD2	1.64	0.78
1:B:37:ALA:HB1	1:B:38:PRO:HD2	1.66	0.78
1:F:21:GLU:HG2	1:F:196:TYR:HB2	1.66	0.78
1:G:101:ASN:HB3	1:H:71:GLN:HG2	1.66	0.78
1:F:9:ILE:HG13	1:F:206:PRO:HG2	1.65	0.77
1:A:164:ASP:HA	1:A:167:ARG:HG3	1.68	0.76
1:H:6:TYR:HA	1:H:59:LEU:HD22	1.66	0.76
1:F:134:MET:HE1	1:F:174:LEU:HA	1.67	0.76
1:A:36:ASP:HA	1:A:40:TYR:CD2	2.21	0.75
1:H:174:LEU:HD21	1:H:184:ILE:HD12	1.66	0.75
1:D:115:TYR:HE1	1:D:212:ALA:HB2	1.52	0.75
1:E:37:ALA:HB1	1:E:38:PRO:HD2	1.68	0.74
1:E:136:HIS:HB3	1:F:55:ASP:O	1.85	0.74
1:G:37:ALA:HB1	1:G:38:PRO:HD2	1.69	0.74
1:B:2:MET:HB2	1:B:63:ILE:O	1.88	0.74
1:B:9:ILE:HG13	1:B:206:PRO:HG2	1.71	0.71
1:E:99:LEU:HD11	1:E:147:PHE:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:GLU:HA	1:F:93:LYS:HD2	1.72	0.71
1:C:6:TYR:HA	1:C:59:LEU:HD22	1.71	0.70
1:D:9:ILE:HG13	1:D:206:PRO:HG2	1.73	0.70
1:B:175:ASP:HA	1:B:181:LYS:HD2	1.73	0.70
1:A:135:GLN:HG2	1:A:177:PHE:CZ	2.25	0.70
1:C:110:LEU:O	1:C:113:VAL:HG22	1.91	0.70
1:C:1:SER:HA	1:C:26:SER:O	1.92	0.70
1:C:144:ARG:HD3	1:C:149:GLY:HA2	1.72	0.70
1:F:6:TYR:CD1	1:F:60:PRO:HG3	2.27	0.70
1:G:164:ASP:HA	1:G:167:ARG:NH1	2.07	0.70
1:D:158:LEU:O	1:D:162:VAL:HG23	1.92	0.70
1:D:160:TYR:HE1	1:D:184:ILE:HG23	1.55	0.70
1:B:114:CYS:SG	1:B:214:TRP:HE3	2.15	0.69
1:D:206:PRO:HB3	1:D:217:LYS:HB2	1.73	0.69
1:G:205:LYS:HG3	1:G:217:LYS:HE2	1.74	0.69
1:A:114:CYS:HG	1:A:214:TRP:HE3	1.38	0.69
1:D:216:ASN:O	1:D:217:LYS:HG3	1.93	0.69
1:C:134:MET:SD	1:C:174:LEU:HD12	2.33	0.69
1:D:6:TYR:O	1:D:31:LYS:HA	1.93	0.68
1:F:54:LEU:HD23	1:F:68:LYS:HB3	1.74	0.68
1:D:167:ARG:HG2	1:D:168:ILE:HD12	1.74	0.68
1:C:2:MET:HB2	1:C:63:ILE:O	1.93	0.68
1:F:163:LEU:HD22	1:F:174:LEU:HD11	1.76	0.68
1:C:110:LEU:HD22	1:C:166:HIS:CE1	2.29	0.68
1:C:130:LEU:HB3	1:C:131:PRO:HD3	1.75	0.68
1:C:99:LEU:HD11	1:C:147:PHE:HB3	1.77	0.68
1:D:123:LYS:HB3	1:D:124:PRO:HD3	1.76	0.68
1:A:64:ASP:HB3	1:A:67:HIS:HB2	1.76	0.67
1:F:110:LEU:HD23	1:F:165:LEU:HD12	1.77	0.67
1:D:29:GLU:HG2	1:D:31:LYS:HE3	1.76	0.67
1:D:96:VAL:HG13	1:D:155:VAL:HG13	1.77	0.67
1:F:73:ASN:HA	1:F:76:LEU:HD12	1.76	0.67
1:F:134:MET:SD	1:F:173:CYS:HB2	2.35	0.67
1:A:167:ARG:HD3	1:A:174:LEU:HD22	1.78	0.66
1:F:217:LYS:HZ2	1:F:217:LYS:HB2	1.60	0.66
1:B:114:CYS:SG	1:B:214:TRP:HB3	2.35	0.66
1:C:164:ASP:O	1:C:167:ARG:HG2	1.94	0.66
1:H:5:GLY:HA3	1:H:61:TYR:HE1	1.58	0.66
1:D:140:PHE:HD2	1:D:147:PHE:HD2	1.44	0.66
1:A:140:PHE:HD2	1:A:147:PHE:HD2	1.44	0.66
1:E:194:SER:O	1:E:198:LYS:HG2	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:HD22	1:E:75:ILE:HG23	1.78	0.65
1:F:9:ILE:HG12	1:F:209:THR:HA	1.78	0.65
1:C:95:ARG:NH2	1:C:144:ARG:HH12	1.95	0.65
1:A:101:ASN:HB3	1:B:71:GLN:OE1	1.96	0.65
1:E:78:TYR:HA	1:E:81:ARG:CZ	2.26	0.65
1:F:37:ALA:HB1	1:F:38:PRO:HD2	1.77	0.65
1:B:159:ALA:O	1:B:163:LEU:HG	1.96	0.65
1:D:148:VAL:HG11	1:D:153:THR:HG23	1.78	0.65
1:C:103:ALA:HB1	1:C:162:VAL:HG21	1.78	0.64
1:D:160:TYR:CE1	1:D:184:ILE:HG23	2.32	0.64
1:G:205:LYS:CG	1:G:217:LYS:HE2	2.28	0.64
1:C:3:THR:HG23	1:C:63:ILE:HB	1.79	0.64
1:C:70:THR:O	1:C:71:GLN:HB2	1.98	0.64
1:H:123:LYS:HB3	1:H:124:PRO:HD3	1.79	0.64
1:H:88:GLU:HG2	1:H:92:GLU:OE2	1.98	0.64
1:H:33:THR:HG22	1:H:210:ARG:HH21	1.63	0.63
1:B:77:CYS:HB3	1:B:81:ARG:HH12	1.61	0.63
1:E:167:ARG:CZ	1:E:184:ILE:HG21	2.28	0.63
1:B:167:ARG:NH2	1:B:184:ILE:HG21	2.12	0.63
1:C:164:ASP:HA	1:C:167:ARG:HD3	1.81	0.63
1:C:119:PHE:HB2	1:C:213:VAL:HG21	1.79	0.63
1:H:79:ILE:O	1:H:83:HIS:HD2	1.82	0.63
1:C:205:LYS:HD3	1:C:217:LYS:NZ	2.14	0.63
1:B:62:LEU:O	1:B:68:LYS:HA	1.99	0.63
1:D:135:GLN:HG2	1:D:139:GLN:OE1	1.99	0.62
1:F:130:LEU:HB3	1:F:131:PRO:HD3	1.81	0.62
1:H:2:MET:SD	1:H:62:LEU:HD21	2.40	0.62
1:F:10:ARG:HD2	1:F:204:PRO:O	1.99	0.62
1:G:7:TRP:HH2	1:G:42:ARG:HG3	1.64	0.62
1:H:63:ILE:HD12	1:H:68:LYS:HG2	1.82	0.62
1:F:67:HIS:HB3	1:F:69:ILE:HD11	1.81	0.61
1:E:73:ASN:HB2	1:F:101:ASN:OD1	2.00	0.61
1:E:101:ASN:OD1	1:F:73:ASN:HB2	1.99	0.61
