Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 02:33 pm BST

PDB ID	:	1E2T
Title	:	Arylamine N-acetyltransferase (NAT) from Salmonella typhimurium
Authors	:	Sinclair, J.C.; Sandy, J.; Delgoda, R.; Sim, E.; Noble, M.E.M.
Deposited on	:	2000-05-24
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

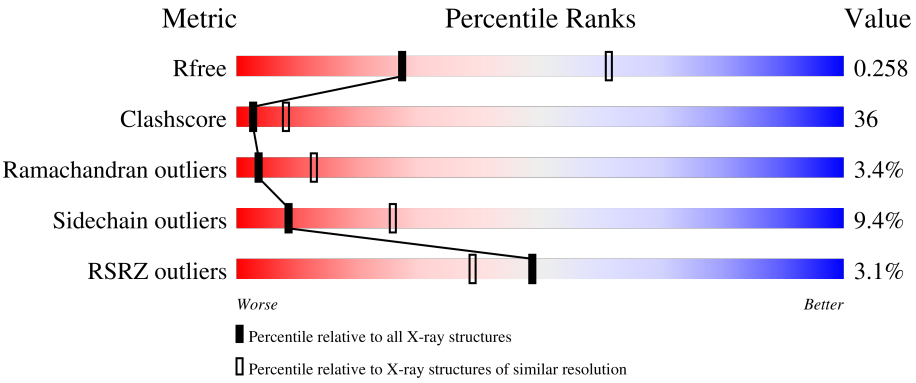
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



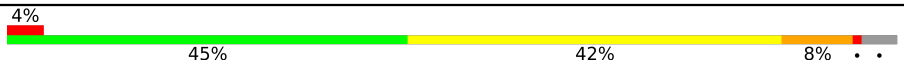
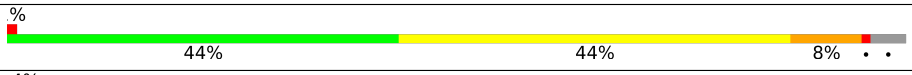
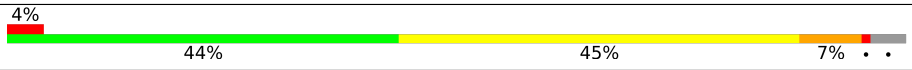
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	284	% 43% 44% 8%
1	B	284	2% 45% 40% 10%
1	C	284	5% 42% 45% 10%
1	D	284	6% 43% 44% 8%
1	E	284	46% 41% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	284	
1	G	284	
1	H	284	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18260 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 N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	B	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	C	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	D	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	E	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	F	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	G	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			
1	H	274	Total	C	N	O	S	0	0	0
			2224	1421	403	389	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	51	Total	O	0	0
			51	51		
2	C	79	Total	O	0	0
			79	79		
2	D	36	Total	O	0	0
			36	36		
2	E	92	Total	O	0	0
			92	92		
2	F	48	Total	O	0	0
			48	48		

Continued on next page...

Continued from previous page...

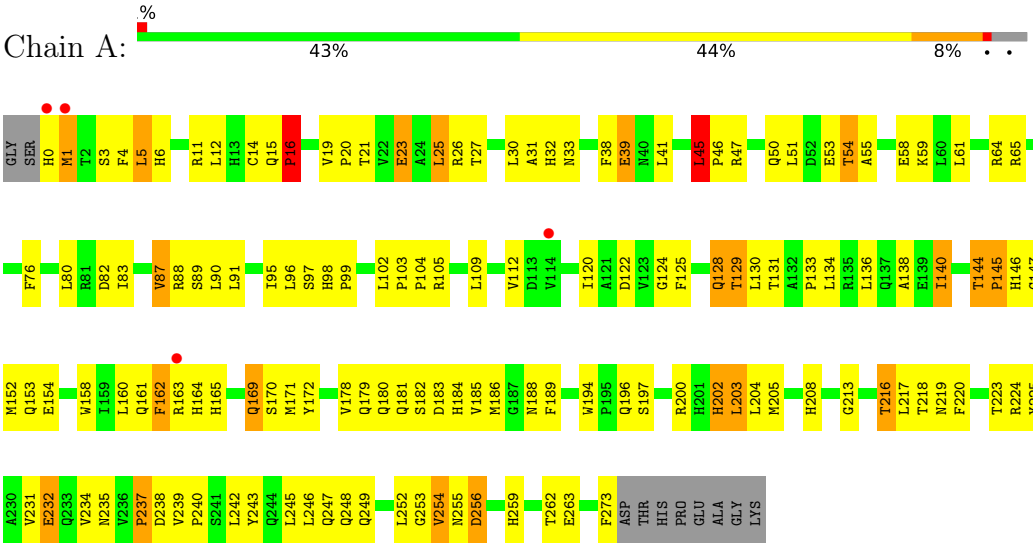
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	56	Total O 56 56	0	0
2	H	50	Total O 50 50	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

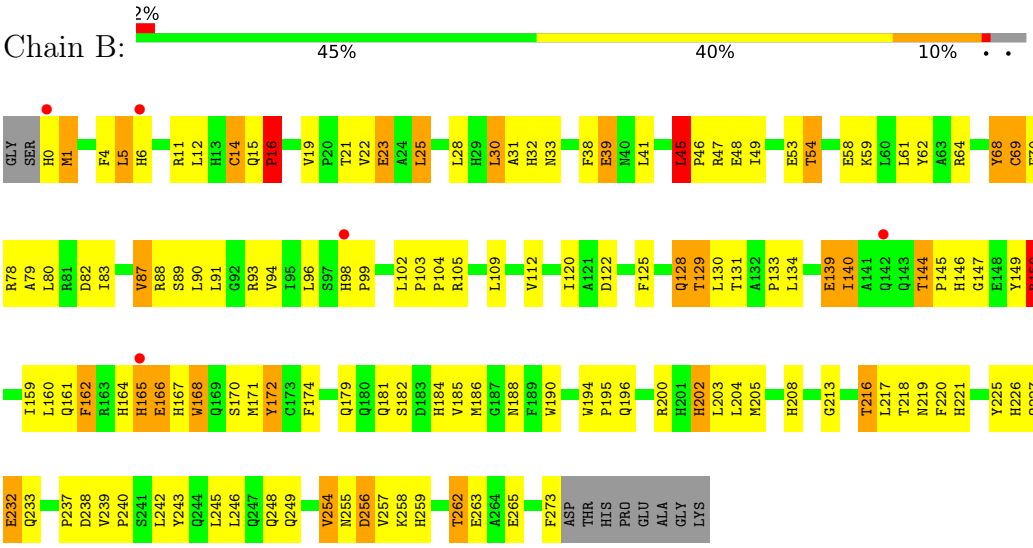
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain A:



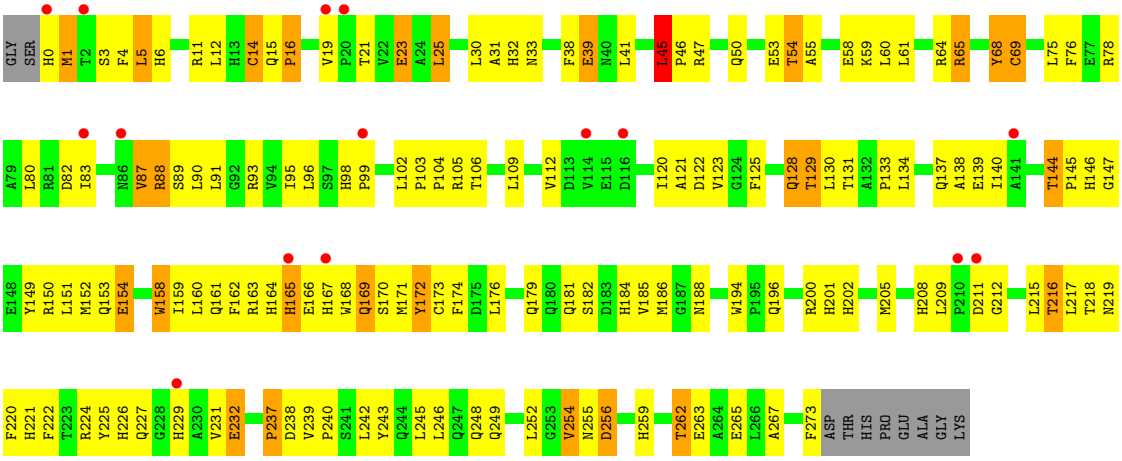
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain B:



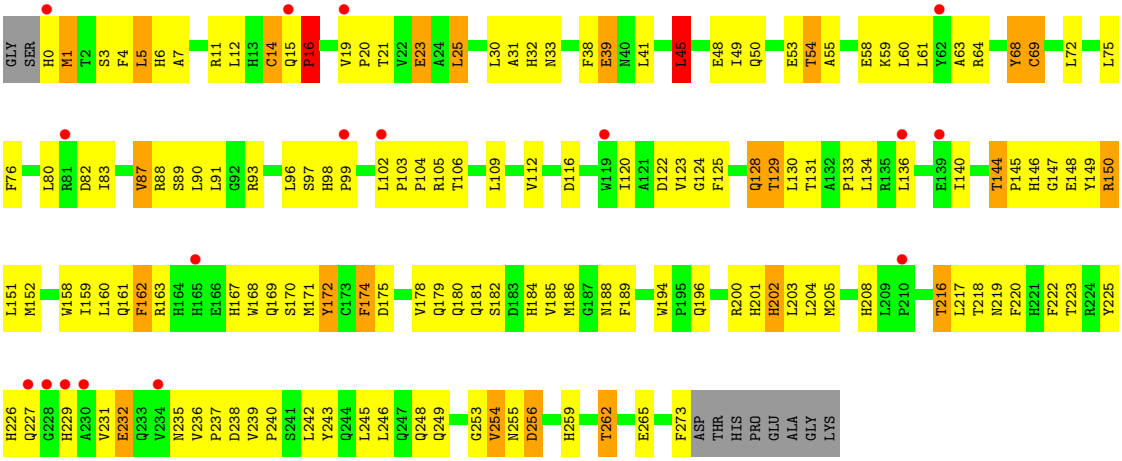
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain C:



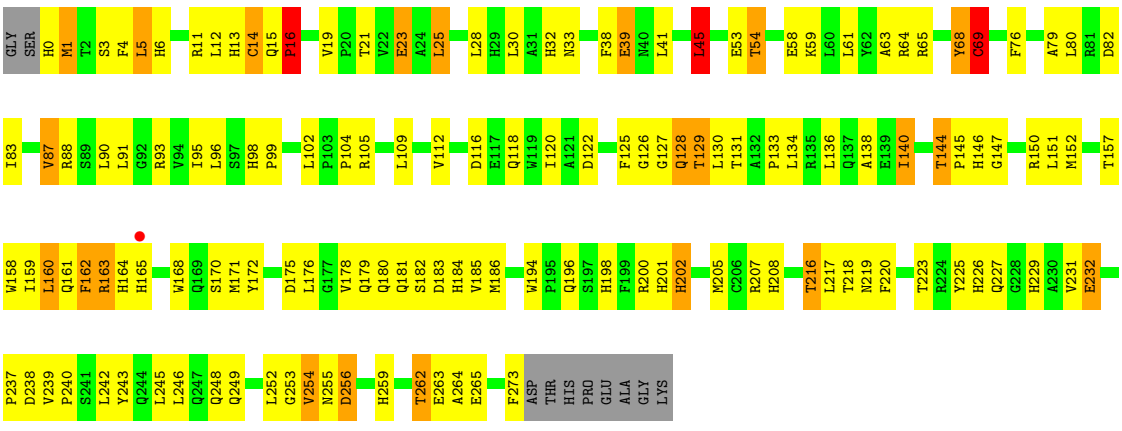
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain D:



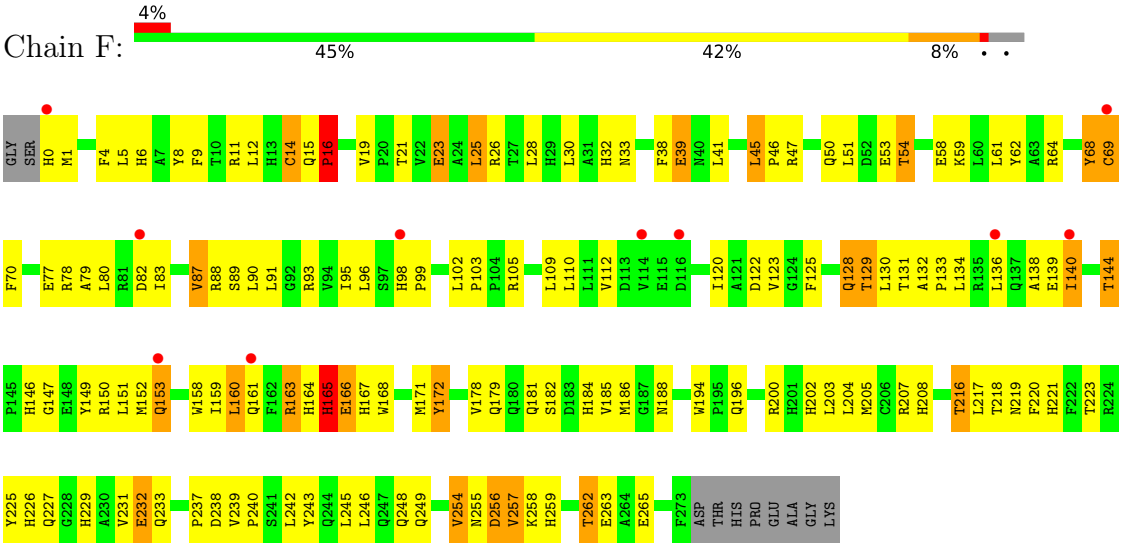
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain E:



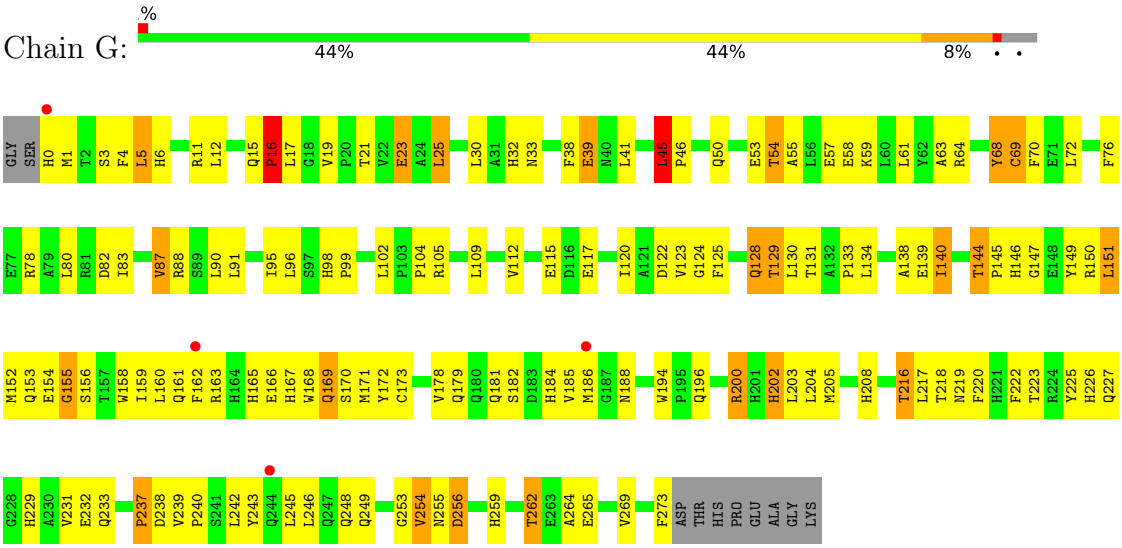
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain F:



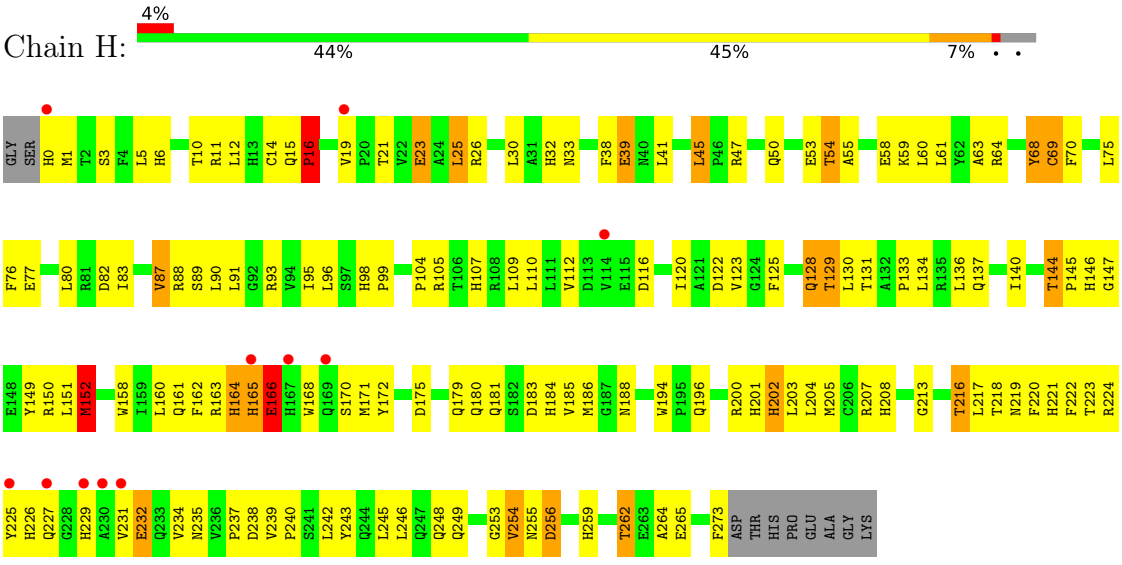
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain G:



• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.53Å 222.42Å 104.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 40.75 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.80) 78.7 (40.75-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.65Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.264 , 0.302 0.267 , 0.258	Depositor DCC
R_{free} test set	6188 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18260	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.78	0/2290	0.87	2/3113 (0.1%)
1	B	0.82	1/2290 (0.0%)	0.91	2/3113 (0.1%)
1	C	0.79	2/2290 (0.1%)	0.90	2/3113 (0.1%)
1	D	0.70	1/2290 (0.0%)	0.85	1/3113 (0.0%)
1	E	0.92	2/2290 (0.1%)	0.94	2/3113 (0.1%)
1	F	0.84	1/2290 (0.0%)	0.88	2/3113 (0.1%)
1	G	0.78	1/2290 (0.0%)	0.88	2/3113 (0.1%)
1	H	0.78	0/2290	0.89	2/3113 (0.1%)
All	All	0.80	8/18320 (0.0%)	0.89	15/24904 (0.1%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	CYS	CB-SG	-8.15	1.68	1.82
1	F	14	CYS	CB-SG	-7.24	1.70	1.82
1	E	14	CYS	CB-SG	-6.82	1.70	1.82
1	G	173	CYS	CB-SG	-6.71	1.70	1.82
1	E	69	CYS	CB-SG	-5.71	1.72	1.81
1	C	158	TRP	CB-CG	-5.54	1.40	1.50
1	D	14	CYS	CB-SG	-5.18	1.73	1.81
1	C	14	CYS	CB-SG	-5.10	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	45	LEU	N-CA-C	-8.12	89.08	111.00
1	A	45	LEU	N-CA-C	-8.07	89.22	111.00
1	B	45	LEU	N-CA-C	-7.72	90.14	111.00
1	C	45	LEU	N-CA-C	-7.62	90.42	111.00
1	B	150	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	G	45	LEU	N-CA-C	-7.60	90.47	111.00
1	H	45	LEU	N-CA-C	-7.59	90.50	111.00
1	F	45	LEU	N-CA-C	-7.55	90.61	111.00
1	D	45	LEU	N-CA-C	-7.50	90.74	111.00
1	G	200	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	F	45	LEU	CA-CB-CG	5.83	128.70	115.30
1	H	45	LEU	CA-CB-CG	5.62	128.23	115.30
1	E	175	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	65	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	A	203	LEU	CB-CG-CD2	-5.08	102.36	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	TYR	Sidechain
1	F	172	TYR	Sidechain

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	2224	0	2149	156	0
1	B	2224	0	2149	179	1
1	C	2224	0	2149	177	2
1	D	2224	0	2149	157	0
1	E	2224	0	2149	145	0
1	F	2224	0	2149	151	1
1	G	2224	0	2149	167	0
1	H	2224	0	2149	161	2
2	A	56	0	0	13	0
2	B	51	0	0	26	0
2	C	79	0	0	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	36	0	0	18	0
2	E	92	0	0	19	0
2	F	48	0	0	13	0
2	G	56	0	0	19	0
2	H	50	0	0	13	0
All	All	18260	0	17192	1252	4

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 36.

