



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:53 AM GMT

PDB ID : 2BX5
Title : Is FR1 the antibody's Achilles heel
Authors : James, L.C.
Deposited on : 2005-07-22
Resolution : 2.70 Å(reported)

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

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

MolProbity : 4.02b-467
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

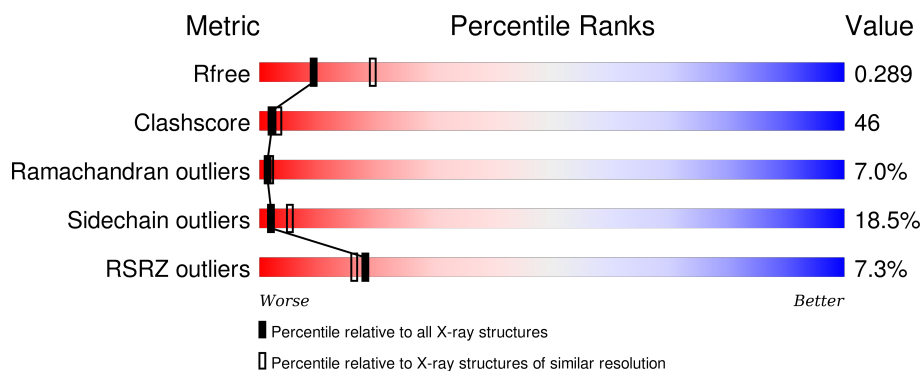
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	107	<div> <div>5%</div> <div>27%</div> <div>53%</div> <div>17%</div> <div>..</div> </div>
1	B	107	<div> <div>5%</div> <div>48%</div> <div>37%</div> <div>14%</div> <div>.</div> </div>
1	C	107	<div> <div>4%</div> <div>36%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>
1	D	107	<div> <div>2%</div> <div>44%</div> <div>44%</div> <div>11%</div> <div>.</div> </div>
1	E	107	<div> <div>2%</div> <div>55%</div> <div>34%</div> <div>9%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	107	
1	G	107	
1	H	107	
1	I	107	
1	J	107	
1	K	107	
1	L	107	
1	M	107	
1	N	107	
1	O	107	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12989 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 VD9 VKI LIGHT-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	B	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	C	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	D	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	E	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	F	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	G	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	H	97	Total	C	N	O	S	0	0	0
			727	456	120	148	3			
1	I	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	J	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	K	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	L	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	M	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	N	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			
1	O	106	Total	C	N	O	S	0	0	0
			801	500	132	166	3			

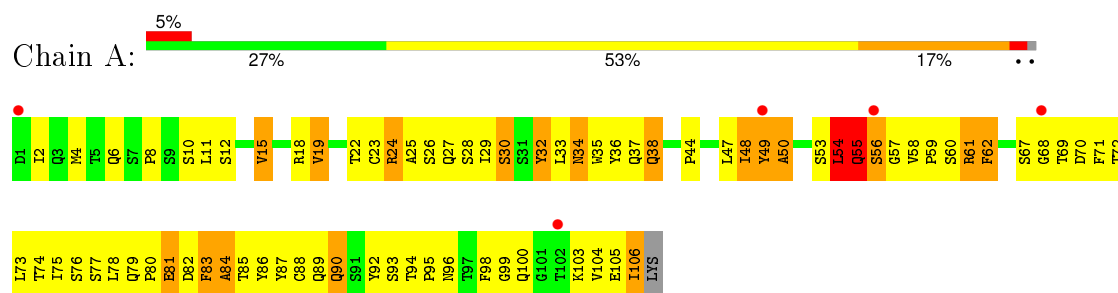
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total 74	O 74	0	0
2	B	77	Total 77	O 77	0	0
2	C	53	Total 53	O 53	0	0
2	D	67	Total 67	O 67	0	0
2	E	64	Total 64	O 64	0	0
2	F	74	Total 74	O 74	0	0
2	G	57	Total 57	O 57	0	0
2	H	68	Total 68	O 68	0	0
2	I	68	Total 68	O 68	0	0
2	J	93	Total 93	O 93	0	0
2	K	75	Total 75	O 75	0	0
2	L	64	Total 64	O 64	0	0
2	M	81	Total 81	O 81	0	0
2	N	68	Total 68	O 68	0	0
2	O	65	Total 65	O 65	0	0

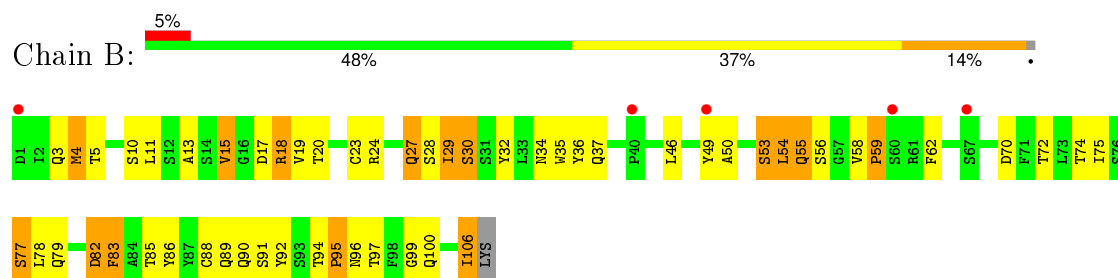
3 Residue-property plots

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

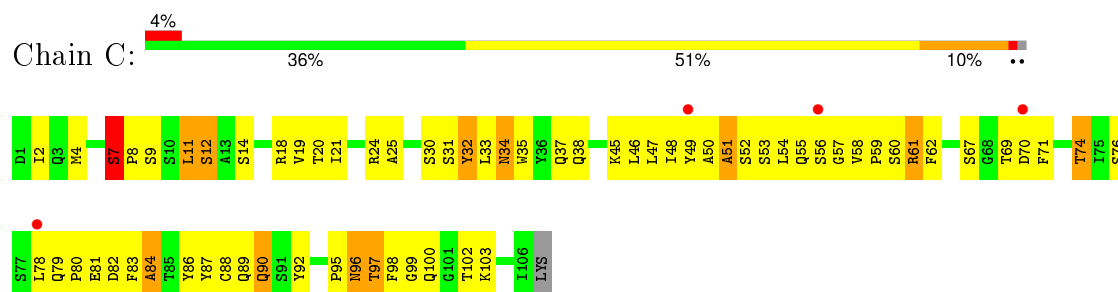
• Molecule 1: VD9 VKI LIGHT-CHAIN



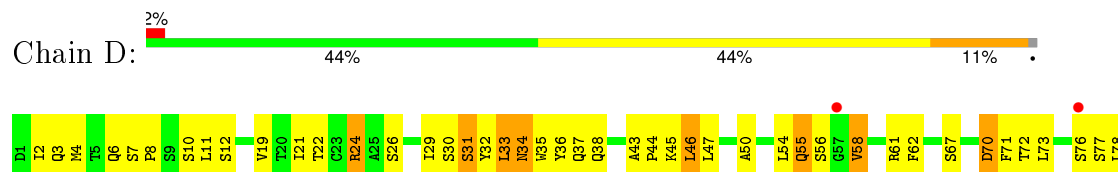
• Molecule 1: VD9 VKI LIGHT-CHAIN



• Molecule 1: VD9 VKI LIGHT-CHAIN

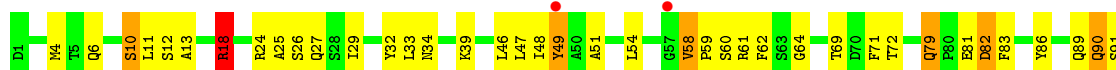


• Molecule 1: VD9 VKI LIGHT-CHAIN

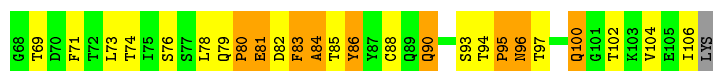
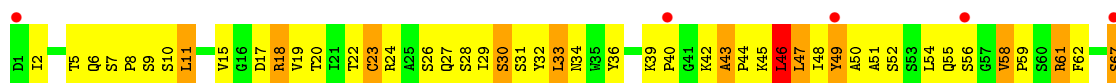




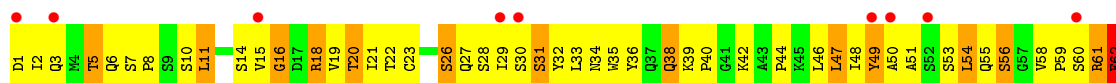
• Molecule 1: VD9 VKI LIGHT-CHAIN



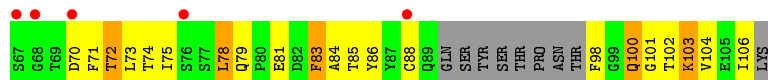
• Molecule 1: VD9 VKI LIGHT-CHAIN



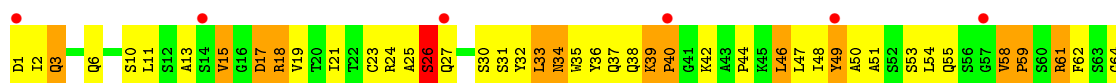
• Molecule 1: VD9 VKI LIGHT-CHAIN

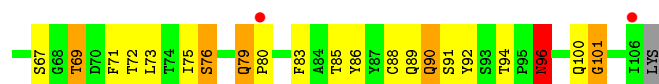


• Molecule 1: VD9 VKI LIGHT-CHAIN

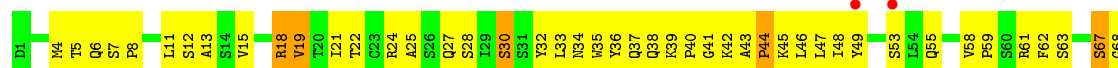


• Molecule 1: VD9 VKI LIGHT-CHAIN

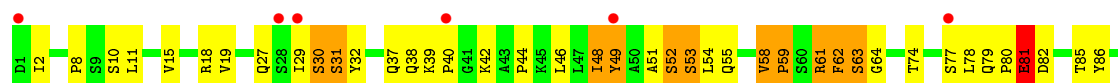




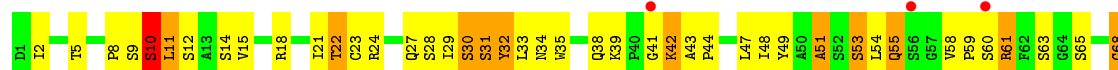
• Molecule 1: VD9 VKI LIGHT-CHAIN



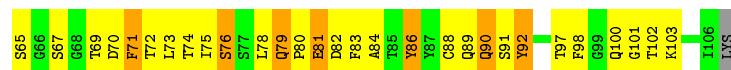
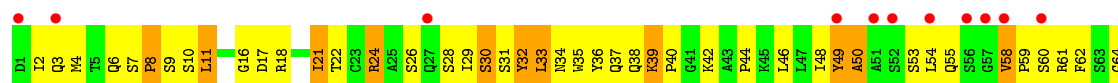
• Molecule 1: VD9 VKI LIGHT-CHAIN



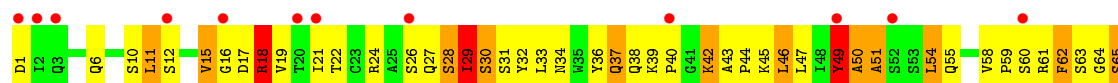
• Molecule 1: VD9 VKI LIGHT-CHAIN

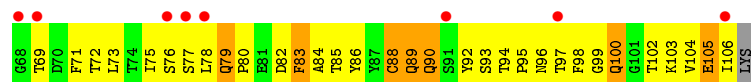


• Molecule 1: VD9 VKI LIGHT-CHAIN



• Molecule 1: VD9 VKI LIGHT-CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	191.93Å 191.93Å 197.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	166.00 – 2.70 25.43 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (166.00-2.70) 99.9 (25.43-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.250 , 0.290 0.286 , 0.289	Depositor DCC
R_{free} test set	2988 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 115.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	18 of 59063 reflections (0.030%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12989	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.76 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6082e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.73	1/818 (0.1%)	0.84	1/1111 (0.1%)
1	B	0.69	0/818	0.82	0/1111
1	C	0.82	3/818 (0.4%)	0.81	0/1111
1	D	0.72	1/818 (0.1%)	0.79	0/1111
1	E	0.78	2/818 (0.2%)	0.89	3/1111 (0.3%)
1	F	0.83	2/818 (0.2%)	0.79	0/1111
1	G	0.73	2/818 (0.2%)	0.87	1/1111 (0.1%)
1	H	0.76	2/741 (0.3%)	0.85	1/1004 (0.1%)
1	I	0.68	1/818 (0.1%)	0.77	0/1111
1	J	0.61	0/818	0.78	0/1111
1	K	0.64	1/818 (0.1%)	0.73	0/1111
1	L	0.80	2/818 (0.2%)	0.79	1/1111 (0.1%)
1	M	0.83	2/818 (0.2%)	0.91	3/1111 (0.3%)
1	N	0.78	2/818 (0.2%)	0.88	3/1111 (0.3%)
1	O	0.75	2/818 (0.2%)	0.80	0/1111
All	All	0.75	23/12193 (0.2%)	0.82	13/16558 (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	A	0	1
1	F	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	2
1	O	0	1
All	All	0	8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	SER	CB-OG	11.32	1.56	1.42
1	O	67	SER	CB-OG	10.46	1.55	1.42
1	F	9	SER	CB-OG	10.22	1.55	1.42
1	L	63	SER	CB-OG	9.81	1.54	1.42
1	D	10	SER	CB-OG	9.04	1.54	1.42
1	L	10	SER	CB-OG	8.38	1.53	1.42
1	E	93	SER	CB-OG	7.49	1.51	1.42
1	N	91	SER	CB-OG	7.16	1.51	1.42
1	A	10	SER	CB-OG	7.02	1.51	1.42
1	F	67	SER	CB-OG	7.01	1.51	1.42
1	G	26	SER	CB-OG	6.51	1.50	1.42
1	K	63	SER	CB-OG	6.35	1.50	1.42
1	M	103	LYS	CE-NZ	6.20	1.64	1.49
1	I	26	SER	CB-OG	5.86	1.49	1.42
1	N	60	SER	CB-OG	5.82	1.49	1.42
1	O	63	SER	CB-OG	5.71	1.49	1.42
1	C	52	SER	CB-OG	5.69	1.49	1.42
1	C	9	SER	CB-OG	5.45	1.49	1.42
1	G	30	SER	CB-OG	5.34	1.49	1.42
1	H	103	LYS	CD-CE	5.33	1.64	1.51
1	H	65	SER	CB-OG	5.20	1.49	1.42
1	E	60	SER	CB-OG	5.19	1.49	1.42
1	M	76	SER	CB-OG	5.06	1.48	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ALA	N-CA-C	-6.08	94.58	111.00
1	M	71	PHE	N-CA-C	5.91	126.96	111.00
1	E	18	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	H	52	SER	N-CA-C	5.74	126.49	111.00
1	N	46	LEU	CB-CG-CD2	-5.67	101.35	111.00
1	M	39	LYS	C-N-CD	5.64	140.25	128.40
1	G	78	LEU	CA-CB-CG	5.54	128.04	115.30
1	M	33	LEU	CA-CB-CG	-5.43	102.81	115.30
1	L	68	GLY	N-CA-C	5.41	126.62	113.10
1	A	54	LEU	CA-CB-CG	5.38	127.69	115.30
1	N	49	TYR	CA-CB-CG	5.09	123.08	113.40
1	E	18	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	N	54	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	GLN	Peptide
1	F	46	LEU	Peptide
1	K	48	ILE	Peptide
1	L	51	ALA	Peptide
1	M	49	TYR	Peptide
1	N	16	GLY	Peptide
1	N	40	PRO	Peptide
1	O	29	ILE	Peptide

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	801	0	775	98	0
1	B	801	0	775	52	0
1	C	801	0	775	69	0
1	D	801	0	775	62	0
1	E	801	0	775	46	0
1	F	801	0	775	75	0
1	G	801	0	775	81	1
1	H	727	0	704	75	0
1	I	801	0	775	97	0
1	J	801	0	775	77	0
1	K	801	0	775	65	0
1	L	801	0	775	79	0
1	M	801	0	775	102	0
1	N	801	0	775	73	1
1	O	801	0	775	80	1
2	A	74	0	0	11	0
2	B	77	0	0	5	0
2	C	53	0	0	6	0
2	D	67	0	0	12	0
2	E	64	0	0	10	0
2	F	74	0	0	11	0
2	G	57	0	0	7	0
2	H	68	0	0	12	0
2	I	68	0	0	13	0
2	J	93	0	0	20	1
2	K	75	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	64	0	0	18	0
2	M	81	0	0	14	0
2	N	68	0	0	4	0
2	O	65	0	0	18	0
All	All	12989	0	11554	1071	3

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 46.