1:F:111:ALA:HA	1:F:208:TYR:HE2	1.64	0.61
1:E:141:LEU:HD13	1:E:147:PHE:CD1	2.36	0.61
1:E:9:ILE:HG12	1:E:209:THR:HA	1.81	0.61
1:D:170:GLU:HB3	1:D:173:CYS:SG	2.40	0.61
1:D:99:LEU:HD12	1:D:155:VAL:HB	1.81	0.61
1:F:2:MET:HA	1:F:63:ILE:O	2.00	0.61
1:E:1:SER:HA	1:E:26:SER:O	2.00	0.61
1:B:21:GLU:HG2	1:B:196:TYR:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ASP:O	1:G:109:GLN:HG3	2.01	0.61
1:H:119:PHE:HB2	1:H:213:VAL:HG21	1.83	0.61
1:D:10:ARG:HG3	1:D:14:HIS:HB2	1.81	0.61
1:B:157:PHE:CD2	1:B:187:PHE:HZ	2.18	0.61
1:A:54:LEU:O	1:A:57:PRO:HD3	2.01	0.61
1:G:144:ARG:HD2	1:G:144:ARG:H	1.64	0.61
1:C:141:LEU:O	1:C:144:ARG:HG2	2.01	0.60
1:G:2:MET:CE	1:G:25:SER:HB3	2.31	0.60
1:B:205:LYS:HB3	1:B:206:PRO:HA	1.82	0.60
1:F:207:LEU:HD12	1:F:208:TYR:HE1	1.65	0.60
1:F:6:TYR:O	1:F:31:LYS:HA	2.01	0.60
1:E:184:ILE:O	1:E:188:GLU:HG2	2.01	0.60
1:C:80:ALA:HB1	1:C:86:CYS:SG	2.41	0.60
1:H:160:TYR:HE1	1:H:184:ILE:HG23	1.67	0.60
1:E:114:CYS:HG	1:E:214:TRP:HE3	1.49	0.60
1:A:101:ASN:OD1	1:B:73:ASN:HB2	2.01	0.60
1:D:64:ASP:HB3	1:D:67:HIS:HB2	1.83	0.60
1:F:6:TYR:HA	1:F:59:LEU:HD22	1.83	0.59
1:F:207:LEU:HD12	1:F:208:TYR:CE1	2.37	0.59
1:H:95:ARG:HB2	1:H:148:VAL:HG23	1.85	0.59
1:E:153:THR:OG1	1:E:155:VAL:HG22	2.02	0.59
1:H:20:LEU:HD21	1:H:79:ILE:HD13	1.84	0.59
1:E:35:GLY:O	1:E:210:ARG:HG3	2.02	0.59
1:D:31:LYS:HE2	1:D:203:LEU:HD11	1.83	0.59
1:E:10:ARG:HB3	1:E:206:PRO:O	2.03	0.59
1:D:134:MET:HG2	1:D:173:CYS:HB3	1.83	0.59
1:A:162:VAL:O	1:A:166:HIS:HD2	1.85	0.59
1:H:112:ARG:HG2	1:H:112:ARG:HH11	1.68	0.59
1:D:6:TYR:HA	1:D:59:LEU:HD22	1.83	0.59
1:A:4:LEU:HD12	1:A:20:LEU:HD21	1.85	0.59
1:G:144:ARG:HG2	1:G:149:GLY:HA2	1.84	0.59
1:H:17:ARG:NH1	1:H:203:LEU:HD23	2.18	0.58
1:C:10:ARG:HA	1:C:17:ARG:HH12	1.66	0.58
1:C:36:ASP:HA	1:C:40:TYR:HD1	1.67	0.58
1:D:115:TYR:CE1	1:D:212:ALA:HB2	2.34	0.58
1:G:9:ILE:HG13	1:G:209:THR:HA	1.85	0.58
1:B:160:TYR:CE1	1:B:184:ILE:HG23	2.38	0.58
1:E:20:LEU:HD23	1:E:79:ILE:HD11	1.84	0.58
1:G:103:ALA:O	1:G:106:VAL:HG22	2.03	0.58
1:C:9:ILE:HG12	1:C:209:THR:HA	1.86	0.58
1:B:40:TYR:O	1:B:42:ARG:HG2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:GLU:HG2	1:H:196:TYR:HB2	1.85	0.58
1:B:119:PHE:HB2	1:B:213:VAL:HG11	1.84	0.58
1:F:217:LYS:NZ	1:F:217:LYS:HB2	2.17	0.58
1:D:119:PHE:HB2	1:D:213:VAL:HG11	1.86	0.58
1:G:63:ILE:HA	1:G:67:HIS:O	2.04	0.58
1:A:9:ILE:HG13	1:A:209:THR:HA	1.85	0.58
1:B:114:CYS:O	1:B:213:VAL:HG12	2.04	0.57
1:E:78:TYR:HA	1:E:81:ARG:NH1	2.19	0.57
1:A:114:CYS:O	1:A:213:VAL:HG22	2.03	0.57
1:E:206:PRO:HG3	1:E:217:LYS:HB2	1.85	0.57
1:H:18:LEU:HD21	1:H:187:PHE:HE2	1.69	0.57
1:H:37:ALA:HB1	1:H:38:PRO:CD	2.34	0.57
1:A:163:LEU:HD23	1:A:184:ILE:HD11	1.87	0.57
1:E:3:THR:HG22	1:E:63:ILE:HB	1.86	0.57
1:A:6:TYR:HA	1:A:59:LEU:HG	1.87	0.57
1:F:140:PHE:O	1:F:144:ARG:NH1	2.38	0.57
1:B:206:PRO:HB3	1:B:217:LYS:CB	2.34	0.57
1:A:205:LYS:HG3	1:A:206:PRO:HA	1.87	0.57
1:F:3:THR:O	1:F:62:LEU:HA	2.04	0.57
1:G:63:ILE:HG12	1:G:68:LYS:HG2	1.87	0.56
1:A:175:ASP:HA	1:A:181:LYS:CE	2.35	0.56
1:A:6:TYR:HD2	1:A:17:ARG:HH22	1.53	0.56
1:C:5:GLY:HA3	1:C:61:TYR:CE2	2.40	0.56
1:C:35:GLY:HA3	1:C:41:ASP:HB2	1.87	0.56
1:A:175:ASP:HA	1:A:181:LYS:HE2	1.87	0.56
1:D:164:ASP:HA	1:D:167:ARG:HD2	1.87	0.56
1:F:22:TYR:HA	1:F:192:LYS:HB3	1.88	0.56
1:F:21:GLU:HG2	1:F:196:TYR:CB	2.35	0.56
1:C:6:TYR:CD1	1:C:60:PRO:HG3	2.40	0.56
1:F:175:ASP:HA	1:F:181:LYS:HD3	1.88	0.56
1:C:110:LEU:HD22	1:C:166:HIS:HE1	1.70	0.56
1:C:210:ARG:HA	1:C:216:ASN:HB2	1.87	0.56
1:G:64:ASP:HB3	1:G:67:HIS:HB2	1.88	0.55
1:E:119:PHE:HB2	1:E:213:VAL:HG21	1.87	0.55
1:C:43:SER:O	1:C:47:ASN:HB2	2.06	0.55
1:D:13:ALA:O	1:D:17:ARG:HG3	2.05	0.55
1:F:110:LEU:HD13	1:F:126:TYR:CE2	2.41	0.55
1:D:114:CYS:HG	1:D:214:TRP:HE3	1.51	0.55
1:C:23:THR:HB	1:C:83:HIS:CD2	2.42	0.55
1:B:45:TRP:CH2	1:B:61:TYR:CE2	2.94	0.55