All (1252) 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:F:46:PRO:HD2	2:F:2011:HOH:O	1.24	1.34
1:F:186:MET:CE	1:H:186:MET:HE3	1.63	1.27
1:F:186:MET:HE2	1:H:186:MET:CE	1.70	1.20
1:B:186:MET:HE3	1:C:186:MET:CE	1.79	1.11
1:B:186:MET:CE	1:C:186:MET:HE3	1.80	1.10
1:B:166:GLU:HG2	1:G:233:GLN:HB2	1.40	1.04
1:A:186:MET:HE1	2:A:2034:HOH:O	1.58	1.03
1:B:128:GLN:HE21	1:B:128:GLN:H	1.03	1.01
1:D:128:GLN:H	1:D:128:GLN:HE21	1.03	1.00
1:E:150:ARG:NH1	1:E:152:MET:SD	2.35	0.99
1:A:128:GLN:H	1:A:128:GLN:HE21	0.99	0.99
1:B:152:MET:HG3	1:B:153:GLN:H	1.26	0.98
1:C:128:GLN:H	1:C:128:GLN:HE21	0.97	0.96
1:G:128:GLN:HE21	1:G:128:GLN:H	1.10	0.94
1:F:128:GLN:H	1:F:128:GLN:HE21	1.07	0.94
1:E:128:GLN:H	1:E:128:GLN:HE21	0.95	0.94
1:A:224:ARG:HD3	2:A:2044:HOH:O	1.66	0.93
1:H:128:GLN:HE21	1:H:128:GLN:N	1.69	0.91
1:E:216:THR:HG22	2:E:2076:HOH:O	1.71	0.91
1:B:25:LEU:HD22	1:B:133:PRO:HG3	1.53	0.90
1:C:104:PRO:HB2	2:C:2032:HOH:O	1.69	0.90
1:F:25:LEU:HD22	1:F:133:PRO:HG3	1.52	0.90
1:H:128:GLN:HE21	1:H:128:GLN:H	0.95	0.89
1:E:128:GLN:H	1:E:128:GLN:NE2	1.69	0.88
1:B:166:GLU:CG	1:G:233:GLN:HB2	2.04	0.88
1:C:161:GLN:HG2	1:C:170:SER:HA	1.56	0.88
1:H:25:LEU:HD22	1:H:133:PRO:HG3	1.56	0.88
1:B:161:GLN:HG2	1:B:170:SER:HA	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LEU:HD22	1:E:133:PRO:HG3	1.57	0.87
1:E:128:GLN:HE21	1:E:128:GLN:N	1.71	0.87
1:A:128:GLN:HE21	1:A:128:GLN:N	1.73	0.86
1:C:128:GLN:HE21	1:C:128:GLN:N	1.73	0.86
1:F:144:THR:HG23	1:F:146:HIS:H	1.40	0.86
1:E:165:HIS:HB2	2:E:2057:HOH:O	1.76	0.85
1:F:58:GLU:HB3	2:F:2014:HOH:O	1.75	0.85
1:E:144:THR:HG23	1:E:146:HIS:H	1.42	0.85
1:H:144:THR:HG23	1:H:146:HIS:H	1.39	0.84
1:G:144:THR:HG23	1:G:146:HIS:H	1.43	0.84
1:B:144:THR:HG23	1:B:146:HIS:H	1.42	0.84
1:F:255:ASN:O	1:F:256:ASP:HB2	1.77	0.84
1:C:144:THR:HG23	1:C:146:HIS:H	1.43	0.83
1:H:128:GLN:H	1:H:128:GLN:NE2	1.74	0.83
1:B:164:HIS:O	1:B:166:GLU:N	2.11	0.82
1:G:273:PHE:HE2	2:G:2044:HOH:O	1.62	0.82
1:G:239:VAL:HG23	2:G:2049:HOH:O	1.79	0.82
1:D:144:THR:HG23	1:D:146:HIS:H	1.44	0.82
1:B:186:MET:HE3	1:C:186:MET:HE3	0.90	0.81
1:C:128:GLN:H	1:C:128:GLN:NE2	1.76	0.81
1:H:161:GLN:HG2	1:H:170:SER:HA	1.62	0.81
1:D:128:GLN:HE21	1:D:128:GLN:N	1.78	0.81
1:A:128:GLN:H	1:A:128:GLN:NE2	1.79	0.80
1:C:138:ALA:HA	1:C:151:LEU:O	1.80	0.80
1:B:255:ASN:O	1:B:256:ASP:HB2	1.81	0.80
1:A:252:LEU:HD13	2:A:2008:HOH:O	1.80	0.80
1:E:186:MET:HE3	1:G:186:MET:HE2	1.63	0.80
1:H:144:THR:HG21	2:H:2026:HOH:O	1.82	0.80
1:G:163:ARG:NE	1:G:166:GLU:O	2.14	0.80
1:G:150:ARG:HB2	1:G:168:TRP:CZ2	2.17	0.80
1:A:144:THR:HG23	1:A:146:HIS:H	1.47	0.79
1:E:163:ARG:HG3	2:E:2053:HOH:O	1.80	0.79
1:F:265:GLU:HB3	2:F:2046:HOH:O	1.82	0.79
1:A:25:LEU:HD22	1:A:133:PRO:HG3	1.64	0.79
1:C:16:PRO:HD3	2:C:2004:HOH:O	1.83	0.79
1:B:165:HIS:O	1:B:166:GLU:HB2	1.81	0.79
1:D:180:GLN:HG2	2:D:2022:HOH:O	1.82	0.79
1:B:128:GLN:HE21	1:B:128:GLN:N	1.79	0.79
1:B:221:HIS:HB2	2:B:2040:HOH:O	1.83	0.79
1:E:160:LEU:HG	1:E:171:MET:HE3	1.63	0.79
1:B:96:LEU:HD23	1:B:171:MET:HA	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ASN:O	1:G:256:ASP:HB2	1.82	0.78
1:C:25:LEU:HD22	1:C:133:PRO:HG3	1.64	0.78
1:B:255:ASN:HB3	2:B:2045:HOH:O	1.83	0.78
1:G:25:LEU:HD22	1:G:133:PRO:HG3	1.65	0.78
1:C:255:ASN:O	1:C:256:ASP:HB2	1.84	0.77
1:G:150:ARG:NE	1:G:152:MET:HG2	1.99	0.77
1:B:128:GLN:H	1:B:128:GLN:NE2	1.81	0.77
1:G:128:GLN:HE21	1:G:128:GLN:N	1.83	0.76
1:A:196:GLN:HG2	2:A:2037:HOH:O	1.85	0.76
1:F:128:GLN:HE21	1:F:128:GLN:N	1.81	0.76
1:A:95:ILE:HG12	1:A:172:TYR:HA	1.65	0.76
1:E:102:LEU:HG	2:E:2037:HOH:O	1.84	0.76
1:C:33:ASN:O	1:C:208:HIS:HB2	1.86	0.76
1:C:186:MET:HE2	2:C:2048:HOH:O	1.87	0.75
1:D:128:GLN:H	1:D:128:GLN:NE2	1.80	0.75
1:E:159:ILE:HD12	1:E:159:ILE:N	2.01	0.75
1:E:161:GLN:HB3	1:E:170:SER:HA	1.66	0.75
1:C:95:ILE:HG12	1:C:172:TYR:HA	1.68	0.75
1:D:25:LEU:HD22	1:D:133:PRO:HG3	1.67	0.74
1:G:91:LEU:HD21	1:G:184:HIS:HD2	1.52	0.74
1:F:164:HIS:O	1:F:165:HIS:HB3	1.87	0.74
1:G:226:HIS:CE1	1:G:227:GLN:HE21	2.05	0.74
1:A:255:ASN:O	1:A:256:ASP:HB2	1.88	0.74
1:H:136:LEU:HD23	1:H:151:LEU:HD13	1.70	0.73
1:A:231:VAL:O	1:A:232:GLU:HB3	1.88	0.73
1:G:115:GLU:HG3	2:G:2029:HOH:O	1.89	0.73
1:C:194:TRP:CZ3	1:C:196:GLN:HB2	2.24	0.73
1:G:231:VAL:O	1:G:232:GLU:HB3	1.88	0.73
1:D:158:TRP:HB2	1:D:174:PHE:CE1	2.23	0.73
1:E:242:LEU:HG	2:E:2083:HOH:O	1.89	0.73
1:C:11:ARG:HD2	1:C:61:LEU:HA	1.70	0.73
1:D:109:LEU:HD21	1:D:174:PHE:CD2	2.23	0.73
1:F:128:GLN:H	1:F:128:GLN:NE2	1.85	0.73
1:B:33:ASN:O	1:B:208:HIS:HB2	1.89	0.72
1:B:46:PRO:HD2	2:D:2027:HOH:O	1.88	0.72
1:C:152:MET:O	1:C:159:ILE:HG22	1.89	0.72
1:B:94:VAL:HG12	2:B:2015:HOH:O	1.88	0.72
1:E:136:LEU:HD22	1:E:158:TRP:CZ2	2.24	0.72
1:B:194:TRP:CZ3	1:B:196:GLN:HB2	2.25	0.72
1:E:226:HIS:CE1	1:E:227:GLN:HE21	2.07	0.72
1:G:217:LEU:HD11	1:G:219:ASN:O	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HD12	2:C:2037:HOH:O	1.89	0.71
1:D:239:VAL:HB	1:D:240:PRO:HD3	1.72	0.71
1:H:255:ASN:O	1:H:256:ASP:HB2	1.90	0.71
1:F:194:TRP:CZ3	1:F:196:GLN:HB2	2.25	0.71
1:H:63:ALA:HB1	2:H:2045:HOH:O	1.89	0.71
1:A:104:PRO:HD3	1:D:182:SER:HB2	1.71	0.71
1:E:144:THR:HG22	1:E:147:GLY:N	2.06	0.70
1:H:144:THR:HG22	1:H:147:GLY:H	1.55	0.70
1:A:226:HIS:CE1	1:A:227:GLN:HE21	2.10	0.70
1:D:55:ALA:HA	2:D:2008:HOH:O	1.90	0.70
1:D:162:PHE:CE1	1:D:169:GLN:HB2	2.27	0.70
1:B:131:THR:HB	2:B:2027:HOH:O	1.91	0.70
1:G:163:ARG:NH2	1:G:167:HIS:HA	2.05	0.70
1:A:186:MET:HE3	1:D:186:MET:HE2	1.74	0.70
1:C:237:PRO:HA	2:C:2068:HOH:O	1.90	0.70
1:F:133:PRO:O	1:F:134:LEU:HD23	1.91	0.69
1:D:255:ASN:O	1:D:256:ASP:HB2	1.90	0.69
1:F:45:LEU:CA	2:F:2011:HOH:O	2.39	0.69
1:C:122:ASP:N	2:C:2037:HOH:O	2.25	0.69
1:D:11:ARG:HD2	1:D:61:LEU:HA	1.73	0.69
1:F:11:ARG:HD2	1:F:61:LEU:HA	1.73	0.69
1:H:11:ARG:HD2	1:H:61:LEU:HA	1.75	0.69
1:C:164:HIS:CG	1:C:165:HIS:H	2.09	0.69
1:F:255:ASN:O	1:F:256:ASP:CB	2.40	0.69
2:A:2017:HOH:O	1:C:46:PRO:HG3	1.90	0.69
2:E:2039:HOH:O	1:G:186:MET:HE1	1.91	0.69
1:G:11:ARG:HD2	1:G:61:LEU:HA	1.74	0.69
1:G:239:VAL:HB	1:G:240:PRO:HD3	1.75	0.69
1:A:152:MET:HG3	1:A:153:GLN:H	1.58	0.69
1:B:152:MET:CG	1:B:153:GLN:H	2.05	0.69
1:F:109:LEU:HD12	1:F:109:LEU:C	2.14	0.69
1:F:25:LEU:HD22	1:F:133:PRO:CG	2.22	0.68
1:D:91:LEU:HD21	1:D:184:HIS:HD2	1.59	0.68
1:E:194:TRP:CZ3	1:E:196:GLN:HB2	2.28	0.68
1:H:39:GLU:OE2	2:H:2007:HOH:O	2.10	0.68
1:D:69:CYS:SG	2:D:2004:HOH:O	2.51	0.68
1:D:150:ARG:HD3	1:D:161:GLN:NE2	2.08	0.68
1:G:217:LEU:HD21	1:G:242:LEU:HD11	1.75	0.68
1:C:239:VAL:HB	1:C:240:PRO:HD3	1.75	0.68
1:F:144:THR:HG22	1:F:147:GLY:H	1.59	0.68
1:H:217:LEU:HD11	1:H:219:ASN:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:TRP:CD2	2:B:2036:HOH:O	2.46	0.68
1:E:144:THR:HG22	1:E:147:GLY:H	1.58	0.68
1:G:128:GLN:H	1:G:128:GLN:NE2	1.86	0.68
1:C:47:ARG:HD2	2:C:2012:HOH:O	1.93	0.67
1:C:217:LEU:HD11	1:C:219:ASN:O	1.94	0.67
1:F:33:ASN:O	1:F:208:HIS:HB2	1.94	0.67
1:F:128:GLN:HB2	1:F:171:MET:CE	2.24	0.67
1:F:216:THR:HG22	1:F:216:THR:O	1.95	0.67
1:A:138:ALA:HA	1:A:151:LEU:O	1.95	0.67
1:H:150:ARG:HB2	1:H:168:TRP:CH2	2.30	0.67
1:B:144:THR:HG22	1:B:147:GLY:H	1.57	0.67
1:E:223:THR:OG1	2:E:2077:HOH:O	2.13	0.67
1:B:39:GLU:HG2	1:B:41:LEU:H	1.59	0.67
1:F:91:LEU:HD21	1:F:184:HIS:HD2	1.58	0.67
1:D:226:HIS:CE1	1:D:227:GLN:HE21	2.13	0.67
1:F:122:ASP:O	1:F:129:THR:HG22	1.94	0.67
1:F:152:MET:HG2	1:F:161:GLN:HE22	1.60	0.67
1:F:159:ILE:HG22	1:F:160:LEU:N	2.10	0.67
1:A:11:ARG:HD2	1:A:61:LEU:HA	1.77	0.67
1:E:181:GLN:O	1:E:185:VAL:HG23	1.95	0.66
1:H:164:HIS:O	1:H:166:GLU:N	2.27	0.66
1:D:33:ASN:O	1:D:208:HIS:HB2	1.95	0.66
1:H:175:ASP:OD1	1:H:175:ASP:N	2.28	0.66
1:H:226:HIS:CE1	1:H:227:GLN:HE21	2.13	0.66
1:H:144:THR:HG22	1:H:147:GLY:N	2.09	0.66
1:A:217:LEU:HD21	1:A:242:LEU:HD11	1.76	0.66
1:B:152:MET:HG3	1:B:153:GLN:N	2.05	0.66
1:F:19:VAL:HG12	1:F:21:THR:HG23	1.78	0.66
1:B:159:ILE:HG22	1:B:160:LEU:H	1.60	0.66
1:F:68:TYR:O	1:F:69:CYS:C	2.31	0.66
1:C:217:LEU:HD21	1:C:242:LEU:HD11	1.77	0.66
1:D:231:VAL:O	1:D:232:GLU:HB3	1.96	0.66
1:E:186:MET:HE2	1:G:186:MET:HE3	1.78	0.66
1:E:231:VAL:O	1:E:232:GLU:HB3	1.94	0.66
1:G:138:ALA:HA	1:G:151:LEU:O	1.94	0.66
1:H:162:PHE:HD2	1:H:171:MET:SD	2.18	0.66
1:B:186:MET:CE	1:C:186:MET:CE	2.54	0.66
1:C:211:ASP:HB3	2:C:2063:HOH:O	1.94	0.66
1:C:249:GLN:HA	2:C:2070:HOH:O	1.95	0.66
1:B:11:ARG:HD2	1:B:61:LEU:HA	1.76	0.66
1:E:255:ASN:O	1:E:256:ASP:HB2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ALA:HA	1:E:151:LEU:O	1.96	0.66
1:E:217:LEU:HD11	1:E:219:ASN:O	1.96	0.66
1:C:160:LEU:HG	1:C:171:MET:CE	2.27	0.65
1:A:194:TRP:CZ3	1:A:196:GLN:HB2	2.32	0.65
1:C:122:ASP:O	1:C:129:THR:HG22	1.97	0.65
1:B:96:LEU:CD2	1:B:171:MET:HA	2.26	0.65
1:A:136:LEU:HD22	1:A:158:TRP:CZ2	2.31	0.65
1:C:144:THR:HG22	1:C:147:GLY:H	1.61	0.65
1:D:162:PHE:HE1	1:D:169:GLN:HB2	1.61	0.65
1:D:216:THR:HG22	2:D:2031:HOH:O	1.96	0.65
1:G:144:THR:HG22	1:G:147:GLY:H	1.61	0.65
1:C:109:LEU:HD12	1:C:109:LEU:C	2.17	0.65
1:H:47:ARG:HG2	2:H:2010:HOH:O	1.97	0.65
1:D:144:THR:HG22	1:D:147:GLY:H	1.62	0.65
1:F:120:ILE:HG13	1:F:120:ILE:O	1.95	0.65
1:F:144:THR:HG22	1:F:147:GLY:N	2.12	0.65
1:B:256:ASP:N	2:B:2045:HOH:O	2.30	0.65
1:F:45:LEU:HA	2:F:2011:HOH:O	1.97	0.65
1:G:151:LEU:HD22	1:G:159:ILE:O	1.96	0.65
1:B:139:GLU:HA	1:B:150:ARG:HH21	1.63	0.64
1:H:239:VAL:HB	1:H:240:PRO:HD3	1.79	0.64
1:A:239:VAL:HB	1:A:240:PRO:HD3	1.78	0.64
1:B:25:LEU:HD22	1:B:133:PRO:CG	2.25	0.64
1:B:217:LEU:HD21	1:B:242:LEU:HD11	1.79	0.64
1:E:109:LEU:C	1:E:109:LEU:HD12	2.17	0.64
1:F:231:VAL:O	1:F:232:GLU:HB3	1.95	0.64
1:G:203:LEU:N	2:G:2044:HOH:O	2.29	0.64
1:F:128:GLN:HB2	1:F:171:MET:HE1	1.79	0.64
1:H:216:THR:HG22	1:H:216:THR:O	1.97	0.64
1:A:91:LEU:HB3	1:A:105:ARG:HB3	1.80	0.64
1:C:226:HIS:CE1	1:C:227:GLN:HE21	2.15	0.64
1:H:130:LEU:HA	2:H:2026:HOH:O	1.98	0.64
1:G:150:ARG:CD	1:G:152:MET:HG2	2.28	0.64
1:B:144:THR:HG22	1:B:147:GLY:N	2.13	0.64
1:C:163:ARG:HH11	1:C:167:HIS:HA	1.63	0.64
1:E:198:HIS:HB2	2:E:2067:HOH:O	1.96	0.64
1:B:109:LEU:C	1:B:109:LEU:HD12	2.17	0.64
1:B:167:HIS:O	1:B:168:TRP:HB2	1.98	0.64
1:G:154:GLU:O	1:G:155:GLY:C	2.36	0.64
1:H:95:ILE:HG12	1:H:172:TYR:HA	1.80	0.64
1:H:150:ARG:NH2	1:H:168:TRP:NE1	2.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ARG:HD2	1:C:168:TRP:CD2	2.33	0.63
1:E:11:ARG:HD2	1:E:61:LEU:HA	1.80	0.63
1:G:194:TRP:CZ3	1:G:196:GLN:HB2	2.33	0.63
1:E:160:LEU:HG	1:E:171:MET:CE	2.29	0.63
1:F:0:HIS:ND1	1:F:1:MET:N	2.47	0.63
1:A:109:LEU:HD12	1:A:109:LEU:C	2.18	0.63
1:B:226:HIS:CE1	1:B:227:GLN:HE21	2.17	0.63
1:D:217:LEU:HD21	1:D:242:LEU:HD11	1.79	0.63
1:F:91:LEU:HD21	1:F:184:HIS:CD2	2.33	0.63
1:F:186:MET:HE2	1:H:186:MET:HE3	0.75	0.63
1:C:39:GLU:HG2	1:C:41:LEU:H	1.64	0.63
1:C:122:ASP:HB3	2:C:2037:HOH:O	1.98	0.63
1:G:91:LEU:HD21	1:G:184:HIS:CD2	2.32	0.63
1:G:144:THR:HG22	1:G:147:GLY:N	2.13	0.63
1:H:194:TRP:CZ3	1:H:196:GLN:HB2	2.34	0.63
1:B:54:THR:O	1:B:58:GLU:HG3	1.98	0.63
1:C:91:LEU:HB3	1:C:105:ARG:HB3	1.80	0.63
1:G:39:GLU:HG2	1:G:41:LEU:H	1.63	0.63
1:A:90:LEU:HD12	1:A:109:LEU:HD11	1.80	0.63
1:C:144:THR:HG22	1:C:147:GLY:N	2.14	0.63
1:G:0:HIS:ND1	1:G:1:MET:N	2.47	0.63
1:H:25:LEU:HD22	1:H:133:PRO:CG	2.28	0.63
1:B:122:ASP:O	1:B:129:THR:HG22	1.99	0.63
1:H:149:TYR:CD2	1:H:162:PHE:HB3	2.34	0.63
1:D:181:GLN:O	1:D:185:VAL:HG23	1.99	0.62
1:E:200:ARG:HH12	1:H:200:ARG:HH12	1.45	0.62
1:D:150:ARG:HB2	1:D:168:TRP:CH2	2.35	0.62
1:F:226:HIS:CE1	1:F:227:GLN:HE21	2.17	0.62
1:G:109:LEU:C	1:G:109:LEU:HD12	2.19	0.62
1:G:150:ARG:HB2	1:G:168:TRP:CH2	2.34	0.62
1:F:39:GLU:HG2	1:F:41:LEU:H	1.62	0.62
1:F:186:MET:CE	1:H:186:MET:CE	2.47	0.62
1:G:33:ASN:O	1:G:208:HIS:HB2	1.98	0.62
1:H:231:VAL:O	1:H:232:GLU:HB3	1.98	0.62
1:A:122:ASP:O	1:A:129:THR:HG22	2.00	0.62
1:A:245:LEU:HD12	1:A:249:GLN:HB2	1.81	0.62
1:B:133:PRO:O	1:B:134:LEU:HD23	1.99	0.62
1:H:125:PHE:H	1:H:129:THR:HG23	1.65	0.62
1:C:125:PHE:H	1:C:129:THR:HG23	1.62	0.62
1:C:153:GLN:O	1:C:154:GLU:HG3	2.00	0.62
1:D:144:THR:HG22	1:D:147:GLY:N	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ILE:HG13	1:E:120:ILE:O	1.98	0.62
1:E:239:VAL:HB	1:E:240:PRO:HD3	1.82	0.62
1:E:182:SER:HB2	1:G:104:PRO:HD3	1.81	0.62
1:A:161:GLN:HA	1:A:169:GLN:O	1.99	0.61
1:B:182:SER:HB2	1:C:104:PRO:HD3	1.81	0.61
1:F:217:LEU:HD11	1:F:219:ASN:O	1.99	0.61
1:F:217:LEU:HD21	1:F:242:LEU:HD11	1.82	0.61
1:G:153:GLN:HB2	1:G:158:TRP:CE3	2.35	0.61
1:B:90:LEU:HD12	1:B:109:LEU:HD11	1.83	0.61
1:A:205:MET:SD	1:A:246:LEU:HD22	2.41	0.61
1:D:87:VAL:CG1	1:D:112:VAL:HG22	2.30	0.61
1:G:165:HIS:O	1:G:166:GLU:HB2	2.00	0.61
1:C:23:GLU:OE1	1:C:23:GLU:HA	2.00	0.61
1:F:152:MET:HG2	1:F:161:GLN:NE2	2.15	0.61
1:F:186:MET:HE3	2:H:2022:HOH:O	1.99	0.61
1:G:163:ARG:HH21	1:G:167:HIS:HA	1.63	0.61
1:G:255:ASN:O	1:G:256:ASP:CB	2.48	0.61
1:C:138:ALA:CA	1:C:151:LEU:O	2.49	0.61
1:E:246:LEU:HD11	2:E:2083:HOH:O	2.01	0.61
1:G:122:ASP:O	1:G:129:THR:HG22	2.01	0.61
1:E:186:MET:CE	1:G:186:MET:CE	2.79	0.61
1:H:120:ILE:O	1:H:120:ILE:HG13	2.00	0.61
1:C:91:LEU:HD21	1:C:184:HIS:HD2	1.66	0.61
1:C:128:GLN:N	1:C:128:GLN:NE2	2.44	0.61
1:E:186:MET:CE	1:G:186:MET:HE2	2.30	0.61
1:H:23:GLU:OE1	1:H:23:GLU:HA	2.01	0.61
1:C:87:VAL:CG1	1:C:112:VAL:HG22	2.31	0.60
1:C:137:GLN:O	1:C:151:LEU:HB2	2.00	0.60
1:D:109:LEU:C	1:D:109:LEU:HD12	2.21	0.60
1:G:128:GLN:HB2	1:G:171:MET:HE1	1.83	0.60
1:B:145:PRO:HB2	2:B:2027:HOH:O	2.00	0.60
1:B:161:GLN:HG2	1:B:170:SER:CA	2.30	0.60
1:E:128:GLN:NE2	1:E:128:GLN:N	2.39	0.60
1:A:144:THR:HG22	1:A:147:GLY:N	2.17	0.60
1:D:194:TRP:CZ3	1:D:196:GLN:HB2	2.36	0.60
1:G:150:ARG:HE	1:G:161:GLN:NE2	1.99	0.60
1:C:87:VAL:HG12	1:C:112:VAL:HG22	1.82	0.60
1:H:19:VAL:HG12	1:H:21:THR:HG23	1.82	0.60
1:C:176:LEU:HD13	2:C:2043:HOH:O	1.99	0.60
1:D:91:LEU:HD21	1:D:184:HIS:CD2	2.37	0.60
1:G:68:TYR:O	1:G:69:CYS:C	2.39	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:NH2	1:B:152:MET:SD	2.66	0.60
1:E:158:TRP:C	1:E:159:ILE:HD12	2.21	0.60
1:E:262:THR:HG23	1:E:265:GLU:OE1	2.02	0.60
1:G:91:LEU:HB3	1:G:105:ARG:HB3	1.83	0.60
1:G:245:LEU:HD12	1:G:249:GLN:HB2	1.83	0.60
1:B:22:VAL:HB	2:B:2022:HOH:O	2.00	0.60
1:B:216:THR:O	1:B:216:THR:HG22	2.00	0.60
1:B:232:GLU:HA	1:F:233:GLN:O	2.02	0.60
1:D:128:GLN:HB2	1:D:171:MET:CE	2.31	0.60
1:G:237:PRO:HG2	1:G:238:ASP:OD1	2.02	0.60
1:A:237:PRO:HG2	1:A:238:ASP:OD1	2.02	0.60
1:D:205:MET:SD	1:D:246:LEU:HD22	2.42	0.60
1:C:160:LEU:HG	1:C:171:MET:HE1	1.84	0.60
1:F:125:PHE:H	1:F:129:THR:HG23	1.66	0.60
1:E:39:GLU:HG2	1:E:41:LEU:H	1.66	0.59
1:A:133:PRO:O	1:A:134:LEU:HD23	2.02	0.59
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.84	0.59
1:D:19:VAL:HG12	1:D:21:THR:HG23	1.83	0.59
1:D:217:LEU:HD11	1:D:219:ASN:O	2.02	0.59
1:B:5:LEU:HD22	1:B:82:ASP:HB3	1.84	0.59
1:C:231:VAL:O	1:C:232:GLU:HB3	2.02	0.59
1:D:54:THR:O	1:D:58:GLU:HG3	2.01	0.59
1:D:87:VAL:HG12	1:D:112:VAL:HG22	1.82	0.59
1:F:159:ILE:HG22	1:F:160:LEU:H	1.68	0.59
1:A:216:THR:HG22	1:A:216:THR:O	2.01	0.59
1:A:14:CYS:SG	1:A:15:GLN:N	2.74	0.59
1:B:0:HIS:ND1	1:B:1:MET:N	2.50	0.59
1:H:128:GLN:N	1:H:128:GLN:NE2	2.41	0.59
1:B:91:LEU:HB3	1:B:105:ARG:HB3	1.85	0.59
1:E:91:LEU:HD21	1:E:184:HIS:HD2	1.68	0.59
1:A:144:THR:HG22	1:A:147:GLY:H	1.67	0.59
1:B:91:LEU:HD21	1:B:184:HIS:HD2	1.68	0.59
1:B:120:ILE:HG13	1:B:120:ILE:O	2.02	0.59
1:E:98:HIS:N	1:E:99:PRO:HD3	2.18	0.59
1:H:5:LEU:HD22	1:H:82:ASP:HB3	1.85	0.59
1:A:162:PHE:CE1	1:A:169:GLN:HB3	2.38	0.59
1:C:0:HIS:ND1	1:C:1:MET:N	2.51	0.59
1:G:5:LEU:HD22	1:G:82:ASP:HB3	1.84	0.59
1:B:231:VAL:O	1:B:232:GLU:HB3	2.03	0.58
1:A:217:LEU:HD11	1:A:219:ASN:O	2.01	0.58
1:B:159:ILE:HG22	1:B:160:LEU:N	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:O	1:C:120:ILE:HG13	2.03	0.58
1:E:136:LEU:HD22	1:E:158:TRP:CE2	2.39	0.58
1:D:23:GLU:HA	1:D:23:GLU:OE1	2.04	0.58
1:D:5:LEU:HD22	1:D:82:ASP:HB3	1.85	0.58
1:D:39:GLU:HG2	1:D:41:LEU:H	1.68	0.58
1:D:91:LEU:HB3	1:D:105:ARG:HB3	1.86	0.58
1:F:38:PHE:O	1:F:205:MET:HA	2.03	0.58
1:A:5:LEU:HD22	1:A:82:ASP:HB3	1.85	0.58
1:G:130:LEU:CD2	1:G:149:TYR:CD2	2.85	0.58
1:A:23:GLU:HA	1:A:23:GLU:OE1	2.03	0.58
1:D:133:PRO:O	1:D:134:LEU:HD23	2.03	0.58
1:G:133:PRO:O	1:G:134:LEU:HD23	2.03	0.58
1:H:96:LEU:HD23	1:H:171:MET:HA	1.86	0.58
1:D:125:PHE:H	1:D:129:THR:HG23	1.67	0.58
1:F:151:LEU:N	1:F:151:LEU:HD23	2.19	0.58
1:G:128:GLN:HB2	1:G:171:MET:CE	2.34	0.58
1:G:169:GLN:HE21	1:G:169:GLN:HA	1.69	0.58
1:H:90:LEU:HD12	1:H:109:LEU:HD11	1.86	0.58
1:G:90:LEU:HD12	1:G:109:LEU:HD11	1.85	0.58
1:H:122:ASP:O	1:H:129:THR:HG22	2.03	0.58
1:A:91:LEU:HD21	1:A:184:HIS:HD2	1.69	0.58
1:E:186:MET:HE3	1:G:186:MET:CE	2.34	0.58
1:F:5:LEU:HD22	1:F:82:ASP:HB3	1.86	0.58
1:E:68:TYR:O	1:E:69:CYS:C	2.41	0.57
1:E:19:VAL:HG12	1:E:21:THR:HG23	1.86	0.57
1:F:45:LEU:HB2	2:F:2011:HOH:O	2.03	0.57
1:C:237:PRO:HG2	1:C:238:ASP:OD1	2.03	0.57
1:F:136:LEU:HD22	1:F:158:TRP:CZ2	2.39	0.57
1:G:19:VAL:HG12	1:G:21:THR:HG23	1.87	0.57
1:D:160:LEU:C	1:D:160:LEU:HD23	2.24	0.57
1:H:11:ARG:HE	1:H:64:ARG:HA	1.69	0.57
1:B:87:VAL:CG1	1:B:112:VAL:HG22	2.33	0.57
1:C:255:ASN:O	1:C:256:ASP:CB	2.53	0.57
1:G:150:ARG:NH2	1:G:168:TRP:CD1	2.72	0.57
1:G:216:THR:O	1:G:216:THR:HG22	2.03	0.57
1:A:33:ASN:O	1:A:208:HIS:HB2	2.04	0.57
1:A:39:GLU:HG2	1:A:41:LEU:H	1.69	0.57
1:A:218:THR:O	1:A:219:ASN:HB2	2.04	0.57
1:B:68:TYR:O	1:B:69:CYS:C	2.42	0.57
1:B:68:TYR:OH	1:B:188:ASN:ND2	2.36	0.57
1:D:0:HIS:ND1	1:D:1:MET:N	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ARG:HA	2:D:2015:HOH:O	2.04	0.57
1:D:122:ASP:O	1:D:129:THR:HG22	2.04	0.57
1:G:25:LEU:HD22	1:G:133:PRO:CG	2.33	0.57
1:A:15:GLN:NE2	1:A:16:PRO:HD2	2.19	0.57
1:A:128:GLN:N	1:A:128:GLN:NE2	2.45	0.57
1:D:150:ARG:O	1:D:161:GLN:HG2	2.05	0.57
1:E:218:THR:O	1:E:219:ASN:HB2	2.05	0.57
1:G:17:LEU:HB3	2:G:2010:HOH:O	2.04	0.57
1:A:130:LEU:HD13	1:A:134:LEU:HG	1.86	0.57
1:E:91:LEU:HD21	1:E:184:HIS:CD2	2.40	0.57
1:B:19:VAL:HG12	1:B:21:THR:HG23	1.87	0.57
1:B:245:LEU:HD12	1:B:249:GLN:HB2	1.87	0.57
1:D:53:GLU:O	1:D:53:GLU:HG3	2.04	0.57
1:D:237:PRO:HG2	1:D:238:ASP:OD1	2.05	0.57
1:E:0:HIS:ND1	1:E:1:MET:N	2.52	0.57
1:E:87:VAL:HG12	1:E:112:VAL:HG22	1.87	0.57
