



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:30 AM GMT

PDB ID : 3ETB
Title : Crystal structure of the engineered neutralizing antibody M18 complexed with anthrax protective antigen domain 4
Authors : Monzingo, A.F.; Leysath, C.E.; Barnett, J.; Iverson, B.L.; Georgiou, G.; Robertus, J.D.
Deposited on : 2008-10-07
Resolution : 3.80 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
<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

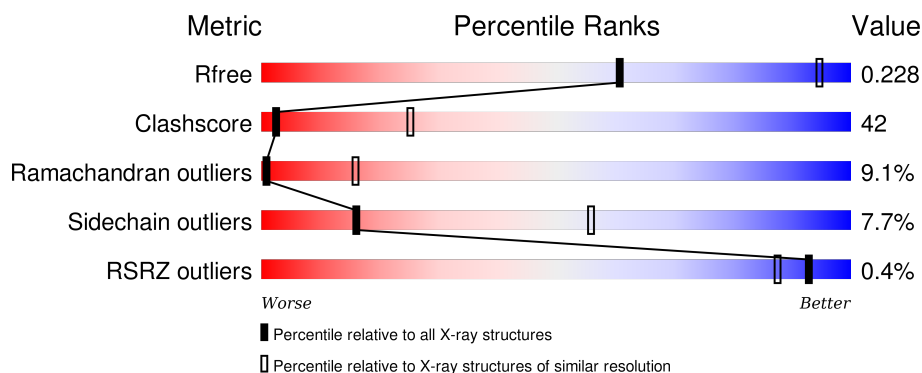
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	F	252	<div> <div>35%</div> <div>44%</div> <div>11%</div> <div>10%</div> </div>
1	G	252	<div> <div>36%</div> <div>45%</div> <div>10%</div> <div>9%</div> </div>
1	H	252	<div> <div>33%</div> <div>47%</div> <div>12%</div> <div>9%</div> </div>
1	I	252	<div> <div>35%</div> <div>46%</div> <div>9%</div> <div>10%</div> </div>
2	J	144	<div> <div>38%</div> <div>51%</div> <div>10%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	144	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>42%</div><div>47%</div><div>10%</div><div>•</div></div></div>
2	L	144	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>41%</div><div>50%</div><div>8%</div><div>••</div></div></div>
2	M	144	<div><div><div></div><div></div><div></div></div><div><div></div><div>44%</div><div>48%</div><div>7%</div><div>•</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11546 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 Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGS)₄ linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	228	Total	C	N	O	S	0	0	1
			1742	1091	296	347	8			
1	G	229	Total	C	N	O	S	0	0	1
			1743	1091	296	348	8			
1	H	229	Total	C	N	O	S	0	0	1
			1743	1091	296	348	8			
1	I	228	Total	C	N	O	S	0	0	1
			1742	1091	296	347	8			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	MET	-	EXPRESSION TAG	PDB 3ETB
F	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
F	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
F	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
F	0	LYS	-	EXPRESSION TAG	PDB 3ETB
F	21	VAL	ILE	ENGINEERED	PDB 3ETB
F	46	PHE	LEU	ENGINEERED	PDB 3ETB
F	56	PRO	SER	ENGINEERED	PDB 3ETB
F	76	ASN	SER	ENGINEERED	PDB 3ETB
F	78	LEU	GLN	ENGINEERED	PDB 3ETB
F	94	PRO	LEU	ENGINEERED	PDB 3ETB
F	109	GLY	-	LINKER	PDB 3ETB
F	110	GLY	-	LINKER	PDB 3ETB
F	111	GLY	-	LINKER	PDB 3ETB
F	112	GLY	-	LINKER	PDB 3ETB
F	113	SER	-	LINKER	PDB 3ETB
F	114	GLY	-	LINKER	PDB 3ETB
F	115	GLY	-	LINKER	PDB 3ETB
F	116	GLY	-	LINKER	PDB 3ETB
F	117	GLY	-	LINKER	PDB 3ETB

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	118	SER	-	LINKER	PDB 3ETB
F	119	GLY	-	LINKER	PDB 3ETB
F	120	GLY	-	LINKER	PDB 3ETB
F	121	GLY	-	LINKER	PDB 3ETB
F	122	GLY	-	LINKER	PDB 3ETB
F	123	SER	-	LINKER	PDB 3ETB
F	124	GLY	-	LINKER	PDB 3ETB
F	125	GLY	-	LINKER	PDB 3ETB
F	126	GLY	-	LINKER	PDB 3ETB
F	127	GLY	-	LINKER	PDB 3ETB
F	128	SER	-	LINKER	PDB 3ETB
F	1030	ASN	SER	ENGINEERED	PDB 3ETB
F	1057	SER	THR	ENGINEERED	PDB 3ETB
F	1064	GLU	LYS	ENGINEERED	PDB 3ETB
F	1068	ILE	THR	ENGINEERED	PDB 3ETB
G	-4	MET	-	EXPRESSION TAG	PDB 3ETB
G	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
G	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
G	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
G	0	LYS	-	EXPRESSION TAG	PDB 3ETB
G	21	VAL	ILE	ENGINEERED	PDB 3ETB
G	46	PHE	LEU	ENGINEERED	PDB 3ETB
G	56	PRO	SER	ENGINEERED	PDB 3ETB
G	76	ASN	SER	ENGINEERED	PDB 3ETB
G	78	LEU	GLN	ENGINEERED	PDB 3ETB
G	94	PRO	LEU	ENGINEERED	PDB 3ETB
G	109	GLY	-	LINKER	PDB 3ETB
G	110	GLY	-	LINKER	PDB 3ETB
G	111	GLY	-	LINKER	PDB 3ETB
G	112	GLY	-	LINKER	PDB 3ETB
G	113	SER	-	LINKER	PDB 3ETB
G	114	GLY	-	LINKER	PDB 3ETB
G	115	GLY	-	LINKER	PDB 3ETB
G	116	GLY	-	LINKER	PDB 3ETB
G	117	GLY	-	LINKER	PDB 3ETB
G	118	SER	-	LINKER	PDB 3ETB
G	119	GLY	-	LINKER	PDB 3ETB
G	120	GLY	-	LINKER	PDB 3ETB
G	121	GLY	-	LINKER	PDB 3ETB
G	122	GLY	-	LINKER	PDB 3ETB
G	123	SER	-	LINKER	PDB 3ETB
G	124	GLY	-	LINKER	PDB 3ETB

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	125	GLY	-	LINKER	PDB 3ETB
G	126	GLY	-	LINKER	PDB 3ETB
G	127	GLY	-	LINKER	PDB 3ETB
G	128	SER	-	LINKER	PDB 3ETB
G	1030	ASN	SER	ENGINEERED	PDB 3ETB
G	1057	SER	THR	ENGINEERED	PDB 3ETB
G	1064	GLU	LYS	ENGINEERED	PDB 3ETB
G	1068	ILE	THR	ENGINEERED	PDB 3ETB
H	-4	MET	-	EXPRESSION TAG	PDB 3ETB
H	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
H	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
H	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
H	0	LYS	-	EXPRESSION TAG	PDB 3ETB
H	21	VAL	ILE	ENGINEERED	PDB 3ETB
H	46	PHE	LEU	ENGINEERED	PDB 3ETB
H	56	PRO	SER	ENGINEERED	PDB 3ETB
H	76	ASN	SER	ENGINEERED	PDB 3ETB
H	78	LEU	GLN	ENGINEERED	PDB 3ETB
H	94	PRO	LEU	ENGINEERED	PDB 3ETB
H	109	GLY	-	LINKER	PDB 3ETB
H	110	GLY	-	LINKER	PDB 3ETB
H	111	GLY	-	LINKER	PDB 3ETB
H	112	GLY	-	LINKER	PDB 3ETB
H	113	SER	-	LINKER	PDB 3ETB
H	114	GLY	-	LINKER	PDB 3ETB
H	115	GLY	-	LINKER	PDB 3ETB
H	116	GLY	-	LINKER	PDB 3ETB
H	117	GLY	-	LINKER	PDB 3ETB
H	118	SER	-	LINKER	PDB 3ETB
H	119	GLY	-	LINKER	PDB 3ETB
H	120	GLY	-	LINKER	PDB 3ETB
H	121	GLY	-	LINKER	PDB 3ETB
H	122	GLY	-	LINKER	PDB 3ETB
H	123	SER	-	LINKER	PDB 3ETB
H	124	GLY	-	LINKER	PDB 3ETB
H	125	GLY	-	LINKER	PDB 3ETB
H	126	GLY	-	LINKER	PDB 3ETB
H	127	GLY	-	LINKER	PDB 3ETB
H	128	SER	-	LINKER	PDB 3ETB
H	1030	ASN	SER	ENGINEERED	PDB 3ETB
H	1057	SER	THR	ENGINEERED	PDB 3ETB
H	1064	GLU	LYS	ENGINEERED	PDB 3ETB

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	1068	ILE	THR	ENGINEERED	PDB 3ETB
I	-4	MET	-	EXPRESSION TAG	PDB 3ETB
I	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
I	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
I	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
I	0	LYS	-	EXPRESSION TAG	PDB 3ETB
I	21	VAL	ILE	ENGINEERED	PDB 3ETB
I	46	PHE	LEU	ENGINEERED	PDB 3ETB
I	56	PRO	SER	ENGINEERED	PDB 3ETB
I	76	ASN	SER	ENGINEERED	PDB 3ETB
I	78	LEU	GLN	ENGINEERED	PDB 3ETB
I	94	PRO	LEU	ENGINEERED	PDB 3ETB
I	109	GLY	-	LINKER	PDB 3ETB
I	110	GLY	-	LINKER	PDB 3ETB
I	111	GLY	-	LINKER	PDB 3ETB
I	112	GLY	-	LINKER	PDB 3ETB
I	113	SER	-	LINKER	PDB 3ETB
I	114	GLY	-	LINKER	PDB 3ETB
I	115	GLY	-	LINKER	PDB 3ETB
I	116	GLY	-	LINKER	PDB 3ETB
I	117	GLY	-	LINKER	PDB 3ETB
I	118	SER	-	LINKER	PDB 3ETB
I	119	GLY	-	LINKER	PDB 3ETB
I	120	GLY	-	LINKER	PDB 3ETB
I	121	GLY	-	LINKER	PDB 3ETB
I	122	GLY	-	LINKER	PDB 3ETB
I	123	SER	-	LINKER	PDB 3ETB
I	124	GLY	-	LINKER	PDB 3ETB
I	125	GLY	-	LINKER	PDB 3ETB
I	126	GLY	-	LINKER	PDB 3ETB
I	127	GLY	-	LINKER	PDB 3ETB
I	128	SER	-	LINKER	PDB 3ETB
I	1030	ASN	SER	ENGINEERED	PDB 3ETB
I	1057	SER	THR	ENGINEERED	PDB 3ETB
I	1064	GLU	LYS	ENGINEERED	PDB 3ETB
I	1068	ILE	THR	ENGINEERED	PDB 3ETB

- Molecule 2 is a protein called Anthrax Protective Antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	144	Total	C	N	O	S	0	0	0
			1146	722	192	231	1			

Continued on next page...

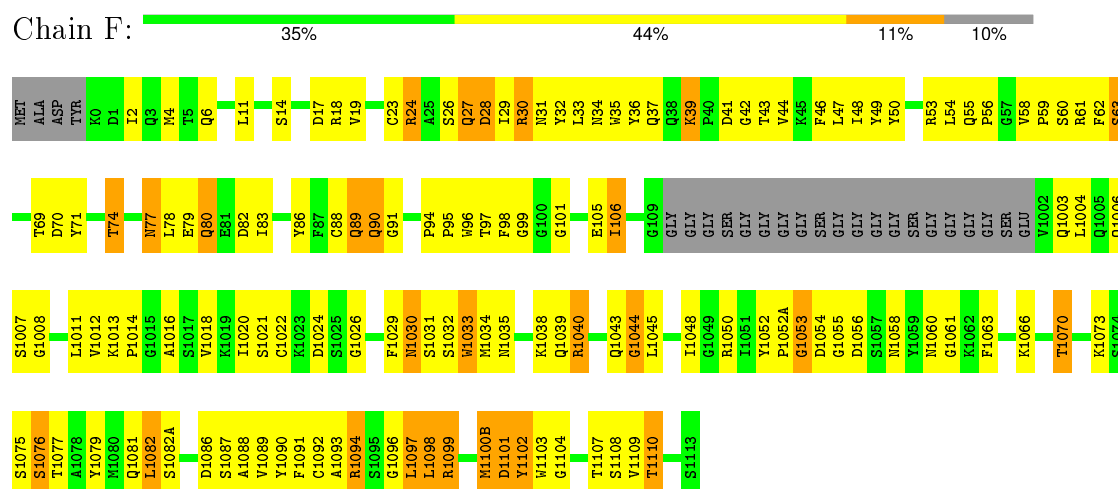
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	144	Total	C	N	O	S	0	0	0
			1146	722	192	231	1			
2	L	143	Total	C	N	O	S	0	0	0
			1138	718	191	228	1			
2	M	144	Total	C	N	O	S	0	0	0
			1146	722	192	231	1			

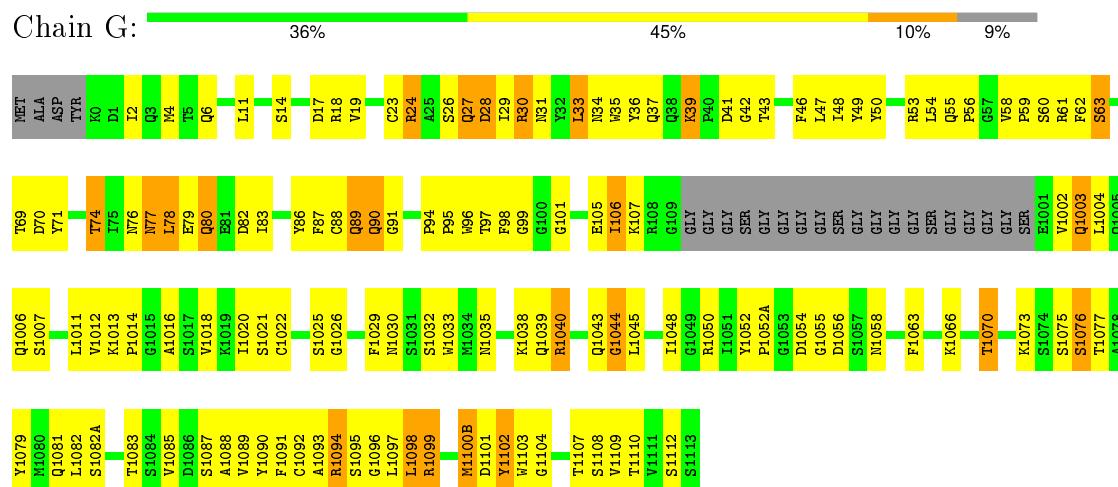
3 Residue-property plots

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.

