



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:22 am GMT

PDB ID : 3F12  
Title : Germline V-genes sculpt the binding site of a family of antibodies neutralizing human cytomegalovirus  
Authors : Thomson, C.A.; Bryson, S.; McLean, G.R.; Creagh, A.L.; Pai, E.F.; Schrader, J.W.  
Deposited on : 2008-10-27  
Resolution : 2.95 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

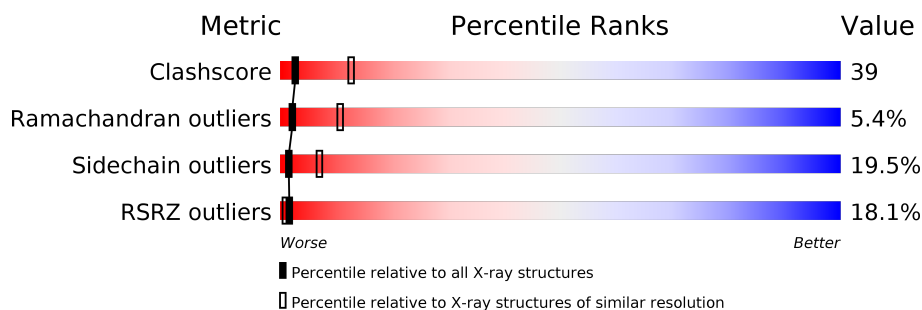
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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  $\geq 3$ , 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	216	<div> <div>13%</div> <div>44%</div> <div>44%</div> <div>9%</div> <div>.</div> </div>
1	C	216	<div> <div>21%</div> <div>36%</div> <div>47%</div> <div>16%</div> <div>.</div> </div>
2	B	242	<div> <div>17%</div> <div>33%</div> <div>37%</div> <div>12%</div> <div>18%</div> </div>
2	D	242	<div> <div>14%</div> <div>31%</div> <div>42%</div> <div>9%</div> <div>.</div> <div>17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6303 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 M2J1 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1630	1024	275	327	4			
1	C	213	Total	C	N	O	S	0	0	0
			1642	1030	277	331	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	PDB 3F12
C	0	MET	-	EXPRESSION TAG	PDB 3F12

- Molecule 2 is a protein called 8f9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total	C	N	O	S	0	0	0
			1508	959	253	290	6			
2	D	202	Total	C	N	O	S	0	0	0
			1523	967	255	295	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	235	LEU	-	EXPRESSION TAG	PDB 3F12
B	236	GLU	-	EXPRESSION TAG	PDB 3F12
B	237	HIS	-	EXPRESSION TAG	PDB 3F12
B	238	HIS	-	EXPRESSION TAG	PDB 3F12
B	239	HIS	-	EXPRESSION TAG	PDB 3F12
B	240	HIS	-	EXPRESSION TAG	PDB 3F12
B	241	HIS	-	EXPRESSION TAG	PDB 3F12
B	242	HIS	-	EXPRESSION TAG	PDB 3F12
D	235	LEU	-	EXPRESSION TAG	PDB 3F12
D	236	GLU	-	EXPRESSION TAG	PDB 3F12

*Continued on next page...*

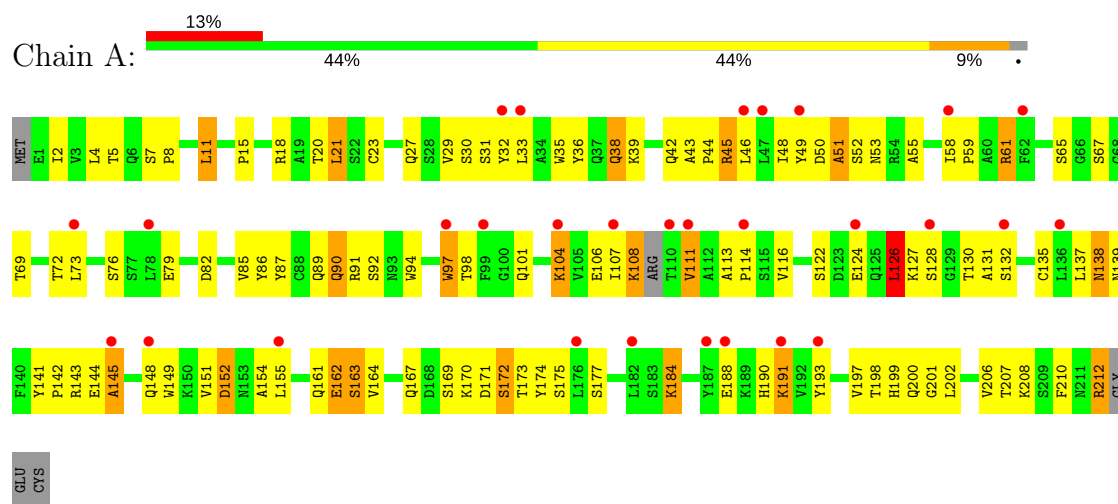
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	237	HIS	-	EXPRESSION TAG	PDB 3F12
D	238	HIS	-	EXPRESSION TAG	PDB 3F12
D	239	HIS	-	EXPRESSION TAG	PDB 3F12
D	240	HIS	-	EXPRESSION TAG	PDB 3F12
D	241	HIS	-	EXPRESSION TAG	PDB 3F12
D	242	HIS	-	EXPRESSION TAG	PDB 3F12