1:H:33:ASN:O	1:H:208:HIS:HB2	2.04	0.57
1:E:226:HIS:HE1	1:E:227:GLN:HE21	1.49	0.57
1:F:96:LEU:HD23	1:F:171:MET:HA	1.87	0.56
1:G:90:LEU:HB2	1:G:109:LEU:CD1	2.35	0.56
1:A:120:ILE:O	1:A:120:ILE:HG13	2.04	0.56
1:C:54:THR:O	1:C:58:GLU:HG3	2.04	0.56
1:G:23:GLU:OE1	1:G:23:GLU:HA	2.04	0.56
1:H:91:LEU:HB3	1:H:105:ARG:HB3	1.86	0.56
1:B:105:ARG:NE	2:B:2019:HOH:O	2.38	0.56
1:B:130:LEU:HD13	1:B:134:LEU:HG	1.87	0.56
1:E:151:LEU:HD23	1:E:160:LEU:HA	1.86	0.56
1:F:91:LEU:HB3	1:F:105:ARG:HB3	1.86	0.56
1:H:137:GLN:HA	2:H:2027:HOH:O	2.06	0.56
1:C:245:LEU:HD12	1:C:249:GLN:HB2	1.87	0.56
1:F:68:TYR:OH	1:F:188:ASN:ND2	2.37	0.56
1:C:68:TYR:O	1:C:69:CYS:C	2.43	0.56
1:F:239:VAL:HB	1:F:240:PRO:HD3	1.86	0.56
1:E:136:LEU:HD22	1:E:158:TRP:CH2	2.40	0.56
1:E:205:MET:SD	1:E:246:LEU:HD22	2.45	0.56
1:B:186:MET:SD	2:C:2032:HOH:O	2.58	0.56
1:E:38:PHE:O	1:E:205:MET:HA	2.05	0.56
1:G:15:GLN:NE2	1:G:16:PRO:HD2	2.21	0.56
1:H:68:TYR:O	1:H:69:CYS:C	2.44	0.56
1:H:218:THR:O	1:H:219:ASN:HB2	2.04	0.56
1:C:47:ARG:CD	2:C:2012:HOH:O	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HA	1:C:167:HIS:O	2.05	0.56
1:F:19:VAL:HG12	1:F:21:THR:CG2	2.36	0.56
1:F:164:HIS:O	1:F:165:HIS:CB	2.53	0.56
1:F:220:PHE:CE1	1:F:242:LEU:HD22	2.41	0.56
1:G:159:ILE:HG22	1:G:160:LEU:N	2.21	0.56
1:H:50:GLN:HG2	2:H:2011:HOH:O	2.06	0.56
1:H:98:HIS:N	1:H:99:PRO:HD3	2.19	0.56
1:B:255:ASN:O	1:B:256:ASP:CB	2.48	0.56
1:E:217:LEU:HD21	1:E:242:LEU:HD11	1.87	0.56
1:H:150:ARG:NH1	1:H:152:MET:CE	2.69	0.56
1:H:0:HIS:ND1	1:H:1:MET:N	2.54	0.56
1:H:150:ARG:HG2	1:H:151:LEU:N	2.21	0.56
1:D:72:LEU:HD12	1:D:124:GLY:HA2	1.88	0.55
1:F:123:VAL:HB	2:F:2025:HOH:O	2.05	0.55
1:F:130:LEU:HD13	1:F:134:LEU:HG	1.88	0.55
1:A:0:HIS:ND1	1:A:1:MET:N	2.54	0.55
1:F:98:HIS:N	1:F:99:PRO:HD3	2.19	0.55
1:G:98:HIS:N	1:G:99:PRO:HD3	2.21	0.55
1:H:161:GLN:HG2	1:H:170:SER:CA	2.34	0.55
1:A:87:VAL:HG12	1:A:112:VAL:HG22	1.88	0.55
1:C:252:LEU:HD13	2:C:2072:HOH:O	2.05	0.55
1:D:6:HIS:CD2	2:D:2001:HOH:O	2.60	0.55
1:A:11:ARG:HE	1:A:64:ARG:HA	1.71	0.55
1:C:176:LEU:CD1	2:C:2043:HOH:O	2.55	0.55
1:D:48:GLU:N	2:D:2005:HOH:O	2.28	0.55
1:B:153:GLN:O	1:B:154:GLU:HB2	2.07	0.55
1:E:220:PHE:CE1	1:E:242:LEU:HD22	2.41	0.55
1:F:165:HIS:O	1:F:167:HIS:N	2.40	0.55
1:C:98:HIS:N	1:C:99:PRO:HD3	2.22	0.55
1:E:90:LEU:HD12	1:E:109:LEU:HD11	1.88	0.55
1:E:122:ASP:O	1:E:129:THR:HG22	2.07	0.55
1:C:205:MET:SD	1:C:246:LEU:HD22	2.47	0.55
1:E:91:LEU:HB3	1:E:105:ARG:HB3	1.89	0.55
1:A:151:LEU:HD23	1:A:160:LEU:HA	1.87	0.54
1:B:194:TRP:CG	2:B:2036:HOH:O	2.58	0.54
1:B:258:LYS:HG2	1:B:259:HIS:CD2	2.42	0.54
1:F:139:GLU:HA	2:F:2029:HOH:O	2.08	0.54
1:G:54:THR:O	1:G:58:GLU:HG3	2.07	0.54
1:G:120:ILE:HG13	1:G:120:ILE:O	2.07	0.54
1:A:19:VAL:HG12	1:A:21:THR:HG23	1.88	0.54
1:G:3:SER:O	1:G:6:HIS:HB3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:ALA:HB3	2:G:2053:HOH:O	2.07	0.54
1:A:87:VAL:CG1	1:A:112:VAL:HG22	2.37	0.54
1:B:150:ARG:HH22	1:B:152:MET:CE	2.20	0.54
1:F:14:CYS:SG	1:F:15:GLN:N	2.80	0.54
1:G:160:LEU:CD2	1:G:171:MET:SD	2.95	0.54
1:G:226:HIS:HE1	1:G:227:GLN:HE21	1.56	0.54
1:H:15:GLN:NE2	1:H:16:PRO:HD2	2.22	0.54
1:H:83:ILE:HG22	1:H:83:ILE:O	2.05	0.54
1:A:27:THR:HG23	2:A:2006:HOH:O	2.06	0.54
1:A:136:LEU:HD22	1:A:158:TRP:CE2	2.43	0.54
1:A:182:SER:HB2	1:D:104:PRO:HD3	1.89	0.54
1:C:121:ALA:C	2:C:2037:HOH:O	2.44	0.54
1:D:245:LEU:HD12	1:D:249:GLN:HB2	1.89	0.54
1:H:205:MET:SD	1:H:246:LEU:HD22	2.47	0.54
1:C:164:HIS:ND1	1:C:165:HIS:N	2.45	0.54
1:E:23:GLU:OE1	1:E:23:GLU:HA	2.07	0.54
1:A:152:MET:HG3	1:A:153:GLN:N	2.22	0.54
1:B:220:PHE:CE1	1:B:242:LEU:HD22	2.43	0.54
1:C:90:LEU:HD12	1:C:109:LEU:HD11	1.88	0.54
1:C:150:ARG:HD2	1:C:168:TRP:CE2	2.43	0.54
1:G:53:GLU:O	1:G:53:GLU:HG3	2.08	0.54
1:A:255:ASN:O	1:A:256:ASP:CB	2.56	0.54
1:G:96:LEU:HD23	1:G:171:MET:HA	1.90	0.54
1:E:245:LEU:HD12	1:E:249:GLN:HB2	1.89	0.54
1:H:245:LEU:HD12	1:H:249:GLN:HB2	1.90	0.54
1:A:186:MET:HE3	1:D:186:MET:CE	2.37	0.54
1:C:19:VAL:HG12	1:C:21:THR:HG23	1.89	0.54
1:C:262:THR:HG23	1:C:265:GLU:OE1	2.07	0.54
1:D:218:THR:O	1:D:219:ASN:HB2	2.06	0.54
1:F:109:LEU:HD23	1:F:172:TYR:CE1	2.43	0.54
1:D:15:GLN:NE2	1:D:16:PRO:HD2	2.24	0.53
1:G:4:PHE:O	1:G:6:HIS:N	2.41	0.53
1:G:125:PHE:H	1:G:129:THR:HG23	1.73	0.53
1:G:203:LEU:HB2	2:G:2044:HOH:O	2.08	0.53
1:D:7:ALA:HB2	2:D:2001:HOH:O	2.08	0.53
1:D:150:ARG:HG2	1:D:151:LEU:O	2.09	0.53
1:H:237:PRO:HG2	1:H:238:ASP:OD1	2.09	0.53
1:B:23:GLU:HA	1:B:23:GLU:OE1	2.09	0.53
1:D:98:HIS:N	1:D:99:PRO:HD3	2.24	0.53
1:E:15:GLN:NE2	1:E:16:PRO:HD2	2.23	0.53
1:F:54:THR:O	1:F:58:GLU:HG3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TYR:O	1:A:69:CYS:C	2.46	0.53
1:D:11:ARG:HE	1:D:64:ARG:HA	1.72	0.53
1:F:53:GLU:HG3	1:F:53:GLU:O	2.08	0.53
1:A:89:SER:O	1:A:90:LEU:HD23	2.09	0.53
1:A:220:PHE:CE1	1:A:242:LEU:HD22	2.44	0.53
1:B:254:VAL:HG13	1:B:254:VAL:O	2.09	0.53
1:D:128:GLN:HB2	1:D:171:MET:HE3	1.90	0.53
1:D:120:ILE:HG13	1:D:120:ILE:O	2.08	0.53
1:F:59:LYS:HG3	1:F:259:HIS:ND1	2.24	0.53
1:H:54:THR:O	1:H:58:GLU:HG3	2.08	0.53
1:A:11:ARG:HH21	1:A:64:ARG:CA	2.22	0.53
1:B:87:VAL:HG12	1:B:112:VAL:HG22	1.90	0.53
1:C:25:LEU:HD22	1:C:133:PRO:CG	2.35	0.53
1:C:38:PHE:O	1:C:205:MET:HA	2.09	0.53
1:E:11:ARG:HH21	1:E:64:ARG:CA	2.22	0.53
1:E:11:ARG:HE	1:E:64:ARG:HA	1.74	0.53
1:E:96:LEU:HD23	1:E:171:MET:HA	1.90	0.53
1:E:133:PRO:O	1:E:134:LEU:HD23	2.07	0.53
1:F:262:THR:HG23	1:F:265:GLU:OE1	2.08	0.53
1:A:200:ARG:HH12	1:C:200:ARG:HH12	1.56	0.53
1:B:98:HIS:N	1:B:99:PRO:HD3	2.23	0.53
1:A:91:LEU:HD21	1:A:184:HIS:CD2	2.44	0.53
1:F:128:GLN:N	1:F:128:GLN:NE2	2.52	0.53
1:G:64:ARG:NH2	2:G:2017:HOH:O	2.42	0.53
1:H:162:PHE:CD2	1:H:171:MET:SD	3.01	0.53
1:H:254:VAL:O	1:H:254:VAL:HG13	2.08	0.53
1:B:59:LYS:HG3	1:B:259:HIS:ND1	2.25	0.52
1:B:238:ASP:OD2	1:B:240:PRO:HD2	2.09	0.52
1:E:53:GLU:O	1:E:53:GLU:HG3	2.09	0.52
1:H:39:GLU:HG2	1:H:41:LEU:H	1.74	0.52
1:B:218:THR:O	1:B:219:ASN:HB2	2.09	0.52
1:D:91:LEU:HG	1:D:179:GLN:HG3	1.90	0.52
1:D:128:GLN:N	1:D:128:GLN:NE2	2.48	0.52
1:D:161:GLN:HB2	1:D:169:GLN:O	2.09	0.52
1:F:238:ASP:OD2	1:F:240:PRO:HD2	2.09	0.52
1:G:128:GLN:N	1:G:128:GLN:NE2	2.52	0.52
1:H:109:LEU:HD12	1:H:109:LEU:C	2.29	0.52
1:C:91:LEU:HD21	1:C:184:HIS:CD2	2.44	0.52
1:F:26:ARG:NH1	2:F:2007:HOH:O	2.43	0.52
1:G:4:PHE:CE2	1:G:78:ARG:HD3	2.44	0.52
1:B:233:GLN:O	1:F:232:GLU:HA	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:HD11	1:D:151:LEU:HD21	1.90	0.52
1:A:153:GLN:O	1:A:153:GLN:HG3	2.08	0.52
1:A:226:HIS:HE1	1:A:227:GLN:HE21	1.56	0.52
1:A:247:GLN:HB3	2:A:2048:HOH:O	2.09	0.52
1:H:136:LEU:HD23	1:H:151:LEU:CD1	2.40	0.52
1:H:161:GLN:CG	1:H:170:SER:HA	2.36	0.52
1:C:202:HIS:HA	1:C:273:PHE:CE2	2.45	0.52
1:E:5:LEU:HD22	1:E:82:ASP:HB3	1.92	0.52
1:F:218:THR:O	1:F:219:ASN:HB2	2.10	0.52
1:B:0:HIS:HA	2:B:2001:HOH:O	2.10	0.52
1:H:12:LEU:HD21	1:H:32:HIS:HA	1.90	0.52
1:H:91:LEU:HD21	1:H:184:HIS:HD2	1.74	0.52
1:E:33:ASN:O	1:E:208:HIS:HB2	2.10	0.52
1:E:237:PRO:HG2	1:E:238:ASP:OD1	2.08	0.52
1:F:160:LEU:C	1:F:161:GLN:HG3	2.30	0.52
1:E:99:PRO:HA	2:E:2034:HOH:O	2.10	0.52
1:F:15:GLN:NE2	1:F:16:PRO:HD2	2.24	0.52
1:B:11:ARG:HE	1:B:64:ARG:HA	1.75	0.52
1:C:11:ARG:HH21	1:C:64:ARG:CA	2.23	0.52
1:C:181:GLN:O	1:C:185:VAL:HG23	2.09	0.52
1:C:226:HIS:HE1	1:C:227:GLN:HE21	1.58	0.52
1:F:128:GLN:CB	1:F:171:MET:HE1	2.40	0.52
1:C:159:ILE:HD11	1:C:170:SER:OG	2.10	0.51
1:E:104:PRO:HD3	1:G:182:SER:HB2	1.92	0.51
1:G:262:THR:HG23	1:G:265:GLU:OE1	2.11	0.51
1:H:181:GLN:O	1:H:185:VAL:HG23	2.10	0.51
1:A:98:HIS:N	1:A:99:PRO:HD3	2.24	0.51
1:D:59:LYS:HG3	1:D:259:HIS:ND1	2.26	0.51
1:D:255:ASN:O	1:D:256:ASP:CB	2.56	0.51
1:E:95:ILE:HG12	1:E:172:TYR:HA	1.92	0.51
1:G:144:THR:HG21	1:G:149:TYR:CE2	2.45	0.51
1:B:150:ARG:NH2	1:B:152:MET:HE1	2.26	0.51
1:C:41:LEU:O	1:C:41:LEU:HD12	2.11	0.51
1:A:150:ARG:NH2	1:A:152:MET:SD	2.83	0.51
1:D:38:PHE:O	1:D:205:MET:HA	2.09	0.51
1:G:203:LEU:O	1:G:204:LEU:HD23	2.11	0.51
1:B:203:LEU:O	1:B:204:LEU:HD23	2.09	0.51
1:C:150:ARG:HH21	1:C:152:MET:CE	2.23	0.51
1:G:223:THR:HG22	1:G:225:TYR:CE1	2.45	0.51
1:H:83:ILE:O	1:H:83:ILE:CG2	2.58	0.51
1:B:46:PRO:HD2	2:B:2007:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HD13	1:C:134:LEU:HG	1.93	0.51
1:C:164:HIS:CG	1:C:165:HIS:N	2.76	0.51
1:D:90:LEU:HD12	1:D:109:LEU:HD11	1.92	0.51
1:D:174:PHE:CD1	1:D:174:PHE:N	2.79	0.51
1:E:91:LEU:HG	1:E:179:GLN:HG3	1.93	0.51
1:E:216:THR:HG22	1:E:216:THR:O	2.11	0.51
1:E:263:GLU:OE2	2:E:2089:HOH:O	2.18	0.51
1:F:12:LEU:HD21	1:F:32:HIS:HA	1.93	0.51
1:H:203:LEU:O	1:H:204:LEU:HD23	2.11	0.51
1:B:83:ILE:HG22	1:B:83:ILE:O	2.09	0.51
1:C:93:ARG:NH2	1:C:105:ARG:NH1	2.59	0.51
1:D:68:TYR:O	1:D:69:CYS:C	2.49	0.51
1:D:239:VAL:HG23	2:D:2033:HOH:O	2.09	0.51
1:E:87:VAL:CG1	1:E:112:VAL:HG22	2.41	0.51
1:E:125:PHE:H	1:E:129:THR:HG23	1.75	0.51
1:F:149:TYR:N	1:F:149:TYR:CD1	2.78	0.51
1:F:150:ARG:HH21	1:F:168:TRP:CB	2.24	0.51
1:A:162:PHE:CD1	1:A:162:PHE:O	2.63	0.51
1:B:128:GLN:N	1:B:128:GLN:NE2	2.50	0.51
1:B:150:ARG:HH12	1:B:152:MET:CE	2.24	0.51
1:H:163:ARG:NH2	1:H:166:GLU:O	2.44	0.51
1:H:217:LEU:HD21	1:H:242:LEU:HD11	1.93	0.51
1:G:130:LEU:HD23	1:G:149:TYR:CE2	2.46	0.51
1:H:150:ARG:NH1	1:H:152:MET:HE2	2.26	0.51
1:G:218:THR:O	1:G:219:ASN:HB2	2.11	0.51
1:H:11:ARG:HH21	1:H:64:ARG:CA	2.24	0.51
1:H:255:ASN:O	1:H:256:ASP:CB	2.56	0.51
1:A:125:PHE:H	1:A:129:THR:HG23	1.75	0.50
1:B:91:LEU:HD21	1:B:184:HIS:CD2	2.45	0.50
1:B:217:LEU:HD11	1:B:219:ASN:O	2.10	0.50
1:F:160:LEU:HD23	1:F:171:MET:SD	2.51	0.50
1:F:245:LEU:HD12	1:F:249:GLN:HB2	1.93	0.50
1:G:95:ILE:HG12	1:G:172:TYR:HA	1.92	0.50
1:A:76:PHE:HE1	1:A:80:LEU:HD21	1.76	0.50
1:F:163:ARG:NH1	2:F:2033:HOH:O	2.43	0.50
1:G:11:ARG:HE	1:G:64:ARG:HA	1.76	0.50
1:H:53:GLU:HG3	1:H:53:GLU:O	2.10	0.50
1:H:166:GLU:C	1:H:166:GLU:OE1	2.50	0.50
1:B:202:HIS:HA	1:B:273:PHE:CE2	2.47	0.50
1:D:174:PHE:N	1:D:174:PHE:HD1	2.09	0.50
1:G:254:VAL:O	1:G:254:VAL:HG13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PRO:N	2:B:2036:HOH:O	2.43	0.50
1:C:216:THR:HG22	1:C:216:THR:O	2.11	0.50
1:H:221:HIS:HD2	2:H:2041:HOH:O	1.93	0.50
1:A:4:PHE:O	1:A:6:HIS:N	2.44	0.50
1:B:166:GLU:HG2	1:G:233:GLN:O	2.11	0.50
1:C:125:PHE:H	1:C:129:THR:CG2	2.23	0.50
1:F:91:LEU:HG	1:F:179:GLN:HG3	1.91	0.50
1:G:90:LEU:HB2	1:G:109:LEU:HD11	1.93	0.50
1:A:53:GLU:HG3	1:A:53:GLU:O	2.12	0.50
1:B:262:THR:HG23	1:B:265:GLU:OE1	2.11	0.50
1:C:172:TYR:CD1	1:C:172:TYR:C	2.85	0.50
1:F:8:TYR:CZ	1:F:12:LEU:HD11	2.47	0.50
1:G:202:HIS:HA	1:G:273:PHE:CE2	2.46	0.50
1:H:90:LEU:HB2	1:H:109:LEU:CD1	2.42	0.50
1:H:133:PRO:O	1:H:134:LEU:HD23	2.12	0.50
1:C:212:GLY:N	2:C:2057:HOH:O	2.30	0.50
1:D:11:ARG:HH21	1:D:64:ARG:CA	2.25	0.50
1:D:184:HIS:CE1	2:D:2023:HOH:O	2.65	0.50
1:F:23:GLU:HA	1:F:23:GLU:OE1	2.12	0.50
1:A:149:TYR:CD2	1:A:162:PHE:HB3	2.47	0.49
1:G:38:PHE:O	1:G:205:MET:HA	2.11	0.49
1:H:144:THR:CG2	1:H:146:HIS:H	2.20	0.49
1:H:163:ARG:HG2	1:H:168:TRP:CE3	2.47	0.49
1:H:165:HIS:O	1:H:166:GLU:CB	2.60	0.49
1:C:220:PHE:CE1	1:C:242:LEU:HD22	2.47	0.49
1:C:254:VAL:HG13	1:C:254:VAL:O	2.12	0.49
1:C:11:ARG:HE	1:C:64:ARG:HA	1.78	0.49
1:G:130:LEU:HD13	1:G:134:LEU:HG	1.93	0.49
1:H:12:LEU:CD2	1:H:32:HIS:HA	2.43	0.49
1:H:76:PHE:CE1	1:H:80:LEU:HD11	2.48	0.49
1:H:220:PHE:CE1	1:H:242:LEU:HD22	2.47	0.49
1:B:11:ARG:HH21	1:B:64:ARG:CA	2.26	0.49
1:B:243:TYR:CG	1:B:263:GLU:HG3	2.48	0.49
1:C:14:CYS:SG	1:C:15:GLN:N	2.84	0.49
1:D:163:ARG:NH1	1:D:167:HIS:HA	2.27	0.49
1:E:54:THR:O	1:E:58:GLU:HG3	2.12	0.49
1:F:123:VAL:C	1:F:129:THR:HG21	2.33	0.49
1:G:202:HIS:HD2	1:G:202:HIS:O	1.95	0.49
1:H:41:LEU:O	1:H:41:LEU:HD12	2.12	0.49
1:A:140:ILE:HD13	2:A:2030:HOH:O	2.12	0.49
1:B:38:PHE:O	1:B:205:MET:HA	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:PHE:H	1:B:129:THR:HG23	1.76	0.49
1:C:15:GLN:NE2	1:C:16:PRO:HD2	2.27	0.49
1:D:220:PHE:CE1	1:D:242:LEU:HD22	2.47	0.49
1:F:205:MET:SD	1:F:246:LEU:HD22	2.53	0.49
1:G:68:TYR:OH	1:G:188:ASN:ND2	2.46	0.49
1:G:128:GLN:CB	1:G:171:MET:HE1	2.41	0.49
1:G:205:MET:SD	1:G:246:LEU:HD22	2.53	0.49
1:A:169:GLN:NE2	1:A:170:SER:H	2.10	0.49
1:E:15:GLN:HE21	1:E:16:PRO:HD2	1.77	0.49
1:G:4:PHE:C	1:G:6:HIS:N	2.65	0.49
1:D:225:TYR:HA	1:D:229:HIS:O	2.13	0.49
1:C:59:LYS:HG3	1:C:259:HIS:ND1	2.27	0.49
1:F:87:VAL:HG12	1:F:112:VAL:HG22	1.95	0.49
1:G:46:PRO:HD2	2:G:2013:HOH:O	2.13	0.49
1:A:162:PHE:HE1	1:A:169:GLN:HB3	1.75	0.49
1:C:88:ARG:NH1	2:C:2028:HOH:O	2.46	0.49
1:D:194:TRP:NE1	2:D:2025:HOH:O	2.11	0.49
1:D:216:THR:HG22	1:D:216:THR:O	2.11	0.49
1:G:178:VAL:HG12	1:G:179:GLN:N	2.28	0.49
1:C:160:LEU:HG	1:C:171:MET:HE2	1.95	0.49
1:F:182:SER:HB2	1:H:104:PRO:HD3	1.94	0.49
1:G:87:VAL:CG1	1:G:112:VAL:HG22	2.43	0.49
1:H:130:LEU:HD13	1:H:134:LEU:HG	1.95	0.49
1:A:178:VAL:HG12	1:A:179:GLN:N	2.28	0.48
1:D:41:LEU:HD12	1:D:41:LEU:O	2.13	0.48
1:F:90:LEU:HD12	1:F:109:LEU:HD11	1.95	0.48
1:B:83:ILE:O	1:B:83:ILE:CG2	2.61	0.48
1:C:53:GLU:O	1:C:53:GLU:HG3	2.13	0.48
1:D:3:SER:O	1:D:6:HIS:HB3	2.13	0.48
1:D:25:LEU:HD22	1:D:133:PRO:CG	2.40	0.48
1:D:96:LEU:HD23	1:D:170:SER:O	2.13	0.48
1:H:19:VAL:HG12	1:H:21:THR:CG2	2.43	0.48
1:D:4:PHE:O	1:D:6:HIS:N	2.47	0.48
1:E:11:ARG:HH21	1:E:64:ARG:HA	1.78	0.48
1:F:5:LEU:HD11	1:F:83:ILE:HG13	1.94	0.48
1:A:253:GLY:HA2	2:A:2015:HOH:O	2.13	0.48
1:B:109:LEU:HD23	1:B:172:TYR:CE1	2.48	0.48
1:C:211:ASP:HA	2:C:2057:HOH:O	2.13	0.48
1:E:225:TYR:HA	1:E:229:HIS:O	2.14	0.48
1:H:15:GLN:HE21	1:H:16:PRO:HD2	1.77	0.48
1:D:184:HIS:HE1	2:D:2023:HOH:O	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:HE21	1:A:16:PRO:HD2	1.79	0.48
1:A:68:TYR:OH	1:A:188:ASN:ND2	2.47	0.48
1:B:104:PRO:HD3	1:C:182:SER:HB2	1.95	0.48
1:C:133:PRO:O	1:C:134:LEU:HD23	2.13	0.48
1:D:222:PHE:CZ	1:D:249:GLN:HG2	2.49	0.48
1:E:41:LEU:HB3	1:E:65:ARG:HH22	1.78	0.48
1:B:30:LEU:HG	2:B:2027:HOH:O	2.12	0.48
1:B:150:ARG:NH2	1:B:152:MET:CE	2.77	0.48
1:F:178:VAL:HG12	1:F:179:GLN:N	2.29	0.48
1:H:109:LEU:HD23	1:H:172:TYR:CE1	2.48	0.48
1:B:14:CYS:SG	1:B:15:GLN:N	2.87	0.48
1:C:89:SER:O	1:C:90:LEU:HD23	2.14	0.48
1:F:77:GLU:HB2	1:F:110:LEU:HD21	1.94	0.48
1:A:87:VAL:HG13	1:A:112:VAL:HG13	1.95	0.48
1:B:93:ARG:NH2	1:B:105:ARG:NH1	2.62	0.48
1:D:203:LEU:O	1:D:204:LEU:HD23	2.14	0.48
1:E:159:ILE:N	1:E:159:ILE:CD1	2.71	0.48
1:E:273:PHE:C	2:E:2092:HOH:O	2.51	0.48
1:H:38:PHE:O	1:H:205:MET:HA	2.14	0.48
1:A:181:GLN:O	1:A:185:VAL:HG23	2.13	0.48
2:A:2040:HOH:O	1:C:201:HIS:HE1	1.97	0.48
1:B:150:ARG:HG2	1:B:168:TRP:CE3	2.49	0.48
1:H:144:THR:HG21	1:H:149:TYR:HE1	1.79	0.48
1:H:202:HIS:HD2	1:H:202:HIS:O	1.96	0.48
1:H:225:TYR:HA	1:H:229:HIS:O	2.13	0.47
1:C:202:HIS:HD2	1:C:202:HIS:O	1.97	0.47
1:F:50:GLN:O	1:F:51:LEU:HD23	2.14	0.47
1:H:202:HIS:HA	1:H:273:PHE:CE2	2.49	0.47
1:H:226:HIS:HE1	1:H:227:GLN:HE21	1.61	0.47
1:A:3:SER:O	1:A:6:HIS:HB3	2.14	0.47
1:B:53:GLU:O	1:B:53:GLU:HG3	2.14	0.47
1:B:225:TYR:HA	1:B:229:HIS:O	2.14	0.47
1:D:262:THR:HG23	1:D:265:GLU:OE1	2.13	0.47
1:A:163:ARG:HG3	1:A:163:ARG:HH11	1.80	0.47
1:D:5:LEU:HD11	1:D:83:ILE:HG13	1.95	0.47
1:E:255:ASN:O	1:E:256:ASP:CB	2.62	0.47
1:F:159:ILE:CG2	1:F:160:LEU:N	2.76	0.47
1:G:181:GLN:O	1:G:185:VAL:HG23	2.15	0.47
1:H:201:HIS:O	1:H:202:HIS:HB3	2.14	0.47
1:B:89:SER:O	1:B:90:LEU:HD23	2.14	0.47
1:D:223:THR:HG22	1:D:225:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:VAL:HG13	1:D:254:VAL:O	2.14	0.47
1:H:93:ARG:NH2	1:H:105:ARG:NH1	2.63	0.47
1:A:91:LEU:HG	1:A:179:GLN:HG3	1.97	0.47
1:B:167:HIS:O	1:B:168:TRP:CB	2.61	0.47
1:B:239:VAL:HG23	2:B:2041:HOH:O	2.15	0.47
1:C:5:LEU:HD22	1:C:82:ASP:HB3	1.97	0.47
1:C:151:LEU:HD23	1:C:160:LEU:HA	1.97	0.47
1:C:162:PHE:CE1	1:C:164:HIS:HB2	2.49	0.47
1:C:273:PHE:CD1	1:C:273:PHE:N	2.80	0.47
1:E:41:LEU:O	1:E:41:LEU:HD12	2.15	0.47
1:E:45:LEU:HD12	1:E:45:LEU:O	2.15	0.47
1:F:203:LEU:O	1:F:204:LEU:HD23	2.13	0.47
1:A:196:GLN:HG3	2:C:2078:HOH:O	2.13	0.47
1:C:83:ILE:HG22	1:C:83:ILE:O	2.15	0.47
1:C:139:GLU:N	1:C:151:LEU:O	2.46	0.47
1:C:176:LEU:HB3	2:C:2028:HOH:O	2.14	0.47
1:F:89:SER:O	1:F:90:LEU:HD23	2.15	0.47
1:G:245:LEU:CD1	1:G:249:GLN:HB2	2.44	0.47
1:D:14:CYS:SG	1:D:15:GLN:N	2.88	0.47
1:D:144:THR:CG2	1:D:149:TYR:HE1	2.27	0.47
1:E:252:LEU:HD13	2:E:2014:HOH:O	2.15	0.47
1:F:87:VAL:CG1	1:F:112:VAL:HG22	2.45	0.47
1:A:186:MET:CE	1:D:186:MET:CE	2.93	0.47
1:C:91:LEU:HG	1:C:179:GLN:HG3	1.97	0.47
1:B:5:LEU:HD12	1:B:5:LEU:HA	1.73	0.46
1:B:19:VAL:HG12	1:B:21:THR:CG2	2.45	0.46
1:D:200:ARG:HB3	2:D:2029:HOH:O	2.15	0.46
1:E:163:ARG:CG	2:E:2053:HOH:O	2.53	0.46
1:A:96:LEU:C	1:A:98:HIS:H	2.18	0.46
1:B:45:LEU:HB2	2:B:2007:HOH:O	2.13	0.46
1:F:150:ARG:HH21	1:F:168:TRP:HB2	1.79	0.46
1:H:11:ARG:HG2	1:H:11:ARG:HH11	1.79	0.46
1:H:33:ASN:OD1	1:H:131:THR:HA	2.14	0.46
1:C:216:THR:HG21	2:C:2062:HOH:O	2.15	0.46
1:C:245:LEU:CD1	1:C:249:GLN:HB2	2.45	0.46
1:D:4:PHE:C	1:D:6:HIS:N	2.69	0.46
1:D:159:ILE:O	1:D:160:LEU:C	2.53	0.46
1:F:12:LEU:CD2	1:F:32:HIS:HA	2.44	0.46
1:F:150:ARG:O	1:F:151:LEU:HB3	2.14	0.46
1:F:243:TYR:CG	1:F:263:GLU:HG3	2.50	0.46
1:H:163:ARG:HG2	1:H:163:ARG:HH11	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:VAL:HG12	1:D:21:THR:CG2	2.44	0.46
1:D:160:LEU:HD23	1:D:161:GLN:N	2.31	0.46
1:E:109:LEU:HD23	1:E:172:TYR:CE1	2.50	0.46
1:F:151:LEU:HB2	1:F:159:ILE:O	2.15	0.46
1:A:38:PHE:O	1:A:205:MET:HA	2.16	0.46
1:G:59:LYS:HG3	1:G:259:HIS:ND1	2.30	0.46
1:G:220:PHE:CE1	1:G:242:LEU:HD22	2.50	0.46
1:H:91:LEU:HD21	1:H:184:HIS:CD2	2.49	0.46
1:H:91:LEU:HG	1:H:179:GLN:HG3	1.98	0.46
1:A:164:HIS:O	1:A:165:HIS:HB2	2.16	0.46
1:B:96:LEU:HD21	1:B:171:MET:CG	2.46	0.46
2:B:2019:HOH:O	1:C:105:ARG:NE	2.48	0.46
1:D:106:THR:HB	2:D:2015:HOH:O	2.15	0.46
1:E:186:MET:HE2	1:G:186:MET:CE	2.41	0.46
1:E:246:LEU:HD21	2:E:2083:HOH:O	2.15	0.46
1:F:254:VAL:O	1:F:254:VAL:HG13	2.16	0.46
1:A:25:LEU:HD22	1:A:133:PRO:CG	2.38	0.46
1:C:76:PHE:CE1	1:C:80:LEU:HD11	2.51	0.46
1:E:130:LEU:HD13	1:E:134:LEU:HG	1.98	0.46
1:F:181:GLN:O	1:F:185:VAL:HG23	2.15	0.46
1:F:221:HIS:HB2	2:F:2016:HOH:O	2.15	0.46
1:G:154:GLU:O	1:G:156:SER:N	2.49	0.46
1:H:76:PHE:HE1	1:H:80:LEU:HD21	1.80	0.46
1:B:144:THR:HG21	1:B:149:TYR:CE1	2.51	0.46