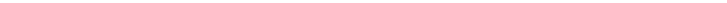
- Molecule 1: Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGGS)₄ linker

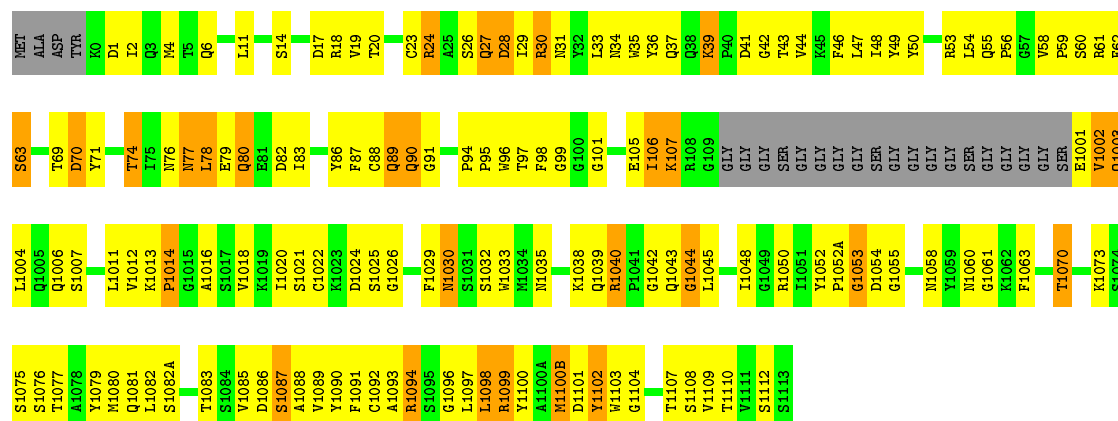


- Molecule 1: Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGGS)₄ linker



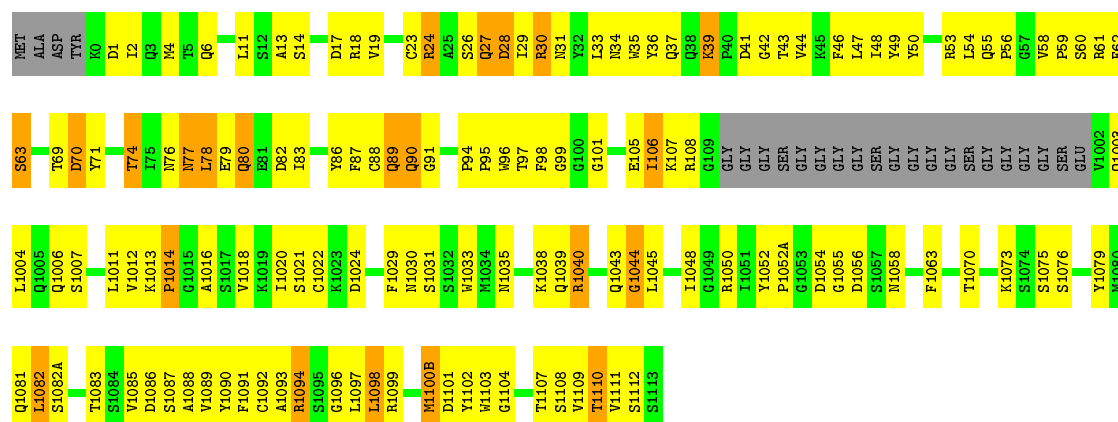
- Molecule 1: Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGGS)₄ linker

Chain H:  33% 47% 12% 9%



- Molecule 1: Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGS)₄ linker

Chain I:  35% 46% 9% 10%

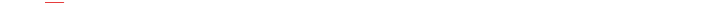


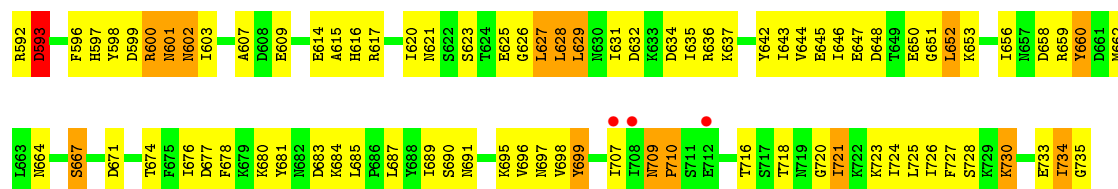
- Molecule 2: Anthrax Protective Antigen

Chain J: 38% 51% 10% •

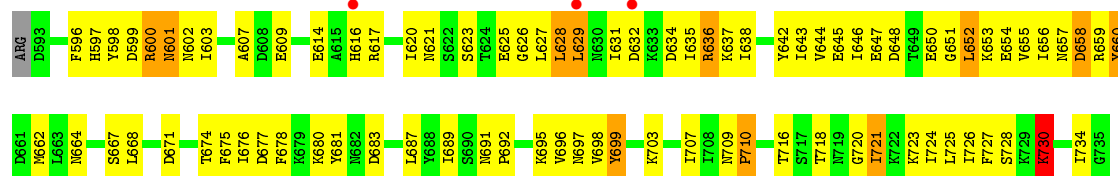


- Molecule 2: Anthrax Protective Antigen

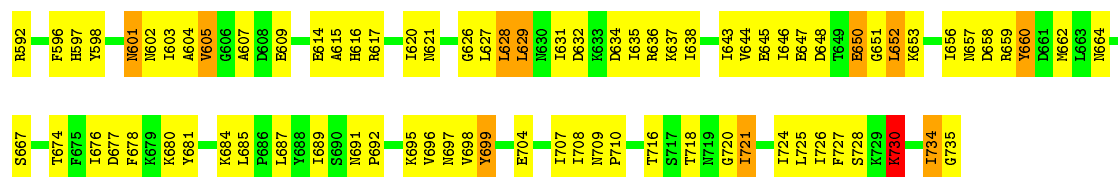
Chain K: 



• Molecule 2: Anthrax Protective Antigen



• Molecule 2: Anthrax Protective Antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.94Å 299.72Å 68.95Å 90.00° 94.45° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 43.84 – 3.81	Depositor EDS
% Data completeness (in resolution range)	83.8 (20.00-3.80) 89.8 (43.84-3.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.276 0.222 , 0.228	Depositor DCC
R_{free} test set	934 reflections (5.73%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 1.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 18322 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F	0.48	0/1781	0.70	0/2413
1	G	0.49	0/1782	0.71	0/2416
1	H	0.49	0/1782	0.70	0/2416
1	I	0.49	0/1781	0.70	0/2413
2	J	0.44	0/1162	0.66	0/1566
2	K	0.47	0/1162	0.69	0/1566
2	L	0.47	0/1154	0.70	0/1555
2	M	0.47	0/1162	0.68	0/1566
All	All	0.48	0/11766	0.69	0/15911