1:C:71:GLN:HG3	1:D:101:ASN:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:ARG:HA	1:E:20:LEU:HD12	1.89	0.55
1:D:14:HIS:O	1:D:18:LEU:HG	2.06	0.55
1:F:134:MET:HE1	1:F:174:LEU:HD13	1.89	0.55
1:A:10:ARG:HG3	1:A:14:HIS:HB2	1.88	0.55
1:G:196:TYR:HE1	1:G:201:ARG:HB2	1.72	0.55
1:G:136:HIS:CD2	1:H:57:PRO:HD2	2.42	0.55
1:F:15:ALA:HA	1:F:18:LEU:HD12	1.89	0.55
1:A:54:LEU:HD23	1:A:68:LYS:HB3	1.88	0.54
1:E:70:THR:O	1:E:71:GLN:HB2	2.07	0.54
1:A:130:LEU:O	1:A:134:MET:HG2	2.07	0.54
1:F:77:CYS:O	1:F:81:ARG:HG3	2.07	0.54
1:F:114:CYS:O	1:F:213:VAL:HG22	2.07	0.54
1:G:4:LEU:CD1	1:G:16:ILE:HG21	2.36	0.54
1:G:70:THR:O	1:G:71:GLN:HB2	2.07	0.54
1:E:92:GLU:O	1:E:96:VAL:HG23	2.08	0.54
1:G:207:LEU:HD12	1:G:208:TYR:CE1	2.42	0.54
1:H:93:LYS:O	1:H:96:VAL:HB	2.07	0.54
1:B:184:ILE:HG22	1:B:184:ILE:O	2.08	0.54
1:E:20:LEU:HD23	1:E:79:ILE:CD1	2.37	0.54
1:D:90:GLU:HG3	1:D:94:ILE:HD11	1.90	0.54
1:A:54:LEU:HD12	1:A:57:PRO:HA	1.89	0.53
1:D:130:LEU:HD21	1:D:173:CYS:SG	2.47	0.53
1:E:93:LYS:HG2	1:F:81:ARG:HE	1.72	0.53
1:F:78:TYR:O	1:F:81:ARG:HB2	2.08	0.53
1:G:12:LEU:HD13	1:G:60:PRO:HD3	1.88	0.53
1:C:10:ARG:HG3	1:C:14:HIS:HB2	1.90	0.53
1:F:129:GLU:O	1:F:133:MET:HG3	2.09	0.53
1:C:114:CYS:O	1:C:213:VAL:HG22	2.09	0.53
1:A:16:ILE:O	1:A:20:LEU:HG	2.09	0.53
1:A:83:HIS:O	1:A:85:LEU:HD12	2.08	0.53
1:A:173:CYS:SG	1:A:174:LEU:N	2.81	0.53
1:E:136:HIS:HB2	1:F:56:PHE:CE1	2.44	0.53
1:D:114:CYS:SG	1:D:214:TRP:CE3	3.01	0.53
1:A:63:ILE:HA	1:A:67:HIS:O	2.09	0.53
1:E:77:CYS:O	1:E:81:ARG:HG2	2.09	0.53
1:E:148:VAL:HG21	1:E:153:THR:OG1	2.09	0.53
1:A:135:GLN:HG2	1:A:177:PHE:HZ	1.74	0.53
1:F:10:ARG:HE	1:F:14:HIS:CG	2.27	0.53
1:F:71:GLN:HA	1:F:71:GLN:OE1	2.08	0.53
1:A:167:ARG:NH1	1:A:184:ILE:HD13	2.24	0.53
1:B:77:CYS:HB3	1:B:81:ARG:NH1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:GLU:O	1:H:52:LEU:HD12	2.09	0.52
1:F:21:GLU:HG2	1:F:196:TYR:CG	2.44	0.52
1:A:42:ARG:HG3	1:A:46:LEU:HD11	1.91	0.52
1:F:134:MET:SD	1:F:174:LEU:HD22	2.50	0.52
1:H:110:LEU:O	1:H:113:VAL:HG22	2.09	0.52
1:B:217:LYS:NZ	1:B:217:LYS:HB2	2.23	0.52
1:G:177:PHE:HB2	1:G:180:LEU:HD12	1.91	0.52
1:G:69:ILE:H	1:G:69:ILE:HD12	1.74	0.52
1:C:45:TRP:CZ2	1:C:49:LYS:HG3	2.44	0.52
1:F:160:TYR:CD1	1:F:184:ILE:HG22	2.45	0.52
1:D:202:PHE:O	1:D:204:PRO:HD3	2.10	0.52
1:G:101:ASN:OD1	1:H:73:ASN:HB2	2.10	0.52
1:G:9:ILE:CD1	1:G:206:PRO:HB3	2.40	0.52
1:A:196:TYR:CE2	1:A:202:PHE:HD1	2.27	0.52
1:B:91:GLU:O	1:B:95:ARG:HG3	2.09	0.52
1:A:123:LYS:HB3	1:A:124:PRO:HD3	1.91	0.52
1:F:4:LEU:HD21	1:F:17:ARG:HG2	1.91	0.52
1:F:102:GLN:O	1:F:106:VAL:HG23	2.10	0.52
1:B:5:GLY:HA2	1:B:30:LYS:O	2.10	0.52
1:H:217:LYS:NZ	1:H:217:LYS:HB2	2.24	0.52
1:F:30:LYS:HE3	1:F:61:TYR:OH	2.10	0.52
1:D:96:VAL:HG13	1:D:155:VAL:CG1	2.39	0.51
1:F:111:ALA:HA	1:F:208:TYR:CE2	2.44	0.51
1:E:54:LEU:HD23	1:E:68:LYS:HB3	1.92	0.51
1:B:64:ASP:HB3	1:B:67:HIS:HB2	1.90	0.51
1:C:10:ARG:HD2	1:C:204:PRO:O	2.10	0.51
1:D:14:HIS:HE1	1:D:202:PHE:CE1	2.28	0.51
1:D:73:ASN:HA	1:D:76:LEU:HD12	1.93	0.51
1:B:16:ILE:HD12	1:B:16:ILE:H	1.75	0.51
1:F:35:GLY:O	1:F:40:TYR:HA	2.10	0.51
1:A:94:ILE:HG23	1:B:69:ILE:HG21	1.93	0.51
1:D:21:GLU:HG3	1:D:196:TYR:CD1	2.45	0.51
1:G:164:ASP:HA	1:G:167:ARG:HH11	1.73	0.51
1:E:164:ASP:O	1:E:167:ARG:HB3	2.10	0.51
1:A:118:ASP:HB3	1:A:121:LYS:HB2	1.92	0.51
1:H:179:ASN:HD22	1:H:179:ASN:N	2.09	0.51
1:E:6:TYR:HA	1:E:59:LEU:CD2	2.37	0.51
1:C:164:ASP:HA	1:C:167:ARG:CD	2.40	0.51
1:E:6:TYR:CE1	1:E:60:PRO:HD3	2.46	0.51
1:D:114:CYS:SG	1:D:214:TRP:HE3	2.33	0.51
1:E:5:GLY:O	1:E:60:PRO:HA	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:CE1	1:B:63:ILE:HD11	2.46	0.50
1:C:36:ASP:O	1:C:37:ALA:HB3	2.11	0.50
1:F:62:LEU:CD2	1:F:69:ILE:HB	2.42	0.50
1:B:6:TYR:HA	1:B:59:LEU:HD22	1.93	0.50
1:G:8:ASP:OD2	1:G:33:THR:HA	2.11	0.50
1:F:110:LEU:CD2	1:F:165:LEU:HD12	2.41	0.50
1:F:146:TRP:CH2	1:F:186:ARG:HG2	2.45	0.50
1:A:115:TYR:HE1	1:A:212:ALA:HB2	1.77	0.50
1:C:94:ILE:HG23	1:D:69:ILE:HD12	1.93	0.50