All (1071) 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:E:4:MET:SD	1:E:4:MET:CE	2.02	1.47
1:C:49:TYR:CE2	1:C:55:GLN:OE1	1.75	1.38
1:L:24:ARG:HG3	1:L:69:THR:O	1.37	1.20
1:L:98:PHE:HA	2:L:2057:HOH:O	1.36	1.20
1:B:82:ASP:HB3	1:B:86:TYR:OH	1.40	1.18
1:N:103:LYS:H	1:N:103:LYS:HD2	1.07	1.15
1:A:15:VAL:HG13	1:A:79:GLN:HE22	1.13	1.14
1:I:59:PRO:HG2	1:I:61:ARG:HH21	1.06	1.12
1:C:24:ARG:HG2	1:C:69:THR:HG22	1.14	1.11
1:L:29:ILE:HD11	1:L:90:GLN:HB2	1.11	1.11
1:F:79:GLN:HB3	1:F:80:PRO:HD2	1.13	1.10
1:H:7:SER:HB2	1:H:8:PRO:HD2	1.11	1.10
1:L:29:ILE:HD11	1:L:90:GLN:CB	1.81	1.09
1:I:79:GLN:OE1	1:N:81:GLU:HG3	1.51	1.09
1:A:54:LEU:HB3	1:A:58:VAL:HG11	1.34	1.09
1:N:29:ILE:HD11	1:N:33:LEU:HB2	1.14	1.08
1:G:18:ARG:HG3	1:G:18:ARG:HH11	1.16	1.08
1:D:85:THR:HG22	2:D:2056:HOH:O	1.55	1.07
1:H:8:PRO:HB3	1:I:11:LEU:HD11	1.09	1.05
1:N:29:ILE:HG12	1:N:29:ILE:O	1.55	1.05
2:L:2009:HOH:O	1:M:8:PRO:HB2	1.54	1.04
1:J:93:SER:HA	2:J:2082:HOH:O	1.57	1.04
1:M:40:PRO:HG3	1:M:83:PHE:HE2	1.16	1.03
1:M:22:THR:HG22	1:M:71:PHE:O	1.60	1.02
1:C:24:ARG:CG	1:C:69:THR:HG22	1.90	1.01
1:G:64:GLY:HA3	2:G:2043:HOH:O	1.60	1.00
1:F:47:LEU:HD23	1:F:58:VAL:HG21	1.42	0.99
1:M:82:ASP:O	1:M:86:TYR:OH	1.82	0.98
1:K:46:LEU:HD21	1:K:49:TYR:HE2	1.28	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:CD2	1:C:55:GLN:OE1	2.16	0.97
1:N:29:ILE:CD1	1:N:33:LEU:HB2	1.95	0.96
1:J:24:ARG:HE	1:J:70:ASP:HB2	1.26	0.96
1:A:33:LEU:HD11	1:A:88:CYS:HB2	1.44	0.95
1:N:33:LEU:HG	1:N:34:ASN:H	1.29	0.95
1:O:8:PRO:HG2	1:O:11:LEU:HD13	1.49	0.95
1:G:11:LEU:HD13	1:G:104:VAL:HG22	1.45	0.94
1:N:46:LEU:HD21	1:N:49:TYR:CZ	2.02	0.94
1:N:83:PHE:HE1	1:N:106:ILE:H	1.12	0.94
1:G:49:TYR:HD1	1:G:49:TYR:H	1.12	0.94
1:M:40:PRO:HG3	1:M:83:PHE:CE2	2.02	0.94
1:O:49:TYR:HD1	1:O:49:TYR:N	1.65	0.94
1:N:64:GLY:HA2	1:N:72:THR:O	1.67	0.94
1:I:30:SER:CB	1:J:49:TYR:HE1	1.80	0.93
1:N:62:PHE:HB2	2:N:2050:HOH:O	1.69	0.93
1:I:59:PRO:CG	1:I:61:ARG:HH21	1.82	0.92
1:L:32:TYR:HD1	2:L:2024:HOH:O	1.49	0.92
1:O:12:SER:HA	1:O:105:GLU:HB2	1.48	0.92
1:C:24:ARG:HG2	1:C:69:THR:CG2	2.01	0.91
1:B:55:GLN:NE2	1:B:55:GLN:HA	1.84	0.91
1:M:79:GLN:HB2	1:M:80:PRO:HD2	1.53	0.90
1:F:94:THR:HA	1:F:96:ASN:H	1.33	0.90
1:B:55:GLN:HE21	1:B:55:GLN:HA	1.34	0.90
1:L:59:PRO:HB2	1:L:61:ARG:HE	1.36	0.90
1:N:103:LYS:H	1:N:103:LYS:CD	1.85	0.90
1:H:7:SER:HB2	1:H:8:PRO:CD	2.01	0.90
1:L:39:LYS:HB2	1:L:42:LYS:HB2	1.52	0.90
1:G:11:LEU:HD22	1:G:19:VAL:HG13	1.53	0.90
1:I:49:TYR:CE2	1:I:55:GLN:OE1	2.23	0.90
1:H:7:SER:CB	1:H:8:PRO:HD2	1.96	0.90
1:E:83:PHE:HA	2:E:2054:HOH:O	1.72	0.90
1:L:89:GLN:HA	2:L:2057:HOH:O	1.72	0.89
1:M:86:TYR:CD1	1:M:86:TYR:N	2.39	0.89
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.37	0.89
1:H:8:PRO:CB	1:I:11:LEU:HD11	2.00	0.89
1:O:49:TYR:CD1	1:O:49:TYR:N	2.39	0.89
1:I:30:SER:OG	1:J:49:TYR:HE1	1.54	0.89
1:N:79:GLN:HB3	1:N:81:GLU:OE1	1.72	0.89
1:F:85:THR:HA	1:F:102:THR:O	1.73	0.88
1:H:8:PRO:HB3	1:I:11:LEU:CD1	2.02	0.88
1:I:31:SER:HA	2:I:2024:HOH:O	1.74	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HB	2:A:2021:HOH:O	1.74	0.87
1:C:49:TYR:HE2	1:C:55:GLN:OE1	1.30	0.87
1:K:30:SER:CB	1:L:49:TYR:HE1	1.88	0.87
1:M:24:ARG:HH11	1:M:24:ARG:HG2	1.39	0.87
1:I:59:PRO:HG2	1:I:61:ARG:NH2	1.90	0.87
1:A:56:SER:HA	2:A:2043:HOH:O	1.75	0.87
1:D:67:SER:OG	2:D:2051:HOH:O	1.92	0.86
1:K:59:PRO:HD2	2:K:2053:HOH:O	1.74	0.86
1:I:30:SER:HG	1:J:49:TYR:HE1	1.13	0.86
1:A:15:VAL:HG13	1:A:79:GLN:NE2	1.89	0.86
1:F:79:GLN:CB	1:F:80:PRO:HD2	2.02	0.86
1:N:33:LEU:HG	1:N:34:ASN:N	1.91	0.85
1:J:27:GLN:HG2	1:J:28:SER:H	1.41	0.85
1:N:103:LYS:HD2	1:N:103:LYS:N	1.92	0.84
1:B:34:ASN:HB2	2:B:2066:HOH:O	1.76	0.84
1:J:69:THR:HA	2:J:2031:HOH:O	1.78	0.83
1:F:79:GLN:HB3	1:F:80:PRO:CD	2.04	0.83
1:C:49:TYR:CE1	1:C:53:SER:OG	2.30	0.83
1:N:59:PRO:HD2	1:N:62:PHE:HE1	1.41	0.83
1:O:9:SER:O	1:O:102:THR:HA	1.78	0.83
1:K:46:LEU:HD21	1:K:49:TYR:CE2	2.13	0.83
1:B:82:ASP:CB	1:B:86:TYR:OH	2.26	0.83
1:C:90:GLN:NE2	1:C:92:TYR:HB3	1.94	0.82
1:I:89:GLN:HG2	1:I:90:GLN:H	1.45	0.82
1:N:78:LEU:CD2	1:N:106:ILE:HG13	2.09	0.82
1:N:90:GLN:HE21	1:N:92:TYR:H	1.26	0.82
1:L:54:LEU:HD11	1:L:58:VAL:HG22	1.62	0.81
1:I:33:LEU:HD11	1:I:88:CYS:HB2	1.61	0.81
1:M:49:TYR:CD1	1:M:55:GLN:NE2	2.48	0.81
1:E:29:ILE:HG22	2:E:2025:HOH:O	1.80	0.81
1:A:83:PHE:HB2	1:A:106:ILE:HG12	1.63	0.81
1:D:83:PHE:HD2	1:D:84:ALA:N	1.78	0.81
1:F:54:LEU:HG	1:F:55:GLN:H	1.46	0.81
1:H:31:SER:O	1:H:50:ALA:HA	1.81	0.81
1:O:94:THR:HA	1:O:95:PRO:C	2.02	0.80
1:L:8:PRO:HB2	2:L:2008:HOH:O	1.79	0.80
1:G:79:GLN:NE2	1:L:59:PRO:HG3	1.96	0.80
1:N:11:LEU:HG	1:O:11:LEU:HD12	1.63	0.79
1:M:89:GLN:HE21	1:M:98:PHE:HE1	1.24	0.79
1:N:83:PHE:CE1	1:N:105:GLU:HA	2.18	0.79
1:G:18:ARG:CG	1:G:18:ARG:HH11	1.94	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:HB3	1:B:86:TYR:HH	1.48	0.79
1:N:83:PHE:HE1	1:N:106:ILE:N	1.79	0.79
1:M:86:TYR:HD1	1:M:86:TYR:N	1.78	0.79
1:I:59:PRO:HB2	1:I:61:ARG:HE	1.48	0.78
1:B:89:GLN:HB3	2:B:2066:HOH:O	1.83	0.78
1:M:44:PRO:HA	2:M:2031:HOH:O	1.84	0.78
1:M:34:ASN:O	1:M:89:GLN:N	2.17	0.78
1:L:12:SER:O	1:M:9:SER:HB3	1.83	0.78
1:A:90:GLN:HE21	1:A:96:ASN:HA	1.49	0.78
1:K:55:GLN:HB3	2:K:2044:HOH:O	1.81	0.78
1:O:11:LEU:HD23	1:O:19:VAL:HG13	1.64	0.77
1:B:90:GLN:HE21	1:B:97:THR:N	1.82	0.77
1:I:30:SER:CB	1:J:49:TYR:CE1	2.67	0.77
1:A:82:ASP:O	1:A:86:TYR:OH	2.01	0.77
1:I:39:LYS:HG2	2:I:2032:HOH:O	1.84	0.77
1:G:11:LEU:HD22	1:G:19:VAL:CG1	2.15	0.77
1:J:21:ILE:O	1:J:72:THR:HG23	1.85	0.77
1:K:79:GLN:HB3	1:K:81:GLU:OE2	1.84	0.77
1:F:19:VAL:HG22	2:F:2009:HOH:O	1.85	0.77
1:I:30:SER:HB2	1:J:49:TYR:CE1	2.20	0.77
1:E:29:ILE:HG13	2:E:2027:HOH:O	1.85	0.77
1:A:8:PRO:HG2	1:A:11:LEU:HD11	1.66	0.77
1:O:8:PRO:HD3	2:O:2012:HOH:O	1.85	0.76
1:N:29:ILE:HD11	1:N:33:LEU:CB	2.07	0.76
1:O:37:GLN:HE21	1:O:86:TYR:HE2	1.27	0.76
1:C:98:PHE:HB3	2:C:2049:HOH:O	1.83	0.76
1:H:54:LEU:HD21	1:H:58:VAL:HG12	1.67	0.76
1:B:46:LEU:HD21	1:B:49:TYR:CE2	2.21	0.75
1:D:8:PRO:HG2	1:D:11:LEU:HD11	1.67	0.75
1:J:4:MET:CE	1:J:25:ALA:HB2	2.15	0.75
1:G:54:LEU:HD23	1:G:58:VAL:HG13	1.68	0.75
1:H:83:PHE:HD2	2:H:2052:HOH:O	1.69	0.75
1:H:33:LEU:HD21	1:H:35:TRP:NE1	2.02	0.74
1:I:86:TYR:O	1:I:101:GLY:HA2	1.87	0.74
1:C:51:ALA:HB2	1:C:71:PHE:HE2	1.51	0.74
1:G:16:GLY:HA2	1:G:78:LEU:N	2.02	0.74
1:B:54:LEU:HD22	1:B:58:VAL:HG13	1.68	0.74
1:D:12:SER:HB2	1:E:10:SER:OG	1.87	0.74
1:D:87:TYR:HD2	1:D:99:GLY:O	1.71	0.74
1:O:49:TYR:H	1:O:49:TYR:HD1	1.35	0.74
1:K:30:SER:HB2	1:L:49:TYR:HE1	1.50	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:LEU:HD11	1:G:8:PRO:HB3	1.70	0.74
1:O:54:LEU:HA	2:O:2031:HOH:O	1.87	0.74
1:I:30:SER:HB2	1:J:49:TYR:HE1	1.51	0.74
1:O:85:THR:HA	1:O:103:LYS:HA	1.68	0.74
1:C:49:TYR:CE1	1:D:30:SER:OG	2.40	0.74
1:A:88:CYS:O	1:A:99:GLY:N	2.20	0.73
1:G:47:LEU:HD13	1:G:62:PHE:HE2	1.54	0.73
1:H:15:VAL:HG23	2:H:2007:HOH:O	1.89	0.73
1:N:6:GLN:NE2	1:N:86:TYR:O	2.22	0.73
1:O:6:GLN:HB2	1:O:23:CYS:SG	2.28	0.73
1:A:72:THR:O	2:A:2058:HOH:O	2.07	0.73
1:O:5:THR:O	1:O:24:ARG:HB2	1.88	0.73
1:N:12:SER:HB2	1:O:10:SER:HB2	1.70	0.73
1:M:35:TRP:CZ3	1:M:88:CYS:HB3	2.24	0.73
1:F:2:ILE:HG12	1:F:27:GLN:HE21	1.54	0.73
1:L:81:GLU:OE1	1:L:82:ASP:OD1	2.06	0.72
1:H:9:SER:HB3	1:I:13:ALA:HA	1.71	0.72
1:G:33:LEU:HG	1:G:34:ASN:H	1.54	0.72
1:I:49:TYR:C	1:I:49:TYR:HD1	1.92	0.72
1:M:35:TRP:CE3	1:M:88:CYS:HB3	2.24	0.72
1:F:47:LEU:HD23	1:F:58:VAL:CG2	2.19	0.72
1:I:32:TYR:CE2	1:J:32:TYR:HE2	2.07	0.72
1:D:83:PHE:HE2	2:D:2055:HOH:O	1.72	0.72
1:H:47:LEU:HD23	2:H:2032:HOH:O	1.88	0.72
1:B:90:GLN:HE21	1:B:97:THR:H	1.36	0.72
1:B:49:TYR:CE1	1:B:55:GLN:NE2	2.57	0.72
1:G:36:TYR:O	1:G:86:TYR:HA	1.90	0.71
1:F:94:THR:HA	1:F:96:ASN:N	2.05	0.71
1:L:65:SER:OG	1:L:72:THR:HG23	1.90	0.71
1:C:31:SER:O	1:C:50:ALA:HA	1.89	0.71
1:L:29:ILE:O	2:L:2024:HOH:O	2.08	0.71
1:F:85:THR:HG23	1:F:102:THR:O	1.90	0.71
1:J:27:GLN:HG2	1:J:28:SER:N	2.06	0.71
1:G:54:LEU:CD2	1:G:58:VAL:HG13	2.20	0.71
1:O:51:ALA:O	1:O:64:GLY:HA3	1.91	0.71
1:A:74:THR:CG2	1:A:76:SER:HB3	2.21	0.71
1:F:2:ILE:CG1	1:F:27:GLN:HE21	2.04	0.71
1:K:30:SER:HB2	1:L:49:TYR:CE1	2.25	0.70
1:K:32:TYR:HB2	1:K:92:TYR:HB2	1.72	0.70
1:K:48:ILE:CG2	1:K:49:TYR:H	2.05	0.70
1:D:83:PHE:O	1:D:84:ALA:HB2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:THR:O	2:G:2015:HOH:O	2.09	0.70
1:N:27:GLN:HE21	1:N:28:SER:H	1.37	0.70
1:N:49:TYR:HD1	1:N:55:GLN:OE1	1.74	0.70
1:B:24:ARG:HH21	1:B:70:ASP:HB2	1.55	0.70
1:E:54:LEU:HD22	1:E:58:VAL:HG11	1.72	0.70
1:I:49:TYR:C	1:I:49:TYR:CD1	2.62	0.70
1:I:46:LEU:CD2	2:J:2015:HOH:O	2.40	0.70
1:H:55:GLN:HA	2:H:2039:HOH:O	1.92	0.69
1:A:61:ARG:HB2	1:A:77:SER:H	1.57	0.69
1:G:33:LEU:HG	1:G:34:ASN:N	2.07	0.69
1:J:49:TYR:CE2	1:J:55:GLN:OE1	2.45	0.69
1:F:49:TYR:C	1:F:49:TYR:CD1	2.64	0.69
1:C:25:ALA:O	1:C:69:THR:HG23	1.93	0.69
1:F:74:THR:HG23	2:F:2018:HOH:O	1.90	0.69
1:G:18:ARG:NH1	1:G:18:ARG:HG3	1.97	0.69
1:B:55:GLN:O	1:B:58:VAL:HG12	1.92	0.69
1:O:90:GLN:C	1:O:92:TYR:H	1.93	0.69
1:C:99:GLY:HA2	2:C:2050:HOH:O	1.91	0.69
1:E:64:GLY:HA2	1:E:72:THR:O	1.91	0.69
1:I:54:LEU:HB3	2:I:2048:HOH:O	1.92	0.69
1:B:36:TYR:HE1	2:B:2066:HOH:O	1.76	0.69
1:I:90:GLN:O	1:I:96:ASN:HA	1.92	0.69
1:D:55:GLN:HB2	1:D:58:VAL:HG11	1.75	0.68
1:M:24:ARG:NH1	1:M:24:ARG:HG2	2.05	0.68