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	F	1742	0	1655	151	0
1	G	1743	0	1646	141	0
1	H	1743	0	1646	151	0
1	I	1742	0	1655	142	0
2	J	1146	0	1134	104	0
2	K	1146	0	1134	94	0
2	L	1138	0	1130	100	0
2	M	1146	0	1134	96	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11546	0	11134	953	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (953) 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:G:1006:GLN:HE22	1:G:1091:PHE:HA	1.29	0.96
1:F:1006:GLN:HE22	1:F:1091:PHE:HA	1.27	0.95
1:G:1011:LEU:HD13	1:G:1110:THR:HG23	1.47	0.95
2:M:629:LEU:HD23	2:M:629:LEU:H	1.32	0.93
1:H:1050:ARG:HE	1:H:1058:ASN:HD22	1.18	0.90
1:H:1011:LEU:HD13	1:H:1110:THR:HG23	1.54	0.90
2:K:629:LEU:HD23	2:K:629:LEU:H	1.37	0.86
1:G:89:GLN:HB2	1:G:98:PHE:CD2	2.10	0.86
1:I:89:GLN:HB2	1:I:98:PHE:CD2	2.10	0.86
1:H:1006:GLN:HE22	1:H:1091:PHE:HA	1.41	0.85
1:H:2:ILE:HB	1:H:90:GLN:HE21	1.41	0.85
1:I:1006:GLN:HE22	1:I:1091:PHE:HA	1.40	0.85
1:F:1011:LEU:HD13	1:F:1110:THR:HG23	1.58	0.85
2:J:629:LEU:H	2:J:629:LEU:HD23	1.42	0.84
1:H:89:GLN:HB2	1:H:98:PHE:CD2	2.12	0.84
1:F:1093:ALA:HB1	1:F:1100(B):MET:HB3	1.59	0.84
1:F:89:GLN:HB2	1:F:98:PHE:CD2	2.13	0.84
1:H:1093:ALA:HB1	1:H:1100(B):MET:HB3	1.60	0.83
2:J:600:ARG:CZ	2:J:601:ASN:H	1.91	0.83
1:I:1011:LEU:HD13	1:I:1110:THR:HG23	1.59	0.83
1:H:2:ILE:HB	1:H:90:GLN:NE2	1.94	0.83
1:H:1050:ARG:HE	1:H:1058:ASN:ND2	1.76	0.82
2:L:629:LEU:H	2:L:629:LEU:HD23	1.46	0.81
1:I:83:ILE:HD11	1:I:106:ILE:HD11	1.63	0.81
1:G:1097:LEU:O	1:G:1098:LEU:HB2	1.80	0.80
1:H:1097:LEU:O	1:H:1098:LEU:HB2	1.79	0.79
1:F:2:ILE:HB	1:F:90:GLN:HE21	1.47	0.79
1:H:83:ILE:HD11	1:H:106:ILE:HD11	1.63	0.79
2:L:662:MET:HG2	2:L:681:TYR:CD1	2.16	0.79
2:K:660:TYR:HB2	2:K:707:ILE:HD11	1.64	0.78
1:G:83:ILE:HD11	1:G:106:ILE:HD11	1.66	0.78
1:F:1097:LEU:O	1:F:1098:LEU:HB2	1.82	0.78
1:F:48:ILE:HG12	1:F:54:LEU:HD23	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:GLN:HE21	1:F:99:GLY:HA3	1.48	0.77
1:F:1050:ARG:HE	1:F:1058:ASN:ND2	1.83	0.77
1:G:1093:ALA:HB1	1:G:1100(B):MET:HB3	1.66	0.77
1:F:83:ILE:HD11	1:F:106:ILE:HD11	1.66	0.77
1:H:48:ILE:HG12	1:H:54:LEU:HD23	1.65	0.77
1:G:1052(A):PRO:O	1:G:1073:LYS:HD3	1.84	0.77
2:M:629:LEU:N	2:M:629:LEU:HD23	2.00	0.77
1:I:48:ILE:HG12	1:I:54:LEU:HD23	1.66	0.76
1:I:6:GLN:HE21	1:I:99:GLY:HA3	1.51	0.76
2:K:596:PHE:CD1	2:K:607:ALA:HB2	2.20	0.76
1:I:1093:ALA:HB1	1:I:1100(B):MET:HB3	1.66	0.75
1:I:2:ILE:HB	1:I:90:GLN:HE21	1.51	0.75
1:G:48:ILE:HG12	1:G:54:LEU:HD23	1.67	0.75
1:H:6:GLN:HE21	1:H:99:GLY:HA3	1.52	0.75
1:G:6:GLN:HE21	1:G:99:GLY:HA3	1.52	0.75
2:M:662:MET:HG2	2:M:681:TYR:CD1	2.21	0.75
2:M:697:ASN:HB3	2:M:699:TYR:HE1	1.52	0.74
1:F:1012:VAL:CG1	1:F:1016:ALA:HB3	2.17	0.74
2:M:660:TYR:HB2	2:M:707:ILE:HD11	1.68	0.74
2:K:662:MET:HG2	2:K:681:TYR:CD1	2.22	0.74
1:F:1050:ARG:HE	1:F:1058:ASN:HD22	1.34	0.74
1:I:1097:LEU:O	1:I:1098:LEU:HB2	1.87	0.74
1:G:39:LYS:HB2	1:G:43:THR:HG22	1.69	0.73
2:L:697:ASN:HB3	2:L:699:TYR:HE1	1.54	0.73
2:M:677:ASP:OD2	2:M:680:LYS:HB2	1.89	0.73
2:M:603:ILE:HG22	2:M:604:ALA:N	2.04	0.73
1:I:39:LYS:HB2	1:I:43:THR:HG22	1.71	0.72
2:K:629:LEU:HD23	2:K:629:LEU:N	2.02	0.72
1:I:80:GLN:O	1:I:83:ILE:HG12	1.88	0.72
1:F:39:LYS:HB2	1:F:43:THR:HG22	1.71	0.72
1:G:80:GLN:O	1:G:83:ILE:HG12	1.90	0.72
1:F:1052(A):PRO:O	1:F:1073:LYS:HD3	1.90	0.71
1:I:1050:ARG:HE	1:I:1058:ASN:HD22	1.36	0.71
2:J:600:ARG:NE	2:J:601:ASN:H	1.88	0.71
1:I:1035:ASN:HD22	1:I:1100(B):MET:HG3	1.56	0.71
1:G:1039:GLN:HB2	1:G:1045:LEU:CD2	2.21	0.71
1:H:39:LYS:HB2	1:H:43:THR:HG22	1.73	0.70
2:M:621:ASN:HB3	2:M:628:LEU:HD23	1.73	0.70
1:G:1035:ASN:HD22	1:G:1100(B):MET:HG3	1.55	0.70
2:K:660:TYR:HB2	2:K:707:ILE:CD1	2.21	0.70
2:J:596:PHE:CD1	2:J:607:ALA:HB2	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1040:ARG:CB	1:I:1040:ARG:HH11	2.04	0.70
2:L:629:LEU:N	2:L:629:LEU:HD23	2.06	0.70
1:G:77:ASN:HB3	2:J:650:GLU:O	1.91	0.70
1:I:50:TYR:HE2	2:M:652:LEU:HD22	1.56	0.69
1:F:1040:ARG:CB	1:F:1040:ARG:HH11	2.04	0.69
2:M:660:TYR:HB2	2:M:707:ILE:CD1	2.22	0.69
2:J:677:ASP:OD2	2:J:680:LYS:HB2	1.92	0.69
2:L:659:ARG:HB3	2:L:662:MET:HB2	1.74	0.69
2:L:696:VAL:O	2:L:696:VAL:HG12	1.93	0.69
2:J:697:ASN:HB3	2:J:699:TYR:HE1	1.58	0.69
2:J:629:LEU:N	2:J:629:LEU:HD23	2.07	0.69
2:L:698:VAL:O	2:L:726:ILE:HG13	1.93	0.69
1:I:1050:ARG:HE	1:I:1058:ASN:ND2	1.90	0.68
1:I:1012:VAL:CG1	1:I:1016:ALA:HB3	2.23	0.68
2:M:603:ILE:HG22	2:M:604:ALA:H	1.56	0.68
1:I:1052(A):PRO:O	1:I:1073:LYS:HD3	1.92	0.68
2:K:697:ASN:HB3	2:K:699:TYR:HE1	1.58	0.68
2:J:660:TYR:HB2	2:J:707:ILE:HD11	1.76	0.68
1:F:50:TYR:HE2	2:J:652:LEU:HD22	1.57	0.68
1:F:77:ASN:HB3	2:K:650:GLU:O	1.94	0.68
1:F:1039:GLN:HB2	1:F:1045:LEU:CD2	2.24	0.68
1:F:1038:LYS:HE2	1:F:1040:ARG:CD	2.23	0.68
2:L:646:ILE:HD11	2:L:687:LEU:HD22	1.75	0.68
2:M:596:PHE:CD1	2:M:607:ALA:HB2	2.28	0.68
1:G:1038:LYS:HE2	1:G:1040:ARG:HD2	1.76	0.68
1:H:80:GLN:O	1:H:83:ILE:HG12	1.95	0.67
2:K:648:ASP:OD2	2:K:652:LEU:HB3	1.94	0.67
1:F:80:GLN:O	1:F:83:ILE:HG12	1.94	0.67
2:L:677:ASP:OD2	2:L:680:LYS:HB2	1.93	0.67
1:G:1056:ASP:HB2	2:K:684:LYS:NZ	2.10	0.67
1:F:1038:LYS:HE2	1:F:1040:ARG:HD2	1.76	0.67
1:G:1040:ARG:HH11	1:G:1040:ARG:CB	2.06	0.67
2:J:662:MET:HG2	2:J:681:TYR:CD1	2.28	0.67
2:L:621:ASN:HB3	2:L:628:LEU:HD23	1.75	0.67
1:G:50:TYR:HE2	2:K:652:LEU:HD22	1.57	0.67
2:J:659:ARG:HH11	2:J:659:ARG:HG2	1.59	0.67
1:I:1107:THR:O	1:I:1109:VAL:HG23	1.95	0.67
2:K:659:ARG:HB3	2:K:662:MET:HB2	1.77	0.67
1:H:1038:LYS:HE2	1:H:1040:ARG:CD	2.25	0.67
2:M:659:ARG:HH11	2:M:659:ARG:HG2	1.59	0.67
1:I:1040:ARG:HB2	1:I:1040:ARG:HH11	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:LEU:HD12	1:H:79:GLU:H	1.60	0.66
1:F:1040:ARG:HB2	1:F:1040:ARG:HH11	1.57	0.66
1:G:1050:ARG:HE	1:G:1058:ASN:HD22	1.43	0.66
1:G:1020:ILE:HD11	1:G:1109:VAL:HG21	1.76	0.66
1:G:1040:ARG:HH11	1:G:1040:ARG:HB2	1.61	0.66
2:K:621:ASN:HB3	2:K:628:LEU:HD23	1.76	0.66
1:H:1011:LEU:CD1	1:H:1110:THR:HG23	2.24	0.66
2:J:659:ARG:HB3	2:J:662:MET:HB2	1.77	0.66
2:J:605:VAL:HG12	2:J:605:VAL:O	1.94	0.66
2:J:660:TYR:HB2	2:J:707:ILE:CD1	2.26	0.65
1:F:2:ILE:HB	1:F:90:GLN:NE2	2.11	0.65
1:H:1006:GLN:HE21	1:H:1104:GLY:HA3	1.60	0.65
1:G:1038:LYS:HE2	1:G:1040:ARG:CD	2.26	0.65
1:I:13:ALA:HA	1:I:107:LYS:HE2	1.77	0.65
1:H:1050:ARG:NE	1:H:1058:ASN:HD22	1.91	0.65
2:K:677:ASP:OD2	2:K:680:LYS:HB2	1.97	0.65
1:I:29:ILE:HD11	1:I:71:TYR:CE1	2.31	0.65
2:J:600:ARG:C	2:J:602:ASN:H	1.98	0.65
1:G:78:LEU:HD12	1:G:79:GLU:H	1.61	0.65
1:H:1043:GLN:O	1:H:1044:GLY:C	2.35	0.65
1:F:1107:THR:O	1:F:1109:VAL:HG23	1.96	0.64
2:K:631:ILE:HD12	2:K:674:THR:HG21	1.80	0.64
1:H:4:MET:HE2	1:H:90:GLN:HG2	1.79	0.64
2:M:601:ASN:N	2:M:601:ASN:HD22	1.95	0.64
1:G:1050:ARG:HE	1:G:1058:ASN:ND2	1.96	0.64
1:F:78:LEU:HD12	1:F:79:GLU:H	1.63	0.64
1:G:1011:LEU:CD1	1:G:1110:THR:HG23	2.25	0.64
2:L:596:PHE:CD1	2:L:607:ALA:HB2	2.32	0.64
1:G:39:LYS:HB2	1:G:43:THR:CG2	2.27	0.64
1:I:78:LEU:HD12	1:I:79:GLU:H	1.62	0.64
2:K:644:VAL:HG22	2:K:698:VAL:HG22	1.80	0.63
1:I:39:LYS:HB2	1:I:43:THR:CG2	2.29	0.63
2:J:698:VAL:O	2:J:726:ILE:HG13	1.98	0.63
2:L:707:ILE:HD11	2:L:721:ILE:HD11	1.81	0.63
1:H:1048:ILE:HA	1:H:1063:PHE:HD1	1.62	0.63
1:H:1035:ASN:HD22	1:H:1100(B):MET:HG3	1.64	0.63
2:L:659:ARG:HG2	2:L:659:ARG:HH11	1.63	0.63
1:F:1035:ASN:HD22	1:F:1100(B):MET:HG3	1.63	0.63
2:K:632:ASP:OD2	2:K:634:ASP:HB2	1.98	0.63
1:I:1038:LYS:HE2	1:I:1040:ARG:CD	2.29	0.62
1:H:29:ILE:HD11	1:H:71:TYR:CE1	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:629:LEU:CD2	2:M:629:LEU:H	2.09	0.62
2:L:600:ARG:C	2:L:602:ASN:H	2.02	0.62
2:K:659:ARG:HG2	2:K:659:ARG:HH11	1.64	0.62
1:H:1038:LYS:HE2	1:H:1040:ARG:HD2	1.82	0.62
1:I:1039:GLN:HB2	1:I:1045:LEU:CD2	2.29	0.62
1:I:1097:LEU:H	2:M:685:LEU:HD13	1.65	0.62
2:L:635:ILE:O	2:L:637:LYS:N	2.33	0.62
2:M:598:TYR:HD1	2:M:604:ALA:HA	1.65	0.62
2:J:621:ASN:HB3	2:J:628:LEU:HD23	1.80	0.62
1:I:1006:GLN:HE21	1:I:1104:GLY:HA3	1.65	0.61
1:G:53:ARG:HG3	1:G:53:ARG:HH11	1.66	0.61
1:G:1107:THR:O	1:G:1109:VAL:HG23	2.00	0.61
2:J:631:ILE:HD12	2:J:674:THR:HG21	1.81	0.61
1:H:1012:VAL:CG1	1:H:1016:ALA:HB3	2.30	0.61
2:J:616:HIS:HA	2:J:629:LEU:HD12	1.83	0.61
1:F:1043:GLN:O	1:F:1044:GLY:C	2.38	0.61
1:H:39:LYS:HB2	1:H:43:THR:CG2	2.30	0.61
1:G:1006:GLN:HE21	1:G:1104:GLY:HA3	1.65	0.61
1:I:1038:LYS:HE2	1:I:1040:ARG:HD2	1.83	0.61
2:M:631:ILE:HD12	2:M:674:THR:HG21	1.83	0.61
1:F:29:ILE:HD11	1:F:71:TYR:CE1	2.35	0.61
1:H:1052(A):PRO:O	1:H:1073:LYS:HD3	2.01	0.61
1:F:54:LEU:HD22	1:F:58:VAL:HG11	1.83	0.60
2:J:603:ILE:HG22	2:J:604:ALA:H	1.66	0.60
2:K:656:ILE:HG13	2:K:687:LEU:HD21	1.83	0.60
1:H:1012:VAL:HG21	1:H:1018:VAL:CG1	2.31	0.60
2:K:616:HIS:HA	2:K:629:LEU:HD12	1.83	0.60
2:L:645:GLU:OE1	2:L:653:LYS:HB3	2.01	0.60
1:I:1048:ILE:HA	1:I:1063:PHE:HD1	1.66	0.60
2:J:644:VAL:HG22	2:J:698:VAL:HG22	1.83	0.60
2:L:601:ASN:HB2	2:L:603:ILE:HG13	1.82	0.60
1:I:53:ARG:HG3	1:I:53:ARG:NH1	2.16	0.60
2:L:697:ASN:ND2	2:L:728:SER:OG	2.34	0.60
1:I:27:GLN:O	1:I:28:ASP:C	2.39	0.60
1:F:39:LYS:HB2	1:F:43:THR:CG2	2.31	0.60
2:M:648:ASP:OD2	2:M:652:LEU:HB3	2.02	0.60
1:G:33:LEU:HD22	1:G:34:ASN:N	2.17	0.60
1:F:1029:PHE:CD2	1:F:1076:SER:HA	2.37	0.60
1:I:53:ARG:HG3	1:I:53:ARG:HH11	1.65	0.60
1:G:53:ARG:HG3	1:G:53:ARG:NH1	2.17	0.60
2:M:698:VAL:O	2:M:726:ILE:HG13	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1012:VAL:CG1	1:G:1016:ALA:HB3	2.32	0.60
1:H:55:GLN:HA	1:H:55:GLN:OE1	2.02	0.59
2:J:730:LYS:O	2:J:734:ILE:HG13	2.02	0.59
2:J:593:ASP:C	2:J:595:ARG:H	2.05	0.59
2:L:648:ASP:OD2	2:L:652:LEU:HB3	2.02	0.59
1:F:1050:ARG:NE	1:F:1058:ASN:HD22	2.00	0.59
1:G:29:ILE:HD11	1:G:71:TYR:CE1	2.36	0.59
2:L:656:ILE:HG13	2:L:687:LEU:HD21	1.84	0.59
2:J:656:ILE:HG13	2:J:687:LEU:HD21	1.83	0.59
2:M:632:ASP:OD2	2:M:634:ASP:HB2	2.03	0.59
1:F:86:TYR:O	1:F:101:GLY:HA2	2.02	0.59
1:F:1006:GLN:HE22	1:F:1091:PHE:CA	2.10	0.59
2:K:629:LEU:CD2	2:K:629:LEU:H	2.12	0.59
1:G:1043:GLN:O	1:G:1044:GLY:C	2.41	0.59
1:G:33:LEU:HD22	1:G:34:ASN:H	1.68	0.59
1:H:53:ARG:NH1	1:H:53:ARG:HG3	2.18	0.59
2:J:629:LEU:H	2:J:629:LEU:CD2	2.14	0.59
2:M:598:TYR:HB3	2:M:602:ASN:HA	1.85	0.59
1:H:1001:GLU:O	1:H:1002:VAL:CB	2.51	0.59
1:I:1048:ILE:HG12	1:I:1063:PHE:CE1	2.38	0.59
2:J:648:ASP:OD2	2:J:652:LEU:HB3	2.03	0.59
1:I:2:ILE:HB	1:I:90:GLN:NE2	2.17	0.58
1:G:54:LEU:HD22	1:G:58:VAL:HG11	1.84	0.58
1:F:33:LEU:HD22	1:F:34:ASN:N	2.18	0.58
1:H:1039:GLN:HB2	1:H:1045:LEU:CD2	2.33	0.58
2:J:644:VAL:HG21	2:J:678:PHE:CD1	2.37	0.58
1:I:33:LEU:HD22	1:I:34:ASN:N	2.18	0.58
1:H:33:LEU:HD22	1:H:34:ASN:N	2.18	0.58
1:F:1097:LEU:H	2:J:685:LEU:HD13	1.67	0.58
1:I:54:LEU:HD22	1:I:58:VAL:HG11	1.85	0.58
2:M:656:ILE:HG13	2:M:687:LEU:HD21	1.84	0.58
1:G:27:GLN:O	1:G:28:ASP:C	2.42	0.58
2:K:696:VAL:HG12	2:K:696:VAL:O	2.03	0.58
2:J:707:ILE:HD11	2:J:721:ILE:HD11	1.85	0.58