1:F:207:LEU:HD11	1:F:214:TRP:CZ3	2.46	0.50
1:G:85:LEU:O	1:G:153:THR:HG22	2.12	0.50
1:G:123:LYS:N	1:G:124:PRO:HD2	2.27	0.50
1:E:210:ARG:HH11	1:E:210:ARG:HB3	1.77	0.50
1:D:77:CYS:O	1:D:81:ARG:HB2	2.10	0.50
1:H:10:ARG:HG2	1:H:14:HIS:HB2	1.93	0.50
1:G:130:LEU:O	1:G:133:MET:HB3	2.12	0.50
1:A:100:GLU:HA	1:A:158:LEU:HD13	1.94	0.50
1:A:114:CYS:SG	1:A:214:TRP:HE3	2.35	0.50
1:B:216:ASN:O	1:B:217:LYS:HD3	2.12	0.50
1:F:22:TYR:HB2	1:F:193:ILE:HD11	1.93	0.50
1:D:78:TYR:HA	1:D:81:ARG:NH1	2.26	0.50
1:C:69:ILE:HG23	1:D:98:ILE:HD11	1.94	0.50
1:B:91:GLU:HG3	1:B:92:GLU:N	2.27	0.50
1:G:119:PHE:CZ	1:G:214:TRP:CD1	3.00	0.50
1:B:130:LEU:O	1:B:133:MET:HB3	2.12	0.50
1:E:58:ASN:HB3	1:E:70:THR:HG22	1.92	0.49
1:B:6:TYR:CE1	1:B:60:PRO:HD3	2.47	0.49
1:B:193:ILE:N	1:B:193:ILE:HD12	2.27	0.49
1:B:197:MET:SD	1:B:202:PHE:CZ	3.04	0.49
1:B:111:ALA:HA	1:B:208:TYR:CE2	2.47	0.49
1:F:23:THR:HB	1:F:83:HIS:CD2	2.47	0.49
1:D:187:PHE:CE2	1:D:193:ILE:HD13	2.46	0.49
1:F:205:LYS:HD3	1:F:217:LYS:CE	2.42	0.49
1:B:111:ALA:HA	1:B:208:TYR:HE2	1.76	0.49
1:E:10:ARG:HD2	1:E:204:PRO:O	2.12	0.49
1:D:22:TYR:HD2	1:D:23:THR:HG23	1.76	0.49
1:C:73:ASN:HB2	1:D:101:ASN:OD1	2.12	0.49
1:H:187:PHE:CD2	1:H:187:PHE:O	2.65	0.49
1:A:108:ASN:HA	1:A:111:ALA:HB3	1.94	0.49
1:A:18:LEU:O	1:A:21:GLU:HB3	2.13	0.49
1:C:77:CYS:O	1:C:80:ALA:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:GLY:HA2	1:H:30:LYS:O	2.13	0.49
1:F:205:LYS:HB2	1:F:206:PRO:HA	1.95	0.49
1:D:14:HIS:HE1	1:D:202:PHE:HE1	1.60	0.49
1:G:3:THR:HB	1:G:28:GLU:HB3	1.94	0.49
1:H:20:LEU:CD2	1:H:79:ILE:HD13	2.42	0.48
1:F:91:GLU:O	1:F:95:ARG:HG3	2.13	0.48
1:A:114:CYS:HG	1:A:214:TRP:HB3	1.78	0.48
1:D:124:PRO:O	1:D:128:GLU:HG3	2.14	0.48
1:B:89:THR:OG1	1:B:92:GLU:HG3	2.13	0.48
1:B:174:LEU:H	1:B:174:LEU:HD12	1.78	0.48
1:G:10:ARG:HG2	1:G:14:HIS:HB2	1.94	0.48
1:D:78:TYR:HA	1:D:81:ARG:HH12	1.78	0.48
1:C:36:ASP:O	1:C:40:TYR:HA	2.14	0.48
1:F:205:LYS:HD3	1:F:217:LYS:HE2	1.94	0.48
1:G:88:GLU:HB2	1:G:92:GLU:OE1	2.13	0.48
1:G:212:ALA:O	1:G:216:ASN:ND2	2.46	0.48
1:E:119:PHE:CZ	1:E:123:LYS:HD3	2.48	0.48
1:G:69:ILE:N	1:G:69:ILE:HD12	2.28	0.48
1:F:62:LEU:HD23	1:F:69:ILE:HB	1.96	0.48
1:D:148:VAL:HG11	1:D:153:THR:CG2	2.42	0.48
1:F:119:PHE:HB2	1:F:213:VAL:HG21	1.95	0.48
1:D:102:GLN:O	1:D:106:VAL:HG23	2.14	0.48
1:B:183:PHE:C	1:B:185:SER:H	2.17	0.48
1:C:25:SER:O	1:C:27:TYR:HD1	1.97	0.48
1:C:63:ILE:HG23	1:C:68:LYS:HE2	1.96	0.48
1:G:103:ALA:HB1	1:G:162:VAL:HG21	1.96	0.48
1:C:93:LYS:HD2	1:D:81:ARG:HD3	1.94	0.48
1:A:114:CYS:SG	1:A:214:TRP:CE3	3.07	0.47
1:B:217:LYS:HZ3	1:B:217:LYS:HB2	1.78	0.47
1:C:123:LYS:HD3	1:C:127:LEU:HD11	1.95	0.47
1:D:118:ASP:HB3	1:D:121:LYS:HD2	1.95	0.47
1:G:9:ILE:HA	1:G:206:PRO:HB2	1.96	0.47
1:A:174:LEU:O	1:A:181:LYS:HE2	2.14	0.47
1:B:21:GLU:HG2	1:B:196:TYR:CG	2.49	0.47
1:B:2:MET:HE2	1:B:62:LEU:HD11	1.97	0.47
1:B:212:ALA:O	1:B:216:ASN:ND2	2.48	0.47
1:B:163:LEU:HB3	1:B:184:ILE:HD11	1.97	0.47
1:E:96:VAL:O	1:E:155:VAL:HG11	2.14	0.47
1:B:8:ASP:HA	1:B:31:LYS:HD2	1.95	0.47
1:G:22:TYR:O	1:G:192:LYS:HD3	2.14	0.47
1:A:180:LEU:O	1:A:183:PHE:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLU:O	1:F:173:CYS:SG	2.64	0.47
1:A:34:MET:HG2	1:A:35:GLY:N	2.30	0.47
1:G:205:LYS:HA	1:G:206:PRO:C	2.35	0.47
1:B:123:LYS:N	1:B:124:PRO:HD2	2.30	0.47
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.80	0.47
1:C:3:THR:HG23	1:C:63:ILE:HD12	1.97	0.47
1:C:49:LYS:HE2	1:C:57:PRO:HB2	1.96	0.47
1:A:141:LEU:HB3	1:A:179:ASN:HD21	1.80	0.47
1:C:181:LYS:O	1:C:184:ILE:HG22	2.14	0.47
1:B:132:THR:O	1:B:135:GLN:HB3	2.15	0.47
1:A:118:ASP:O	1:A:122:LEU:HD13	2.15	0.47
1:H:140:PHE:HD2	1:H:147:PHE:HD1	1.61	0.47
1:D:159:ALA:O	1:D:163:LEU:HG	2.15	0.47
1:E:70:THR:O	1:E:71:GLN:CB	2.62	0.47
1:B:132:THR:O	1:B:136:HIS:ND1	2.47	0.47
1:H:126:TYR:CE1	1:H:133:MET:HE1	2.50	0.47
1:A:105:ASP:O	1:A:109:GLN:HG3	2.15	0.47