1:M:21:ILE:HD12	1:M:73:LEU:HD23	1.74	0.68
1:D:38:GLN:NE2	1:D:44:PRO:HG3	2.08	0.68
1:J:25:ALA:HB3	2:J:2031:HOH:O	1.92	0.68
1:L:29:ILE:O	1:L:31:SER:N	2.27	0.68
1:M:89:GLN:NE2	1:M:98:PHE:CE1	2.53	0.68
1:G:93:SER:O	1:G:96:ASN:OD1	2.12	0.68
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.76	0.68
1:B:94:THR:HG22	1:B:96:ASN:HD21	1.59	0.68
1:A:35:TRP:HA	1:A:87:TYR:O	1.94	0.68
1:K:30:SER:OG	1:L:49:TYR:HE1	1.76	0.67
1:D:89:GLN:HG2	1:D:90:GLN:N	2.09	0.67
1:D:83:PHE:CD2	1:D:84:ALA:N	2.62	0.67
1:I:21:ILE:HD12	1:I:73:LEU:HD23	1.75	0.67
1:H:106:ILE:HG21	2:H:2051:HOH:O	1.94	0.67
1:A:90:GLN:OE1	1:A:92:TYR:HB3	1.94	0.67
1:G:54:LEU:HD11	1:G:60:SER:HA	1.77	0.67
1:G:66:GLY:HA3	1:G:71:PHE:HA	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ARG:HB2	1:D:76:SER:OG	1.95	0.67
1:O:8:PRO:HG2	1:O:11:LEU:CD1	2.23	0.67
1:M:24:ARG:HD2	1:M:70:ASP:HA	1.75	0.67
1:I:90:GLN:HG2	1:I:92:TYR:HB3	1.76	0.67
1:H:78:LEU:HD23	1:H:106:ILE:HD12	1.75	0.67
1:D:24:ARG:CD	1:D:70:ASP:OD1	2.42	0.66
1:M:16:GLY:HA2	1:M:78:LEU:H	1.59	0.66
1:F:82:ASP:HB3	1:F:86:TYR:OH	1.96	0.66
1:O:37:GLN:NE2	1:O:86:TYR:HE2	1.93	0.66
1:M:21:ILE:HB	1:M:73:LEU:HB3	1.77	0.66
1:H:62:PHE:CE2	1:H:75:ILE:HG12	2.30	0.66
1:I:3:GLN:HB2	1:I:26:SER:HB3	1.78	0.66
1:H:61:ARG:HG2	1:H:61:ARG:HH11	1.60	0.66
1:I:79:GLN:OE1	1:N:81:GLU:CG	2.36	0.66
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.07	0.66
1:G:90:GLN:HG3	1:G:92:TYR:N	2.10	0.66
1:J:8:PRO:HG2	1:K:11:LEU:HD11	1.78	0.66
1:F:24:ARG:HG2	1:F:69:THR:HG22	1.76	0.66
1:M:49:TYR:HB3	1:M:53:SER:HB3	1.77	0.66
1:L:9:SER:HB2	2:M:2006:HOH:O	1.94	0.66
1:M:89:GLN:HG3	1:M:98:PHE:CD1	2.31	0.66
1:C:90:GLN:O	1:C:96:ASN:HA	1.96	0.66
1:J:8:PRO:CG	1:K:11:LEU:HD11	2.26	0.66
1:K:32:TYR:HE2	1:L:32:TYR:HD2	1.43	0.66
1:G:11:LEU:CD2	1:G:19:VAL:HG13	2.23	0.66
1:E:90:GLN:HG2	1:E:92:TYR:H	1.61	0.66
1:O:22:THR:HG22	1:O:72:THR:HG23	1.78	0.66
1:J:69:THR:HB	2:J:2027:HOH:O	1.95	0.65
1:D:29:ILE:HG13	2:D:2029:HOH:O	1.94	0.65
1:O:79:GLN:O	1:O:82:ASP:HB2	1.96	0.65
1:C:51:ALA:HB2	1:C:71:PHE:CE2	2.32	0.65
1:N:27:GLN:HG3	1:N:28:SER:N	2.11	0.65
1:B:83:PHE:HB3	2:B:2063:HOH:O	1.96	0.65
1:A:61:ARG:H	1:A:61:ARG:CD	2.10	0.65
1:F:2:ILE:HG12	1:F:27:GLN:NE2	2.11	0.65
1:K:46:LEU:CD2	1:K:49:TYR:CE2	2.79	0.65
1:A:71:PHE:HZ	2:A:2052:HOH:O	1.79	0.65
1:K:61:ARG:HG2	1:K:62:PHE:H	1.61	0.65
1:E:33:LEU:HG	1:E:34:ASN:N	2.11	0.65
1:A:61:ARG:HG3	1:A:77:SER:O	1.95	0.64
1:J:36:TYR:HB3	2:J:2050:HOH:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:LEU:HD12	1:I:34:ASN:N	2.12	0.64
1:L:32:TYR:HB3	1:L:91:SER:HB2	1.79	0.64
1:D:31:SER:O	1:D:50:ALA:HA	1.98	0.64
1:D:83:PHE:CE2	2:D:2055:HOH:O	2.46	0.64
1:J:42:LYS:HB3	2:J:2046:HOH:O	1.96	0.64
1:J:47:LEU:HD11	1:J:86:TYR:HE2	1.63	0.64
1:C:34:ASN:HB3	1:C:46:LEU:HD11	1.78	0.64
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.79	0.64
1:A:89:GLN:HB2	1:A:98:PHE:CE2	2.33	0.64
1:F:106:ILE:HG12	2:F:2073:HOH:O	1.97	0.64
1:M:86:TYR:HD1	1:M:86:TYR:H	1.45	0.64
1:K:46:LEU:CD2	1:K:49:TYR:HE2	2.07	0.64
1:H:54:LEU:HD21	1:H:58:VAL:CG1	2.27	0.64
1:A:15:VAL:CG1	1:A:79:GLN:HE22	2.01	0.63
1:I:18:ARG:HG2	1:I:76:SER:HA	1.80	0.63
1:K:48:ILE:CG2	1:K:49:TYR:N	2.60	0.63
1:I:33:LEU:CD1	1:I:88:CYS:HB2	2.28	0.63
1:J:6:GLN:HE22	1:J:87:TYR:HA	1.63	0.63
1:I:89:GLN:HG2	1:I:90:GLN:N	2.12	0.63
1:A:30:SER:O	1:A:67:SER:HB2	1.98	0.63
1:I:46:LEU:HD21	2:J:2015:HOH:O	1.99	0.63
1:C:25:ALA:O	1:C:69:THR:CG2	2.47	0.63
1:A:90:GLN:NE2	1:A:96:ASN:HA	2.13	0.63
1:I:34:ASN:HD21	1:I:91:SER:H	1.47	0.63
1:J:92:TYR:HB2	2:J:2039:HOH:O	1.97	0.63
1:L:24:ARG:HD2	1:L:70:ASP:HB3	1.81	0.63
1:N:59:PRO:HD2	1:N:62:PHE:CE1	2.28	0.63
1:J:6:GLN:HG2	1:J:7:SER:H	1.63	0.63
1:D:55:GLN:HB2	1:D:58:VAL:CG1	2.29	0.63
1:C:95:PRO:HA	2:C:2047:HOH:O	1.98	0.63
1:G:47:LEU:O	1:G:55:GLN:HG2	1.99	0.63
1:B:49:TYR:CD1	1:B:55:GLN:OE1	2.51	0.63
1:L:30:SER:O	1:L:31:SER:HB2	1.99	0.63
1:I:51:ALA:CB	2:I:2029:HOH:O	2.45	0.63
1:K:79:GLN:HA	1:K:79:GLN:NE2	2.13	0.63
1:M:3:GLN:HG2	1:M:26:SER:HB3	1.81	0.63
1:O:39:LYS:HG2	1:O:84:ALA:HB2	1.81	0.62
2:K:2030:HOH:O	1:L:32:TYR:HA	1.98	0.62
1:A:49:TYR:HB2	2:A:2040:HOH:O	1.98	0.62
1:L:32:TYR:CB	1:L:91:SER:HB2	2.30	0.62
1:G:11:LEU:N	1:G:11:LEU:HD12	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:HB2	1:L:76:SER:HB2	1.80	0.62
1:I:49:TYR:CZ	1:I:55:GLN:OE1	2.52	0.62
1:O:55:GLN:HB2	1:O:58:VAL:CG1	2.29	0.62
1:D:87:TYR:CD2	1:D:99:GLY:O	2.53	0.62
1:G:27:GLN:O	1:G:29:ILE:HG23	2.00	0.62
1:H:75:ILE:HG21	1:H:78:LEU:HD12	1.80	0.62
1:N:24:ARG:HA	1:N:69:THR:O	1.98	0.62
1:G:86:TYR:OH	2:G:2050:HOH:O	2.14	0.62
1:O:31:SER:OG	2:O:2023:HOH:O	2.11	0.62
1:I:44:PRO:HD3	2:I:2035:HOH:O	1.99	0.62
1:N:81:GLU:H	1:N:81:GLU:CD	2.02	0.62
1:I:33:LEU:HD23	1:I:71:PHE:CD1	2.35	0.62
1:I:39:LYS:O	1:I:42:LYS:HB2	1.99	0.61
1:A:36:TYR:CD1	1:A:98:PHE:HE2	2.17	0.61
1:F:34:ASN:O	1:F:88:CYS:HA	2.00	0.61
1:M:49:TYR:CB	1:M:53:SER:HB3	2.30	0.61
1:J:6:GLN:OE1	1:J:35:TRP:HZ3	1.82	0.61
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.83	0.61
1:A:58:VAL:HG13	1:A:58:VAL:O	1.99	0.61
1:H:100:GLN:NE2	2:H:2061:HOH:O	2.22	0.61
1:E:71:PHE:HZ	2:E:2027:HOH:O	1.82	0.61
1:L:5:THR:HA	1:L:100:GLN:OE1	1.99	0.61
1:M:46:LEU:HG	1:M:49:TYR:CZ	2.35	0.61
1:O:94:THR:HA	1:O:96:ASN:N	2.16	0.61
1:K:38:GLN:HB3	1:K:44:PRO:HA	1.82	0.61
1:M:40:PRO:CG	1:M:83:PHE:CE2	2.81	0.61
1:I:49:TYR:HD1	1:I:49:TYR:O	1.81	0.61
1:O:82:ASP:O	1:O:84:ALA:N	2.33	0.61
1:L:33:LEU:HD12	1:L:89:GLN:O	1.99	0.61
1:F:20:THR:HB	1:G:20:THR:HB	1.83	0.61
1:A:79:GLN:NE2	1:A:79:GLN:HA	2.15	0.61
1:M:34:ASN:N	1:M:89:GLN:O	2.32	0.61
1:G:35:TRP:N	1:G:48:ILE:O	2.34	0.61
1:L:59:PRO:HG2	1:L:61:ARG:HH21	1.66	0.61
1:D:35:TRP:CZ3	1:D:88:CYS:HB3	2.36	0.61
1:F:43:ALA:HB1	1:F:44:PRO:CD	2.31	0.60
1:H:33:LEU:HD21	1:H:35:TRP:HE1	1.66	0.60
1:H:49:TYR:CE1	1:H:55:GLN:OE1	2.54	0.60
1:L:31:SER:O	1:L:33:LEU:N	2.31	0.60
1:B:94:THR:HG22	1:B:96:ASN:ND2	2.16	0.60
1:I:17:ASP:HB2	2:I:2013:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:61:ARG:NH2	1:N:79:GLN:HB2	2.16	0.60
1:O:31:SER:CB	2:O:2023:HOH:O	2.50	0.60
1:C:54:LEU:HB3	1:C:58:VAL:HG13	1.83	0.60
1:G:11:LEU:CD2	1:G:19:VAL:CG1	2.80	0.60
1:H:50:ALA:HB3	2:H:2037:HOH:O	2.01	0.60
1:G:83:PHE:O	1:G:84:ALA:HB2	2.02	0.60
1:L:68:GLY:HA2	1:L:71:PHE:CZ	2.37	0.60
1:L:2:ILE:HG23	1:L:27:GLN:HB3	1.83	0.60
1:K:30:SER:HG	1:L:49:TYR:HE1	1.43	0.60
1:K:59:PRO:CB	1:K:61:ARG:HE	2.14	0.60
1:M:32:TYR:O	1:M:90:GLN:HA	2.02	0.60
1:I:90:GLN:CG	1:I:92:TYR:HB3	2.31	0.59
1:E:29:ILE:HD13	1:E:90:GLN:HB2	1.84	0.59
1:L:86:TYR:HB3	2:L:2056:HOH:O	2.01	0.59
1:C:55:GLN:O	1:C:57:GLY:N	2.35	0.59
1:G:2:ILE:HD12	1:G:29:ILE:HG22	1.84	0.59
1:K:80:PRO:C	1:K:82:ASP:H	2.03	0.59
1:A:85:THR:HG23	1:A:103:LYS:HG2	1.84	0.59
1:I:90:GLN:C	1:I:92:TYR:H	2.04	0.59
1:C:33:LEU:HG	1:C:89:GLN:O	2.01	0.59
1:I:33:LEU:HD11	1:I:88:CYS:CB	2.32	0.59
1:C:49:TYR:CE1	1:D:30:SER:CB	2.86	0.59
1:A:54:LEU:HB3	1:A:58:VAL:CG1	2.22	0.59
1:G:78:LEU:HD12	1:G:82:ASP:HB2	1.85	0.59
1:M:58:VAL:HG23	1:M:62:PHE:CD1	2.37	0.59
1:H:6:GLN:OE1	1:H:88:CYS:SG	2.59	0.59
1:L:43:ALA:HB1	1:L:44:PRO:CD	2.33	0.59
1:I:67:SER:HA	1:I:71:PHE:CE2	2.38	0.58
1:A:24:ARG:HG3	1:A:70:ASP:OD1	2.03	0.58
1:B:78:LEU:HG	1:B:106:ILE:HD11	1.85	0.58
1:K:48:ILE:HG22	1:K:49:TYR:N	2.18	0.58
1:G:47:LEU:HD13	1:G:62:PHE:CE2	2.38	0.58
1:A:8:PRO:CG	1:A:11:LEU:HD11	2.32	0.58
1:M:24:ARG:HD2	1:M:70:ASP:CA	2.33	0.58
1:J:8:PRO:HG2	1:K:11:LEU:CD1	2.34	0.58
1:H:24:ARG:HD3	1:H:70:ASP:HA	1.83	0.58
1:O:80:PRO:HA	1:O:106:ILE:HG21	1.85	0.58
1:L:42:LYS:HE2	2:L:2035:HOH:O	2.04	0.58
1:H:85:THR:HG22	1:H:102:THR:H	1.67	0.58
1:A:61:ARG:HD3	1:A:61:ARG:H	1.67	0.58
1:O:31:SER:O	1:O:33:LEU:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HB2	2:A:2073:HOH:O	2.03	0.58
1:J:47:LEU:HD22	1:J:58:VAL:HG21	1.86	0.58
1:G:38:GLN:HG3	1:G:42:LYS:O	2.04	0.58
1:D:36:TYR:HD1	2:D:2057:HOH:O	1.86	0.58
1:N:46:LEU:HD12	2:N:2033:HOH:O	2.04	0.57
1:E:90:GLN:OE1	1:E:97:THR:OG1	2.17	0.57
1:A:8:PRO:HG2	1:A:11:LEU:CD1	2.32	0.57
1:K:44:PRO:HB2	2:K:2041:HOH:O	2.03	0.57
1:M:83:PHE:CD2	1:M:83:PHE:C	2.77	0.57
1:F:47:LEU:CD2	1:F:58:VAL:HG21	2.25	0.57
1:L:59:PRO:CB	1:L:61:ARG:HE	2.13	0.57
1:G:11:LEU:HD11	1:G:102:THR:CG2	2.34	0.57
1:G:86:TYR:O	1:G:101:GLY:HA2	2.04	0.57
1:H:33:LEU:HD13	1:H:71:PHE:CD1	2.39	0.57
1:N:49:TYR:CD1	1:N:55:GLN:OE1	2.55	0.57
1:J:90:GLN:O	1:J:96:ASN:HB3	2.05	0.57
1:G:16:GLY:HA2	1:G:78:LEU:H	1.67	0.57
1:M:31:SER:H	1:M:32:TYR:HD1	1.51	0.57
1:G:11:LEU:H	1:G:11:LEU:HD12	1.69	0.57
1:H:37:GLN:HE21	1:H:47:LEU:HD21	1.68	0.57
1:D:2:ILE:HB	1:D:90:GLN:NE2	2.20	0.57
1:J:90:GLN:HE21	1:J:93:SER:H	1.53	0.57
1:J:4:MET:HE3	1:J:25:ALA:HB2	1.85	0.57
1:F:49:TYR:C	1:F:49:TYR:HD1	2.08	0.57
1:G:59:PRO:O	1:G:62:PHE:HB2	2.05	0.57
1:D:38:GLN:HE21	1:D:44:PRO:HG3	1.70	0.57
1:N:24:ARG:HG2	1:N:69:THR:HG22	1.85	0.57
1:N:17:ASP:H	1:N:78:LEU:N	2.02	0.57
1:N:33:LEU:HD22	1:N:71:PHE:CD2	2.40	0.57
1:L:73:LEU:HD23	1:L:73:LEU:O	2.05	0.57
1:J:49:TYR:HE2	1:J:55:GLN:OE1	1.86	0.56
1:C:35:TRP:CH2	1:C:88:CYS:HB3	2.40	0.56
1:J:98:PHE:HD2	2:J:2076:HOH:O	1.87	0.56
1:C:21:ILE:HG12	1:C:102:THR:HG21	1.86	0.56
1:M:55:GLN:O	1:M:58:VAL:HG13	2.04	0.56
1:M:29:ILE:HG23	1:M:29:ILE:O	2.06	0.56
1:I:49:TYR:CD1	1:I:49:TYR:O	2.58	0.56