1:F:55:GLN:HA	1:F:55:GLN:OE1	2.03	0.57
1:F:1048:ILE:HA	1:F:1063:PHE:HD1	1.67	0.57
1:H:54:LEU:HD22	1:H:58:VAL:HG11	1.86	0.57
1:F:4:MET:HE2	1:F:90:GLN:HG2	1.86	0.57
2:J:632:ASP:OD2	2:J:634:ASP:HB2	2.05	0.57
2:L:614:GLU:O	2:L:617:ARG:HB3	2.05	0.57
1:I:55:GLN:OE1	1:I:55:GLN:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:GLN:HA	1:F:98:PHE:HA	1.87	0.57
2:J:643:ILE:HD13	2:J:718:THR:HB	1.86	0.57
2:K:647:GLU:HG3	2:K:653:LYS:HG2	1.87	0.57
1:H:1040:ARG:HH11	1:H:1040:ARG:CB	2.17	0.57
1:G:1012:VAL:HG21	1:G:1018:VAL:CG1	2.35	0.57
2:J:614:GLU:O	2:J:617:ARG:HB3	2.05	0.57
2:L:631:ILE:HD12	2:L:674:THR:HG21	1.85	0.57
2:L:629:LEU:H	2:L:629:LEU:CD2	2.17	0.57
1:H:33:LEU:HD22	1:H:34:ASN:H	1.69	0.57
1:H:1099:ARG:HB3	2:L:683:ASP:HB2	1.87	0.57
2:M:697:ASN:ND2	2:M:728:SER:OG	2.38	0.57
2:M:616:HIS:HA	2:M:629:LEU:HD12	1.86	0.57
1:F:1020:ILE:HD11	1:F:1109:VAL:HG21	1.87	0.57
1:F:33:LEU:HD22	1:F:34:ASN:H	1.70	0.57
1:H:86:TYR:O	1:H:101:GLY:HA2	2.04	0.57
2:M:605:VAL:HB	2:M:704:GLU:HB3	1.85	0.57
2:J:600:ARG:CD	2:J:601:ASN:H	2.18	0.56
2:J:600:ARG:CZ	2:J:601:ASN:N	2.65	0.56
2:M:659:ARG:HB3	2:M:662:MET:HB2	1.85	0.56
2:M:645:GLU:OE1	2:M:653:LYS:HB3	2.05	0.56
1:I:1050:ARG:NE	1:I:1058:ASN:HD22	2.03	0.56
2:K:643:ILE:HD13	2:K:718:THR:HB	1.87	0.56
2:L:628:LEU:O	2:L:628:LEU:HG	2.05	0.56
1:G:1012:VAL:HG12	1:G:1013:LYS:N	2.21	0.56
1:F:19:VAL:HG21	1:F:78:LEU:HD22	1.87	0.56
1:F:27:GLN:O	1:F:28:ASP:C	2.43	0.56
1:I:89:GLN:HA	1:I:98:PHE:HA	1.88	0.56
1:F:53:ARG:HH11	1:F:53:ARG:HG3	1.71	0.56
1:F:53:ARG:HG3	1:F:53:ARG:NH1	2.21	0.56
1:G:1039:GLN:HB2	1:G:1045:LEU:HD23	1.88	0.56
1:I:33:LEU:HD22	1:I:34:ASN:H	1.70	0.56
2:J:635:ILE:O	2:J:637:LYS:N	2.39	0.56
1:F:1040:ARG:NH1	1:F:1040:ARG:HB2	2.21	0.56
2:K:635:ILE:O	2:K:637:LYS:N	2.39	0.56
1:F:1006:GLN:HE21	1:F:1104:GLY:HA3	1.70	0.56
1:H:53:ARG:HG3	1:H:53:ARG:HH11	1.67	0.56
1:H:27:GLN:O	1:H:28:ASP:C	2.44	0.56
1:G:1048:ILE:HA	1:G:1063:PHE:HD1	1.70	0.56
1:F:1012:VAL:HG11	1:F:1016:ALA:HB3	1.88	0.56
2:J:645:GLU:OE1	2:J:653:LYS:HB3	2.06	0.56
1:I:86:TYR:O	1:I:101:GLY:HA2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:VAL:HG21	1:G:78:LEU:HD22	1.88	0.55
2:M:646:ILE:HD11	2:M:687:LEU:HD22	1.88	0.55
1:I:61:ARG:HH21	1:I:82:ASP:CG	2.09	0.55
2:K:734:ILE:HG22	2:K:735:GLY:N	2.21	0.55
1:H:89:GLN:HA	1:H:98:PHE:HA	1.88	0.55
1:H:1020:ILE:HD11	1:H:1109:VAL:HG21	1.88	0.55
2:K:646:ILE:HD11	2:K:687:LEU:HD22	1.86	0.55
2:K:596:PHE:HB2	2:K:598:TYR:CE1	2.42	0.55
1:H:19:VAL:HG21	1:H:78:LEU:HD22	1.87	0.55
1:I:1043:GLN:O	1:I:1044:GLY:C	2.45	0.55
1:G:86:TYR:O	1:G:101:GLY:HA2	2.06	0.55
1:G:1097:LEU:O	1:G:1098:LEU:CB	2.54	0.55
1:F:1003:GLN:HB3	1:F:1102:TYR:CE1	2.41	0.55
1:G:89:GLN:HA	1:G:98:PHE:HA	1.89	0.55
1:H:1097:LEU:O	1:H:1098:LEU:CB	2.54	0.55
2:K:645:GLU:OE1	2:K:653:LYS:HB3	2.06	0.55
2:K:696:VAL:HB	2:K:734:ILE:HD11	1.87	0.55
1:I:1054:ASP:OD1	1:I:1055:GLY:N	2.40	0.55
1:G:1006:GLN:HE22	1:G:1091:PHE:CA	2.13	0.55
1:I:4:MET:HE2	1:I:90:GLN:HG2	1.89	0.55
1:I:1012:VAL:HG21	1:I:1018:VAL:CG1	2.37	0.55
2:L:627:LEU:HD21	2:L:727:PHE:CE2	2.42	0.54
1:H:1107:THR:O	1:H:1109:VAL:HG23	2.07	0.54
1:I:19:VAL:HG21	1:I:78:LEU:HD22	1.88	0.54
2:L:616:HIS:HA	2:L:629:LEU:HD12	1.88	0.54
2:M:696:VAL:HB	2:M:734:ILE:HD11	1.89	0.54
2:M:726:ILE:HD12	2:M:727:PHE:N	2.23	0.54
2:L:696:VAL:HB	2:L:734:ILE:HD11	1.89	0.54
1:G:4:MET:HE2	1:G:90:GLN:HG2	1.89	0.54
1:G:55:GLN:HA	1:G:55:GLN:OE1	2.07	0.54
2:J:697:ASN:ND2	2:J:728:SER:OG	2.40	0.54
2:M:696:VAL:O	2:M:696:VAL:HG12	2.08	0.54
2:K:698:VAL:O	2:K:726:ILE:HG13	2.08	0.54
1:G:106:ILE:O	1:G:107:LYS:C	2.45	0.54
2:L:660:TYR:HB2	2:L:707:ILE:HD11	1.89	0.54
2:M:697:ASN:HB3	2:M:699:TYR:CE1	2.39	0.53
1:I:77:ASN:HB3	2:L:650:GLU:O	2.08	0.53
2:K:644:VAL:HG21	2:K:678:PHE:CD1	2.43	0.53
1:H:1040:ARG:HH11	1:H:1040:ARG:HB2	1.72	0.53
1:G:1011:LEU:HD13	1:G:1110:THR:CG2	2.31	0.53
2:L:644:VAL:HG22	2:L:698:VAL:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:PHE:O	1:G:63:SER:HB3	2.08	0.53
1:H:46:PHE:CZ	1:H:49:TYR:HB3	2.43	0.53
1:I:1038:LYS:HB2	1:I:1048:ILE:HD11	1.91	0.53
2:K:697:ASN:ND2	2:K:728:SER:OG	2.41	0.53
2:J:734:ILE:HG22	2:J:735:GLY:N	2.23	0.53
1:F:1039:GLN:HB2	1:F:1045:LEU:HD23	1.90	0.53
1:F:30:ARG:O	1:F:31:ASN:HB2	2.08	0.53
2:J:600:ARG:C	2:J:602:ASN:N	2.58	0.53
1:I:1040:ARG:HB2	1:I:1040:ARG:NH1	2.23	0.53
2:L:657:ASN:O	2:L:659:ARG:N	2.42	0.53
1:G:46:PHE:CD2	1:G:55:GLN:NE2	2.76	0.53
1:G:46:PHE:CZ	1:G:49:TYR:HB3	2.43	0.53
2:J:696:VAL:HG12	2:J:696:VAL:O	2.08	0.53
2:K:626:GLY:HA2	2:K:678:PHE:CD2	2.44	0.53
1:G:90:GLN:OE1	1:G:91:GLY:N	2.42	0.53
1:G:61:ARG:HH21	1:G:82:ASP:CG	2.12	0.52
1:H:1089:VAL:HG12	1:H:1090:TYR:N	2.24	0.52
1:F:1097:LEU:O	1:F:1098:LEU:CB	2.56	0.52
1:I:46:PHE:CD2	1:I:55:GLN:NE2	2.78	0.52
1:H:61:ARG:HH21	1:H:82:ASP:CG	2.11	0.52
2:L:600:ARG:HG2	2:L:601:ASN:H	1.75	0.52
2:J:696:VAL:HB	2:J:734:ILE:HD11	1.91	0.52
1:G:1003:GLN:HB3	1:G:1102:TYR:CE1	2.45	0.52
1:H:1011:LEU:HD13	1:H:1110:THR:CG2	2.34	0.52
1:I:46:PHE:CZ	1:I:49:TYR:HB3	2.44	0.52
1:H:1012:VAL:HG12	1:H:1013:LYS:N	2.25	0.52
2:M:644:VAL:HG22	2:M:698:VAL:HG22	1.91	0.52
1:F:1012:VAL:HG12	1:F:1013:LYS:N	2.25	0.52
2:J:646:ILE:HD11	2:J:687:LEU:HD22	1.90	0.52
2:M:726:ILE:HD12	2:M:727:PHE:HB3	1.92	0.52
1:H:49:TYR:CD1	1:H:1098:LEU:HD11	2.45	0.52
1:F:46:PHE:CZ	1:F:49:TYR:HB3	2.44	0.52
1:G:1039:GLN:HB2	1:G:1045:LEU:HD21	1.90	0.52
1:H:1038:LYS:HE2	1:H:1040:ARG:HD3	1.92	0.52
1:I:90:GLN:OE1	1:I:91:GLY:N	2.43	0.52
1:F:46:PHE:CD2	1:F:55:GLN:NE2	2.77	0.52
1:F:1012:VAL:HG21	1:F:1018:VAL:CG1	2.40	0.52
1:G:23:CYS:HB2	1:G:35:TRP:CH2	2.45	0.52
2:L:644:VAL:HG21	2:L:678:PHE:CD1	2.45	0.52
2:K:720:GLY:O	2:K:721:ILE:C	2.48	0.52
1:H:48:ILE:HG23	1:H:53:ARG:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:627:LEU:HD21	2:J:727:PHE:CE2	2.44	0.51
1:G:1022:CYS:O	1:G:1077:THR:HG23	2.10	0.51
1:F:90:GLN:OE1	1:F:91:GLY:N	2.43	0.51
2:M:662:MET:HG2	2:M:681:TYR:CG	2.45	0.51
1:I:62:PHE:O	1:I:63:SER:HB3	2.10	0.51
2:K:662:MET:HG2	2:K:681:TYR:CG	2.44	0.51
2:J:720:GLY:O	2:J:721:ILE:C	2.48	0.51
2:L:660:TYR:HB2	2:L:707:ILE:CD1	2.40	0.51
1:H:30:ARG:O	1:H:31:ASN:HB2	2.09	0.51
2:M:627:LEU:HD12	2:M:676:ILE:HD12	1.92	0.51
1:H:89:GLN:HE21	1:H:96:TRP:HB3	1.76	0.51
2:L:616:HIS:CD2	2:L:629:LEU:HD11	2.45	0.51
2:M:699:TYR:N	2:M:699:TYR:CD1	2.79	0.51
1:G:30:ARG:O	1:G:31:ASN:HB2	2.10	0.51
2:J:689:ILE:HD11	2:J:696:VAL:HG21	1.92	0.51
2:L:662:MET:HG2	2:L:681:TYR:CE1	2.45	0.51
2:M:707:ILE:HD11	2:M:721:ILE:HD11	1.92	0.51
2:L:643:ILE:HD13	2:L:718:THR:HB	1.93	0.51
1:F:1048:ILE:HG12	1:F:1063:PHE:CE1	2.45	0.51
1:F:62:PHE:O	1:F:63:SER:HB3	2.10	0.51
1:H:1:ASP:HB3	1:H:95:PRO:HG2	1.92	0.51
1:I:1035:ASN:ND2	1:I:1100(B):MET:HG3	2.23	0.51
2:M:614:GLU:O	2:M:617:ARG:HB3	2.11	0.51
1:I:1012:VAL:HG12	1:I:1016:ALA:HB3	1.92	0.51
1:H:1029:PHE:CD2	1:H:1076:SER:HA	2.46	0.51
1:F:35:TRP:CE3	1:F:88:CYS:HB3	2.46	0.51
2:K:699:TYR:CD1	2:K:699:TYR:N	2.79	0.51
1:F:1089:VAL:HG12	1:F:1090:TYR:N	2.25	0.51
1:F:24:ARG:HE	1:G:24:ARG:HH21	1.58	0.51
1:G:1097:LEU:H	2:K:685:LEU:HD13	1.75	0.50
1:F:23:CYS:HB2	1:F:35:TRP:CH2	2.45	0.50
2:L:662:MET:HG2	2:L:681:TYR:CG	2.46	0.50
1:H:1002:VAL:O	1:H:1004:LEU:N	2.45	0.50
2:K:600:ARG:HG2	2:K:601:ASN:N	2.26	0.50
1:I:1082:LEU:HD11	1:I:1090:TYR:CE2	2.46	0.50
1:H:53:ARG:HH22	2:L:654:GLU:HB3	1.76	0.50
1:F:78:LEU:HD11	1:F:82:ASP:HB2	1.93	0.50
2:L:635:ILE:C	2:L:637:LYS:N	2.64	0.50
2:K:614:GLU:O	2:K:617:ARG:HB3	2.11	0.50
1:G:1029:PHE:CD2	1:G:1076:SER:HA	2.46	0.50
1:G:1035:ASN:ND2	1:G:1100(B):MET:HG3	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1097:LEU:O	1:I:1098:LEU:CB	2.59	0.50
2:L:699:TYR:N	2:L:699:TYR:CD1	2.79	0.50
1:F:61:ARG:HH21	1:F:82:ASP:CG	2.13	0.50
1:H:23:CYS:HB2	1:H:35:TRP:CH2	2.46	0.50
2:M:664:ASN:O	2:M:664:ASN:CG	2.49	0.50
2:L:621:ASN:HB3	2:L:628:LEU:HB3	1.93	0.50
1:I:30:ARG:O	1:I:31:ASN:HB2	2.11	0.50
1:I:78:LEU:HD11	1:I:82:ASP:HB2	1.93	0.50
1:G:78:LEU:HD11	1:G:82:ASP:HB2	1.94	0.50
2:L:638:ILE:O	2:L:703:LYS:HG3	2.11	0.50
1:H:77:ASN:HB3	2:M:650:GLU:O	2.12	0.50
2:J:699:TYR:N	2:J:699:TYR:CD1	2.80	0.50
1:G:1040:ARG:HB2	1:G:1040:ARG:NH1	2.27	0.50
1:F:89:GLN:HE21	1:F:96:TRP:HB3	1.77	0.50
1:I:105:GLU:O	1:I:106:ILE:HG12	2.12	0.50
1:H:46:PHE:CD2	1:H:55:GLN:NE2	2.80	0.50
1:I:48:ILE:HG23	1:I:53:ARG:O	2.12	0.50
2:M:643:ILE:HD13	2:M:718:THR:HB	1.94	0.50
2:J:627:LEU:HD12	2:J:676:ILE:HD12	1.93	0.50
1:F:1038:LYS:HE2	1:F:1040:ARG:HD3	1.94	0.50
1:H:1007:SER:HB3	1:H:1021:SER:H	1.76	0.50
1:G:1097:LEU:N	1:G:1097:LEU:HD22	2.26	0.49
1:H:1096:GLY:O	1:H:1097:LEU:HB2	2.11	0.49
1:G:31:ASN:O	1:G:33:LEU:N	2.45	0.49
1:G:35:TRP:CE3	1:G:88:CYS:HB3	2.46	0.49
1:F:35:TRP:CZ3	1:F:88:CYS:HB3	2.47	0.49
1:G:36:TYR:HE1	1:G:89:GLN:HB3	1.76	0.49
2:J:600:ARG:NH1	2:J:601:ASN:H	2.11	0.49
1:F:48:ILE:HG23	1:F:53:ARG:O	2.12	0.49
1:H:2:ILE:CB	1:H:90:GLN:HE21	2.18	0.49
1:F:49:TYR:CD1	1:F:1098:LEU:HD11	2.47	0.49
2:J:635:ILE:C	2:J:637:LYS:N	2.66	0.49
1:H:62:PHE:O	1:H:63:SER:HB3	2.12	0.49
1:F:24:ARG:HH21	1:G:24:ARG:HE	1.59	0.49
2:M:691:ASN:OD1	2:M:691:ASN:C	2.51	0.49
2:L:697:ASN:HB3	2:L:699:TYR:CE1	2.40	0.49
1:I:1012:VAL:HG11	1:I:1016:ALA:HB3	1.93	0.49
2:J:605:VAL:HG12	2:J:704:GLU:HB3	1.93	0.49
1:I:23:CYS:HB2	1:I:35:TRP:CH2	2.47	0.49
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.94	0.49
1:G:1007:SER:HB3	1:G:1021:SER:H	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:604:ALA:HB1	2:M:638:ILE:CG2	2.42	0.49
1:H:1038:LYS:O	1:H:1038:LYS:HG2	2.12	0.49
1:H:78:LEU:HD11	1:H:82:ASP:HB2	1.94	0.49
2:J:726:ILE:HD12	2:J:727:PHE:HB3	1.95	0.49
2:J:691:ASN:C	2:J:691:ASN:OD1	2.51	0.49
2:J:616:HIS:CD2	2:J:629:LEU:HD11	2.48	0.49
1:F:41:ASP:O	1:F:43:THR:N	2.46	0.49
1:I:31:ASN:O	1:I:33:LEU:N	2.45	0.49
1:F:41:ASP:OD1	1:F:41:ASP:O	2.31	0.49
2:J:643:ILE:HB	2:J:699:TYR:HB2	1.94	0.49
1:I:49:TYR:CD1	1:I:1098:LEU:HD11	2.47	0.49
2:K:628:LEU:HG	2:K:628:LEU:O	2.13	0.49
1:H:1052:TYR:O	1:H:1052(A):PRO:C	2.51	0.49
1:I:26:SER:O	1:I:27:GLN:HB3	2.13	0.49
2:K:599:ASP:O	2:K:602:ASN:N	2.46	0.49
1:H:35:TRP:CE3	1:H:88:CYS:HB3	2.48	0.49
1:F:18:ARG:NH2	1:F:74:THR:HG21	2.28	0.49
2:K:697:ASN:HB3	2:K:699:TYR:CE1	2.44	0.48
2:L:720:GLY:O	2:L:721:ILE:C	2.52	0.48
1:H:26:SER:O	1:H:27:GLN:HB3	2.13	0.48
1:G:1004:LEU:HD22	1:G:1022:CYS:SG	2.53	0.48
1:G:1096:GLY:O	1:G:1097:LEU:HB2	2.13	0.48
2:L:600:ARG:O	2:L:602:ASN:N	2.46	0.48
1:G:2:ILE:HB	1:G:90:GLN:HE21	1.77	0.48
2:M:628:LEU:O	2:M:628:LEU:HG	2.13	0.48
2:L:620:ILE:H	2:L:629:LEU:HA	1.78	0.48
2:M:659:ARG:NH1	2:M:659:ARG:HG2	2.28	0.48
2:M:734:ILE:HG22	2:M:735:GLY:N	2.27	0.48
1:G:49:TYR:CD1	1:G:1098:LEU:HD11	2.48	0.48
2:J:699:TYR:N	2:J:699:TYR:HD1	2.12	0.48
1:G:1038:LYS:O	1:G:1038:LYS:HG2	2.13	0.48
2:J:598:TYR:CD2	2:J:603:ILE:O	2.67	0.48
2:K:664:ASN:O	2:K:664:ASN:CG	2.51	0.48
2:J:600:ARG:NH1	2:J:601:ASN:N	2.61	0.48