1:B:6:TYR:O	1:B:31:LYS:HA	2.16	0.46
1:A:115:TYR:CE1	1:A:212:ALA:HB2	2.50	0.46
1:G:9:ILE:HD12	1:G:206:PRO:HB3	1.97	0.46
1:E:113:VAL:HG13	1:E:122:LEU:HB3	1.98	0.46
1:A:144:ARG:HD3	1:A:149:GLY:CA	2.34	0.46
1:F:43:SER:HA	1:F:46:LEU:HB2	1.97	0.46
1:F:157:PHE:CD2	1:F:187:PHE:HZ	2.33	0.46
1:E:22:TYR:HD1	1:E:192:LYS:HB2	1.80	0.46
1:G:102:GLN:O	1:G:105:ASP:HB3	2.16	0.46
1:D:40:TYR:CG	1:D:211:VAL:HG12	2.49	0.46
1:C:13:ALA:O	1:C:15:ALA:N	2.49	0.46
1:H:174:LEU:HG	1:H:181:LYS:CD	2.41	0.46
1:F:69:ILE:N	1:F:69:ILE:HD12	2.31	0.46
1:F:15:ALA:O	1:F:18:LEU:HB2	2.16	0.46
1:G:62:LEU:O	1:G:68:LYS:HA	2.16	0.46
1:F:64:ASP:HB3	1:F:67:HIS:HB2	1.98	0.46
1:B:62:LEU:HD22	1:B:75:ILE:HG23	1.98	0.46
1:B:9:ILE:HG13	1:B:206:PRO:CG	2.43	0.46
1:H:33:THR:HG22	1:H:210:ARG:NH2	2.29	0.46
1:D:134:MET:HB3	1:D:177:PHE:CE2	2.51	0.46
1:B:88:GLU:CD	1:B:151:LYS:HE3	2.37	0.46
1:F:6:TYR:HE2	1:F:9:ILE:O	1.99	0.46
1:G:10:ARG:CG	1:G:14:HIS:HB2	2.46	0.46
1:G:130:LEU:N	1:G:131:PRO:HD2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:ALA:O	1:H:163:LEU:HG	2.16	0.46
1:H:207:LEU:HD22	1:H:207:LEU:N	2.31	0.46
1:G:99:LEU:HD22	1:G:99:LEU:HA	1.51	0.46
1:C:106:VAL:O	1:C:109:GLN:HB3	2.16	0.46
1:F:110:LEU:HD13	1:F:126:TYR:HE2	1.81	0.45
1:F:141:LEU:HD21	1:F:183:PHE:HB2	1.97	0.45
1:E:196:TYR:O	1:E:202:PHE:HB2	2.16	0.45
1:E:130:LEU:N	1:E:131:PRO:HD2	2.31	0.45
1:G:94:ILE:HD13	1:H:69:ILE:HD11	1.97	0.45
1:B:173:CYS:SG	1:B:174:LEU:HD12	2.57	0.45
1:H:107:SER:OG	1:H:162:VAL:HG22	2.17	0.45
1:G:207:LEU:HD12	1:G:208:TYR:HE1	1.79	0.45
1:A:129:GLU:O	1:A:132:THR:HG22	2.16	0.45
1:C:209:THR:OG1	1:C:211:VAL:HG12	2.17	0.45
1:B:182:ASP:O	1:B:185:SER:HB2	2.17	0.45
1:A:127:LEU:HD22	1:A:170:GLU:OE1	2.17	0.45
1:F:138:SER:O	1:F:179:ASN:ND2	2.49	0.45
1:H:43:SER:HA	1:H:46:LEU:HB2	1.99	0.45
1:A:106:VAL:HG13	1:A:162:VAL:HG11	1.99	0.45
1:B:22:TYR:CD1	1:B:193:ILE:HD11	2.51	0.45
1:E:179:ASN:HD22	1:E:179:ASN:N	2.15	0.45
1:G:157:PHE:HA	1:G:187:PHE:CE2	2.52	0.45
1:A:99:LEU:HD12	1:A:155:VAL:HB	1.98	0.45
1:E:80:ALA:CB	1:E:86:CYS:SG	2.95	0.45
1:C:95:ARG:NH1	1:C:140:PHE:CE2	2.85	0.45
1:G:71:GLN:HE21	1:H:102:GLN:HA	1.82	0.45
1:F:148:VAL:HG12	1:F:151:LYS:O	2.15	0.45
1:A:119:PHE:HB2	1:A:213:VAL:HG21	1.98	0.45
1:B:157:PHE:CE2	1:B:187:PHE:HZ	2.35	0.45
1:A:79:ILE:O	1:A:83:HIS:HD2	1.99	0.45
1:D:70:THR:O	1:D:71:GLN:HB2	2.16	0.45
1:D:49:LYS:O	1:D:57:PRO:HB3	2.16	0.45
1:F:22:TYR:O	1:F:192:LYS:HE3	2.16	0.44
1:C:49:LYS:HD3	1:C:50:PHE:CZ	2.52	0.44
1:B:5:GLY:HA2	1:B:30:LYS:HB3	1.98	0.44
1:E:167:ARG:NH1	1:E:184:ILE:HG21	2.32	0.44
1:B:125:GLU:O	1:B:128:GLU:HG2	2.17	0.44
1:A:77:CYS:O	1:A:81:ARG:HB2	2.17	0.44
1:C:5:GLY:HA3	1:C:61:TYR:CZ	2.52	0.44
1:G:134:MET:HB2	1:G:177:PHE:CE2	2.51	0.44
1:D:54:LEU:HD12	1:D:57:PRO:HA	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ASP:O	1:F:120:GLU:N	2.51	0.44
1:F:122:LEU:HD12	1:F:122:LEU:H	1.82	0.44
1:G:2:MET:O	1:G:28:GLU:N	2.50	0.44
1:B:106:VAL:HG23	1:B:162:VAL:HG21	1.98	0.44
1:F:144:ARG:HD3	1:F:149:GLY:HA2	2.00	0.44
1:B:59:LEU:HA	1:B:60:PRO:C	2.38	0.44
1:C:125:GLU:O	1:C:128:GLU:HG2	2.17	0.44
1:C:132:THR:O	1:C:135:GLN:HB3	2.18	0.44
1:C:7:TRP:C	1:C:9:ILE:H	2.21	0.44
1:H:7:TRP:HH2	1:H:42:ARG:HB3	1.82	0.44
1:C:101:ASN:HB3	1:D:71:GLN:OE1	2.18	0.44
1:G:193:ILE:HG22	1:G:197:MET:SD	2.57	0.44
1:G:140:PHE:HD2	1:G:147:PHE:HD1	1.66	0.44
1:C:70:THR:H	1:D:98:ILE:HD11	1.83	0.44
1:C:183:PHE:HA	1:C:186:ARG:NH1	2.33	0.44
1:C:8:ASP:HB3	1:C:31:LYS:HG2	1.98	0.44
1:E:78:TYR:HE1	1:F:94:ILE:HD11	1.83	0.44
1:H:177:PHE:HA	1:H:178:PRO:HD2	1.83	0.44
1:A:62:LEU:HD22	1:A:75:ILE:HG23	2.00	0.44
1:A:36:ASP:HA	1:A:40:TYR:CE2	2.52	0.44
1:D:86:CYS:O	1:D:153:THR:HG22	2.18	0.44
1:F:16:ILE:O	1:F:20:LEU:HB2	2.18	0.44
1:G:12:LEU:CD1	1:G:60:PRO:HD3	2.47	0.44
1:E:109:GLN:O	1:E:113:VAL:HG23	2.18	0.44
1:F:123:LYS:N	1:F:124:PRO:HD2	2.33	0.44
1:E:163:LEU:HB2	1:E:184:ILE:HD11	2.00	0.43