1:K:11:LEU:O	1:K:105:GLU:HB2	2.05	0.56
1:A:49:TYR:CE1	1:B:30:SER:HB2	2.40	0.56
1:A:85:THR:CG2	1:A:103:LYS:HG2	2.35	0.56
1:E:86:TYR:O	1:E:101:GLY:HA2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:HD22	1:E:58:VAL:CG1	2.35	0.56
1:C:82:ASP:O	1:C:86:TYR:OH	2.18	0.56
1:F:83:PHE:O	1:F:84:ALA:HB2	2.05	0.56
1:I:11:LEU:HD23	1:I:19:VAL:HG13	1.87	0.56
1:K:48:ILE:HG23	1:K:49:TYR:H	1.71	0.56
1:D:83:PHE:CD2	1:D:83:PHE:C	2.77	0.56
1:A:53:SER:HB2	2:A:2041:HOH:O	2.04	0.56
1:A:29:ILE:HD11	1:A:33:LEU:HB2	1.87	0.56
1:M:29:ILE:HD11	1:M:92:TYR:HB3	1.88	0.56
1:A:85:THR:OG1	1:A:103:LYS:HE2	2.05	0.56
1:L:43:ALA:HB1	1:L:44:PRO:HD2	1.88	0.56
1:G:5:THR:OG1	2:G:2005:HOH:O	2.18	0.56
1:B:49:TYR:O	1:B:50:ALA:C	2.44	0.56
1:I:90:GLN:HG2	1:I:92:TYR:CB	2.35	0.56
1:E:61:ARG:NH2	1:E:82:ASP:CG	2.59	0.56
1:D:43:ALA:HB1	1:D:44:PRO:CD	2.36	0.56
1:M:29:ILE:O	1:M:30:SER:C	2.44	0.56
1:E:46:LEU:HD21	1:E:49:TYR:CZ	2.41	0.56
1:H:49:TYR:O	1:H:52:SER:N	2.38	0.55
1:C:100:GLN:N	1:C:100:GLN:OE1	2.26	0.55
1:K:49:TYR:O	1:K:53:SER:HB3	2.06	0.55
1:J:4:MET:HE1	1:J:25:ALA:HB2	1.89	0.55
1:B:18:ARG:HD3	1:B:75:ILE:O	2.06	0.55
1:O:25:ALA:CB	1:O:29:ILE:HG12	2.36	0.55
1:B:27:GLN:O	1:B:29:ILE:N	2.39	0.55
1:L:89:GLN:HG3	1:L:98:PHE:CZ	2.42	0.55
1:O:11:LEU:HD22	2:O:2012:HOH:O	2.06	0.55
1:J:49:TYR:CE1	1:J:53:SER:HB3	2.42	0.55
1:F:49:TYR:CZ	1:F:55:GLN:OE1	2.60	0.55
1:O:37:GLN:NE2	1:O:86:TYR:CE2	2.61	0.55
1:D:2:ILE:HD12	1:D:90:GLN:NE2	2.21	0.55
1:M:32:TYR:N	1:M:32:TYR:CD1	2.74	0.55
1:M:29:ILE:CD1	1:M:92:TYR:HB3	2.37	0.55
1:K:90:GLN:O	1:K:96:ASN:HB3	2.06	0.55
1:O:73:LEU:HD23	2:O:2006:HOH:O	2.06	0.55
1:M:84:ALA:C	1:M:86:TYR:HE1	2.10	0.55
1:B:37:GLN:HG3	1:B:86:TYR:CE2	2.41	0.55
1:D:61:ARG:HG2	1:D:62:PHE:CD1	2.42	0.55
1:A:60:SER:HA	2:A:2046:HOH:O	2.07	0.55
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.42	0.55
1:M:79:GLN:O	1:M:82:ASP:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:GLN:NE2	1:F:102:THR:OG1	2.40	0.55
1:E:25:ALA:C	1:E:27:GLN:H	2.10	0.55
1:M:34:ASN:HB2	1:M:89:GLN:HB3	1.89	0.54
1:O:46:LEU:O	1:O:55:GLN:CG	2.56	0.54
1:N:46:LEU:HD21	1:N:49:TYR:CE1	2.42	0.54
1:I:48:ILE:HG21	1:I:51:ALA:O	2.08	0.54
1:H:38:GLN:C	1:H:84:ALA:HB1	2.28	0.54
1:C:59:PRO:O	1:C:61:ARG:N	2.39	0.54
1:G:6:GLN:HG3	1:G:23:CYS:HB2	1.88	0.54
1:M:65:SER:O	1:M:72:THR:HB	2.07	0.54
1:L:54:LEU:HD23	2:L:2040:HOH:O	2.07	0.54
1:F:59:PRO:HG2	1:F:62:PHE:HE1	1.72	0.54
1:K:29:ILE:O	1:K:31:SER:N	2.41	0.54
1:M:49:TYR:HD1	1:M:55:GLN:NE2	2.00	0.54
1:H:6:GLN:O	1:H:7:SER:O	2.25	0.54
1:L:102:THR:HG23	2:L:2008:HOH:O	2.07	0.54
1:N:30:SER:O	1:N:67:SER:HA	2.08	0.54
1:L:29:ILE:HD11	1:L:90:GLN:HB3	1.82	0.54
1:I:64:GLY:HA2	1:I:72:THR:O	2.08	0.54
1:K:11:LEU:HD23	1:K:104:VAL:HG22	1.90	0.54
1:F:33:LEU:HD22	1:F:71:PHE:CD2	2.43	0.54
1:L:24:ARG:CG	1:L:69:THR:O	2.32	0.53
1:K:55:GLN:O	1:K:58:VAL:HG12	2.08	0.53
1:L:68:GLY:HA2	1:L:71:PHE:HZ	1.72	0.53
1:M:79:GLN:HB2	1:M:80:PRO:CD	2.34	0.53
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.43	0.53
1:C:47:LEU:O	1:C:58:VAL:HG11	2.08	0.53
1:A:49:TYR:CE1	1:B:30:SER:CB	2.91	0.53
1:F:61:ARG:HH21	1:F:82:ASP:CG	2.11	0.53
1:A:35:TRP:CE3	1:A:73:LEU:HD22	2.43	0.53
1:A:79:GLN:HG3	1:F:80:PRO:HG3	1.90	0.53
1:K:61:ARG:O	1:K:62:PHE:C	2.47	0.53
1:E:33:LEU:HD22	1:E:71:PHE:CB	2.39	0.53
1:A:6:GLN:HB2	1:A:23:CYS:SG	2.49	0.53
1:M:44:PRO:CA	2:M:2031:HOH:O	2.48	0.53
1:M:84:ALA:C	1:M:86:TYR:CE1	2.82	0.53
1:A:79:GLN:O	1:A:82:ASP:HB2	2.09	0.53
1:H:34:ASN:O	1:H:88:CYS:HA	2.08	0.53
1:N:46:LEU:HD21	1:N:49:TYR:CE2	2.43	0.53
1:J:8:PRO:HB3	2:K:2014:HOH:O	2.09	0.53
1:E:4:MET:CG	1:E:4:MET:CE	2.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:44:PRO:C	2:J:2050:HOH:O	2.48	0.53
1:M:38:GLN:HE21	1:M:44:PRO:HD3	1.74	0.52
1:F:2:ILE:O	1:F:97:THR:HG21	2.09	0.52
1:J:6:GLN:OE1	1:J:35:TRP:CZ3	2.61	0.52
1:M:3:GLN:HB2	1:M:26:SER:HB3	1.91	0.52
1:F:2:ILE:CG1	1:F:27:GLN:NE2	2.69	0.52
1:J:34:ASN:HB3	1:J:46:LEU:HD11	1.92	0.52
1:A:47:LEU:C	1:A:48:ILE:HG12	2.29	0.52
1:B:17:ASP:OD2	1:C:7:SER:HB2	2.09	0.52
1:C:49:TYR:HE1	1:D:30:SER:OG	1.88	0.52
1:M:81:GLU:C	1:M:83:PHE:N	2.62	0.52
1:F:48:ILE:HD11	1:F:62:PHE:HB3	1.90	0.52
1:H:11:LEU:HD21	2:H:2012:HOH:O	2.08	0.52
1:I:49:TYR:CE2	1:I:55:GLN:CD	2.81	0.52
1:G:89:GLN:HA	2:G:2053:HOH:O	2.10	0.52
1:A:19:VAL:HG21	1:A:78:LEU:HD13	1.92	0.52
1:C:79:GLN:OE1	1:H:59:PRO:HB3	2.08	0.52
1:J:38:GLN:HE21	1:J:44:PRO:HD3	1.74	0.52
1:O:54:LEU:HD23	2:O:2031:HOH:O	2.08	0.52
1:C:49:TYR:HE1	1:C:53:SER:OG	1.88	0.52
1:I:58:VAL:O	1:I:59:PRO:O	2.27	0.52
1:O:10:SER:O	1:O:11:LEU:HD13	2.09	0.52
1:K:61:ARG:O	1:K:63:SER:N	2.43	0.52
1:L:88:CYS:O	2:L:2057:HOH:O	2.19	0.52
1:N:83:PHE:CE1	1:N:106:ILE:N	2.57	0.52
1:I:36:TYR:CZ	1:I:46:LEU:HD22	2.45	0.52
1:D:83:PHE:O	1:D:84:ALA:CB	2.57	0.52
1:A:2:ILE:HG12	1:A:27:GLN:HG3	1.91	0.52
1:N:34:ASN:HB3	1:N:49:TYR:HA	1.92	0.52
1:I:30:SER:OG	1:J:49:TYR:CE1	2.40	0.52
1:O:12:SER:CA	1:O:105:GLU:HB2	2.30	0.52
1:D:24:ARG:NE	1:D:70:ASP:OD1	2.43	0.52
1:N:12:SER:HB2	1:O:10:SER:CB	2.38	0.52
1:C:90:GLN:HE21	1:C:92:TYR:HB3	1.70	0.52
1:M:44:PRO:HB3	2:M:2031:HOH:O	2.09	0.52
1:I:6:GLN:NE2	1:I:86:TYR:O	2.38	0.52
1:H:9:SER:O	1:H:102:THR:HA	2.09	0.52
1:G:27:GLN:HG3	1:G:28:SER:N	2.25	0.52
1:J:87:TYR:HB3	2:J:2076:HOH:O	2.08	0.52
1:F:23:CYS:O	1:F:71:PHE:HB2	2.10	0.52
1:C:58:VAL:HG21	1:C:62:PHE:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:GLN:HG2	1:N:38:GLN:N	2.24	0.52
1:M:34:ASN:O	1:M:88:CYS:HA	2.09	0.51
1:A:34:ASN:N	1:A:34:ASN:ND2	2.57	0.51
1:E:81:GLU:OE1	1:J:80:PRO:HG2	2.10	0.51
1:D:106:ILE:HG22	2:D:2067:HOH:O	2.09	0.51
1:C:49:TYR:CE1	1:D:30:SER:HB2	2.46	0.51
1:M:84:ALA:HB3	1:M:86:TYR:CZ	2.44	0.51
1:G:47:LEU:HB2	1:G:48:ILE:HD12	1.92	0.51
1:G:82:ASP:HA	2:G:2050:HOH:O	2.09	0.51
1:A:80:PRO:HD2	1:A:81:GLU:OE2	2.10	0.51
1:M:22:THR:CG2	1:M:71:PHE:O	2.48	0.51
1:E:51:ALA:O	1:E:64:GLY:HA3	2.09	0.51
1:G:86:TYR:O	1:G:102:THR:N	2.43	0.51
1:A:33:LEU:HG	1:A:34:ASN:N	2.25	0.51
1:M:59:PRO:O	1:M:61:ARG:N	2.40	0.51
1:E:71:PHE:CZ	2:E:2027:HOH:O	2.54	0.51
1:O:46:LEU:O	1:O:55:GLN:HG2	2.11	0.51
1:A:25:ALA:HB3	1:A:69:THR:HA	1.92	0.51
1:L:29:ILE:CD1	1:L:90:GLN:CB	2.72	0.51
1:K:37:GLN:HE21	1:K:86:TYR:HE2	1.54	0.51
1:A:94:THR:HA	1:A:95:PRO:C	2.30	0.51
1:N:105:GLU:N	2:N:2068:HOH:O	2.32	0.51
1:A:29:ILE:HA	1:A:92:TYR:CE1	2.46	0.51
1:A:90:GLN:O	1:A:96:ASN:HB3	2.10	0.51
1:G:19:VAL:HG12	1:G:21:ILE:HG13	1.93	0.51
1:J:72:THR:CG2	2:J:2067:HOH:O	2.59	0.51
1:G:38:GLN:HB2	1:G:44:PRO:HA	1.92	0.51
1:E:24:ARG:HA	1:E:69:THR:O	2.10	0.51
1:C:25:ALA:H	1:C:69:THR:HG23	1.75	0.51
1:I:58:VAL:HG23	1:I:62:PHE:HD1	1.76	0.51
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.59	0.51
1:B:55:GLN:CA	1:B:55:GLN:NE2	2.61	0.51
1:C:8:PRO:CG	1:C:11:LEU:HD11	2.41	0.51
1:H:24:ARG:NH1	2:H:2014:HOH:O	2.44	0.50
1:H:11:LEU:HD13	1:H:19:VAL:CG1	2.40	0.50
1:O:93:SER:HB2	2:O:2061:HOH:O	2.10	0.50
1:C:49:TYR:HE2	1:C:55:GLN:CD	2.10	0.50
1:G:35:TRP:O	1:G:46:LEU:HD12	2.12	0.50
1:K:30:SER:CB	1:L:49:TYR:CE1	2.79	0.50
1:J:91:SER:N	2:J:2039:HOH:O	2.44	0.50
1:A:62:PHE:N	1:A:62:PHE:CD1	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:ALA:HB1	2:I:2029:HOH:O	2.07	0.50
1:J:72:THR:HG22	2:J:2067:HOH:O	2.11	0.50
1:D:2:ILE:HD12	1:D:90:GLN:HE21	1.77	0.50
1:B:35:TRP:CZ3	1:B:88:CYS:HB3	2.45	0.50
1:F:10:SER:O	1:G:11:LEU:HA	2.11	0.50
1:E:47:LEU:HD22	1:E:58:VAL:HG23	1.94	0.50
1:G:32:TYR:O	1:G:90:GLN:HA	2.11	0.50
1:G:3:GLN:O	1:G:26:SER:N	2.45	0.50
1:M:67:SER:HA	1:M:71:PHE:CZ	2.45	0.50
1:A:83:PHE:HD1	1:A:104:VAL:O	1.93	0.50
1:B:24:ARG:NH2	1:B:70:ASP:HB2	2.26	0.50
1:D:33:LEU:HD11	1:D:88:CYS:HB2	1.93	0.50
1:N:17:ASP:H	1:N:78:LEU:H	1.59	0.50
1:B:34:ASN:ND2	1:B:91:SER:HB2	2.26	0.50
1:E:33:LEU:HD22	1:E:71:PHE:CG	2.47	0.50
1:O:90:GLN:C	1:O:92:TYR:N	2.64	0.50
1:M:36:TYR:HB3	2:M:2031:HOH:O	2.12	0.50
1:F:86:TYR:CD1	1:F:86:TYR:N	2.79	0.50
1:N:12:SER:HA	2:N:2068:HOH:O	2.11	0.50
1:O:63:SER:N	2:O:2043:HOH:O	2.38	0.50
1:A:34:ASN:HD22	1:A:34:ASN:N	2.10	0.50
1:I:32:TYR:CE2	1:J:32:TYR:CE2	2.95	0.50
1:F:29:ILE:O	1:F:31:SER:N	2.45	0.50
1:O:73:LEU:HD12	2:O:2043:HOH:O	2.11	0.50
1:G:36:TYR:CE2	1:G:46:LEU:HB2	2.47	0.50
1:B:90:GLN:NE2	1:B:97:THR:OG1	2.45	0.50
1:I:25:ALA:O	1:I:69:THR:HG23	2.12	0.50
1:F:59:PRO:O	1:F:62:PHE:HD1	1.95	0.50
1:I:34:ASN:O	1:I:89:GLN:N	2.43	0.49
1:M:49:TYR:O	1:M:53:SER:N	2.42	0.49
1:G:94:THR:HA	1:G:95:PRO:C	2.31	0.49
1:D:73:LEU:HD12	2:D:2048:HOH:O	2.12	0.49
1:M:18:ARG:CD	2:M:2009:HOH:O	2.60	0.49
1:L:11:LEU:HD22	2:L:2008:HOH:O	2.10	0.49
1:A:36:TYR:CD1	1:A:98:PHE:CE2	2.99	0.49
1:J:7:SER:HA	1:J:8:PRO:O	2.12	0.49
1:M:79:GLN:CB	1:M:80:PRO:HD2	2.30	0.49
2:L:2015:HOH:O	1:M:8:PRO:HG3	2.13	0.49
1:J:55:GLN:O	1:J:58:VAL:HG12	2.12	0.49
1:D:24:ARG:NH1	1:D:24:ARG:CG	2.72	0.49
1:C:2:ILE:HG13	1:C:90:GLN:NE2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ALA:HB3	2:E:2021:HOH:O	2.12	0.49
1:F:15:VAL:HG13	1:F:79:GLN:HA	1.93	0.49
1:M:84:ALA:O	1:M:86:TYR:HE1	1.94	0.49
1:N:62:PHE:CE2	1:N:75:ILE:HG23	2.48	0.49
1:M:49:TYR:CD2	1:M:49:TYR:N	2.79	0.49
1:C:89:GLN:HA	1:C:97:THR:O	2.12	0.49
1:L:9:SER:O	1:L:10:SER:HB2	2.12	0.49
1:J:13:ALA:HB2	1:K:8:PRO:HB3	1.94	0.49
1:A:37:GLN:HG2	1:A:38:GLN:N	2.27	0.49
1:O:54:LEU:HD21	1:O:62:PHE:O	2.13	0.49