2:J:659:ARG:HG2	2:J:659:ARG:NH1	2.27	0.48
1:F:1004:LEU:HD22	1:F:1022:CYS:SG	2.53	0.48
1:F:1094:ARG:O	1:F:1094:ARG:HG2	2.13	0.48
2:K:596:PHE:HD1	2:K:607:ALA:HB2	1.77	0.48
2:M:699:TYR:N	2:M:699:TYR:HD1	2.10	0.48
2:L:699:TYR:N	2:L:699:TYR:HD1	2.11	0.48
1:G:1089:VAL:HG12	1:G:1090:TYR:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1056:ASP:HB2	2:J:684:LYS:NZ	2.28	0.48
1:H:36:TYR:HE1	1:H:89:GLN:HB3	1.77	0.48
1:H:46:PHE:HZ	1:H:49:TYR:HB3	1.79	0.48
2:K:709:ASN:HB2	2:K:710:PRO:CD	2.43	0.48
1:G:1099:ARG:HB3	2:K:683:ASP:HB2	1.95	0.48
1:H:37:GLN:HB2	1:H:47:LEU:HD11	1.96	0.48
2:L:691:ASN:C	2:L:691:ASN:OD1	2.52	0.48
2:M:621:ASN:HB3	2:M:628:LEU:HB3	1.96	0.48
2:K:645:GLU:HG2	2:K:697:ASN:HB2	1.95	0.48
2:J:626:GLY:HA2	2:J:678:PHE:CD2	2.49	0.48
2:K:635:ILE:C	2:K:637:LYS:N	2.67	0.48
1:G:1050:ARG:NE	1:G:1058:ASN:HD22	2.11	0.48
2:M:726:ILE:HD12	2:M:726:ILE:C	2.34	0.48
2:K:627:LEU:HD12	2:K:676:ILE:HD12	1.96	0.48
2:M:647:GLU:HG3	2:M:653:LYS:HG2	1.94	0.48
2:J:697:ASN:HB3	2:J:699:TYR:CE1	2.44	0.48
2:J:605:VAL:HG12	2:J:704:GLU:N	2.29	0.48
2:K:627:LEU:HD21	2:K:727:PHE:CD2	2.49	0.47
1:G:89:GLN:HE21	1:G:96:TRP:HB3	1.79	0.47
2:K:691:ASN:OD1	2:K:691:ASN:C	2.53	0.47
1:I:1012:VAL:HG12	1:I:1013:LYS:N	2.29	0.47
1:H:35:TRP:CZ3	1:H:88:CYS:HB3	2.49	0.47
1:F:1030:ASN:HB3	1:F:1053:GLY:HA2	1.96	0.47
2:M:597:HIS:CD2	2:M:597:HIS:N	2.82	0.47
1:I:1056:ASP:HB2	2:M:684:LYS:NZ	2.29	0.47
2:M:726:ILE:HD12	2:M:727:PHE:CB	2.44	0.47
2:M:627:LEU:HD21	2:M:727:PHE:CE2	2.49	0.47
2:L:627:LEU:HD12	2:L:676:ILE:HD12	1.95	0.47
1:F:36:TYR:HE1	1:F:89:GLN:HB3	1.78	0.47
2:K:699:TYR:HD1	2:K:699:TYR:N	2.11	0.47
1:G:26:SER:O	1:G:27:GLN:HB3	2.15	0.47
2:K:600:ARG:C	2:K:602:ASN:H	2.18	0.47
2:J:664:ASN:CG	2:J:664:ASN:O	2.52	0.47
2:K:609:GLU:HG2	2:K:724:ILE:HG23	1.95	0.47
1:F:46:PHE:HZ	1:F:49:TYR:HB3	1.80	0.47
2:L:699:TYR:HB3	2:L:723:LYS:HB2	1.95	0.47
2:L:730:LYS:O	2:L:734:ILE:HG13	2.15	0.47
1:H:31:ASN:O	1:H:33:LEU:N	2.46	0.47
1:F:26:SER:O	1:F:27:GLN:HB3	2.14	0.47
1:H:90:GLN:OE1	1:H:91:GLY:N	2.47	0.47
2:L:599:ASP:O	2:L:600:ARG:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1089:VAL:HG12	1:I:1090:TYR:N	2.30	0.47
2:K:627:LEU:HD21	2:K:727:PHE:CE2	2.48	0.47
1:I:36:TYR:HE1	1:I:89:GLN:HB3	1.80	0.47
1:H:106:ILE:O	1:H:107:LYS:C	2.53	0.47
1:F:1096:GLY:O	1:F:1097:LEU:HB2	2.14	0.47
1:I:1096:GLY:O	1:I:1097:LEU:HB2	2.15	0.47
1:I:1097:LEU:HD22	1:I:1097:LEU:N	2.29	0.47
1:I:46:PHE:HZ	1:I:49:TYR:HB3	1.79	0.47
1:I:55:GLN:HG3	1:I:56:PRO:HD2	1.97	0.47
2:J:647:GLU:HG3	2:J:653:LYS:HG2	1.97	0.47
1:F:31:ASN:O	1:F:33:LEU:N	2.48	0.47
1:G:1048:ILE:HG12	1:G:1063:PHE:CE1	2.50	0.47
1:G:4:MET:CE	1:G:90:GLN:HB3	2.45	0.47
1:G:35:TRP:CZ3	1:G:88:CYS:HB3	2.50	0.47
2:K:601:ASN:C	2:K:603:ILE:H	2.17	0.47
1:G:1032:SER:N	1:G:1052:TYR:HE1	2.13	0.47
1:F:1099:ARG:HB3	2:J:683:ASP:HB2	1.95	0.47
2:K:623:SER:C	2:K:625:GLU:H	2.18	0.47
2:L:632:ASP:OD2	2:L:634:ASP:HB2	2.15	0.47
1:F:4:MET:CE	1:F:90:GLN:HB3	2.45	0.47
1:G:1093:ALA:CB	1:G:1100(B):MET:HB3	2.41	0.47
2:M:660:TYR:CD2	2:M:716:THR:HG22	2.50	0.47
2:M:601:ASN:ND2	2:M:601:ASN:N	2.62	0.47
2:L:601:ASN:O	2:L:602:ASN:C	2.53	0.47
1:H:1012:VAL:HG21	1:H:1018:VAL:HG13	1.97	0.47
1:H:1080:MET:HE3	1:H:1090:TYR:CD2	2.50	0.47
1:F:37:GLN:CB	1:F:47:LEU:HD11	2.45	0.47
1:G:46:PHE:HD2	1:G:55:GLN:NE2	2.12	0.47
1:G:105:GLU:O	1:G:106:ILE:HG12	2.15	0.47
1:F:1040:ARG:HB3	1:F:1088:ALA:HB2	1.97	0.47
1:H:1048:ILE:HA	1:H:1063:PHE:CD1	2.48	0.47
1:H:1048:ILE:HG12	1:H:1063:PHE:CE1	2.49	0.47
2:K:599:ASP:HB3	2:K:603:ILE:HB	1.96	0.47
1:G:1081:GLN:O	1:G:1082(A):SER:N	2.48	0.47
2:K:597:HIS:CD2	2:K:597:HIS:N	2.81	0.47
1:G:46:PHE:HZ	1:G:49:TYR:HB3	1.78	0.47
2:K:596:PHE:CE1	2:K:607:ALA:HB2	2.49	0.47
2:L:726:ILE:HD12	2:L:727:PHE:HB3	1.96	0.47
1:H:1004:LEU:HD22	1:H:1022:CYS:SG	2.54	0.47
1:H:37:GLN:CB	1:H:47:LEU:HD11	2.45	0.47
1:H:1003:GLN:CB	1:H:1102:TYR:CE1	2.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:603:ILE:CG2	2:M:604:ALA:H	2.25	0.46
1:I:1039:GLN:HB2	1:I:1045:LEU:HD23	1.98	0.46
1:H:1003:GLN:HA	1:H:1025:SER:OG	2.15	0.46
1:F:1097:LEU:HD22	1:F:1097:LEU:N	2.30	0.46
1:F:46:PHE:HD2	1:F:55:GLN:NE2	2.13	0.46
1:F:1048:ILE:HG23	1:F:1063:PHE:CD1	2.49	0.46
2:J:644:VAL:HG21	2:J:678:PHE:HD1	1.77	0.46
1:H:1087:SER:HA	1:H:1109:VAL:O	2.16	0.46
1:I:35:TRP:CE3	1:I:88:CYS:HB3	2.50	0.46
1:I:1029:PHE:CD2	1:I:1076:SER:HA	2.50	0.46
1:I:69:THR:C	1:I:70:ASP:OD1	2.53	0.46
2:M:620:ILE:H	2:M:629:LEU:HA	1.80	0.46
2:K:616:HIS:CD2	2:K:629:LEU:HD11	2.51	0.46
2:M:720:GLY:O	2:M:721:ILE:C	2.53	0.46
1:F:1040:ARG:HB3	1:F:1088:ALA:CB	2.44	0.46
1:F:1094:ARG:HH11	1:F:1094:ARG:HG2	1.80	0.46
2:L:655:VAL:HB	2:L:658:ASP:HB2	1.97	0.46
2:M:644:VAL:HG21	2:M:678:PHE:CD1	2.50	0.46
2:J:621:ASN:HB3	2:J:628:LEU:HB3	1.98	0.46
1:I:1048:ILE:HG23	1:I:1063:PHE:CD1	2.50	0.46
1:I:4:MET:CE	1:I:90:GLN:HB3	2.45	0.46
2:M:603:ILE:CG2	2:M:604:ALA:N	2.73	0.46
2:L:626:GLY:HA2	2:L:678:PHE:CD2	2.50	0.46
1:H:4:MET:CE	1:H:90:GLN:HB3	2.45	0.46
1:H:105:GLU:HB3	1:H:106:ILE:H	1.47	0.46
2:L:643:ILE:HB	2:L:699:TYR:HB2	1.96	0.46
1:G:1003:GLN:HA	1:G:1025:SER:OG	2.16	0.46
1:F:1024:ASP:OD1	1:F:1026:GLY:N	2.49	0.46
1:I:89:GLN:HE21	1:I:96:TRP:HB3	1.80	0.46
2:L:659:ARG:NH1	2:L:659:ARG:HG2	2.31	0.46
1:F:1054:ASP:OD1	1:F:1055:GLY:N	2.49	0.46
1:F:1006:GLN:NE2	1:F:1092:CYS:H	2.13	0.46
2:M:620:ILE:HG22	2:M:620:ILE:O	2.16	0.46
1:H:89:GLN:HG2	1:H:90:GLN:O	2.16	0.46
2:L:627:LEU:HD21	2:L:727:PHE:CD2	2.51	0.46
1:G:1004:LEU:HD11	1:G:1094:ARG:HB3	1.98	0.46
2:K:726:ILE:C	2:K:726:ILE:HD12	2.36	0.46
1:G:1044:GLY:O	1:G:1045:LEU:HG	2.16	0.46
1:H:69:THR:C	1:H:70:ASP:OD1	2.54	0.46
1:F:1035:ASN:ND2	1:F:1100(B):MET:HG3	2.30	0.45
2:K:660:TYR:CD2	2:K:716:THR:HG22	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:ILE:HG23	1:G:53:ARG:O	2.17	0.45
2:L:596:PHE:HB2	2:L:598:TYR:OH	2.15	0.45
2:K:689:ILE:HD11	2:K:696:VAL:HG21	1.97	0.45
2:K:662:MET:CE	2:K:681:TYR:HB3	2.46	0.45
2:L:725:LEU:HD12	2:L:726:ILE:H	1.81	0.45
1:I:1089:VAL:C	1:I:1090:TYR:CD1	2.89	0.45
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.99	0.45
2:J:699:TYR:HB3	2:J:723:LYS:HB2	1.98	0.45
1:F:1039:GLN:HB2	1:F:1045:LEU:HD21	1.96	0.45
1:I:78:LEU:CD1	1:I:82:ASP:HB2	2.46	0.45
1:H:1075:SER:O	1:H:1076:SER:C	2.53	0.45
1:H:50:TYR:HE2	2:L:652:LEU:HD22	1.81	0.45
1:H:59:PRO:O	1:H:61:ARG:N	2.49	0.45
1:G:1012:VAL:HG11	1:G:1016:ALA:HB3	1.99	0.45
2:M:615:ALA:C	2:M:617:ARG:H	2.19	0.45
1:F:14:SER:O	1:F:17:ASP:OD2	2.33	0.45
1:I:18:ARG:NH2	1:I:74:THR:HG21	2.30	0.45
1:I:41:ASP:O	1:I:41:ASP:OD1	2.35	0.45
1:G:59:PRO:O	1:G:61:ARG:N	2.50	0.45
2:L:660:TYR:CD2	2:L:716:THR:HG22	2.52	0.45
1:G:1012:VAL:HG21	1:G:1018:VAL:HG11	1.99	0.45
2:J:623:SER:C	2:J:625:GLU:H	2.19	0.45
1:H:18:ARG:NH2	1:H:74:THR:HG21	2.31	0.45
2:M:621:ASN:CB	2:M:628:LEU:HD23	2.43	0.45
2:K:626:GLY:HA2	2:K:678:PHE:CE2	2.51	0.45
2:K:615:ALA:C	2:K:617:ARG:H	2.19	0.45
1:I:1004:LEU:HD22	1:I:1022:CYS:SG	2.56	0.45
1:F:1012:VAL:HG12	1:F:1016:ALA:HB3	1.93	0.45
1:I:1040:ARG:HB3	1:I:1088:ALA:CB	2.47	0.45
2:K:695:LYS:HA	2:K:730:LYS:HA	1.99	0.45
1:I:44:VAL:HG11	1:I:1103:TRP:CD2	2.52	0.45
1:G:1098:LEU:HD23	1:G:1098:LEU:HA	1.68	0.45
2:J:699:TYR:CD2	2:J:723:LYS:HD2	2.52	0.45
2:J:597:HIS:N	2:J:606:GLY:O	2.40	0.45
2:M:601:ASN:O	2:M:602:ASN:HB2	2.17	0.45
1:I:1020:ILE:HD11	1:I:1109:VAL:HG21	1.98	0.45
2:J:725:LEU:HD11	2:J:727:PHE:O	2.17	0.45
1:G:1070:THR:HG23	1:G:1079:TYR:HB2	1.98	0.45
1:F:44:VAL:HG11	1:F:1103:TRP:CD2	2.52	0.45
1:G:69:THR:C	1:G:70:ASP:OD1	2.56	0.45
1:H:1030:ASN:HB3	1:H:1053:GLY:HA2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:627:LEU:HD21	2:M:727:PHE:CD2	2.52	0.45
1:G:1097:LEU:N	1:G:1097:LEU:CD2	2.80	0.45
2:L:699:TYR:CD2	2:L:723:LYS:HD2	2.51	0.45
1:H:41:ASP:OD1	1:H:41:ASP:O	2.35	0.45
1:H:78:LEU:CD1	1:H:82:ASP:HB2	2.47	0.45
1:G:1092:CYS:O	1:G:1092:CYS:SG	2.75	0.44
1:F:1093:ALA:CB	1:F:1100(B):MET:HB3	2.41	0.44
1:H:105:GLU:O	1:H:106:ILE:HG12	2.17	0.44
1:I:46:PHE:HD2	1:I:55:GLN:NE2	2.14	0.44
2:L:689:ILE:HD11	2:L:696:VAL:HG21	1.99	0.44
2:K:643:ILE:HB	2:K:699:TYR:HB2	1.98	0.44
2:J:605:VAL:CG1	2:J:704:GLU:HB3	2.47	0.44
1:I:71:TYR:N	1:I:71:TYR:CD1	2.84	0.44
1:G:18:ARG:NH2	1:G:74:THR:HG21	2.32	0.44
1:F:1006:GLN:HG2	1:F:1092:CYS:SG	2.57	0.44
2:J:600:ARG:HA	2:J:600:ARG:HD2	1.62	0.44
2:M:659:ARG:HH11	2:M:659:ARG:CG	2.30	0.44
2:M:662:MET:HG2	2:M:681:TYR:CE1	2.51	0.44
1:H:1040:ARG:HB3	1:H:1088:ALA:CB	2.47	0.44
2:K:599:ASP:HB3	2:K:603:ILE:O	2.16	0.44
1:F:69:THR:C	1:F:70:ASP:OD1	2.55	0.44
1:F:1070:THR:HG23	1:F:1079:TYR:HB2	1.99	0.44
1:I:1006:GLN:HG2	1:I:1092:CYS:SG	2.56	0.44
1:I:105:GLU:HB3	1:I:106:ILE:H	1.48	0.44
1:G:41:ASP:OD1	1:G:41:ASP:O	2.36	0.44
2:L:621:ASN:CB	2:L:628:LEU:HD23	2.46	0.44
1:H:14:SER:O	1:H:17:ASP:OD2	2.36	0.44
1:F:1033:TRP:HB3	1:F:1034:MET:H	1.68	0.44
1:G:89:GLN:HB2	1:G:98:PHE:CE2	2.52	0.44
1:I:1098:LEU:HA	1:I:1098:LEU:HD23	1.73	0.44
1:I:1038:LYS:HE2	1:I:1040:ARG:HD3	1.99	0.44
1:I:1004:LEU:HD23	1:I:1004:LEU:HA	1.80	0.44
1:I:14:SER:O	1:I:17:ASP:OD2	2.35	0.44
2:L:709:ASN:HB2	2:L:710:PRO:CD	2.48	0.44
2:K:644:VAL:HG21	2:K:678:PHE:HD1	1.81	0.44
1:H:46:PHE:HD2	1:H:55:GLN:NE2	2.15	0.44
1:H:106:ILE:O	1:H:107:LYS:O	2.36	0.44
1:F:1097:LEU:N	2:J:685:LEU:HD13	2.30	0.44
1:F:105:GLU:O	1:F:106:ILE:HG12	2.17	0.44
1:F:1004:LEU:HD11	1:F:1094:ARG:HB3	2.00	0.44
2:J:620:ILE:H	2:J:629:LEU:HA	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1100(B):MET:CE	1:F:1100(B):MET:N	2.80	0.44
1:F:1098:LEU:HA	1:F:1098:LEU:HD23	1.76	0.44
1:F:55:GLN:HG3	1:F:56:PRO:HD2	1.99	0.44
2:J:662:MET:HG2	2:J:681:TYR:CG	2.53	0.44
1:F:78:LEU:CD1	1:F:82:ASP:HB2	2.47	0.44
1:I:35:TRP:CZ3	1:I:88:CYS:HB3	2.52	0.44
2:J:597:HIS:CD2	2:J:597:HIS:N	2.85	0.44
1:H:1070:THR:HG23	1:H:1079:TYR:HB2	1.99	0.44
2:M:627:LEU:HD13	2:M:629:LEU:HD22	1.99	0.44
1:H:89:GLN:HB2	1:H:98:PHE:CE2	2.53	0.44
1:I:55:GLN:CD	1:I:56:PRO:HD2	2.38	0.44
2:K:621:ASN:HB3	2:K:628:LEU:HB3	2.00	0.44
1:F:1003:GLN:CB	1:F:1102:TYR:CE1	3.00	0.44
1:I:37:GLN:CB	1:I:47:LEU:HD11	2.48	0.44
1:G:55:GLN:HG3	1:G:56:PRO:HD2	1.99	0.44
1:I:55:GLN:CG	1:I:56:PRO:HD2	2.48	0.44
1:H:1004:LEU:HD23	1:H:1004:LEU:HA	1.82	0.44
1:H:1024:ASP:OD1	1:H:1026:GLY:N	2.50	0.44
2:J:655:VAL:HB	2:J:658:ASP:HB2	2.00	0.44
2:L:647:GLU:HG3	2:L:653:LYS:HG2	2.00	0.44
1:I:41:ASP:O	1:I:43:THR:N	2.51	0.44
2:L:644:VAL:HG21	2:L:678:PHE:HD1	1.83	0.44
1:F:59:PRO:O	1:F:61:ARG:N	2.51	0.44
2:L:596:PHE:HA	2:L:607:ALA:HA	1.99	0.44
1:H:1032:SER:N	1:H:1052:TYR:HE1	2.15	0.44
1:F:1029:PHE:CE2	1:F:1076:SER:HA	2.53	0.44
2:J:615:ALA:C	2:J:617:ARG:H	2.20	0.44
1:I:1075:SER:O	1:I:1076:SER:C	2.54	0.44
2:L:668:LEU:HD12	2:L:668:LEU:HA	1.81	0.44
1:H:1014:PRO:CG	1:H:1112:SER:O	2.66	0.44
2:M:616:HIS:CD2	2:M:629:LEU:HD11	2.53	0.43
1:H:1006:GLN:NE2	1:H:1092:CYS:H	2.15	0.43