1:C:174:PHE:HA	2:C:2045:HOH:O	2.15	0.46
1:C:218:THR:O	1:C:219:ASN:HB2	2.15	0.46
1:D:178:VAL:HG12	1:D:179:GLN:N	2.30	0.46
1:H:64:ARG:HD2	2:H:2016:HOH:O	2.15	0.46
1:B:48:GLU:HA	2:B:2008:HOH:O	2.15	0.46
1:B:153:GLN:O	1:B:154:GLU:CB	2.64	0.46
1:B:194:TRP:C	2:B:2036:HOH:O	2.54	0.46
1:B:205:MET:SD	1:B:246:LEU:HD22	2.55	0.46
1:E:12:LEU:CD2	1:E:32:HIS:HA	2.45	0.46
1:F:93:ARG:NH2	1:F:105:ARG:NH1	2.64	0.46
1:F:96:LEU:CD2	1:F:171:MET:HA	2.46	0.46
1:G:5:LEU:HD11	1:G:83:ILE:HG13	1.98	0.46
1:G:96:LEU:CD2	1:G:171:MET:HA	2.46	0.46
1:H:87:VAL:HG12	1:H:112:VAL:HG22	1.97	0.46
1:H:224:ARG:NH2	2:H:2040:HOH:O	2.24	0.46
1:A:161:GLN:CA	1:A:169:GLN:O	2.64	0.46
1:B:12:LEU:HD21	1:B:32:HIS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:O	1:D:45:LEU:HG	2.16	0.46
1:G:12:LEU:HD21	1:G:32:HIS:HA	1.97	0.46
1:G:19:VAL:HG12	1:G:21:THR:CG2	2.46	0.46
1:G:87:VAL:HG12	1:G:112:VAL:HG22	1.98	0.46
1:G:130:LEU:HD23	1:G:149:TYR:CD2	2.51	0.46
1:H:89:SER:O	1:H:90:LEU:HD23	2.16	0.46
1:A:136:LEU:HD22	1:A:158:TRP:CH2	2.51	0.45
1:C:45:LEU:HD12	1:C:45:LEU:O	2.16	0.45
1:D:89:SER:O	1:D:90:LEU:HD23	2.16	0.45
1:F:225:TYR:HA	1:F:229:HIS:O	2.16	0.45
1:B:79:ALA:O	1:B:80:LEU:C	2.54	0.45
1:C:11:ARG:HH21	1:C:64:ARG:HA	1.80	0.45
1:D:202:HIS:HA	1:D:273:PHE:CE2	2.52	0.45
1:E:3:SER:O	1:E:6:HIS:HB3	2.16	0.45
1:H:160:LEU:HD23	1:H:171:MET:CE	2.46	0.45
1:A:138:ALA:O	1:A:140:ILE:N	2.46	0.45
1:A:152:MET:HG2	1:A:154:GLU:HG3	1.99	0.45
1:A:245:LEU:CD1	1:A:249:GLN:HB2	2.44	0.45
1:C:12:LEU:HD21	1:C:32:HIS:HA	1.97	0.45
1:C:123:VAL:C	1:C:129:THR:HG21	2.37	0.45
1:D:15:GLN:HE21	1:D:16:PRO:HD2	1.82	0.45
1:E:138:ALA:O	1:E:140:ILE:N	2.46	0.45
1:E:178:VAL:HA	2:E:2027:HOH:O	2.15	0.45
1:E:178:VAL:HG12	1:E:179:GLN:N	2.30	0.45
1:G:144:THR:HG21	1:G:149:TYR:HE2	1.78	0.45
1:H:60:LEU:HD12	1:H:75:LEU:HD22	1.97	0.45
1:H:243:TYR:CZ	1:H:254:VAL:HG21	2.52	0.45
1:A:96:LEU:HD23	1:A:171:MET:HA	1.98	0.45
1:A:202:HIS:HA	1:A:273:PHE:CE2	2.52	0.45
1:B:237:PRO:HG2	1:B:238:ASP:OD1	2.16	0.45
1:E:186:MET:CE	1:G:186:MET:HE3	2.43	0.45
1:G:262:THR:HG21	2:G:2021:HOH:O	2.16	0.45
1:B:45:LEU:HD12	1:B:45:LEU:O	2.17	0.45
1:B:200:ARG:HH12	1:D:200:ARG:HH12	1.65	0.45
1:E:96:LEU:CD2	1:E:171:MET:HA	2.47	0.45
1:E:201:HIS:O	1:E:202:HIS:HB3	2.16	0.45
1:G:11:ARG:HH21	1:G:64:ARG:CA	2.29	0.45
1:G:222:PHE:CZ	1:G:249:GLN:HG2	2.52	0.45
1:H:68:TYR:OH	1:H:188:ASN:ND2	2.50	0.45
1:B:33:ASN:OD1	1:B:131:THR:HA	2.16	0.45
1:B:46:PRO:HG3	2:D:2011:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:TYR:HA	1:C:229:HIS:O	2.17	0.45
1:D:243:TYR:CE1	1:D:254:VAL:HG21	2.51	0.45
1:E:11:ARG:HG2	1:E:11:ARG:HH11	1.80	0.45
1:E:150:ARG:HG2	1:E:168:TRP:CZ3	2.52	0.45
1:F:41:LEU:HD12	1:F:41:LEU:O	2.16	0.45
1:F:144:THR:CG2	1:F:146:HIS:H	2.22	0.45
1:A:12:LEU:HD13	1:A:31:ALA:HB3	1.98	0.45
1:B:15:GLN:NE2	1:B:16:PRO:HD2	2.31	0.45
1:B:150:ARG:NH1	1:B:152:MET:CE	2.80	0.45
1:F:69:CYS:HB2	1:F:70:PHE:H	1.61	0.45
1:F:163:ARG:HD2	1:F:166:GLU:HA	1.99	0.45
1:F:237:PRO:HG2	1:F:238:ASP:OD1	2.16	0.45
1:G:41:LEU:HD12	1:G:41:LEU:O	2.17	0.45
1:H:107:HIS:CE1	1:H:125:PHE:HD1	2.35	0.45
1:B:46:PRO:O	1:B:47:ARG:HB2	2.17	0.45
1:B:220:PHE:CD1	1:B:242:LEU:HD22	2.52	0.45
1:C:144:THR:HG21	1:C:149:TYR:HE2	1.82	0.45
1:E:160:LEU:CG	1:E:171:MET:HE3	2.41	0.45
1:B:91:LEU:HG	1:B:179:GLN:HG3	1.99	0.45
1:B:262:THR:N	1:B:265:GLU:OE1	2.46	0.45
1:C:106:THR:HG21	2:C:2018:HOH:O	2.15	0.45
1:D:125:PHE:H	1:D:129:THR:CG2	2.29	0.45
1:F:11:ARG:HE	1:F:64:ARG:HA	1.80	0.45
1:G:152:MET:CG	1:G:161:GLN:NE2	2.80	0.45
1:A:186:MET:HE2	1:D:186:MET:HE3	1.99	0.45
1:G:45:LEU:HD12	1:G:45:LEU:O	2.17	0.45
1:H:55:ALA:HA	2:H:2013:HOH:O	2.17	0.45
1:D:96:LEU:C	1:D:98:HIS:H	2.20	0.44
1:D:201:HIS:CE1	2:D:2030:HOH:O	2.69	0.44
1:G:15:GLN:HE21	1:G:16:PRO:HD2	1.81	0.44
1:H:222:PHE:CZ	1:H:249:GLN:HG2	2.52	0.44
1:A:223:THR:HG22	1:A:225:TYR:CE1	2.51	0.44
1:F:4:PHE:CE2	1:F:78:ARG:HD3	2.53	0.44
1:F:258:LYS:HG2	1:F:259:HIS:CD2	2.52	0.44
1:G:117:GLU:HB2	2:G:2029:HOH:O	2.16	0.44
1:H:96:LEU:CD2	1:H:171:MET:HA	2.46	0.44
1:A:254:VAL:O	1:A:254:VAL:HG13	2.17	0.44
1:B:87:VAL:HG13	1:B:112:VAL:HG13	1.99	0.44
1:D:76:PHE:HE1	1:D:80:LEU:HD21	1.80	0.44
1:D:102:LEU:HA	1:D:103:PRO:HD3	1.72	0.44
1:D:149:TYR:N	1:D:149:TYR:CD1	2.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:CD1	1:D:249:GLN:HB2	2.46	0.44
1:E:105:ARG:HG3	2:E:2039:HOH:O	2.17	0.44
1:E:126:GLY:O	1:E:127:GLY:C	2.56	0.44
1:E:176:LEU:HD12	1:E:176:LEU:N	2.33	0.44
1:H:23:GLU:OE1	1:H:26:ARG:HG3	2.17	0.44
1:H:180:GLN:O	1:H:183:ASP:N	2.50	0.44
1:H:223:THR:HG22	1:H:225:TYR:CE1	2.52	0.44
1:B:144:THR:CG2	1:B:149:TYR:HE1	2.30	0.44
1:B:181:GLN:O	1:B:185:VAL:HG23	2.17	0.44
1:D:226:HIS:HE1	1:D:227:GLN:HE21	1.65	0.44
1:F:33:ASN:OD1	1:F:131:THR:HA	2.18	0.44
1:A:11:ARG:HH21	1:A:64:ARG:HA	1.82	0.44
1:B:78:ARG:HD2	2:B:2010:HOH:O	2.16	0.44
1:C:11:ARG:HG2	1:C:11:ARG:HH11	1.83	0.44
1:C:15:GLN:HE21	1:C:16:PRO:HD2	1.81	0.44
1:C:102:LEU:HA	1:C:103:PRO:HD3	1.77	0.44
1:F:11:ARG:HH21	1:F:64:ARG:CA	2.31	0.44
1:F:163:ARG:HD3	1:F:166:GLU:O	2.18	0.44
1:G:33:ASN:OD1	1:G:131:THR:HA	2.17	0.44
1:H:5:LEU:HD11	1:H:83:ILE:HG13	2.00	0.44
1:A:23:GLU:OE1	1:A:26:ARG:HG3	2.17	0.44
1:A:245:LEU:HD12	1:A:245:LEU:O	2.18	0.44
1:B:41:LEU:HD12	1:B:41:LEU:O	2.17	0.44
1:H:3:SER:O	1:H:6:HIS:HB3	2.18	0.44
1:A:4:PHE:C	1:A:6:HIS:N	2.68	0.44
1:C:12:LEU:CD2	1:C:32:HIS:HA	2.47	0.44
1:D:262:THR:N	1:D:265:GLU:OE1	2.49	0.44
1:F:46:PRO:O	1:F:47:ARG:HB2	2.18	0.44
1:F:140:ILE:O	1:F:140:ILE:HG22	2.17	0.44
1:F:220:PHE:CD1	1:F:242:LEU:HD22	2.53	0.44
1:H:123:VAL:C	1:H:129:THR:HG21	2.37	0.44
1:B:15:GLN:NE2	2:B:2003:HOH:O	2.37	0.44
1:C:5:LEU:HD11	1:C:83:ILE:HG13	2.00	0.44
1:C:60:LEU:HB2	1:C:75:LEU:HD22	2.00	0.44
1:C:150:ARG:NH1	1:C:168:TRP:CG	2.86	0.44
1:D:7:ALA:HB1	2:D:2002:HOH:O	2.17	0.44
1:D:130:LEU:HD13	1:D:134:LEU:HG	1.99	0.44
1:E:12:LEU:HD21	1:E:32:HIS:HA	2.00	0.44
1:G:163:ARG:NH2	1:G:166:GLU:O	2.51	0.44
1:H:0:HIS:CE1	2:H:2004:HOH:O	2.71	0.44
1:H:11:ARG:HH21	1:H:64:ARG:HA	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:CG2	1:A:208:HIS:ND1	2.80	0.44
1:A:197:SER:HA	2:A:2039:HOH:O	2.18	0.44
1:A:243:TYR:CE1	1:A:254:VAL:HG21	2.53	0.44
1:A:273:PHE:N	1:A:273:PHE:CD1	2.82	0.44
1:B:150:ARG:HH12	1:B:152:MET:HE2	1.82	0.44
1:D:136:LEU:HD22	1:D:158:TRP:CE2	2.53	0.44
1:F:159:ILE:CG2	1:F:160:LEU:H	2.30	0.44
1:G:125:PHE:H	1:G:129:THR:CG2	2.31	0.44
1:A:1:MET:HE1	1:A:6:HIS:ND1	2.33	0.43
1:A:12:LEU:CD2	1:A:32:HIS:HA	2.48	0.43
1:A:50:GLN:O	1:A:51:LEU:HD23	2.18	0.43
1:B:69:CYS:HB2	1:B:70:PHE:H	1.62	0.43
1:B:164:HIS:N	2:B:2030:HOH:O	2.49	0.43
1:C:4:PHE:C	1:C:6:HIS:N	2.71	0.43
1:C:4:PHE:O	1:C:6:HIS:N	2.50	0.43
1:D:160:LEU:CD2	1:D:171:MET:SD	3.06	0.43
1:E:160:LEU:HD21	1:E:171:MET:HE1	2.00	0.43
1:G:50:GLN:HB2	1:G:55:ALA:CB	2.48	0.43
1:G:243:TYR:CE1	1:G:254:VAL:HG21	2.53	0.43
1:H:25:LEU:HD13	1:H:133:PRO:CG	2.48	0.43
1:C:3:SER:O	1:C:6:HIS:HB3	2.18	0.43
1:C:83:ILE:O	1:C:83:ILE:CG2	2.67	0.43
1:D:109:LEU:HD21	1:D:174:PHE:CE2	2.54	0.43
1:E:223:THR:HG22	1:E:225:TYR:CE1	2.53	0.43
1:F:79:ALA:O	1:F:80:LEU:C	2.54	0.43
1:G:202:HIS:O	1:G:202:HIS:CD2	2.72	0.43
1:B:245:LEU:CD1	1:B:249:GLN:HB2	2.47	0.43
1:E:262:THR:OG1	1:E:264:ALA:N	2.52	0.43
1:G:72:LEU:HD12	1:G:124:GLY:HA2	2.00	0.43
1:G:76:PHE:HE1	1:G:80:LEU:HD21	1.83	0.43
1:G:91:LEU:HG	1:G:179:GLN:HG3	2.00	0.43
1:G:102:LEU:HB2	2:G:2027:HOH:O	2.17	0.43
1:G:131:THR:CG2	1:G:208:HIS:ND1	2.82	0.43
1:B:140:ILE:HG22	1:B:140:ILE:O	2.17	0.43
1:C:25:LEU:HD13	1:C:133:PRO:CG	2.49	0.43
1:E:14:CYS:SG	1:E:15:GLN:N	2.92	0.43
1:E:243:TYR:CZ	1:E:254:VAL:HG21	2.53	0.43
1:F:15:GLN:HE21	1:F:16:PRO:HD2	1.82	0.43
1:F:223:THR:HG22	1:F:225:TYR:CE1	2.53	0.43
1:H:238:ASP:OD2	1:H:240:PRO:HD2	2.19	0.43
1:A:103:PRO:HA	2:A:2024:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:SER:HB2	1:C:104:PRO:CD	2.47	0.43
1:C:4:PHE:CE2	1:C:78:ARG:HD3	2.54	0.43
1:F:125:PHE:O	1:F:125:PHE:CD2	2.72	0.43
1:H:245:LEU:CD1	1:H:249:GLN:HB2	2.48	0.43
1:A:172:TYR:O	1:A:172:TYR:CD1	2.71	0.43
1:A:243:TYR:CG	1:A:263:GLU:HG3	2.53	0.43
1:B:28:LEU:O	1:B:31:ALA:HB3	2.19	0.43
1:C:19:VAL:HG12	1:C:21:THR:CG2	2.49	0.43
1:C:262:THR:N	1:C:265:GLU:OE1	2.49	0.43
1:E:4:PHE:C	1:E:6:HIS:N	2.72	0.43
1:F:207:ARG:NH1	1:F:249:GLN:O	2.49	0.43
1:F:153:GLN:HE21	1:F:153:GLN:HB3	1.51	0.43
1:C:200:ARG:NH1	2:C:2052:HOH:O	2.49	0.43
1:C:221:HIS:HB2	2:C:2066:HOH:O	2.19	0.43
1:E:5:LEU:HD12	1:E:5:LEU:HA	1.79	0.43
1:G:96:LEU:C	1:G:98:HIS:H	2.22	0.43
1:H:125:PHE:H	1:H:129:THR:CG2	2.30	0.43
1:A:83:ILE:O	1:A:83:ILE:HG22	2.18	0.43
1:B:165:HIS:ND1	1:B:165:HIS:C	2.72	0.43
1:B:174:PHE:CD1	1:B:174:PHE:N	2.87	0.43
1:C:139:GLU:OE2	1:C:152:MET:SD	2.76	0.43
1:F:11:ARG:CD	1:F:61:LEU:HA	2.43	0.43
1:H:77:GLU:HB2	1:H:110:LEU:HD21	2.01	0.43
1:H:162:PHE:CD2	1:H:171:MET:HG3	2.53	0.43
1:A:54:THR:O	1:A:58:GLU:HG3	2.19	0.43
1:A:225:TYR:HA	1:A:229:HIS:O	2.19	0.43
1:C:93:ARG:N	1:C:173:CYS:O	2.48	0.43
1:D:11:ARG:HH21	1:D:64:ARG:HA	1.83	0.43
1:D:68:TYR:OH	1:D:188:ASN:ND2	2.52	0.43
1:D:76:PHE:CE1	1:D:80:LEU:HD21	2.54	0.43
1:D:96:LEU:HD23	1:D:171:MET:HA	2.01	0.43
1:F:226:HIS:HE1	1:F:227:GLN:HE21	1.66	0.43
1:G:149:TYR:HD1	1:G:162:PHE:CB	2.32	0.43
1:H:14:CYS:SG	1:H:15:GLN:N	2.92	0.43
1:A:180:GLN:O	1:A:181:GLN:C	2.57	0.42
1:B:130:LEU:HD23	1:B:149:TYR:CE2	2.54	0.42
1:D:49:ILE:O	1:D:49:ILE:HG22	2.18	0.42
1:E:19:VAL:HG12	1:E:21:THR:CG2	2.48	0.42
1:E:33:ASN:OD1	1:E:131:THR:HA	2.18	0.42
1:F:200:ARG:HH12	1:G:200:ARG:HH12	1.66	0.42
1:A:76:PHE:CE1	1:A:80:LEU:HD21	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:HIS:ND1	1:A:165:HIS:CD2	2.88	0.42
1:B:49:ILE:O	1:B:49:ILE:HG22	2.19	0.42
1:B:190:TRP:CH2	1:B:194:TRP:CE2	3.07	0.42
1:C:68:TYR:OH	1:C:188:ASN:ND2	2.51	0.42
1:E:93:ARG:NH2	1:E:105:ARG:NH1	2.67	0.42
1:E:162:PHE:HD1	1:E:162:PHE:H	1.66	0.42
1:E:207:ARG:NH1	1:E:249:GLN:O	2.51	0.42
1:B:256:ASP:O	1:B:257:VAL:C	2.56	0.42
1:F:125:PHE:H	1:F:129:THR:CG2	2.31	0.42
1:F:256:ASP:O	1:F:257:VAL:C	2.56	0.42
1:G:159:ILE:CG2	1:G:160:LEU:N	2.82	0.42
1:H:87:VAL:CG1	1:H:112:VAL:HG22	2.48	0.42
1:H:150:ARG:HD3	1:H:152:MET:SD	2.59	0.42
1:A:12:LEU:HD21	1:A:32:HIS:HA	2.00	0.42
1:B:144:THR:HG21	1:B:149:TYR:HE1	1.84	0.42
1:D:231:VAL:O	1:D:232:GLU:CB	2.66	0.42
1:E:200:ARG:NH1	1:H:200:ARG:HH12	2.15	0.42
1:E:262:THR:HG23	1:E:265:GLU:CD	2.40	0.42
1:H:207:ARG:NH1	1:H:249:GLN:O	2.50	0.42
1:A:72:LEU:HD12	1:A:124:GLY:HA2	2.01	0.42
1:A:125:PHE:H	1:A:129:THR:CG2	2.32	0.42
1:B:11:ARG:CD	1:B:61:LEU:HA	2.48	0.42
1:B:202:HIS:HB2	1:B:219:ASN:OD1	2.20	0.42
1:C:150:ARG:NH1	1:C:168:TRP:CB	2.82	0.42
1:D:45:LEU:HD12	1:D:45:LEU:O	2.20	0.42
1:D:87:VAL:HG13	1:D:112:VAL:HG13	2.01	0.42
1:D:160:LEU:HD21	1:D:171:MET:SD	2.60	0.42
1:G:5:LEU:HD12	1:G:5:LEU:HA	1.82	0.42
1:A:46:PRO:O	1:A:47:ARG:HB2	2.20	0.42
1:B:109:LEU:C	1:B:109:LEU:CD1	2.87	0.42
1:B:161:GLN:CG	1:B:170:SER:HA	2.38	0.42
1:D:60:LEU:HB2	1:D:75:LEU:HD22	2.01	0.42
1:G:12:LEU:CD2	1:G:32:HIS:HA	2.50	0.42
1:G:178:VAL:HA	2:G:2020:HOH:O	2.19	0.42
1:G:225:TYR:HA	1:G:229:HIS:O	2.20	0.42
1:H:136:LEU:HD22	1:H:158:TRP:CZ2	2.54	0.42
1:B:259:HIS:CD2	1:B:259:HIS:N	2.85	0.42
1:C:158:TRP:NE1	2:C:2043:HOH:O	2.32	0.42
1:G:45:LEU:HB2	2:G:2013:HOH:O	2.20	0.42
1:G:87:VAL:HG13	1:G:112:VAL:HG13	2.01	0.42
1:A:76:PHE:CE1	1:A:80:LEU:HD11	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CD1	1:A:242:LEU:HD22	2.55	0.42
1:C:150:ARG:HH21	1:C:152:MET:HE1	1.82	0.42
1:D:33:ASN:OD1	1:D:131:THR:HA	2.20	0.42
1:E:4:PHE:O	1:E:6:HIS:N	2.53	0.42
1:E:12:LEU:O	1:E:13:HIS:C	2.57	0.42
1:E:273:PHE:CD1	1:E:273:PHE:N	2.84	0.42
1:F:5:LEU:HG	1:F:9:PHE:CE2	2.55	0.42
1:F:45:LEU:CB	2:F:2011:HOH:O	2.61	0.42
1:F:46:PRO:CD	2:F:2011:HOH:O	2.11	0.42
1:F:122:ASP:O	1:F:129:THR:CG2	2.66	0.42
1:C:130:LEU:HD23	1:C:149:TYR:CE2	2.55	0.42
1:C:150:ARG:NH2	1:C:152:MET:HE2	2.35	0.42
1:D:50:GLN:HB2	1:D:55:ALA:CB	2.50	0.42
1:H:163:ARG:NH1	1:H:168:TRP:CG	2.88	0.42
1:A:45:LEU:O	1:A:45:LEU:HD12	2.18	0.41
1:A:59:LYS:HA	1:A:259:HIS:ND1	2.34	0.41
1:A:234:VAL:HG12	1:A:235:ASN:N	2.34	0.41
1:H:262:THR:OG1	1:H:264:ALA:N	2.53	0.41
1:A:33:ASN:OD1	1:A:131:THR:HA	2.20	0.41
1:D:12:LEU:HD21	1:D:32:HIS:HA	2.02	0.41
1:D:123:VAL:C	1:D:129:THR:HG21	2.40	0.41
1:F:132:ALA:O	1:F:133:PRO:O	2.38	0.41
1:G:163:ARG:CZ	1:G:166:GLU:O	2.65	0.41
1:H:163:ARG:NH1	1:H:168:TRP:CD1	2.88	0.41
1:A:102:LEU:HA	1:A:103:PRO:HD3	1.74	0.41
1:A:138:ALA:HB2	1:A:153:GLN:HB2	2.03	0.41
1:A:231:VAL:O	1:A:232:GLU:CB	2.60	0.41
1:B:146:HIS:CE1	2:B:2027:HOH:O	2.72	0.41
1:D:12:LEU:CD2	1:D:32:HIS:HA	2.51	0.41
1:D:202:HIS:HD2	1:D:202:HIS:O	2.04	0.41
1:G:53:GLU:HA	2:G:2016:HOH:O	2.21	0.41
1:G:76:PHE:CE1	1:G:80:LEU:HD21	2.56	0.41
1:G:96:LEU:HD23	1:G:170:SER:O	2.20	0.41
1:H:11:ARG:HH21	1:H:64:ARG:C	2.24	0.41
1:H:243:TYR:CE1	1:H:254:VAL:HG21	2.55	0.41
1:A:4:PHE:O	1:A:5:LEU:C	2.58	0.41
1:A:5:LEU:HD12	1:A:5:LEU:HA	1.84	0.41
1:A:19:VAL:HA	1:A:20:PRO:HD2	1.89	0.41
1:A:243:TYR:CZ	1:A:254:VAL:HG21	2.55	0.41
1:B:12:LEU:CD2	1:B:32:HIS:HA	2.51	0.41
1:B:53:GLU:HB3	2:B:2010:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PHE:HE1	1:B:80:LEU:HD21	1.86	0.41
1:D:172:TYR:O	1:D:172:TYR:HD1	2.03	0.41
1:F:109:LEU:C	1:F:109:LEU:CD1	2.85	0.41
1:H:60:LEU:HB2	1:H:75:LEU:HD22	2.02	0.41
1:A:180:GLN:O	1:A:183:ASP:N	2.53	0.41
1:B:5:LEU:HD11	1:B:83:ILE:HG13	2.02	0.41
1:B:11:ARG:HH21	1:B:64:ARG:HA	1.85	0.41
1:C:50:GLN:HB2	1:C:55:ALA:CB	2.51	0.41
1:C:60:LEU:CB	1:C:75:LEU:HD22	2.51	0.41
1:D:5:LEU:HD12	1:D:5:LEU:HA	1.87	0.41
1:D:220:PHE:CD1	1:D:242:LEU:HD22	2.55	0.41
1:E:125:PHE:H	1:E:129:THR:CG2	2.34	0.41
1:E:131:THR:CG2	1:E:208:HIS:ND1	2.83	0.41
1:G:59:LYS:HA	1:G:259:HIS:ND1	2.36	0.41
1:G:109:LEU:C	1:G:109:LEU:CD1	2.88	0.41
1:H:234:VAL:CG1	1:H:235:ASN:N	2.83	0.41
1:A:19:VAL:HG12	1:A:21:THR:CG2	2.49	0.41
1:A:213:GLY:HA2	1:A:225:TYR:O	2.21	0.41
1:B:4:PHE:CE2	1:B:78:ARG:HD3	2.55	0.41
1:C:93:ARG:NH2	1:C:105:ARG:HH12	2.19	0.41
1:C:144:THR:CG2	1:C:146:HIS:H	2.25	0.41
1:C:243:TYR:CZ	1:C:254:VAL:HG21	2.56	0.41
1:D:63:ALA:O	1:D:253:GLY:HA3	2.20	0.41
1:G:223:THR:CG2	1:G:225:TYR:CE1	3.04	0.41
1:A:12:LEU:HD13	1:A:31:ALA:CB	2.51	0.41
1:A:96:LEU:C	1:A:98:HIS:N	2.74	0.41
1:B:144:THR:CG2	1:B:146:HIS:H	2.22	0.41
1:D:1:MET:HE1	1:D:6:HIS:ND1	2.34	0.41
1:E:63:ALA:O	1:E:253:GLY:HA3	2.20	0.41
1:E:200:ARG:HH12	1:H:200:ARG:NH1	2.14	0.41
1:E:238:ASP:OD2	1:E:240:PRO:HD2	2.20	0.41
1:F:245:LEU:CD1	1:F:249:GLN:HB2	2.51	0.41
1:H:213:GLY:HA2	1:H:225:TYR:O	2.20	0.41
1:B:4:PHE:C	1:B:6:HIS:N	2.74	0.41
1:B:162:PHE:CD1	1:B:162:PHE:N	2.88	0.41
1:C:41:LEU:HB3	1:C:65:ARG:HH22	1.86	0.41
1:E:59:LYS:HB2	1:E:259:HIS:CE1	2.55	0.41
1:G:54:THR:N	2:G:2016:HOH:O	2.53	0.41
1:H:59:LYS:HG3	1:H:259:HIS:ND1	2.35	0.41
1:A:5:LEU:HD11	1:A:83:ILE:HG13	2.02	0.41
1:A:50:GLN:HB2	1:A:55:ALA:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CD1	1:A:172:TYR:C	2.93	0.41
1:B:102:LEU:HA	1:B:103:PRO:HD3	1.79	0.41
1:B:122:ASP:O	1:B:129:THR:CG2	2.67	0.41
1:B:200:ARG:NH1	1:D:200:ARG:HH12	2.18	0.41
1:C:12:LEU:HD13	1:C:31:ALA:CB	2.51	0.41
1:C:176:LEU:CB	2:C:2028:HOH:O	2.69	0.41
1:C:215:LEU:CD2	1:C:224:ARG:HG3	2.51	0.41
1:C:262:THR:HG23	1:C:265:GLU:CD	2.41	0.41
1:D:90:LEU:HB2	1:D:109:LEU:CD1	2.51	0.41
1:E:118:GLN:N	2:E:2044:HOH:O	2.52	0.41
1:E:180:GLN:O	1:E:183:ASP:N	2.53	0.41
1:E:202:HIS:HA	1:E:273:PHE:CE2	2.56	0.41
1:F:28:LEU:HD23	1:F:28:LEU:HA	1.94	0.41
1:G:57:GLU:N	2:G:2016:HOH:O	2.53	0.41
1:G:69:CYS:HB2	1:G:70:PHE:H	1.61	0.41
1:G:269:VAL:HG13	2:G:2054:HOH:O	2.20	0.41
1:H:63:ALA:O	1:H:253:GLY:HA3	2.21	0.41
1:A:162:PHE:CD1	1:A:162:PHE:N	2.89	0.41
1:C:163:ARG:NH1	1:C:167:HIS:HA	2.32	0.41
1:C:222:PHE:CZ	1:C:249:GLN:HG2	2.56	0.41
1:C:243:TYR:CG	1:C:263:GLU:HG3	2.56	0.41
1:D:150:ARG:HB2	1:D:168:TRP:CZ3	2.56	0.41
1:H:69:CYS:HB2	1:H:70:PHE:H	1.70	0.41
1:H:234:VAL:HG12	1:H:235:ASN:N	2.35	0.41
1:A:41:LEU:HB3	1:A:65:ARG:HH22	1.86	0.40
1:A:55:ALA:HB1	2:A:2052:HOH:O	2.21	0.40
1:B:15:GLN:HB3	2:B:2002:HOH:O	2.20	0.40
1:B:61:LEU:HD21	1:B:75:LEU:HD21	2.02	0.40
1:B:195:PRO:HD2	2:B:2036:HOH:O	2.21	0.40
1:D:148:GLU:HB3	1:D:163:ARG:HB2	2.03	0.40
1:E:239:VAL:N	1:E:240:PRO:CD	2.84	0.40
1:F:95:ILE:HG12	1:F:172:TYR:HA	2.02	0.40
1:H:144:THR:CG2	1:H:149:TYR:HE1	2.33	0.40
1:H:162:PHE:CE2	1:H:171:MET:HG3	2.56	0.40
1:B:90:LEU:HB2	1:B:109:LEU:CD1	2.51	0.40
1:C:239:VAL:HB	1:C:240:PRO:CD	2.49	0.40
1:D:162:PHE:CD1	1:D:169:GLN:HB2	2.55	0.40
1:E:243:TYR:CE1	1:E:254:VAL:HG21	2.57	0.40
1:F:87:VAL:HG13	1:F:112:VAL:HG13	2.02	0.40
1:F:90:LEU:HB2	1:F:109:LEU:CD1	2.52	0.40
1:F:243:TYR:CE1	1:F:254:VAL:HG21	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:GLU:O	1:G:140:ILE:C	2.60	0.40
1:C:12:LEU:HD13	1:C:31:ALA:HB3	2.03	0.40
1:C:41:LEU:O	1:C:45:LEU:HG	2.21	0.40
1:C:96:LEU:C	1:C:98:HIS:H	2.23	0.40
1:C:232:GLU:HB2	2:C:2065:HOH:O	2.22	0.40
1:C:239:VAL:HG11	1:C:267:ALA:HB2	2.04	0.40
1:D:12:LEU:HD13	1:D:31:ALA:HB3	2.03	0.40
1:D:235:ASN:O	1:D:236:VAL:C	2.58	0.40
1:E:79:ALA:O	1:E:80:LEU:C	2.59	0.40
1:E:83:ILE:O	1:E:83:ILE:HG22	2.20	0.40
1:G:63:ALA:HB1	2:G:2052:HOH:O	2.22	0.40
1:G:123:VAL:C	1:G:129:THR:HG21	2.42	0.40
1:G:259:HIS:CD2	1:G:259:HIS:N	2.89	0.40
1:H:149:TYR:HD2	1:H:162:PHE:HB3	1.83	0.40
1:A:189:PHE:CE2	1:D:189:PHE:CE2	3.10	0.40
1:B:96:LEU:C	1:B:98:HIS:H	2.25	0.40
1:B:166:GLU:HG2	1:G:233:GLN:CB	2.29	0.40
1:C:125:PHE:CB	1:C:129:THR:HG23	2.52	0.40
1:C:161:GLN:HB3	1:C:169:GLN:O	2.21	0.40
1:F:102:LEU:HA	1:F:103:PRO:HD3	1.72	0.40
1:F:138:ALA:HA	1:F:151:LEU:O	2.22	0.40
1:H:273:PHE:CD1	1:H:273:PHE:N	2.88	0.40
1:A:161:GLN:HB3	1:A:169:GLN:O	2.22	0.40
1:A:203:LEU:O	1:A:204:LEU:HD23	2.22	0.40
1:B:213:GLY:HA2	1:B:225:TYR:O	2.22	0.40
1:C:33:ASN:OD1	1:C:131:THR:HA	2.22	0.40
1:C:243:TYR:CE1	1:C:254:VAL:HG21	2.56	0.40
1:D:19:VAL:HA	1:D:20:PRO:HD2	1.92	0.40
1:E:28:LEU:HD23	1:E:28:LEU:HA	1.91	0.40
1:E:59:LYS:HG3	1:E:259:HIS:ND1	2.37	0.40
1:E:205:MET:HG2	2:E:2014:HOH:O	2.20	0.40
1:G:63:ALA:O	1:G:253:GLY:HA3	2.21	0.40
1:H:1:MET:HE1	1:H:6:HIS:ND1	2.36	0.40
1:H:87:VAL:HG13	1:H:112:VAL:HG13	2.02	0.40
1:H:262:THR:HG23	1:H:265:GLU:OE1	2.22	0.40