1:E:2:MET:O	1:E:27:TYR:HA	2.17	0.43
1:F:5:GLY:HA3	1:F:61:TYR:CZ	2.53	0.43
1:A:81:ARG:HH22	1:B:94:ILE:HG22	1.82	0.43
1:C:92:GLU:HG3	1:C:148:VAL:CG1	2.48	0.43
1:G:184:ILE:HG23	1:G:188:GLU:OE2	2.17	0.43
1:C:192:LYS:NZ	1:C:192:LYS:HB2	2.33	0.43
1:E:74:ALA:HA	1:F:97:ASP:HB3	1.99	0.43
1:H:167:ARG:HD3	1:H:168:ILE:HG13	2.01	0.43
1:H:160:TYR:CE1	1:H:184:ILE:HG23	2.51	0.43
1:H:49:LYS:HD3	1:H:57:PRO:CB	2.48	0.43
1:F:164:ASP:O	1:F:167:ARG:HB3	2.18	0.43
1:C:196:TYR:HD1	1:C:201:ARG:HH21	1.65	0.43
1:H:153:THR:OG1	1:H:155:VAL:HG22	2.18	0.43
1:A:216:ASN:HD22	1:A:216:ASN:H	1.66	0.43
1:G:207:LEU:HB3	1:G:208:TYR:HD1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:TYR:HB3	1:F:70:THR:HG22	2.00	0.43
1:C:87:GLY:HA2	1:C:92:GLU:HB3	2.00	0.43
1:B:115:TYR:CE1	1:B:212:ALA:HB2	2.53	0.43
1:G:2:MET:HE2	1:G:25:SER:HB3	1.99	0.43
1:E:114:CYS:O	1:E:213:VAL:HG22	2.17	0.43
1:H:143:LYS:HD3	1:H:143:LYS:N	2.34	0.43
1:F:153:THR:OG1	1:F:155:VAL:HG22	2.18	0.43
1:C:95:ARG:NH1	1:C:147:PHE:O	2.51	0.43
1:C:71:GLN:CG	1:D:101:ASN:HB3	2.48	0.43
1:C:21:GLU:HG3	1:C:196:TYR:CD1	2.54	0.43
1:E:64:ASP:N	1:E:67:HIS:O	2.50	0.43
1:F:49:LYS:HD3	1:F:50:PHE:CE1	2.54	0.43
1:D:10:ARG:HG2	1:D:11:GLY:N	2.34	0.43
1:A:13:ALA:HA	1:A:16:ILE:HD12	2.00	0.43
1:F:164:ASP:HA	1:F:167:ARG:CB	2.49	0.43
1:F:10:ARG:HH21	1:F:14:HIS:CD2	2.36	0.43
1:F:19:LEU:HG	1:F:79:ILE:HG21	2.00	0.43
1:E:10:ARG:HB2	1:E:204:PRO:O	2.19	0.43
1:C:196:TYR:CZ	1:C:202:PHE:HA	2.54	0.43
1:H:105:ASP:O	1:H:109:GLN:HB2	2.18	0.43
1:C:64:ASP:HB3	1:C:67:HIS:HB2	2.00	0.43
1:E:98:ILE:HD11	1:F:69:ILE:HG23	2.00	0.43
1:H:89:THR:OG1	1:H:92:GLU:HB2	2.19	0.43
1:E:49:LYS:HE3	1:E:57:PRO:HB2	2.00	0.43
1:E:132:THR:O	1:E:135:GLN:HB3	2.18	0.43
1:G:54:LEU:HD12	1:G:57:PRO:HA	2.01	0.43
1:E:32:TYR:HH	1:E:61:TYR:HH	1.65	0.43
1:B:206:PRO:HB3	1:B:217:LYS:HB3	2.00	0.43
1:E:141:LEU:O	1:E:144:ARG:HG2	2.18	0.43
1:D:56:PHE:O	1:D:70:THR:HG21	2.18	0.43
1:H:141:LEU:O	1:H:144:ARG:NH1	2.52	0.43
1:H:75:ILE:HD12	1:H:75:ILE:H	1.84	0.43
1:D:180:LEU:O	1:D:184:ILE:HD12	2.18	0.42
1:A:10:ARG:CG	1:A:14:HIS:HB2	2.49	0.42
1:C:31:LYS:HB2	1:C:31:LYS:HE3	1.86	0.42
1:H:144:ARG:HA	1:H:145:PRO:HD3	1.86	0.42
1:F:108:ASN:HA	1:F:108:ASN:HD22	1.67	0.42
1:C:91:GLU:O	1:C:95:ARG:HG3	2.19	0.42
1:G:10:ARG:HB3	1:G:206:PRO:O	2.19	0.42
1:E:163:LEU:CB	1:E:184:ILE:HD11	2.48	0.42
1:H:82:LYS:O	1:H:83:HIS:CG	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:LEU:HD12	1:F:79:ILE:HG12	2.01	0.42
1:G:92:GLU:O	1:G:96:VAL:HG23	2.19	0.42
1:H:140:PHE:HD2	1:H:147:PHE:CD1	2.36	0.42
1:A:89:THR:OG1	1:A:92:GLU:HG3	2.19	0.42
1:C:123:LYS:N	1:C:124:PRO:HD2	2.34	0.42
1:A:216:ASN:HD22	1:A:216:ASN:N	2.17	0.42
1:E:182:ASP:O	1:E:186:ARG:HB2	2.19	0.42
1:A:9:ILE:HA	1:A:206:PRO:HG2	2.01	0.42
1:H:130:LEU:HD12	1:H:133:MET:SD	2.59	0.42
1:G:206:PRO:HA	1:G:217:LYS:NZ	2.34	0.42
1:F:23:THR:HB	1:F:83:HIS:NE2	2.34	0.42
1:B:138:SER:OG	1:B:180:LEU:HG	2.19	0.42
1:E:144:ARG:NH1	1:E:144:ARG:HG2	2.35	0.42
1:H:119:PHE:O	1:H:123:LYS:N	2.53	0.42
1:F:188:GLU:HG2	1:F:197:MET:HE1	2.01	0.42
1:H:167:ARG:HH21	1:H:184:ILE:HG21	1.85	0.42
1:H:70:THR:O	1:H:71:GLN:HB2	2.20	0.42
1:A:99:LEU:HD11	1:A:159:ALA:HB2	2.02	0.42
1:G:211:VAL:O	1:G:211:VAL:HG22	2.20	0.42
1:D:16:ILE:H	1:D:16:ILE:HD12	1.84	0.42
1:F:141:LEU:O	1:F:144:ARG:HG2	2.20	0.42
1:H:42:ARG:O	1:H:46:LEU:HD23	2.19	0.42
1:D:62:LEU:O	1:D:68:LYS:HA	2.19	0.42
1:D:146:TRP:HB3	1:D:156:ASP:OD2	2.19	0.42
1:C:8:ASP:OD2	1:C:33:THR:HA	2.20	0.41
1:B:79:ILE:O	1:B:83:HIS:CD2	2.73	0.41
1:E:33:THR:H	1:E:44:GLN:HE22	1.68	0.41
1:A:140:PHE:CD2	1:A:147:PHE:HD2	2.32	0.41
1:D:114:CYS:O	1:D:213:VAL:HG12	2.19	0.41
1:H:126:TYR:HE1	1:H:133:MET:HE1	1.85	0.41
1:H:130:LEU:HD11	1:H:166:HIS:CD2	2.55	0.41
1:G:94:ILE:HD11	1:H:78:TYR:CE1	2.55	0.41
1:C:183:PHE:HA	1:C:186:ARG:HH11	1.85	0.41
1:A:125:GLU:O	1:A:128:GLU:HB3	2.19	0.41
1:D:144:ARG:HA	1:D:145:PRO:HD3	1.74	0.41