1:M:49:TYR:HD1	1:M:55:GLN:CD	2.16	0.49
1:O:4:MET:O	1:O:100:GLN:OE1	2.30	0.49
1:K:42:LYS:HG3	2:K:2038:HOH:O	2.12	0.49
1:G:18:ARG:HD3	2:G:2045:HOH:O	2.13	0.49
1:M:33:LEU:HD22	1:M:71:PHE:CD2	2.47	0.49
1:F:78:LEU:HD11	1:F:104:VAL:HG11	1.95	0.49
1:B:34:ASN:HB3	1:B:46:LEU:HD11	1.94	0.49
1:H:85:THR:CG2	1:H:102:THR:H	2.26	0.49
1:J:33:LEU:HD21	1:J:88:CYS:HB2	1.93	0.49
1:L:54:LEU:HG	1:L:58:VAL:HG13	1.93	0.48
1:G:31:SER:OG	1:G:51:ALA:HB2	2.12	0.48
1:M:89:GLN:NE2	1:M:98:PHE:HE1	2.02	0.48
1:M:62:PHE:CD2	1:M:75:ILE:HG12	2.49	0.48
1:D:54:LEU:HD21	1:D:58:VAL:HG22	1.94	0.48
1:A:78:LEU:HD11	1:A:104:VAL:HG11	1.95	0.48
1:O:34:ASN:HB2	1:O:89:GLN:HB3	1.95	0.48
1:J:6:GLN:O	1:J:7:SER:HB3	2.14	0.48
1:L:60:SER:OG	2:L:2045:HOH:O	2.20	0.48
1:O:75:ILE:HG22	1:O:77:SER:O	2.13	0.48
1:F:6:GLN:HB3	1:F:100:GLN:H	1.79	0.48
1:O:61:ARG:HD3	1:O:61:ARG:H	1.78	0.48
1:H:85:THR:OG1	1:H:103:LYS:HD3	2.14	0.48
1:H:61:ARG:NH1	1:H:61:ARG:HG2	2.27	0.48
1:L:35:TRP:HB2	1:L:48:ILE:HB	1.96	0.48
1:I:59:PRO:CG	1:I:61:ARG:NH2	2.63	0.48
1:N:61:ARG:HD2	1:N:77:SER:O	2.13	0.48
1:A:38:GLN:HB2	1:A:44:PRO:HA	1.95	0.48
1:J:59:PRO:HG2	1:J:62:PHE:CE1	2.49	0.48
1:M:59:PRO:C	1:M:61:ARG:H	2.17	0.48
1:J:24:ARG:HD3	1:J:69:THR:HG22	1.96	0.48
1:A:83:PHE:HB2	1:A:106:ILE:CG1	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:TYR:OH	1:I:46:LEU:HD22	2.14	0.48
1:O:48:ILE:HG13	2:O:2031:HOH:O	2.14	0.48
1:I:90:GLN:HE21	1:I:96:ASN:HA	1.79	0.48
1:F:49:TYR:O	1:F:49:TYR:HD1	1.96	0.48
1:A:59:PRO:HB2	1:A:61:ARG:HD3	1.96	0.48
1:M:18:ARG:HD3	2:M:2009:HOH:O	2.13	0.48
1:D:79:GLN:O	1:D:82:ASP:HB2	2.13	0.48
1:I:25:ALA:O	1:I:26:SER:C	2.52	0.47
1:A:49:TYR:O	1:A:50:ALA:C	2.52	0.47
1:N:33:LEU:HD11	1:N:88:CYS:HB2	1.96	0.47
1:G:34:ASN:HA	1:G:49:TYR:HA	1.95	0.47
1:A:78:LEU:HD21	1:A:106:ILE:HD13	1.96	0.47
1:A:19:VAL:HG23	1:A:75:ILE:HB	1.96	0.47
1:M:38:GLN:HG2	1:M:39:LYS:O	2.14	0.47
1:J:38:GLN:NE2	1:J:44:PRO:HD3	2.29	0.47
1:B:49:TYR:CD1	1:B:55:GLN:NE2	2.81	0.47
1:C:58:VAL:CG2	1:C:62:PHE:HB2	2.45	0.47
1:D:21:ILE:O	1:D:73:LEU:N	2.40	0.47
1:B:19:VAL:O	1:B:74:THR:HA	2.14	0.47
1:C:19:VAL:O	1:C:74:THR:HA	2.14	0.47
1:I:58:VAL:CG2	1:I:62:PHE:HD1	2.28	0.47
1:N:78:LEU:HD21	1:N:106:ILE:HG13	1.90	0.47
1:H:63:SER:O	1:H:73:LEU:HD12	2.14	0.47
1:K:11:LEU:HD21	1:K:19:VAL:HG13	1.95	0.47
1:E:82:ASP:OD1	1:E:82:ASP:N	2.48	0.47
1:G:88:CYS:O	1:G:99:GLY:N	2.48	0.47
1:H:22:THR:HG23	1:H:72:THR:HG23	1.95	0.47
1:M:44:PRO:CB	2:M:2031:HOH:O	2.63	0.47
1:H:7:SER:CB	1:H:8:PRO:CD	2.70	0.47
1:N:78:LEU:HD23	1:N:106:ILE:HG13	1.92	0.47
1:G:49:TYR:N	1:G:49:TYR:CD1	2.62	0.47
1:A:83:PHE:CB	1:A:106:ILE:HG12	2.41	0.47
1:M:24:ARG:HH11	1:M:24:ARG:CG	2.18	0.47
1:O:32:TYR:O	1:O:90:GLN:HA	2.15	0.47
1:O:37:GLN:HB3	1:O:47:LEU:HG	1.97	0.47
1:H:83:PHE:CG	1:H:83:PHE:O	2.68	0.47
1:F:84:ALA:HB3	2:F:2059:HOH:O	2.15	0.47
1:F:18:ARG:HH11	1:F:76:SER:HA	1.79	0.47
1:A:29:ILE:HA	1:A:92:TYR:CD1	2.50	0.47
1:D:71:PHE:HZ	2:D:2029:HOH:O	1.98	0.47
1:O:66:GLY:HA3	1:O:71:PHE:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:SER:O	1:H:8:PRO:C	2.53	0.46
1:E:59:PRO:HG2	1:E:62:PHE:CE1	2.50	0.46
1:O:18:ARG:HG3	1:O:76:SER:HA	1.97	0.46
1:H:47:LEU:HB2	1:H:48:ILE:HG12	1.97	0.46
1:D:31:SER:N	2:D:2029:HOH:O	2.47	0.46
1:M:30:SER:HB3	1:M:32:TYR:CE1	2.50	0.46
1:O:16:GLY:O	1:O:77:SER:HA	2.16	0.46
1:K:61:ARG:HD3	1:K:61:ARG:H	1.81	0.46
1:I:33:LEU:HD23	1:I:71:PHE:CG	2.50	0.46
1:O:31:SER:HB3	2:O:2023:HOH:O	2.14	0.46
1:F:31:SER:HB2	2:F:2050:HOH:O	2.14	0.46
1:C:34:ASN:ND2	1:C:89:GLN:OE1	2.48	0.46
1:A:49:TYR:CE1	1:B:30:SER:OG	2.66	0.46
1:K:94:THR:HA	1:K:95:PRO:C	2.35	0.46
1:M:6:GLN:NE2	1:M:102:THR:H	2.14	0.46
1:A:32:TYR:HE2	1:B:32:TYR:HE2	1.64	0.46
1:G:11:LEU:HD11	1:G:102:THR:HG21	1.98	0.46
1:F:73:LEU:HD12	1:F:74:THR:H	1.81	0.46
1:H:4:MET:O	1:H:100:GLN:NE2	2.49	0.46
1:M:2:ILE:HB	1:M:90:GLN:HE21	1.81	0.46
1:A:57:GLY:O	1:A:58:VAL:C	2.54	0.46
1:B:34:ASN:OD1	1:B:50:ALA:N	2.37	0.46
1:G:1:ASP:C	1:G:2:ILE:HG12	2.36	0.46
1:M:72:THR:HG22	1:M:74:THR:OG1	2.16	0.46
1:K:27:GLN:O	1:K:29:ILE:HG23	2.16	0.46
1:I:94:THR:HG21	2:I:2065:HOH:O	2.14	0.46
1:O:21:ILE:HA	2:O:2012:HOH:O	2.16	0.46
1:G:11:LEU:HD11	1:G:102:THR:HG22	1.98	0.46
1:H:49:TYR:CZ	1:H:55:GLN:OE1	2.69	0.46
1:B:62:PHE:CE2	1:B:75:ILE:HG12	2.51	0.46
1:O:18:ARG:HA	1:O:75:ILE:O	2.16	0.46
1:H:41:GLY:N	2:H:2025:HOH:O	2.40	0.46
1:I:50:ALA:HB1	2:I:2026:HOH:O	2.15	0.46
1:I:30:SER:OG	1:I:31:SER:N	2.49	0.45
1:F:102:THR:HB	2:F:2061:HOH:O	2.15	0.45
1:H:5:THR:HA	1:H:100:GLN:HE22	1.81	0.45
1:A:25:ALA:H	1:A:69:THR:HG23	1.81	0.45
1:K:85:THR:HA	1:K:102:THR:O	2.16	0.45
1:J:27:GLN:CG	1:J:28:SER:H	2.20	0.45
1:J:32:TYR:O	2:J:2039:HOH:O	2.21	0.45
1:A:89:GLN:HB2	1:A:98:PHE:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:PRO:HG3	1:G:83:PHE:CE2	2.51	0.45
1:F:61:ARG:NH2	1:F:82:ASP:OD1	2.50	0.45
1:B:55:GLN:O	1:B:56:SER:C	2.54	0.45
1:M:36:TYR:C	2:M:2031:HOH:O	2.54	0.45
1:C:80:PRO:HB3	2:C:2043:HOH:O	2.16	0.45
1:K:39:LYS:O	1:K:40:PRO:C	2.55	0.45
1:C:49:TYR:CE1	1:C:53:SER:CB	2.98	0.45
1:M:81:GLU:HG2	1:M:82:ASP:N	2.31	0.45
1:C:4:MET:CE	1:C:90:GLN:HB3	2.46	0.45
1:O:5:THR:HA	2:O:2063:HOH:O	2.17	0.45
1:F:30:SER:OG	1:F:31:SER:N	2.48	0.45
1:J:18:ARG:HG2	1:J:19:VAL:N	2.32	0.45
1:A:47:LEU:HD13	1:A:62:PHE:HD2	1.81	0.45
1:D:36:TYR:CE2	1:D:46:LEU:HD22	2.52	0.45
1:N:50:ALA:O	1:N:51:ALA:HB3	2.16	0.45
1:J:48:ILE:CD1	1:J:63:SER:HA	2.46	0.45
1:N:77:SER:O	1:N:78:LEU:C	2.54	0.45
1:G:34:ASN:HA	1:G:48:ILE:O	2.17	0.45
1:E:83:PHE:CE1	1:E:105:GLU:HG3	2.51	0.45
1:M:3:GLN:CG	1:M:26:SER:HB3	2.47	0.45
1:K:38:GLN:NE2	1:K:44:PRO:HD3	2.31	0.45
1:A:6:GLN:CB	1:A:23:CYS:SG	3.05	0.45
1:A:25:ALA:N	1:A:69:THR:HG23	2.31	0.45
2:J:2018:HOH:O	1:K:8:PRO:HA	2.15	0.45
1:L:29:ILE:CD1	1:L:90:GLN:HB2	2.07	0.45
1:M:7:SER:HA	1:M:8:PRO:HA	1.54	0.45
1:G:48:ILE:HA	1:G:53:SER:O	2.16	0.45
1:M:76:SER:HA	2:M:2065:HOH:O	2.16	0.45
1:D:3:GLN:HB2	1:D:26:SER:HB3	1.98	0.45
1:N:39:LYS:HG2	1:N:83:PHE:O	2.17	0.45
1:C:35:TRP:HA	1:C:87:TYR:O	2.17	0.45
1:I:40:PRO:HG2	2:I:2060:HOH:O	2.16	0.45
1:M:33:LEU:HD22	1:M:71:PHE:CG	2.52	0.45
1:E:34:ASN:HD21	1:E:91:SER:HB2	1.82	0.45
1:F:36:TYR:HA	1:F:45:LYS:O	2.17	0.45
1:L:103:LYS:HG2	2:L:2064:HOH:O	2.16	0.45
1:K:78:LEU:HG	1:K:106:ILE:HD11	1.99	0.45
1:B:100:GLN:N	1:B:100:GLN:OE1	2.49	0.45
1:M:21:ILE:N	2:M:2014:HOH:O	2.40	0.44
1:F:33:LEU:HG	1:F:34:ASN:N	2.32	0.44
1:H:24:ARG:HE	1:H:70:ASP:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD21	1:B:19:VAL:HG22	1.99	0.44
1:D:22:THR:HA	1:D:72:THR:HA	1.98	0.44
1:A:74:THR:HG22	1:A:76:SER:HB3	1.99	0.44
1:F:7:SER:HA	1:F:8:PRO:C	2.38	0.44
1:D:34:ASN:HD21	1:D:91:SER:HG	1.64	0.44
1:G:48:ILE:HG23	1:G:53:SER:N	2.31	0.44
1:F:54:LEU:HG	1:F:55:GLN:N	2.25	0.44
1:K:80:PRO:C	1:K:82:ASP:N	2.70	0.44
1:F:31:SER:HB2	1:F:51:ALA:HB2	1.99	0.44
1:A:78:LEU:CD2	1:A:106:ILE:HD13	2.47	0.44
1:D:61:ARG:HG2	1:D:62:PHE:CE1	2.52	0.44
1:H:7:SER:HB3	1:H:22:THR:CB	2.48	0.44
1:F:11:LEU:HD11	2:F:2009:HOH:O	2.16	0.44
1:F:95:PRO:O	1:F:96:ASN:C	2.56	0.44
1:O:89:GLN:HA	1:O:97:THR:O	2.17	0.44
1:O:75:ILE:HG21	1:O:78:LEU:HD12	1.98	0.44
1:M:37:GLN:NE2	2:M:2070:HOH:O	2.50	0.44
1:K:59:PRO:HB3	1:K:61:ARG:HE	1.83	0.44
1:M:58:VAL:HA	1:M:59:PRO:HD3	1.80	0.44
1:O:46:LEU:O	1:O:55:GLN:HG3	2.17	0.44
1:N:84:ALA:O	1:N:86:TYR:CD1	2.71	0.44
1:I:44:PRO:CD	2:I:2035:HOH:O	2.63	0.44
1:M:30:SER:HB3	1:M:32:TYR:HE1	1.83	0.44
1:N:27:GLN:CG	1:N:28:SER:N	2.80	0.44
1:O:29:ILE:O	1:O:31:SER:N	2.51	0.44
1:H:5:THR:O	1:H:24:ARG:N	2.40	0.44
1:G:8:PRO:HG2	1:G:11:LEU:HG	2.00	0.44
1:B:4:MET:CE	1:B:90:GLN:HB3	2.47	0.44
1:F:20:THR:HG21	1:G:20:THR:HG21	1.99	0.44
1:K:38:GLN:HB3	1:K:44:PRO:CA	2.47	0.44
1:A:25:ALA:C	1:A:27:GLN:N	2.69	0.44
1:D:6:GLN:H	1:D:100:GLN:HE21	1.64	0.44
1:H:7:SER:HB3	1:H:22:THR:HB	2.00	0.44
1:N:61:ARG:CZ	1:N:79:GLN:HB2	2.48	0.44
1:O:48:ILE:CG2	1:O:49:TYR:N	2.81	0.44
1:F:49:TYR:CD1	1:F:49:TYR:N	2.86	0.44
1:D:33:LEU:HD22	1:D:71:PHE:CD2	2.53	0.44
1:M:40:PRO:C	1:M:42:LYS:H	2.20	0.43
1:A:29:ILE:HG13	2:A:2052:HOH:O	2.18	0.43
1:I:49:TYR:C	1:I:51:ALA:N	2.71	0.43
1:O:47:LEU:HD22	1:O:58:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:LEU:HA	2:F:2030:HOH:O	2.17	0.43
1:J:15:VAL:HA	2:J:2070:HOH:O	2.16	0.43
1:I:61:ARG:HB2	1:I:76:SER:N	2.33	0.43
1:A:96:ASN:HB2	2:A:2068:HOH:O	2.17	0.43
1:E:106:ILE:CD1	2:E:2054:HOH:O	2.66	0.43
1:I:32:TYR:O	1:I:34:ASN:ND2	2.50	0.43
1:L:55:GLN:HB2	1:L:58:VAL:HG12	1.99	0.43
1:H:48:ILE:HG23	2:H:2033:HOH:O	2.18	0.43
1:J:6:GLN:HG2	1:J:7:SER:N	2.32	0.43
1:O:29:ILE:HD11	1:O:33:LEU:HD13	2.00	0.43
1:L:38:GLN:HE21	1:L:44:PRO:HD3	1.82	0.43
1:H:19:VAL:O	1:H:74:THR:HA	2.17	0.43
1:B:10:SER:OG	1:C:12:SER:HB2	2.17	0.43
1:N:15:VAL:HG12	1:N:80:PRO:HG3	2.00	0.43
1:C:18:ARG:HD2	1:C:76:SER:O	2.18	0.43
1:K:52:SER:HA	1:K:64:GLY:O	2.18	0.43
1:A:34:ASN:O	1:A:88:CYS:HA	2.17	0.43
1:D:54:LEU:HD11	1:D:58:VAL:O	2.18	0.43
1:J:30:SER:O	1:J:67:SER:HB2	2.18	0.43
1:K:92:TYR:CD2	1:K:92:TYR:O	2.72	0.43
1:N:55:GLN:HB2	1:N:58:VAL:CG1	2.48	0.43
1:L:47:LEU:HB3	1:L:58:VAL:HG21	2.01	0.43
1:M:3:GLN:CB	1:M:26:SER:HB3	2.48	0.43
1:N:85:THR:HA	1:N:102:THR:O	2.18	0.43
1:L:54:LEU:HD11	1:L:58:VAL:CG2	2.41	0.43
1:J:8:PRO:HG3	1:K:11:LEU:HD11	1.99	0.43
1:E:81:GLU:H	1:E:81:GLU:HG2	1.30	0.43