All (4) 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)
1:F:6:HIS:ND1	1:F:62:TYR:OH[2_665]	1.90	0.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASP:OD2	1:H:10:THR:O[4_556]	1.92	0.28
1:B:6:HIS:ND1	1:B:62:TYR:OH[2_665]	1.98	0.22
1:C:209:LEU:CD1	1:H:6:HIS:NE2[4_556]	2.19	0.01

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	272/284 (96%)	225 (83%)	38 (14%)	9 (3%)	4 13
1	B	272/284 (96%)	216 (79%)	44 (16%)	12 (4%)	2 8
1	C	272/284 (96%)	223 (82%)	41 (15%)	8 (3%)	4 15
1	D	272/284 (96%)	217 (80%)	46 (17%)	9 (3%)	4 13
1	E	272/284 (96%)	229 (84%)	35 (13%)	8 (3%)	4 15
1	F	272/284 (96%)	223 (82%)	40 (15%)	9 (3%)	4 13
1	G	272/284 (96%)	221 (81%)	44 (16%)	7 (3%)	5 18
1	H	272/284 (96%)	226 (83%)	35 (13%)	11 (4%)	3 9
All	All	2176/2272 (96%)	1780 (82%)	323 (15%)	73 (3%)	3 13

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
1	A	256	ASP
1	B	69	CYS
1	B	140	ILE
1	B	165	HIS
1	B	166	GLU
1	B	256	ASP
1	C	54	THR
1	C	69	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	140	ILE
1	C	256	ASP
1	D	54	THR
1	D	69	CYS
1	D	140	ILE
1	D	256	ASP
1	E	54	THR
1	E	256	ASP
1	F	69	CYS
1	F	140	ILE
1	F	166	GLU
1	F	256	ASP
1	G	54	THR
1	G	69	CYS
1	G	140	ILE
1	G	256	ASP
1	H	69	CYS
1	H	140	ILE
1	H	164	HIS
1	H	165	HIS
1	H	256	ASP
1	A	54	THR
1	A	140	ILE
1	B	54	THR
1	E	69	CYS
1	E	140	ILE
1	F	54	THR
1	G	5	LEU
1	G	155	GLY
1	H	54	THR
1	H	166	GLU
1	B	154	GLU
1	B	168	TRP
1	C	165	HIS
1	D	5	LEU
1	F	165	HIS
1	H	152	MET
1	A	5	LEU
1	C	5	LEU
1	C	154	GLU
1	D	97	SER
1	D	116	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	16	PRO
1	H	116	ASP
1	A	97	SER
1	B	139	GLU
1	B	232	GLU
1	E	5	LEU
1	E	116	ASP
1	E	232	GLU
1	F	232	GLU
1	H	232	GLU
1	A	232	GLU
1	B	5	LEU
1	C	232	GLU
1	D	16	PRO
1	D	232	GLU
1	A	16	PRO
1	E	16	PRO
1	B	16	PRO
1	A	145	PRO
1	F	16	PRO
1	H	16	PRO
1	F	257	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	236/243 (97%)	213 (90%)	23 (10%)	8 24
1	B	236/243 (97%)	215 (91%)	21 (9%)	9 28
1	C	236/243 (97%)	214 (91%)	22 (9%)	9 26
1	D	236/243 (97%)	211 (89%)	25 (11%)	6 20
1	E	236/243 (97%)	211 (89%)	25 (11%)	6 20
1	F	236/243 (97%)	216 (92%)	20 (8%)	10 31
1	G	236/243 (97%)	215 (91%)	21 (9%)	9 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	236/243 (97%)	216 (92%)	20 (8%)	10 31
All	All	1888/1944 (97%)	1711 (91%)	177 (9%)	8 26