2:J:660:TYR:CD2	2:J:716:THR:HG22	2.53	0.43
1:F:1075:SER:O	1:F:1076:SER:C	2.56	0.43
2:K:599:ASP:O	2:K:600:ARG:C	2.56	0.43
2:J:600:ARG:HG2	2:L:662:MET:CE	2.48	0.43
1:H:41:ASP:O	1:H:43:THR:N	2.51	0.43
2:J:596:PHE:HD1	2:J:607:ALA:HB2	1.80	0.43
1:H:1042:GLY:C	1:H:1043:GLN:HE21	2.22	0.43
2:J:627:LEU:HD21	2:J:727:PHE:CD2	2.54	0.43
1:F:1022:CYS:O	1:F:1077:THR:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLN:HB2	1:G:47:LEU:HD11	2.00	0.43
1:I:1007:SER:HB3	1:I:1021:SER:H	1.83	0.43
2:M:645:GLU:HG2	2:M:697:ASN:HB2	2.00	0.43
1:F:1038:LYS:HB2	1:F:1048:ILE:HD11	2.00	0.43
1:G:78:LEU:CD1	1:G:82:ASP:HB2	2.48	0.43
2:J:678:PHE:CD2	2:J:687:LEU:HD12	2.53	0.43
2:L:599:ASP:O	2:L:602:ASN:N	2.50	0.43
1:H:1012:VAL:HG12	1:H:1016:ALA:HB3	1.99	0.43
2:K:592:ARG:O	2:K:593:ASP:HB2	2.17	0.43
1:H:49:TYR:CG	1:H:1098:LEU:HD11	2.53	0.43
1:I:1086:ASP:O	1:I:1088:ALA:N	2.51	0.43
1:G:1056:ASP:CB	2:K:684:LYS:NZ	2.80	0.43
1:I:1020:ILE:O	1:I:1079:TYR:HA	2.19	0.43
1:F:71:TYR:N	1:F:71:TYR:CD1	2.85	0.43
2:J:593:ASP:C	2:J:595:ARG:N	2.71	0.43
2:M:635:ILE:O	2:M:637:LYS:N	2.51	0.43
2:L:597:HIS:N	2:L:597:HIS:CD2	2.86	0.43
1:I:1014:PRO:HG3	1:I:1111:VAL:HG12	2.01	0.43
2:L:623:SER:C	2:L:625:GLU:H	2.21	0.43
1:H:2:ILE:CB	1:H:90:GLN:NE2	2.75	0.43
2:J:600:ARG:O	2:J:601:ASN:HB2	2.19	0.43
1:F:1048:ILE:HA	1:F:1063:PHE:CD1	2.52	0.43
2:J:652:LEU:HD23	2:J:653:LYS:N	2.33	0.43
2:J:726:ILE:C	2:J:726:ILE:HD12	2.39	0.43
1:I:106:ILE:HG22	1:I:106:ILE:O	2.19	0.43
1:F:105:GLU:HB3	1:F:106:ILE:H	1.50	0.43
2:L:652:LEU:HD23	2:L:653:LYS:N	2.34	0.43
2:M:657:ASN:O	2:M:659:ARG:N	2.52	0.43
1:I:1052:TYR:O	1:I:1052(A):PRO:C	2.57	0.43
1:G:1020:ILE:HD11	1:G:1109:VAL:CG2	2.45	0.43
2:M:605:VAL:CG2	2:M:704:GLU:HB3	2.48	0.43
1:G:1035:ASN:ND2	1:G:1095:SER:OG	2.52	0.43
1:F:1012:VAL:HG21	1:F:1018:VAL:HG13	2.00	0.43
2:L:628:LEU:CG	2:L:628:LEU:O	2.67	0.43
1:H:59:PRO:HG2	1:H:62:PHE:CD1	2.54	0.43
1:I:59:PRO:O	1:I:61:ARG:N	2.52	0.43
2:L:601:ASN:HB2	2:L:603:ILE:CG1	2.48	0.43
1:G:1048:ILE:HG23	1:G:1063:PHE:CD1	2.54	0.43
1:G:1003:GLN:CB	1:G:1102:TYR:CE1	3.02	0.43
1:F:1082:LEU:HD11	1:F:1090:TYR:CE2	2.54	0.43
1:F:1006:GLN:NE2	1:F:1092:CYS:N	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:627:LEU:HD13	2:K:629:LEU:HD22	2.01	0.43
1:H:55:GLN:CD	1:H:56:PRO:HD2	2.39	0.43
2:M:659:ARG:CB	2:M:662:MET:SD	3.06	0.43
1:H:19:VAL:CG2	1:H:78:LEU:HD22	2.49	0.43
1:F:1004:LEU:HD23	1:F:1024:ASP:HA	2.00	0.43
2:L:616:HIS:HD2	2:L:629:LEU:HD11	1.84	0.43
1:F:1097:LEU:CD2	1:F:1097:LEU:N	2.82	0.43
1:G:54:LEU:HD22	1:G:58:VAL:CG1	2.49	0.43
1:G:6:GLN:HE22	1:G:87:PHE:HA	1.83	0.43
1:F:1086:ASP:O	1:F:1088:ALA:N	2.52	0.43
1:H:1012:VAL:HG11	1:H:1016:ALA:HB3	2.00	0.43
2:J:603:ILE:HG22	2:J:604:ALA:N	2.32	0.43
1:I:88:CYS:SG	1:I:88:CYS:O	2.77	0.43
1:G:6:GLN:NE2	1:G:99:GLY:HA3	2.29	0.43
2:L:601:ASN:HD22	2:L:603:ILE:HD11	1.84	0.43
1:G:71:TYR:CD1	1:G:71:TYR:N	2.86	0.43
2:L:609:GLU:HG2	2:L:724:ILE:HG23	2.00	0.43
1:F:55:GLN:CD	1:F:56:PRO:HD2	2.39	0.42
1:G:1040:ARG:HB3	1:G:1088:ALA:CB	2.49	0.42
2:J:726:ILE:HD12	2:J:727:PHE:CB	2.49	0.42
1:H:71:TYR:CD1	1:H:71:TYR:N	2.87	0.42
2:M:725:LEU:HD12	2:M:726:ILE:H	1.84	0.42
2:K:620:ILE:HG22	2:K:620:ILE:O	2.18	0.42
1:G:41:ASP:O	1:G:43:THR:N	2.51	0.42
1:I:1040:ARG:HB3	1:I:1088:ALA:HB2	2.00	0.42
1:H:1040:ARG:HB2	1:H:1040:ARG:NH1	2.34	0.42
2:J:598:TYR:HD2	2:J:603:ILE:O	2.02	0.42
1:I:1029:PHE:C	1:I:1031:SER:H	2.23	0.42
1:F:1007:SER:HB3	1:F:1021:SER:H	1.83	0.42
1:G:1083:THR:C	1:G:1085:VAL:N	2.73	0.42
2:L:662:MET:HE2	2:L:681:TYR:HB3	2.01	0.42
1:I:1100(B):MET:N	1:I:1100(B):MET:CE	2.83	0.42
2:L:601:ASN:HB2	2:L:603:ILE:CD1	2.49	0.42
1:G:1004:LEU:HD23	1:G:1004:LEU:HA	1.78	0.42
1:F:1081:GLN:O	1:F:1082(A):SER:N	2.52	0.42
2:K:662:MET:HE2	2:K:681:TYR:HB3	2.02	0.42
1:G:94:PRO:HA	1:G:95:PRO:C	2.40	0.42
1:G:105:GLU:HB3	1:G:106:ILE:H	1.49	0.42
1:F:1032:SER:N	1:F:1052:TYR:HE1	2.17	0.42
2:J:657:ASN:O	2:J:659:ARG:N	2.53	0.42
1:F:19:VAL:CG2	1:F:78:LEU:HD22	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1039:GLN:HB2	1:H:1045:LEU:HD21	2.00	0.42
1:G:1075:SER:O	1:G:1076:SER:C	2.58	0.42
1:G:37:GLN:CB	1:G:47:LEU:HD11	2.49	0.42
1:G:1006:GLN:NE2	1:G:1092:CYS:H	2.16	0.42
2:M:628:LEU:CG	2:M:628:LEU:O	2.68	0.42
2:M:626:GLY:HA2	2:M:678:PHE:CD2	2.55	0.42
1:F:55:GLN:CG	1:F:56:PRO:HD2	2.50	0.42
1:I:1048:ILE:HA	1:I:1063:PHE:CD1	2.52	0.42
2:L:678:PHE:CD2	2:L:687:LEU:HD12	2.55	0.42
1:F:1060:ASN:OD1	1:F:1061:GLY:N	2.52	0.42
2:K:659:ARG:NH1	2:K:659:ARG:HG2	2.33	0.42
1:G:59:PRO:HG2	1:G:62:PHE:CD1	2.55	0.42
1:G:1012:VAL:HG12	1:G:1013:LYS:H	1.82	0.42
1:I:1083:THR:C	1:I:1085:VAL:H	2.23	0.42
1:H:1098:LEU:HA	1:H:1098:LEU:HD23	1.76	0.42
1:H:55:GLN:HG3	1:H:56:PRO:HD2	2.02	0.42
1:F:54:LEU:HD22	1:F:58:VAL:CG1	2.49	0.42
1:I:6:GLN:NE2	1:I:99:GLY:HA3	2.27	0.42
2:M:598:TYR:HB3	2:M:603:ILE:O	2.19	0.42
2:M:598:TYR:CD1	2:M:604:ALA:HA	2.51	0.42
2:L:627:LEU:O	2:L:675:PHE:CD1	2.73	0.42
1:I:76:ASN:O	1:I:77:ASN:C	2.58	0.42
1:H:1:ASP:HB3	1:H:95:PRO:CG	2.49	0.42
2:L:709:ASN:HB2	2:L:710:PRO:HD2	2.02	0.42
1:H:1060:ASN:OD1	1:H:1061:GLY:N	2.52	0.42
2:M:616:HIS:HB3	2:M:629:LEU:HD13	2.02	0.42
2:L:600:ARG:HG2	2:L:601:ASN:N	2.33	0.42
2:J:692:PRO:HB3	2:J:732:TYR:HB3	2.02	0.42
1:I:89:GLN:HG2	1:I:90:GLN:O	2.19	0.42
1:I:1039:GLN:HB2	1:I:1045:LEU:HD21	2.01	0.42
1:H:1083:THR:C	1:H:1085:VAL:H	2.23	0.42
1:H:6:GLN:HE22	1:H:87:PHE:HA	1.85	0.41
2:K:699:TYR:HB3	2:K:723:LYS:HB2	2.02	0.41
1:I:19:VAL:CG2	1:I:78:LEU:HD22	2.50	0.41
2:K:730:LYS:HB2	2:K:733:GLU:OE1	2.20	0.41
2:J:635:ILE:O	2:J:636:ARG:C	2.58	0.41
1:H:1054:ASP:OD1	1:H:1055:GLY:N	2.53	0.41
1:G:55:GLN:CG	1:G:56:PRO:HD2	2.50	0.41
1:I:59:PRO:HG2	1:I:62:PHE:CD1	2.55	0.41
1:H:1048:ILE:HG23	1:H:1063:PHE:CD1	2.54	0.41
1:H:20:THR:OG1	1:H:74:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:PRO:HA	1:F:95:PRO:C	2.41	0.41
1:H:1006:GLN:HE22	1:H:1091:PHE:CA	2.21	0.41
2:K:723:LYS:HG2	2:K:723:LYS:H	1.63	0.41
1:G:1048:ILE:HA	1:G:1063:PHE:CD1	2.54	0.41
1:G:1083:THR:C	1:G:1085:VAL:H	2.22	0.41
2:J:640:SER:OG	2:J:706:THR:OG1	2.37	0.41
2:M:601:ASN:O	2:M:602:ASN:CB	2.69	0.41
1:H:1081:GLN:O	1:H:1082(A):SER:N	2.53	0.41
2:K:726:ILE:HD12	2:K:727:PHE:CB	2.51	0.41
1:I:89:GLN:HB2	1:I:98:PHE:CE2	2.54	0.41
1:G:49:TYR:CG	1:G:1098:LEU:HD11	2.56	0.41
2:M:598:TYR:HB3	2:M:602:ASN:C	2.40	0.41
1:F:59:PRO:HG2	1:F:62:PHE:CD1	2.56	0.41
2:J:725:LEU:HD12	2:J:726:ILE:H	1.84	0.41
1:H:1022:CYS:O	1:H:1077:THR:HG23	2.20	0.41
1:H:1097:LEU:N	1:H:1097:LEU:HD22	2.35	0.41
2:M:643:ILE:HB	2:M:699:TYR:HB2	2.03	0.41
1:F:1052:TYR:O	1:F:1052(A):PRO:C	2.59	0.41
2:L:726:ILE:HD12	2:L:727:PHE:CB	2.50	0.41
1:I:1012:VAL:HG21	1:I:1018:VAL:HG13	2.02	0.41
1:H:1012:VAL:HG21	1:H:1018:VAL:HG11	2.02	0.41
2:K:730:LYS:O	2:K:734:ILE:HG13	2.20	0.41
2:L:631:ILE:HD13	2:L:642:TYR:OH	2.21	0.41
2:M:730:LYS:O	2:M:734:ILE:HG13	2.21	0.41
2:K:690:SER:O	2:K:691:ASN:HB2	2.21	0.41
1:I:1004:LEU:HD23	1:I:1024:ASP:HA	2.03	0.41
2:M:620:ILE:O	2:M:621:ASN:HB2	2.21	0.41
1:H:1093:ALA:CB	1:H:1100(B):MET:HB3	2.41	0.41
1:G:1093:ALA:HB2	1:G:1103:TRP:CD2	2.56	0.41
2:M:718:THR:HA	2:M:721:ILE:HD12	2.02	0.41
1:I:1048:ILE:HG12	1:I:1063:PHE:CD1	2.56	0.41
1:G:76:ASN:O	1:G:77:ASN:C	2.59	0.41
2:L:695:LYS:HA	2:L:730:LYS:HA	2.02	0.41
1:G:1038:LYS:HE2	1:G:1040:ARG:HD3	2.02	0.41
2:K:631:ILE:HD13	2:K:642:TYR:OH	2.20	0.41
1:H:94:PRO:HA	1:H:95:PRO:C	2.41	0.41
2:K:620:ILE:H	2:K:629:LEU:HA	1.86	0.41
1:H:1093:ALA:HB2	1:H:1103:TRP:CD2	2.56	0.41
1:F:49:TYR:CG	1:F:1098:LEU:HD11	2.56	0.41
1:I:6:GLN:HE22	1:I:87:PHE:HA	1.86	0.41
1:I:1097:LEU:CD2	1:I:1097:LEU:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:592:ARG:N	2:M:596:PHE:CE2	2.89	0.41
1:I:62:PHE:O	1:I:63:SER:CB	2.69	0.41
2:K:696:VAL:HG21	2:K:734:ILE:HD12	2.02	0.41
1:F:1089:VAL:C	1:F:1090:TYR:CD1	2.94	0.41
1:F:1007:SER:OG	1:F:1008:GLY:N	2.53	0.41
1:F:1021:SER:HB3	1:F:1079:TYR:CD2	2.54	0.41
1:I:94:PRO:HA	1:I:95:PRO:C	2.40	0.41
1:I:1081:GLN:O	1:I:1082(A):SER:N	2.54	0.41
2:J:621:ASN:CB	2:J:628:LEU:HD23	2.50	0.41
1:F:89:GLN:HG2	1:F:90:GLN:O	2.20	0.41
1:F:46:PHE:HB2	1:F:1101:ASP:HA	2.03	0.41
1:I:54:LEU:HD22	1:I:58:VAL:CG1	2.51	0.41
1:H:1039:GLN:HB2	1:H:1045:LEU:HD23	2.02	0.41
1:H:1089:VAL:CG1	1:H:1090:TYR:N	2.84	0.41
1:F:88:CYS:SG	1:F:88:CYS:O	2.79	0.41
1:G:14:SER:O	1:G:17:ASP:OD2	2.38	0.41
1:H:1100:TYR:O	1:H:1100:TYR:CD1	2.74	0.41
2:K:678:PHE:CD2	2:K:687:LEU:HD12	2.56	0.41
2:K:726:ILE:HD12	2:K:727:PHE:N	2.35	0.41
2:K:725:LEU:HD11	2:K:727:PHE:O	2.21	0.41
1:H:44:VAL:HG11	1:H:1103:TRP:CD2	2.55	0.41
2:M:659:ARG:NH1	2:M:659:ARG:CG	2.84	0.41
2:J:726:ILE:HD12	2:J:727:PHE:N	2.36	0.41
2:M:689:ILE:HD11	2:M:696:VAL:HG21	2.03	0.41
1:F:1004:LEU:HA	1:F:1004:LEU:HD23	1.83	0.41
1:F:1006:GLN:CG	1:F:1092:CYS:SG	3.09	0.40
2:L:662:MET:CE	2:L:681:TYR:HB3	2.51	0.40
1:I:1011:LEU:CD1	1:I:1110:THR:HG23	2.42	0.40
1:I:1097:LEU:N	2:M:685:LEU:HD13	2.32	0.40
2:K:628:LEU:O	2:K:628:LEU:CG	2.70	0.40
1:G:4:MET:HE3	1:G:90:GLN:HB3	2.02	0.40
1:F:1089:VAL:CG1	1:F:1090:TYR:N	2.84	0.40
1:G:98:PHE:CD1	1:G:98:PHE:N	2.90	0.40
1:I:1006:GLN:NE2	1:I:1092:CYS:H	2.19	0.40
1:H:1086:ASP:O	1:H:1088:ALA:N	2.54	0.40
1:F:1029:PHE:C	1:F:1031:SER:H	2.24	0.40
2:M:609:GLU:HG2	2:M:724:ILE:HG23	2.02	0.40
1:H:24:ARG:HH21	1:I:24:ARG:HE	1.68	0.40
1:H:55:GLN:CG	1:H:56:PRO:HD2	2.51	0.40
1:H:50:TYR:CZ	2:L:654:GLU:HB2	2.55	0.40
2:K:662:MET:HG2	2:K:681:TYR:CE1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:596:PHE:HB2	2:L:598:TYR:CZ	2.56	0.40
2:L:635:ILE:O	2:L:636:ARG:C	2.59	0.40
2:J:603:ILE:CG2	2:J:604:ALA:H	2.29	0.40
2:M:695:LYS:HA	2:M:730:LYS:HA	2.04	0.40
1:H:76:ASN:O	1:H:77:ASN:C	2.60	0.40
2:J:709:ASN:HB2	2:J:710:PRO:CD	2.51	0.40
1:I:29:ILE:O	1:I:30:ARG:HG3	2.21	0.40
2:L:637:LYS:O	2:L:703:LYS:HD2	2.22	0.40
1:I:1004:LEU:HD11	1:I:1094:ARG:HB3	2.04	0.40
1:G:1054:ASP:OD1	1:G:1055:GLY:N	2.54	0.40
2:M:708:ILE:HG13	2:M:709:ASN:ND2	2.36	0.40
1:I:1006:GLN:CG	1:I:1092:CYS:SG	3.09	0.40
2:J:620:ILE:O	2:J:621:ASN:HB2	2.21	0.40
2:J:660:TYR:CE1	2:J:709:ASN:HA	2.57	0.40
2:L:600:ARG:C	2:L:602:ASN:N	2.71	0.40
1:G:1012:VAL:HG12	1:G:1016:ALA:HB3	2.03	0.40
2:L:664:ASN:O	2:L:664:ASN:CG	2.59	0.40
1:H:1094:ARG:O	1:H:1094:ARG:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	224/252 (89%)	168 (75%)	36 (16%)	20 (9%)	1	16
1	G	225/252 (89%)	165 (73%)	37 (16%)	23 (10%)	1	13
1	H	225/252 (89%)	164 (73%)	40 (18%)	21 (9%)	1	15
1	I	224/252 (89%)	165 (74%)	39 (17%)	20 (9%)	1	16
2	J	142/144 (99%)	100 (70%)	28 (20%)	14 (10%)	1	13
2	K	142/144 (99%)	100 (70%)	28 (20%)	14 (10%)	1	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	141/144 (98%)	105 (74%)	26 (18%)	10 (7%)	1	23
2	M	142/144 (99%)	100 (70%)	30 (21%)	12 (8%)	1	17
All	All	1465/1584 (92%)	1067 (73%)	264 (18%)	134 (9%)	1	16