1:K:15:VAL:HA	1:K:78:LEU:O	2.18	0.43
1:O:95:PRO:O	1:O:97:THR:HG23	2.19	0.43
1:A:18:ARG:HA	1:A:76:SER:HA	2.01	0.43
1:D:55:GLN:HB3	1:D:56:SER:H	1.53	0.43
1:F:30:SER:OG	1:F:32:TYR:HD1	2.00	0.43
1:I:61:ARG:HD3	1:I:61:ARG:H	1.83	0.43
1:A:34:ASN:H	1:A:34:ASN:HD22	1.66	0.43
1:G:16:GLY:HA2	1:G:78:LEU:O	2.18	0.43
1:G:83:PHE:O	1:G:84:ALA:CB	2.67	0.43
1:J:43:ALA:O	1:J:45:LYS:N	2.51	0.43
1:C:87:TYR:HD2	1:C:99:GLY:O	2.01	0.43
1:C:8:PRO:HB2	1:C:11:LEU:CD1	2.48	0.43
1:J:12:SER:CB	1:K:10:SER:HG	2.32	0.43
1:M:82:ASP:O	1:M:83:PHE:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:O	1:C:33:LEU:N	2.52	0.43
1:K:30:SER:OG	1:L:49:TYR:CE1	2.58	0.42
1:O:6:GLN:OE1	1:O:99:GLY:HA3	2.19	0.42
1:C:58:VAL:HG23	1:C:62:PHE:CD1	2.54	0.42
1:J:48:ILE:HD11	1:J:63:SER:HA	2.01	0.42
1:N:18:ARG:HG2	1:N:74:THR:HG23	2.00	0.42
1:M:10:SER:O	1:M:11:LEU:HB2	2.19	0.42
1:C:48:ILE:HA	1:C:53:SER:O	2.19	0.42
1:J:24:ARG:HG2	1:J:69:THR:O	2.18	0.42
1:E:29:ILE:CG2	2:E:2025:HOH:O	2.52	0.42
1:M:18:ARG:HG3	2:M:2013:HOH:O	2.19	0.42
1:C:89:GLN:HG3	1:C:98:PHE:CE1	2.54	0.42
1:J:37:GLN:OE1	1:J:39:LYS:HE3	2.19	0.42
1:H:47:LEU:O	1:H:55:GLN:HB2	2.19	0.42
1:I:21:ILE:HB	1:I:73:LEU:HB3	2.00	0.42
1:O:3:GLN:HB2	2:O:2019:HOH:O	2.19	0.42
1:D:45:LYS:HB2	1:D:45:LYS:HE2	1.76	0.42
1:I:18:ARG:C	1:I:18:ARG:HD2	2.40	0.42
1:C:25:ALA:N	1:C:69:THR:HG23	2.35	0.42
1:M:82:ASP:O	1:M:84:ALA:N	2.52	0.42
1:G:11:LEU:CD1	1:G:104:VAL:HG22	2.33	0.42
1:L:41:GLY:C	1:L:42:LYS:O	2.58	0.42
1:M:49:TYR:CD1	1:M:55:GLN:CD	2.92	0.42
1:H:49:TYR:HD2	1:H:49:TYR:HA	1.68	0.42
1:G:2:ILE:HG13	1:G:93:SER:HB3	2.02	0.42
1:H:78:LEU:HG	1:H:79:GLN:H	1.84	0.42
1:N:37:GLN:O	1:N:45:LYS:HB2	2.20	0.42
1:I:54:LEU:HD21	1:I:62:PHE:HB2	2.02	0.42
1:L:39:LYS:O	1:L:41:GLY:N	2.51	0.42
1:E:83:PHE:CA	2:E:2054:HOH:O	2.47	0.42
1:K:59:PRO:HB2	1:K:61:ARG:HE	1.81	0.42
1:O:90:GLN:NE2	1:O:97:THR:OG1	2.49	0.42
1:C:51:ALA:CB	1:C:71:PHE:HE2	2.27	0.42
1:N:19:VAL:O	1:N:74:THR:HA	2.19	0.42
1:I:34:ASN:HB3	1:I:46:LEU:HD11	2.00	0.42
1:K:58:VAL:HB	2:K:2044:HOH:O	2.18	0.42
1:H:35:TRP:HB2	1:H:48:ILE:CG1	2.50	0.42
1:H:54:LEU:HD13	1:H:55:GLN:O	2.19	0.42
1:O:24:ARG:HB3	1:O:24:ARG:HE	1.55	0.42
1:N:26:SER:O	1:N:27:GLN:HB2	2.20	0.42
1:H:59:PRO:O	1:H:62:PHE:HD1	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:64:GLY:HA2	1:M:72:THR:O	2.20	0.42
1:I:85:THR:C	2:I:2061:HOH:O	2.57	0.42
1:B:77:SER:HA	2:B:2017:HOH:O	2.20	0.42
1:F:86:TYR:N	1:F:86:TYR:HD1	2.17	0.42
1:F:19:VAL:HG21	1:F:78:LEU:HD13	2.02	0.42
1:J:58:VAL:HA	1:J:59:PRO:HD2	1.76	0.42
1:J:59:PRO:HG2	1:J:62:PHE:HE1	1.83	0.42
1:A:83:PHE:O	1:A:84:ALA:HB2	2.20	0.42
1:O:89:GLN:HG3	1:O:98:PHE:CE1	2.54	0.42
1:H:62:PHE:HE2	1:H:75:ILE:HG12	1.78	0.42
1:J:8:PRO:HG2	1:J:11:LEU:HD13	2.01	0.42
1:H:38:GLN:O	1:H:84:ALA:HB1	2.20	0.42
1:F:18:ARG:HB2	1:F:18:ARG:CZ	2.50	0.42
1:A:55:GLN:CD	2:A:2042:HOH:O	2.57	0.42
1:I:23:CYS:HB3	1:I:35:TRP:CH2	2.54	0.42
1:I:61:ARG:H	1:I:61:ARG:CD	2.32	0.42
1:N:77:SER:O	1:N:79:GLN:NE2	2.53	0.42
1:A:83:PHE:CB	1:A:106:ILE:CG1	2.97	0.42
1:O:34:ASN:O	1:O:88:CYS:HA	2.19	0.42
1:I:37:GLN:HG3	1:I:86:TYR:CE2	2.54	0.42
1:L:22:THR:HG22	1:L:72:THR:HB	2.01	0.42
1:G:2:ILE:HG21	1:G:29:ILE:HG21	2.01	0.42
1:G:90:GLN:HB2	1:G:92:TYR:H	1.85	0.42
1:L:9:SER:O	1:L:10:SER:CB	2.68	0.42
1:E:86:TYR:O	1:E:101:GLY:CA	2.68	0.42
1:E:6:GLN:HB3	1:E:100:GLN:OE1	2.20	0.42
1:K:32:TYR:CE2	1:L:32:TYR:HD2	2.30	0.42
1:C:92:TYR:C	1:C:92:TYR:CD2	2.93	0.42
1:E:33:LEU:HD22	1:E:71:PHE:HB3	2.01	0.42
1:F:46:LEU:HD12	1:F:49:TYR:HB3	2.02	0.42
1:B:95:PRO:O	1:B:97:THR:HG23	2.19	0.42
1:E:79:GLN:N	1:E:82:ASP:OD2	2.52	0.42
1:E:61:ARG:NH2	1:E:82:ASP:OD2	2.53	0.42
1:I:94:THR:HG23	2:I:2063:HOH:O	2.20	0.42
1:A:12:SER:CB	1:A:105:GLU:HB3	2.50	0.42
1:F:2:ILE:HD13	1:F:90:GLN:OE1	2.20	0.41
1:F:80:PRO:O	1:F:82:ASP:N	2.53	0.41
1:G:50:ALA:HB1	1:H:31:SER:HB2	2.02	0.41
1:A:61:ARG:NH1	2:F:2058:HOH:O	2.53	0.41
1:C:8:PRO:HG3	1:C:11:LEU:HD11	2.01	0.41
1:O:73:LEU:CD2	2:O:2006:HOH:O	2.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:37:GLN:CB	1:O:47:LEU:HG	2.50	0.41
1:E:58:VAL:HG13	1:E:59:PRO:O	2.20	0.41
1:M:6:GLN:CD	1:M:101:GLY:H	2.23	0.41
1:B:4:MET:HE1	1:B:90:GLN:HB3	2.03	0.41
1:C:32:TYR:HD1	2:C:2018:HOH:O	2.03	0.41
1:L:14:SER:HB2	2:L:2013:HOH:O	2.18	0.41
1:L:15:VAL:HG23	2:L:2013:HOH:O	2.20	0.41
1:M:33:LEU:HG	1:M:34:ASN:N	2.35	0.41
1:H:56:SER:C	1:H:58:VAL:H	2.24	0.41
1:F:84:ALA:CB	2:F:2059:HOH:O	2.68	0.41
1:O:44:PRO:HB2	2:O:2028:HOH:O	2.21	0.41
1:J:61:ARG:HB2	1:J:76:SER:OG	2.20	0.41
1:A:58:VAL:CG1	1:A:58:VAL:O	2.68	0.41
1:M:9:SER:O	1:M:102:THR:HA	2.21	0.41
1:G:7:SER:HA	1:G:8:PRO:C	2.41	0.41
1:D:12:SER:CB	1:E:10:SER:OG	2.64	0.41
1:O:85:THR:HG23	1:O:103:LYS:HG2	2.02	0.41
1:D:73:LEU:CD1	2:D:2048:HOH:O	2.67	0.41
1:C:45:LYS:HE3	2:C:2024:HOH:O	2.20	0.41
1:L:23:CYS:HB3	1:L:35:TRP:CH2	2.55	0.41
1:L:49:TYR:CZ	1:L:53:SER:OG	2.74	0.41
1:F:29:ILE:O	1:F:30:SER:C	2.58	0.41
1:O:66:GLY:C	1:O:71:PHE:CD2	2.94	0.41
1:M:50:ALA:HA	2:M:2029:HOH:O	2.20	0.41
1:L:30:SER:O	1:L:31:SER:CB	2.67	0.41
1:L:90:GLN:HG2	1:L:97:THR:OG1	2.21	0.41
1:J:93:SER:HB3	2:J:2001:HOH:O	2.21	0.41
1:B:32:TYR:CD1	1:B:92:TYR:HD1	2.39	0.41
1:F:36:TYR:CE2	1:F:46:LEU:HD22	2.55	0.41
1:C:35:TRP:O	1:C:46:LEU:HD12	2.20	0.41
1:B:94:THR:HA	1:B:96:ASN:N	2.35	0.41
1:G:39:LYS:O	1:G:40:PRO:C	2.59	0.41
1:E:81:GLU:CD	1:J:80:PRO:HG2	2.41	0.41
1:N:50:ALA:O	1:N:51:ALA:CB	2.69	0.41
1:D:93:SER:OG	2:D:2059:HOH:O	2.22	0.41
1:I:11:LEU:HA	1:I:11:LEU:HD12	1.73	0.41
1:N:31:SER:O	1:N:33:LEU:N	2.54	0.41
1:N:33:LEU:CG	1:N:34:ASN:H	2.16	0.41
1:G:54:LEU:HD23	1:G:55:GLN:H	1.86	0.41
1:B:46:LEU:CD2	1:B:49:TYR:CE2	3.00	0.41
1:F:85:THR:CG2	1:F:102:THR:O	2.65	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:MET:HE1	1:C:90:GLN:HB3	2.03	0.41
1:H:37:GLN:HB2	1:H:86:TYR:CE2	2.56	0.41
1:C:30:SER:O	1:C:71:PHE:HZ	2.04	0.41
1:C:79:GLN:C	1:C:81:GLU:H	2.24	0.41
1:I:25:ALA:O	1:I:27:GLN:N	2.54	0.41
1:I:24:ARG:HA	1:I:69:THR:O	2.21	0.41
1:J:36:TYR:CZ	1:J:46:LEU:HD13	2.56	0.41
1:H:100:GLN:HG2	1:H:101:GLY:H	1.86	0.41
1:L:100:GLN:HG2	2:L:2061:HOH:O	2.21	0.41
1:L:21:ILE:HD12	1:L:73:LEU:HD22	2.02	0.41
1:K:32:TYR:HD1	1:K:92:TYR:CD1	2.39	0.41
1:L:33:LEU:HD11	1:L:88:CYS:HB2	2.02	0.41
1:A:29:ILE:O	1:A:32:TYR:HB2	2.21	0.41
1:D:19:VAL:HG21	1:D:78:LEU:HD13	2.03	0.41
1:H:8:PRO:HD3	1:I:19:VAL:HA	2.03	0.40
1:O:21:ILE:HB	2:O:2006:HOH:O	2.21	0.40
1:G:85:THR:HA	1:G:102:THR:O	2.20	0.40
1:E:29:ILE:C	2:E:2027:HOH:O	2.59	0.40
1:I:38:GLN:HB2	1:I:44:PRO:HB3	2.03	0.40
1:F:33:LEU:HD11	1:F:88:CYS:HB2	2.03	0.40
1:F:67:SER:HB3	2:F:2050:HOH:O	2.20	0.40
1:A:105:GLU:OE1	1:A:105:GLU:HA	2.21	0.40
1:K:89:GLN:HG3	1:K:98:PHE:CZ	2.56	0.40
1:N:42:LYS:HB3	1:N:43:ALA:H	1.77	0.40
1:L:32:TYR:HB2	1:L:91:SER:HB2	2.03	0.40
1:H:8:PRO:HG3	1:I:11:LEU:HD21	2.03	0.40
1:N:36:TYR:CE2	1:N:46:LEU:HD13	2.56	0.40
1:K:49:TYR:HB2	1:K:53:SER:O	2.22	0.40
1:M:54:LEU:HD11	1:M:62:PHE:O	2.20	0.40
1:H:49:TYR:CE1	1:H:55:GLN:CD	2.94	0.40
1:C:79:GLN:HE21	1:C:80:PRO:CD	2.33	0.40
1:D:29:ILE:O	1:D:32:TYR:HB2	2.21	0.40
1:L:15:VAL:HG22	1:L:80:PRO:HD3	2.02	0.40
1:I:79:GLN:HB2	1:I:80:PRO:CD	2.50	0.40
1:M:6:GLN:NE2	1:M:86:TYR:O	2.53	0.40
1:K:48:ILE:HG22	1:K:49:TYR:H	1.78	0.40
1:A:90:GLN:NE2	1:A:93:SER:O	2.54	0.40
1:F:11:LEU:HD22	1:F:11:LEU:HA	1.94	0.40
1:K:61:ARG:NH1	1:K:77:SER:O	2.55	0.40
1:J:28:SER:HA	1:J:68:GLY:O	2.21	0.40
1:J:91:SER:HB2	2:J:2078:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:HB3	1:E:58:VAL:HG11	2.04	0.40
1:N:19:VAL:O	1:N:74:THR:HG23	2.20	0.40
1:N:21:ILE:CG2	1:N:22:THR:N	2.84	0.40
1:E:103:LYS:HB2	1:E:103:LYS:HE3	1.68	0.40
1:N:29:ILE:HD13	1:N:71:PHE:CZ	2.56	0.40
1:B:58:VAL:HG23	1:B:59:PRO:HD2	2.03	0.40
1:C:34:ASN:O	1:C:88:CYS:HA	2.21	0.40
1:H:35:TRP:CD2	1:H:73:LEU:HB2	2.57	0.40
1:O:4:MET:HB3	1:O:99:GLY:HA2	2.02	0.40
1:A:30:SER:HB3	1:B:53:SER:CB	2.51	0.40
1:C:38:GLN:O	1:C:84:ALA:HB1	2.20	0.40
1:D:7:SER:OG	1:E:18:ARG:O	2.34	0.40
1:I:67:SER:HA	1:I:71:PHE:HE2	1.86	0.40
1:I:91:SER:HA	1:I:96:ASN:HD22	1.86	0.40
1:H:53:SER:HB2	2:H:2037:HOH:O	2.21	0.40
1:H:85:THR:HA	1:H:102:THR:O	2.21	0.40
1:A:28:SER:HA	1:A:68:GLY:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2015:HOH:O	2:J:2085:HOH:O[4_765]	2.14	0.06
1:G:94:THR:OG1	1:N:92:TYR:O[11_656]	2.17	0.03
1:O:30:SER:OG	1:O:53:SER:OG[9_765]	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	104/107 (97%)	82 (79%)	17 (16%)	5 (5%)	3 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	104/107 (97%)	78 (75%)	16 (15%)	10 (10%)	1	1
1	C	104/107 (97%)	82 (79%)	15 (14%)	7 (7%)	1	2
1	D	104/107 (97%)	84 (81%)	16 (15%)	4 (4%)	4	9
1	E	104/107 (97%)	88 (85%)	14 (14%)	2 (2%)	10	25
1	F	104/107 (97%)	82 (79%)	10 (10%)	12 (12%)	0	0
1	G	104/107 (97%)	80 (77%)	15 (14%)	9 (9%)	1	1
1	H	93/107 (87%)	71 (76%)	17 (18%)	5 (5%)	2	4
1	I	104/107 (97%)	82 (79%)	13 (12%)	9 (9%)	1	1
1	J	104/107 (97%)	83 (80%)	16 (15%)	5 (5%)	3	5
1	K	104/107 (97%)	79 (76%)	15 (14%)	10 (10%)	1	1
1	L	104/107 (97%)	78 (75%)	19 (18%)	7 (7%)	1	2
1	M	104/107 (97%)	76 (73%)	23 (22%)	5 (5%)	3	5
1	N	104/107 (97%)	74 (71%)	17 (16%)	13 (12%)	0	0
1	O	104/107 (97%)	82 (79%)	16 (15%)	6 (6%)	2	3
All	All	1549/1605 (96%)	1201 (78%)	239 (15%)	109 (7%)	1	2