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	PRO
1	A	23	GLU
1	A	25	LEU
1	A	30	LEU
1	A	39	GLU
1	A	45	LEU
1	A	68	TYR
1	A	87	VAL
1	A	88	ARG
1	A	128	GLN
1	A	129	THR
1	A	144	THR
1	A	145	PRO
1	A	150	ARG
1	A	162	PHE
1	A	169	GLN
1	A	202	HIS
1	A	216	THR
1	A	237	PRO
1	A	248	GLN
1	A	254	VAL
1	A	262	THR
1	B	1	MET
1	B	16	PRO
1	B	23	GLU
1	B	25	LEU
1	B	30	LEU
1	B	39	GLU
1	B	45	LEU
1	B	68	TYR
1	B	87	VAL
1	B	88	ARG
1	B	128	GLN
1	B	129	THR
1	B	144	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	150	ARG
1	B	152	MET
1	B	162	PHE
1	B	202	HIS
1	B	216	THR
1	B	248	GLN
1	B	254	VAL
1	B	262	THR
1	C	1	MET
1	C	16	PRO
1	C	23	GLU
1	C	25	LEU
1	C	30	LEU
1	C	39	GLU
1	C	45	LEU
1	C	68	TYR
1	C	87	VAL
1	C	88	ARG
1	C	128	GLN
1	C	129	THR
1	C	144	THR
1	C	145	PRO
1	C	166	GLU
1	C	169	GLN
1	C	172	TYR
1	C	216	THR
1	C	237	PRO
1	C	248	GLN
1	C	254	VAL
1	C	262	THR
1	D	1	MET
1	D	16	PRO
1	D	23	GLU
1	D	25	LEU
1	D	30	LEU
1	D	39	GLU
1	D	45	LEU
1	D	68	TYR
1	D	87	VAL
1	D	88	ARG
1	D	128	GLN
1	D	129	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	144	THR
1	D	145	PRO
1	D	150	ARG
1	D	152	MET
1	D	162	PHE
1	D	172	TYR
1	D	174	PHE
1	D	175	ASP
1	D	202	HIS
1	D	216	THR
1	D	248	GLN
1	D	254	VAL
1	D	262	THR
1	E	1	MET
1	E	16	PRO
1	E	23	GLU
1	E	25	LEU
1	E	30	LEU
1	E	39	GLU
1	E	45	LEU
1	E	68	TYR
1	E	76	PHE
1	E	87	VAL
1	E	88	ARG
1	E	128	GLN
1	E	129	THR
1	E	144	THR
1	E	145	PRO
1	E	157	THR
1	E	160	LEU
1	E	162	PHE
1	E	163	ARG
1	E	164	HIS
1	E	202	HIS
1	E	216	THR
1	E	248	GLN
1	E	254	VAL
1	E	262	THR
1	F	16	PRO
1	F	23	GLU
1	F	25	LEU
1	F	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	39	GLU
1	F	68	TYR
1	F	87	VAL
1	F	88	ARG
1	F	128	GLN
1	F	129	THR
1	F	144	THR
1	F	153	GLN
1	F	160	LEU
1	F	163	ARG
1	F	165	HIS
1	F	202	HIS
1	F	216	THR
1	F	248	GLN
1	F	254	VAL
1	F	262	THR
1	G	16	PRO
1	G	23	GLU
1	G	25	LEU
1	G	30	LEU
1	G	39	GLU
1	G	45	LEU
1	G	68	TYR
1	G	87	VAL
1	G	88	ARG
1	G	128	GLN
1	G	129	THR
1	G	144	THR
1	G	145	PRO
1	G	151	LEU
1	G	169	GLN
1	G	202	HIS
1	G	216	THR
1	G	237	PRO
1	G	248	GLN
1	G	254	VAL
1	G	262	THR
1	H	16	PRO
1	H	23	GLU
1	H	25	LEU
1	H	30	LEU
1	H	39	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	45	LEU
1	H	68	TYR
1	H	87	VAL
1	H	88	ARG
1	H	128	GLN
1	H	129	THR
1	H	144	THR
1	H	145	PRO
1	H	152	MET
1	H	166	GLU
1	H	202	HIS
1	H	216	THR
1	H	248	GLN
1	H	254	VAL
1	H	262	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	86	ASN
1	A	128	GLN
1	A	153	GLN
1	A	165	HIS
1	A	167	HIS
1	A	169	GLN
1	A	184	HIS
1	A	188	ASN
1	A	198	HIS
1	A	202	HIS
1	A	226	HIS
1	A	244	GLN
1	B	15	GLN
1	B	86	ASN
1	B	128	GLN
1	B	153	GLN
1	B	184	HIS
1	B	188	ASN
1	B	198	HIS
1	B	202	HIS
1	B	221	HIS
1	B	226	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	244	GLN
1	C	15	GLN
1	C	86	ASN
1	C	128	GLN
1	C	169	GLN
1	C	184	HIS
1	C	188	ASN
1	C	198	HIS
1	C	202	HIS
1	C	226	HIS
1	C	244	GLN
1	D	15	GLN
1	D	86	ASN
1	D	128	GLN
1	D	161	GLN
1	D	184	HIS
1	D	188	ASN
1	D	198	HIS
1	D	202	HIS
1	D	226	HIS
1	D	244	GLN
1	E	15	GLN
1	E	86	ASN
1	E	128	GLN
1	E	184	HIS
1	E	188	ASN
1	E	226	HIS
1	E	244	GLN
1	F	15	GLN
1	F	86	ASN
1	F	128	GLN
1	F	153	GLN
1	F	161	GLN
1	F	184	HIS
1	F	188	ASN
1	F	198	HIS
1	F	221	HIS
1	F	226	HIS
1	F	244	GLN
1	G	15	GLN
1	G	86	ASN
1	G	128	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	161	GLN
1	G	169	GLN
1	G	184	HIS
1	G	188	ASN
1	G	198	HIS
1	G	202	HIS
1	G	226	HIS
1	G	244	GLN
1	H	15	GLN
1	H	86	ASN
1	H	128	GLN
1	H	161	GLN
1	H	165	HIS
1	H	184	HIS
1	H	188	ASN
1	H	198	HIS
1	H	202	HIS
1	H	221	HIS
1	H	226	HIS