1:E:103:ALA:HB1	1:E:162:VAL:HG21	2.02	0.41
1:A:63:ILE:HG23	1:A:68:LYS:HD2	2.02	0.41
1:C:94:ILE:O	1:C:98:ILE:HG13	2.20	0.41
1:G:119:PHE:CZ	1:G:214:TRP:HD1	2.38	0.41
1:A:92:GLU:O	1:A:96:VAL:HG23	2.20	0.41
1:G:108:ASN:O	1:G:112:ARG:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:CYS:HG	1:H:214:TRP:HE3	1.64	0.41
1:F:7:TRP:O	1:F:31:LYS:HG2	2.21	0.41
1:B:61:TYR:CD1	1:B:63:ILE:HD11	2.55	0.41
1:B:212:ALA:HB3	1:B:216:ASN:HB3	2.03	0.41
1:F:146:TRP:O	1:F:149:GLY:N	2.50	0.41
1:H:49:LYS:HD3	1:H:57:PRO:HB3	2.02	0.41
1:F:177:PHE:HA	1:F:178:PRO:HD2	1.84	0.41
1:E:58:ASN:HB3	1:E:70:THR:CG2	2.50	0.41
1:G:89:THR:OG1	1:G:92:GLU:HG3	2.21	0.41
1:C:21:GLU:HG3	1:C:196:TYR:CG	2.55	0.41
1:B:98:ILE:HG22	1:B:99:LEU:N	2.35	0.41
1:C:19:LEU:O	1:C:22:TYR:HB3	2.20	0.41
1:B:208:TYR:HB3	1:B:212:ALA:HB2	2.02	0.41
1:C:70:THR:O	1:C:71:GLN:CB	2.66	0.41
1:A:205:LYS:HA	1:A:206:PRO:C	2.41	0.41
1:C:145:PRO:HG2	1:C:150:ASP:HA	2.03	0.41
1:B:45:TRP:CH2	1:B:61:TYR:HE2	2.38	0.41
1:H:20:LEU:HD21	1:H:79:ILE:CD1	2.50	0.41
1:E:22:TYR:CD1	1:E:192:LYS:HB2	2.56	0.41
1:D:80:ALA:HB2	1:D:154:PHE:HB3	2.02	0.41
1:B:10:ARG:NE	1:B:165:LEU:HD21	2.36	0.41
1:G:4:LEU:HB3	1:G:62:LEU:HD13	2.02	0.41
1:E:212:ALA:O	1:E:216:ASN:ND2	2.54	0.41
1:B:37:ALA:HB1	1:B:38:PRO:CD	2.43	0.41
1:F:16:ILE:HG13	1:F:16:ILE:H	1.75	0.41
1:B:21:GLU:HG2	1:B:196:TYR:CB	2.49	0.41
1:E:20:LEU:HD13	1:E:27:TYR:CD2	2.56	0.41
1:A:5:GLY:O	1:A:60:PRO:HA	2.21	0.41
1:B:206:PRO:HB3	1:B:217:LYS:HB2	2.02	0.41
1:F:160:TYR:HD1	1:F:184:ILE:HG22	1.86	0.41
1:D:71:GLN:O	1:D:75:ILE:HG13	2.21	0.41
1:A:69:ILE:HG22	1:A:75:ILE:HG12	2.03	0.41
1:G:6:TYR:O	1:G:31:LYS:HA	2.21	0.41
1:F:125:GLU:O	1:F:128:GLU:HB2	2.20	0.41
1:G:181:LYS:HB3	1:G:181:LYS:HE3	1.89	0.41
1:A:163:LEU:O	1:A:167:ARG:HG2	2.21	0.40
1:C:134:MET:SD	1:C:174:LEU:CD1	3.04	0.40
1:A:217:LYS:HE2	1:A:217:LYS:HB2	1.96	0.40
1:B:7:TRP:C	1:B:9:ILE:H	2.24	0.40
1:B:5:GLY:O	1:B:60:PRO:HA	2.21	0.40
1:A:64:ASP:N	1:A:67:HIS:O	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:TYR:CZ	1:B:208:TYR:HD2	2.39	0.40
1:B:65:GLY:C	1:B:67:HIS:H	2.25	0.40
1:D:21:GLU:OE2	1:D:196:TYR:HB2	2.21	0.40
1:C:206:PRO:CG	1:C:217:LYS:HB3	2.37	0.40
1:A:95:ARG:NH2	1:A:144:ARG:NH2	2.69	0.40
1:B:2:MET:HE1	1:B:62:LEU:HD21	2.03	0.40
1:F:10:ARG:HG2	1:F:14:HIS:HB2	2.03	0.40
1:H:17:ARG:HH12	1:H:203:LEU:HD23	1.86	0.40
1:A:130:LEU:N	1:A:131:PRO:HD2	2.36	0.40
1:F:157:PHE:CE2	1:F:187:PHE:HZ	2.39	0.40
1:G:98:ILE:HD11	1:H:69:ILE:HG23	2.02	0.40
1:G:59:LEU:HA	1:G:59:LEU:HD23	1.91	0.40
1:F:96:VAL:O	1:F:100:GLU:HB2	2.22	0.40
1:G:64:ASP:O	1:G:66:ALA:N	2.54	0.40
1:F:2:MET:HE1	1:F:20:LEU:HD11	2.02	0.40
1:E:108:ASN:O	1:E:112:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	215/217 (99%)	184 (86%)	24 (11%)	7 (3%)	5 30
1	B	215/217 (99%)	176 (82%)	28 (13%)	11 (5%)	2 19
1	C	215/217 (99%)	180 (84%)	29 (14%)	6 (3%)	6 34
1	D	215/217 (99%)	183 (85%)	27 (13%)	5 (2%)	8 39
1	E	215/217 (99%)	188 (87%)	20 (9%)	7 (3%)	5 30
1	F	215/217 (99%)	183 (85%)	25 (12%)	7 (3%)	5 30
1	G	215/217 (99%)	182 (85%)	23 (11%)	10 (5%)	3 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	215/217 (99%)	184 (86%)	22 (10%)	9 (4%)	3 23
All	All	1720/1736 (99%)	1460 (85%)	198 (12%)	62 (4%)	4 28

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	B	147	PHE
1	B	204	PRO
1	C	14	HIS
1	C	71	GLN
1	E	71	GLN
1	F	119	PHE
1	G	206	PRO
1	A	147	PHE
1	B	40	TYR
1	B	41	ASP
1	B	71	GLN
1	B	142	GLY
1	C	49	LYS
1	D	204	PRO
1	E	65	GLY
1	E	204	PRO
1	F	147	PHE
1	G	142	GLY
1	H	37	ALA
1	B	37	ALA
1	B	184	ILE
1	D	40	TYR
1	E	210	ARG
1	G	41	ASP
1	H	36	ASP
1	H	40	TYR
1	H	188	GLU
1	H	191	GLU
1	H	204	PRO
1	A	57	PRO
1	A	65	GLY
1	B	6	TYR
1	B	119	PHE
1	F	46	LEU
1	G	52	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	71	GLN
1	A	40	TYR
1	A	210	ARG
1	B	72	SER
1	C	37	ALA
1	C	145	PRO
1	D	45	TRP
1	D	141	LEU
1	E	52	LEU
1	G	40	TYR
1	G	215	GLY
1	H	25	SER