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1033	TRP
1	F	1098	LEU
1	G	1002	VAL
1	G	1033	TRP
1	G	1098	LEU
1	H	60	SER
1	H	1002	VAL
1	H	1003	GLN
1	H	1033	TRP
1	H	1098	LEU
1	I	108	ARG
1	I	1033	TRP
1	I	1098	LEU
2	J	628	LEU
2	J	710	PRO
2	J	730	LYS
2	K	593	ASP
2	K	628	LEU
2	K	710	PRO
2	K	721	ILE
2	L	628	LEU
2	L	658	ASP
2	L	710	PRO
2	M	628	LEU
2	M	629	LEU
2	M	710	PRO
1	F	42	GLY
1	F	60	SER
1	F	63	SER
1	F	77	ASN
1	F	1044	GLY
1	F	1087	SER
1	F	1108	SER
1	G	42	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	60	SER
1	G	63	SER
1	G	1044	GLY
1	G	1082	LEU
1	G	1087	SER
1	G	1108	SER
1	H	42	GLY
1	H	63	SER
1	H	77	ASN
1	H	107	LYS
1	H	1044	GLY
1	H	1082	LEU
1	H	1087	SER
1	H	1108	SER
1	I	42	GLY
1	I	60	SER
1	I	63	SER
1	I	77	ASN
1	I	1003	GLN
1	I	1044	GLY
1	I	1087	SER
1	I	1108	SER
2	J	598	TYR
2	J	599	ASP
2	J	629	LEU
2	J	636	ARG
2	J	658	ASP
2	J	721	ILE
2	K	629	LEU
2	K	636	ARG
2	K	658	ASP
2	L	601	ASN
2	L	629	LEU
2	L	636	ARG
2	L	721	ILE
2	L	730	LYS
2	M	658	ASP
2	M	721	ILE
1	F	27	GLN
1	F	1014	PRO
1	F	1066	LYS
1	F	1082	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	27	GLN
1	G	77	ASN
1	G	1003	GLN
1	G	1014	PRO
1	H	27	GLN
1	I	27	GLN
1	I	1014	PRO
1	I	1082	LEU
2	J	603	ILE
2	K	600	ARG
2	K	627	LEU
2	M	636	ARG
2	M	651	GLY
2	M	730	LYS
1	F	28	ASP
1	F	80	GLN
1	G	28	ASP
1	G	80	GLN
1	G	106	ILE
1	H	28	ASP
1	H	80	GLN
1	H	1014	PRO
1	I	28	ASP
2	J	651	GLY
2	K	601	ASN
2	K	602	ASN
2	L	651	GLY
1	F	32	TYR
1	F	1076	SER
1	G	78	LEU
1	G	1066	LYS
1	G	1076	SER
1	G	1112	SER
1	I	78	LEU
1	I	80	GLN
1	I	106	ILE
1	I	1112	SER
2	J	610	SER
2	K	651	GLY
2	K	667	SER
2	K	734	ILE
2	M	650	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1053	GLY
1	G	1026	GLY
1	H	78	LEU
1	H	106	ILE
1	F	106	ILE
1	H	1053	GLY
2	M	605	VAL
2	M	692	PRO
1	F	39	LYS
1	I	39	LYS
2	J	734	ILE
1	G	39	LYS
1	H	39	LYS
2	J	692	PRO
2	L	692	PRO
2	M	734	ILE