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 monosaccharides 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 (i)

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	274/284 (96%)	0.22	4 (1%)	73	68	47, 79, 110, 122	0
1	B	274/284 (96%)	0.23	6 (2%)	62	52	54, 77, 106, 119	0
1	C	274/284 (96%)	0.30	15 (5%)	25	16	54, 79, 113, 121	0
1	D	274/284 (96%)	0.45	17 (6%)	20	13	49, 93, 116, 121	0
1	E	274/284 (96%)	-0.09	1 (0%)	92	91	37, 59, 87, 119	0
1	F	274/284 (96%)	0.23	10 (3%)	42	32	45, 70, 104, 119	0
1	G	274/284 (96%)	0.13	4 (1%)	73	68	39, 77, 106, 120	0
1	H	274/284 (96%)	0.16	11 (4%)	38	28	47, 78, 109, 120	0
All	All	2192/2272 (96%)	0.20	68 (3%)	49	39	37, 76, 110, 122	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.5
1	A	0	HIS	6.5
1	H	0	HIS	5.7
1	F	0	HIS	5.3
1	G	0	HIS	5.2
1	D	0	HIS	5.1
1	C	211	ASP	4.9
1	B	0	HIS	4.7
1	D	165	HIS	4.5
1	D	15	GLN	4.4
1	D	19	VAL	4.3
1	C	114	VAL	4.0
1	B	165	HIS	3.9
1	H	19	VAL	3.9
1	E	165	HIS	3.7
1	C	0	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	165	HIS	3.3
1	F	116	ASP	3.2
1	D	230	ALA	3.1
1	F	98	HIS	3.0
1	D	227	GLN	2.9
1	D	119	TRP	2.9
1	F	114	VAL	2.9
1	D	229	HIS	2.8
1	F	136	LEU	2.8
1	C	86	ASN	2.7
1	H	225	TYR	2.7
1	C	141	ALA	2.7
1	B	152	MET	2.7
1	C	167	HIS	2.7
1	F	140	ILE	2.6
1	H	169	GLN	2.6
1	C	20	PRO	2.6
1	H	165	HIS	2.6
1	H	114	VAL	2.6
1	H	227	GLN	2.6
1	A	114	VAL	2.5
1	F	69	CYS	2.5
1	C	210	PRO	2.4
1	A	163	ARG	2.4
1	C	99	PRO	2.4
1	D	210	PRO	2.4
1	D	62	TYR	2.4
1	F	161	GLN	2.3
1	G	162	PHE	2.3
1	D	99	PRO	2.3
1	H	167	HIS	2.3
1	H	231	VAL	2.2
1	D	102	LEU	2.2
1	D	228	GLY	2.2
1	B	142	GLN	2.2
1	C	83	ILE	2.2
1	D	139	GLU	2.2
1	C	19	VAL	2.2
1	H	230	ALA	2.1
1	B	6	HIS	2.1
1	G	244	GLN	2.1
1	C	229	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	98	HIS	2.1
1	F	82	ASP	2.1
1	D	234	VAL	2.1
1	C	116	ASP	2.0
1	F	153	GLN	2.0
1	H	229	HIS	2.0
1	G	186	MET	2.0
1	D	81	ARG	2.0
1	A	1	MET	2.0
1	D	136	LEU	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.