1	A	37	ALA
1	D	37	ALA
1	E	37	ALA
1	F	37	ALA
1	F	71	GLN
1	G	37	ALA
1	G	43	SER
1	G	71	GLN
1	G	65	GLY
1	H	38	PRO
1	F	11	GLY
1	C	171	PRO
1	F	204	PRO
1	E	98	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	195/195 (100%)	183 (94%)	12 (6%)	23 61
1	B	195/195 (100%)	180 (92%)	15 (8%)	16 51
1	C	195/195 (100%)	176 (90%)	19 (10%)	10 38
1	D	195/195 (100%)	177 (91%)	18 (9%)	11 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	195/195 (100%)	175 (90%)	20 (10%)	9 34
1	F	195/195 (100%)	172 (88%)	23 (12%)	6 27
1	G	195/195 (100%)	175 (90%)	20 (10%)	9 34
1	H	195/195 (100%)	177 (91%)	18 (9%)	11 40
All	All	1560/1560 (100%)	1415 (91%)	145 (9%)	11 40

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	25	SER
1	A	36	ASP
1	A	68	LYS
1	A	70	THR
1	A	99	LEU
1	A	135	GLN
1	A	158	LEU
1	A	165	LEU
1	A	182	ASP
1	A	201	ARG
1	A	216	ASN
1	B	3	THR
1	B	9	ILE
1	B	39	ASP
1	B	44	GLN
1	B	55	ASP
1	B	59	LEU
1	B	69	ILE
1	B	70	THR
1	B	114	CYS
1	B	132	THR
1	B	138	SER
1	B	144	ARG
1	B	186	ARG
1	B	201	ARG
1	B	217	LYS
1	C	2	MET
1	C	3	THR
1	C	24	ASP
1	C	34	MET
1	C	39	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	44	GLN
1	C	68	LYS
1	C	72	SER
1	C	77	CYS
1	C	84	ASN
1	C	123	LYS
1	C	150	ASP
1	C	166	HIS
1	C	167	ARG
1	C	177	PHE
1	C	179	ASN
1	C	184	ILE
1	C	197	MET
1	C	205	LYS
1	D	2	MET
1	D	9	ILE
1	D	21	GLU
1	D	24	ASP
1	D	39	ASP
1	D	42	ARG
1	D	72	SER
1	D	97	ASP
1	D	105	ASP
1	D	113	VAL
1	D	127	LEU
1	D	132	THR
1	D	134	MET
1	D	137	PHE
1	D	167	ARG
1	D	179	ASN
1	D	192	LYS
1	D	201	ARG
1	E	1	SER
1	E	2	MET
1	E	12	LEU
1	E	41	ASP
1	E	42	ARG
1	E	50	PHE
1	E	52	LEU
1	E	84	ASN
1	E	93	LYS
1	E	118	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	136	HIS
1	E	137	PHE
1	E	144	ARG
1	E	179	ASN
1	E	182	ASP
1	E	197	MET
1	E	198	LYS
1	E	201	ARG
1	E	205	LYS
1	E	210	ARG
1	F	26	SER
1	F	43	SER
1	F	47	ASN
1	F	55	ASP
1	F	84	ASN
1	F	90	GLU
1	F	95	ARG
1	F	99	LEU
1	F	104	MET
1	F	105	ASP
1	F	106	VAL
1	F	122	LEU
1	F	123	LYS
1	F	132	THR
1	F	147	PHE
1	F	148	VAL
1	F	164	ASP
1	F	165	LEU
1	F	182	ASP
1	F	201	ARG
1	F	203	LEU
1	F	205	LYS
1	F	207	LEU
1	G	4	LEU
1	G	10	ARG
1	G	12	LEU
1	G	16	ILE
1	G	39	ASP
1	G	47	ASN
1	G	84	ASN
1	G	90	GLU
1	G	99	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	112	ARG
1	G	136	HIS
1	G	143	LYS
1	G	153	THR
1	G	158	LEU
1	G	165	LEU
1	G	175	ASP
1	G	182	ASP
1	G	201	ARG
1	G	207	LEU
1	G	217	LYS
1	H	31	LYS
1	H	33	THR
1	H	44	GLN
1	H	49	LYS
1	H	52	LEU
1	H	61	TYR
1	H	70	THR
1	H	71	GLN
1	H	105	ASP
1	H	127	LEU
1	H	147	PHE
1	H	151	LYS
1	H	167	ARG
1	H	175	ASP
1	H	179	ASN
1	H	185	SER
1	H	209	THR
1	H	217	LYS

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	83	HIS
1	A	135	GLN
1	A	166	HIS
1	A	179	ASN
1	A	216	ASN
1	B	44	GLN
1	B	58	ASN
1	B	172	ASN
1	C	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	14	HIS
1	D	108	ASN
1	D	179	ASN
1	D	216	ASN
1	E	44	GLN
1	E	179	ASN
1	F	108	ASN
1	F	179	ASN
1	G	71	GLN
1	G	108	ASN
1	H	83	HIS
1	H	84	ASN
1	H	179	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	217/217 (100%)	-0.22	0 100 100	6, 18, 29, 35	0
1	B	217/217 (100%)	-0.21	1 (0%) 91 90	5, 17, 28, 35	0
1	C	217/217 (100%)	-0.24	1 (0%) 91 90	5, 18, 28, 34	0
1	D	217/217 (100%)	-0.24	2 (0%) 85 82	5, 17, 28, 35	0
1	E	217/217 (100%)	-0.15	1 (0%) 91 90	6, 17, 29, 34	0
1	F	217/217 (100%)	-0.22	2 (0%) 85 82	5, 18, 29, 34	0
1	G	217/217 (100%)	-0.22	1 (0%) 91 90	5, 17, 29, 34	0
1	H	217/217 (100%)	-0.31	0 100 100	4, 17, 28, 34	0
All	All	1736/1736 (100%)	-0.23	8 (0%) 91 90	4, 18, 29, 35	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	ASP	4.0
1	D	38	PRO	3.4
1	F	38	PRO	2.8
1	B	38	PRO	2.8
1	D	39	ASP	2.6
1	G	25	SER	2.5
1	E	122	LEU	2.5
1	C	84	ASN	2.4

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

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

6.3 Carbohydrates (i)

There are no 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.