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	F	188/201 (94%)	171 (91%)	17 (9%)	12	49
1	G	187/201 (93%)	171 (91%)	16 (9%)	13	51
1	H	187/201 (93%)	171 (91%)	16 (9%)	13	51
1	I	188/201 (94%)	170 (90%)	18 (10%)	10	46
2	J	128/131 (98%)	119 (93%)	9 (7%)	19	60
2	K	128/131 (98%)	120 (94%)	8 (6%)	22	63
2	L	127/131 (97%)	120 (94%)	7 (6%)	27	68
2	M	128/131 (98%)	122 (95%)	6 (5%)	32	72
All	All	1261/1328 (95%)	1164 (92%)	97 (8%)	16	56

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	11	LEU
1	F	24	ARG
1	F	30	ARG
1	F	74	THR
1	F	89	GLN
1	F	90	GLN
1	F	97	THR
1	F	1030	ASN
1	F	1040	ARG
1	F	1070	THR
1	F	1094	ARG
1	F	1097	LEU
1	F	1099	ARG
1	F	1100(B)	MET
1	F	1101	ASP
1	F	1102	TYR
1	F	1110	THR
1	G	11	LEU
1	G	24	ARG
1	G	30	ARG
1	G	33	LEU
1	G	74	THR
1	G	89	GLN
1	G	90	GLN
1	G	97	THR
1	G	1030	ASN
1	G	1040	ARG
1	G	1070	THR
1	G	1094	ARG
1	G	1099	ARG
1	G	1100(B)	MET
1	G	1101	ASP
1	G	1102	TYR
1	H	11	LEU
1	H	24	ARG
1	H	30	ARG
1	H	70	ASP
1	H	74	THR
1	H	89	GLN
1	H	90	GLN
1	H	97	THR
1	H	1030	ASN
1	H	1040	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	1070	THR
1	H	1094	ARG
1	H	1099	ARG
1	H	1100(B)	MET
1	H	1101	ASP
1	H	1102	TYR
1	I	1	ASP
1	I	11	LEU
1	I	24	ARG
1	I	30	ARG
1	I	70	ASP
1	I	74	THR
1	I	89	GLN
1	I	90	GLN
1	I	97	THR
1	I	1030	ASN
1	I	1040	ARG
1	I	1070	THR
1	I	1094	ARG
1	I	1099	ARG
1	I	1100(B)	MET
1	I	1101	ASP
1	I	1102	TYR
1	I	1110	THR
2	J	600	ARG
2	J	602	ASN
2	J	652	LEU
2	J	660	TYR
2	J	667	SER
2	J	671	ASP
2	J	699	TYR
2	J	713	ASN
2	J	730	LYS
2	K	593	ASP
2	K	652	LEU
2	K	660	TYR
2	K	667	SER
2	K	671	ASP
2	K	699	TYR
2	K	709	ASN
2	K	730	LYS
2	L	600	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	652	LEU
2	L	660	TYR
2	L	667	SER
2	L	671	ASP
2	L	699	TYR
2	L	730	LYS
2	M	601	ASN
2	M	652	LEU
2	M	660	TYR
2	M	667	SER
2	M	699	TYR
2	M	730	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	6	GLN
1	F	37	GLN
1	F	1006	GLN
1	F	1035	ASN
1	F	1039	GLN
1	F	1043	GLN
1	F	1058	ASN
1	G	6	GLN
1	G	37	GLN
1	G	38	GLN
1	G	77	ASN
1	G	1006	GLN
1	G	1035	ASN
1	G	1043	GLN
1	G	1058	ASN
1	H	6	GLN
1	H	37	GLN
1	H	38	GLN
1	H	1006	GLN
1	H	1043	GLN
1	H	1058	ASN
1	I	6	GLN
1	I	37	GLN
1	I	38	GLN
1	I	77	ASN
1	I	1006	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1035	ASN
1	I	1043	GLN
1	I	1058	ASN
2	J	630	ASN
2	J	697	ASN
2	J	705	ASN
2	J	709	ASN
2	J	713	ASN
2	K	601	ASN
2	K	630	ASN
2	K	697	ASN
2	K	705	ASN
2	K	709	ASN
2	K	713	ASN
2	L	601	ASN
2	L	630	ASN
2	L	697	ASN
2	L	705	ASN
2	L	709	ASN
2	L	713	ASN
2	M	601	ASN
2	M	630	ASN
2	M	697	ASN
2	M	705	ASN
2	M	709	ASN
2	M	713	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	F	228/252 (90%)	-0.32	0	100	100	10, 10, 25, 100	0
1	G	229/252 (90%)	-0.26	0	100	100	10, 10, 28, 70	0
1	H	229/252 (90%)	-0.31	0	100	100	10, 10, 23, 75	0
1	I	228/252 (90%)	-0.31	0	100	100	10, 10, 21, 64	0
2	J	144/144 (100%)	0.17	0	100	100	10, 10, 38, 87	0
2	K	144/144 (100%)	-0.18	3 (2%)	67	51	10, 10, 42, 78	0
2	L	143/144 (99%)	0.32	3 (2%)	67	51	10, 10, 53, 80	0
2	M	144/144 (100%)	-0.24	0	100	100	10, 10, 30, 75	0
All	All	1489/1584 (94%)	-0.18	6 (0%)	93	87	10, 10, 33, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	707	ILE	3.0
2	L	629	LEU	2.9
2	L	616	HIS	2.4
2	K	708	ILE	2.3
2	K	712	GLU	2.1
2	L	632	ASP	2.1

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.