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	SER
1	B	77	SER
1	C	56	SER
1	C	60	SER
1	D	31	SER
1	F	80	PRO
1	F	81	GLU
1	G	15	VAL
1	H	7	SER
1	I	15	VAL
1	I	59	PRO
1	I	83	PHE
1	J	30	SER
1	K	62	PHE
1	L	30	SER
1	L	31	SER
1	L	42	LYS
1	M	30	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	32	TYR
1	N	51	ALA
1	O	30	SER
1	O	32	TYR
1	O	59	PRO
1	O	83	PHE
1	B	83	PHE
1	C	32	TYR
1	C	51	ALA
1	D	81	GLU
1	E	26	SER
1	F	96	ASN
1	G	61	ARG
1	G	84	ALA
1	H	8	PRO
1	H	27	GLN
1	I	96	ASN
1	I	101	GLY
1	J	67	SER
1	K	51	ALA
1	K	52	SER
1	K	54	LEU
1	K	81	GLU
1	L	28	SER
1	M	50	ALA
1	N	18	ARG
1	N	28	SER
1	N	47	LEU
1	N	54	LEU
1	O	31	SER
1	O	47	LEU
1	A	26	SER
1	C	78	LEU
1	D	55	GLN
1	D	84	ALA
1	F	30	SER
1	F	40	PRO
1	F	50	ALA
1	G	10	SER
1	G	62	PHE
1	G	83	PHE
1	J	41	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	30	SER
1	L	32	TYR
1	L	51	ALA
1	N	30	SER
1	N	42	LYS
1	N	83	PHE
1	A	30	SER
1	A	50	ALA
1	B	30	SER
1	B	59	PRO
1	B	95	PRO
1	B	99	GLY
1	C	84	ALA
1	F	28	SER
1	F	52	SER
1	F	84	ALA
1	F	95	PRO
1	H	104	VAL
1	K	53	SER
1	M	8	PRO
1	M	60	SER
1	N	50	ALA
1	A	84	ALA
1	G	56	SER
1	H	51	ALA
1	I	26	SER
1	I	40	PRO
1	I	76	SER
1	K	59	PRO
1	K	103	LYS
1	L	10	SER
1	N	29	ILE
1	N	65	SER
1	B	13	ALA
1	E	101	GLY
1	F	43	ALA
1	F	47	LEU
1	G	14	SER
1	K	31	SER
1	M	11	LEU
1	A	15	VAL
1	G	16	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	75	ILE
1	J	44	PRO
1	J	40	PRO
1	N	44	PRO
1	B	15	VAL
1	B	29	ILE
1	C	7	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/93 (99%)	73 (79%)	19 (21%)	1	4
1	B	92/93 (99%)	76 (83%)	16 (17%)	2	6
1	C	92/93 (99%)	77 (84%)	15 (16%)	3	7
1	D	92/93 (99%)	81 (88%)	11 (12%)	6	14
1	E	92/93 (99%)	76 (83%)	16 (17%)	2	6
1	F	92/93 (99%)	71 (77%)	21 (23%)	1	3
1	G	92/93 (99%)	74 (80%)	18 (20%)	1	4
1	H	82/93 (88%)	60 (73%)	22 (27%)	0	2
1	I	92/93 (99%)	72 (78%)	20 (22%)	1	3
1	J	92/93 (99%)	82 (89%)	10 (11%)	8	18
1	K	92/93 (99%)	79 (86%)	13 (14%)	4	10
1	L	92/93 (99%)	77 (84%)	15 (16%)	3	7
1	M	92/93 (99%)	75 (82%)	17 (18%)	2	5
1	N	92/93 (99%)	74 (80%)	18 (20%)	1	4
1	O	92/93 (99%)	70 (76%)	22 (24%)	1	2
All	All	1370/1395 (98%)	1117 (82%)	253 (18%)	2	5

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	19	VAL
1	A	22	THR
1	A	24	ARG
1	A	32	TYR
1	A	34	ASN
1	A	38	GLN
1	A	48	ILE
1	A	49	TYR
1	A	54	LEU
1	A	55	GLN
1	A	56	SER
1	A	61	ARG
1	A	62	PHE
1	A	81	GLU
1	A	83	PHE
1	A	90	GLN
1	A	100	GLN
1	A	106	ILE
1	B	3	GLN
1	B	4	MET
1	B	5	THR
1	B	15	VAL
1	B	18	ARG
1	B	20	THR
1	B	23	CYS
1	B	27	GLN
1	B	53	SER
1	B	54	LEU
1	B	55	GLN
1	B	72	THR
1	B	79	GLN
1	B	82	ASP
1	B	85	THR
1	B	106	ILE
1	C	7	SER
1	C	11	LEU
1	C	12	SER
1	C	20	THR
1	C	34	ASN
1	C	37	GLN
1	C	61	ARG
1	C	67	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	70	ASP
1	C	74	THR
1	C	83	PHE
1	C	90	GLN
1	C	96	ASN
1	C	97	THR
1	C	103	LYS
1	D	4	MET
1	D	24	ARG
1	D	33	LEU
1	D	34	ASN
1	D	46	LEU
1	D	58	VAL
1	D	70	ASP
1	D	77	SER
1	D	83	PHE
1	D	90	GLN
1	D	100	GLN
1	E	10	SER
1	E	11	LEU
1	E	12	SER
1	E	18	ARG
1	E	32	TYR
1	E	39	LYS
1	E	48	ILE
1	E	49	TYR
1	E	58	VAL
1	E	79	GLN
1	E	82	ASP
1	E	89	GLN
1	E	90	GLN
1	E	100	GLN
1	E	103	LYS
1	E	105	GLU
1	F	5	THR
1	F	11	LEU
1	F	17	ASP
1	F	18	ARG
1	F	22	THR
1	F	23	CYS
1	F	26	SER
1	F	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	39	LYS
1	F	42	LYS
1	F	46	LEU
1	F	49	TYR
1	F	56	SER
1	F	58	VAL
1	F	61	ARG
1	F	81	GLU
1	F	83	PHE
1	F	86	TYR
1	F	90	GLN
1	F	93	SER
1	F	100	GLN
1	G	5	THR
1	G	11	LEU
1	G	18	ARG
1	G	20	THR
1	G	22	THR
1	G	31	SER
1	G	38	GLN
1	G	47	LEU
1	G	49	TYR
1	G	54	LEU
1	G	56	SER
1	G	61	ARG
1	G	62	PHE
1	G	69	THR
1	G	82	ASP
1	G	94	THR
1	G	100	GLN
1	G	105	GLU
1	H	2	ILE
1	H	15	VAL
1	H	18	ARG
1	H	21	ILE
1	H	22	THR
1	H	24	ARG
1	H	26	SER
1	H	27	GLN
1	H	33	LEU
1	H	37	GLN
1	H	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	46	LEU
1	H	47	LEU
1	H	49	TYR
1	H	55	GLN
1	H	61	ARG
1	H	72	THR
1	H	78	LEU
1	H	81	GLU
1	H	83	PHE
1	H	98	PHE
1	H	100	GLN
1	I	1	ASP
1	I	2	ILE
1	I	3	GLN
1	I	10	SER
1	I	15	VAL
1	I	17	ASP
1	I	18	ARG
1	I	33	LEU
1	I	34	ASN
1	I	39	LYS
1	I	46	LEU
1	I	49	TYR
1	I	53	SER
1	I	58	VAL
1	I	61	ARG
1	I	69	THR
1	I	79	GLN
1	I	90	GLN
1	I	96	ASN
1	I	100	GLN
1	J	5	THR
1	J	18	ARG
1	J	19	VAL
1	J	22	THR
1	J	81	GLU
1	J	89	GLN
1	J	90	GLN
1	J	94	THR
1	J	105	GLU
1	J	106	ILE
1	K	2	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	18	ARG
1	K	49	TYR
1	K	58	VAL
1	K	61	ARG
1	K	74	THR
1	K	81	GLU
1	K	89	GLN
1	K	90	GLN
1	K	94	THR
1	K	100	GLN
1	K	105	GLU
1	K	106	ILE
1	L	11	LEU
1	L	18	ARG
1	L	22	THR
1	L	34	ASN
1	L	53	SER
1	L	55	GLN
1	L	61	ARG
1	L	72	THR
1	L	73	LEU
1	L	74	THR
1	L	81	GLU
1	L	83	PHE
1	L	89	GLN
1	L	94	THR
1	L	100	GLN
1	M	4	MET
1	M	17	ASP
1	M	21	ILE
1	M	24	ARG
1	M	28	SER
1	M	32	TYR
1	M	48	ILE
1	M	58	VAL
1	M	69	THR
1	M	79	GLN
1	M	81	GLU
1	M	86	TYR
1	M	90	GLN
1	M	91	SER
1	M	92	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	97	THR
1	M	100	GLN
1	N	1	ASP
1	N	10	SER
1	N	11	LEU
1	N	15	VAL
1	N	18	ARG
1	N	29	ILE
1	N	37	GLN
1	N	49	TYR
1	N	62	PHE
1	N	63	SER
1	N	65	SER
1	N	67	SER
1	N	79	GLN
1	N	81	GLU
1	N	85	THR
1	N	90	GLN
1	N	103	LYS
1	N	106	ILE
1	O	1	ASP
1	O	3	GLN
1	O	4	MET
1	O	6	GLN
1	O	11	LEU
1	O	23	CYS
1	O	24	ARG
1	O	46	LEU
1	O	47	LEU
1	O	49	TYR
1	O	58	VAL
1	O	61	ARG
1	O	67	SER
1	O	69	THR
1	O	79	GLN
1	O	83	PHE
1	O	88	CYS
1	O	89	GLN
1	O	90	GLN
1	O	100	GLN
1	O	104	VAL
1	O	105	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	79	GLN
1	B	3	GLN
1	B	55	GLN
1	B	79	GLN
1	B	90	GLN
1	B	96	ASN
1	C	55	GLN
1	C	79	GLN
1	D	34	ASN
1	D	38	GLN
1	D	55	GLN
1	D	79	GLN
1	D	89	GLN
1	D	90	GLN
1	D	100	GLN
1	E	38	GLN
1	E	79	GLN
1	F	6	GLN
1	F	27	GLN
1	F	100	GLN
1	G	38	GLN
1	G	79	GLN
1	G	96	ASN
1	H	37	GLN
1	H	38	GLN
1	I	34	ASN
1	J	6	GLN
1	J	38	GLN
1	J	55	GLN
1	J	79	GLN
1	K	38	GLN
1	K	79	GLN
1	K	90	GLN
1	L	34	ASN
1	L	38	GLN
1	L	79	GLN
1	M	34	ASN
1	M	38	GLN
1	M	55	GLN
1	M	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	96	ASN
1	M	100	GLN
1	N	27	GLN
1	N	37	GLN
1	N	79	GLN
1	N	90	GLN
1	O	27	GLN
1	O	37	GLN
1	O	79	GLN
1	O	89	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	106/107 (99%)	0.58	5 (4%) 35 34	24, 42, 50, 53	0
1	B	106/107 (99%)	0.41	5 (4%) 35 34	17, 34, 45, 47	0
1	C	106/107 (99%)	0.38	4 (3%) 44 44	20, 37, 50, 53	0
1	D	106/107 (99%)	0.23	2 (1%) 70 70	16, 30, 43, 48	0
1	E	106/107 (99%)	0.17	2 (1%) 70 70	14, 28, 35, 44	0
1	F	106/107 (99%)	0.45	5 (4%) 35 34	28, 40, 47, 50	0
1	G	106/107 (99%)	0.76	13 (12%) 5 4	27, 45, 56, 63	0
1	H	97/107 (90%)	0.94	12 (12%) 5 4	35, 48, 60, 63	0
1	I	106/107 (99%)	0.63	8 (7%) 17 15	30, 43, 55, 64	0
1	J	106/107 (99%)	0.50	4 (3%) 44 44	16, 38, 49, 57	0
1	K	106/107 (99%)	0.56	6 (5%) 27 26	21, 37, 49, 55	0
1	L	106/107 (99%)	0.56	4 (3%) 44 44	20, 41, 47, 52	0
1	M	106/107 (99%)	0.91	11 (10%) 8 6	30, 46, 62, 66	0
1	N	106/107 (99%)	1.10	20 (18%) 2 1	40, 56, 67, 69	0
1	O	106/107 (99%)	1.10	15 (14%) 4 3	32, 53, 63, 67	0
All	All	1581/1605 (98%)	0.62	116 (7%) 18 16	14, 41, 59, 69	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	68	GLY	5.7
1	O	106	ILE	4.9
1	M	57	GLY	4.6
1	O	76	SER	4.5
1	K	49	TYR	4.5
1	I	57	GLY	4.2
1	H	70	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	40	PRO	4.1
1	H	68	GLY	4.1
1	H	49	TYR	4.1
1	O	67	SER	3.9
1	G	60	SER	3.7
1	N	68	GLY	3.6
1	M	1	ASP	3.6
1	G	49	TYR	3.5
1	K	28	SER	3.3
1	M	51	ALA	3.2
1	N	49	TYR	3.2
1	N	2	ILE	3.2
1	O	12	SER	3.2
1	H	52	SER	3.1
1	N	40	PRO	3.1
1	N	3	GLN	3.1
1	G	67	SER	3.1
1	C	70	ASP	3.1
1	C	49	TYR	3.1
1	J	99	GLY	3.0
1	M	49	TYR	3.0
1	I	14	SER	3.0
1	O	60	SER	2.9
1	B	1	ASP	2.9
1	F	56	SER	2.9
1	O	56	SER	2.9
1	O	46	LEU	2.8
1	C	56	SER	2.8
1	H	28	SER	2.8
1	M	58	VAL	2.8
1	F	1	ASP	2.8
1	M	52	SER	2.8
1	N	104	VAL	2.8
1	E	49	TYR	2.7
1	L	56	SER	2.7
1	N	60	SER	2.7
1	I	80	PRO	2.7
1	G	78	LEU	2.7
1	F	40	PRO	2.7
1	O	91	SER	2.7
1	O	77	SER	2.7
1	N	106	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	TYR	2.6
1	J	49	TYR	2.6
1	O	69	THR	2.6
1	L	106	ILE	2.6
1	H	67	SER	2.5
1	I	27	GLN	2.5
1	N	21	ILE	2.5
1	M	60	SER	2.5
1	F	49	TYR	2.5
1	H	76	SER	2.5
1	G	3	GLN	2.5
1	G	30	SER	2.4
1	A	68	GLY	2.4
1	N	1	ASP	2.4
1	N	83	PHE	2.4
1	N	105	GLU	2.4
1	K	29	ILE	2.4
1	G	50	ALA	2.4
1	H	40	PRO	2.4
1	M	3	GLN	2.4
1	D	57	GLY	2.4
1	N	67	SER	2.4
1	B	49	TYR	2.4
1	J	106	ILE	2.3
1	K	1	ASP	2.3
1	G	52	SER	2.3
1	J	53	SER	2.3
1	G	83	PHE	2.3
1	H	25	ALA	2.3
1	I	49	TYR	2.3
1	O	78	LEU	2.3
1	K	77	SER	2.3
1	N	16	GLY	2.3
1	I	1	ASP	2.2
1	N	26	SER	2.2
1	N	52	SER	2.2
1	O	97	THR	2.2
1	O	1	ASP	2.2
1	B	40	PRO	2.2
1	I	106	ILE	2.2
1	G	1	ASP	2.2
1	M	54	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	102	THR	2.2
1	G	15	VAL	2.2
1	N	20	THR	2.2
1	G	29	ILE	2.2
1	N	97	THR	2.2
1	E	57	GLY	2.1
1	I	40	PRO	2.1
1	B	60	SER	2.1
1	F	67	SER	2.1
1	M	56	SER	2.1
1	H	88	CYS	2.1
1	N	12	SER	2.1
1	M	27	GLN	2.1
1	N	86	TYR	2.1
1	L	41	GLY	2.1
1	O	26	SER	2.1
1	B	67	SER	2.1
1	H	66	GLY	2.1
1	D	76	SER	2.1
1	G	91	SER	2.1
1	A	56	SER	2.0
1	C	78	LEU	2.0
1	A	1	ASP	2.0
1	L	60	SER	2.0
1	H	8	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.