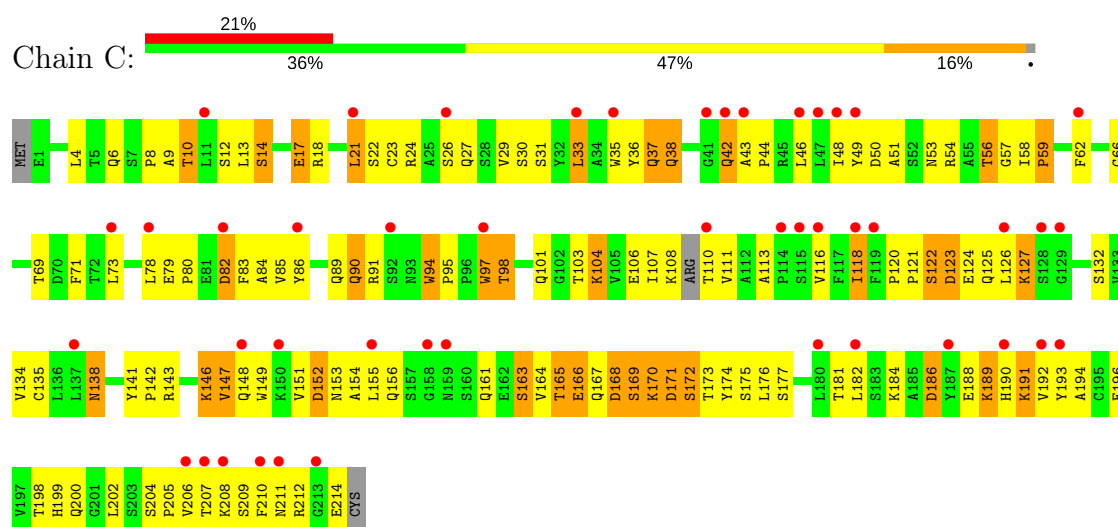
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: M2J1 Fab

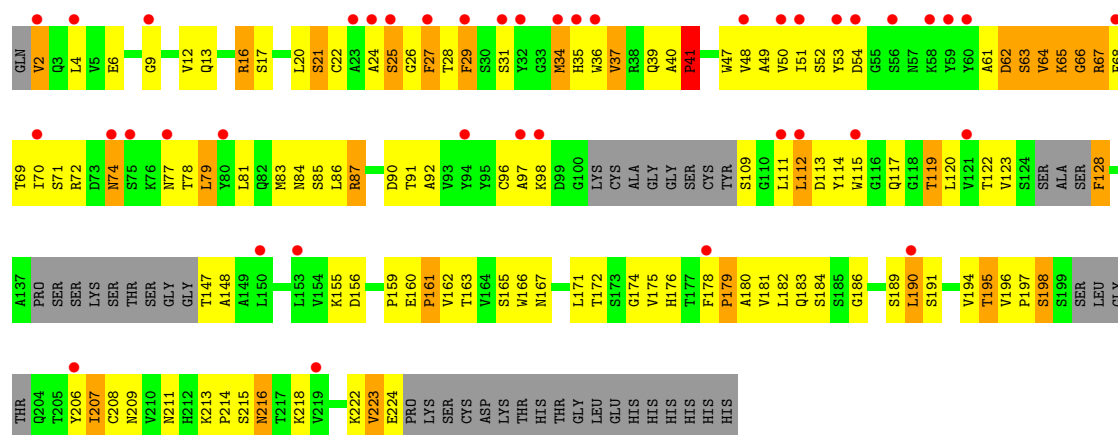


#### • Molecule 1: M2J1 Fab

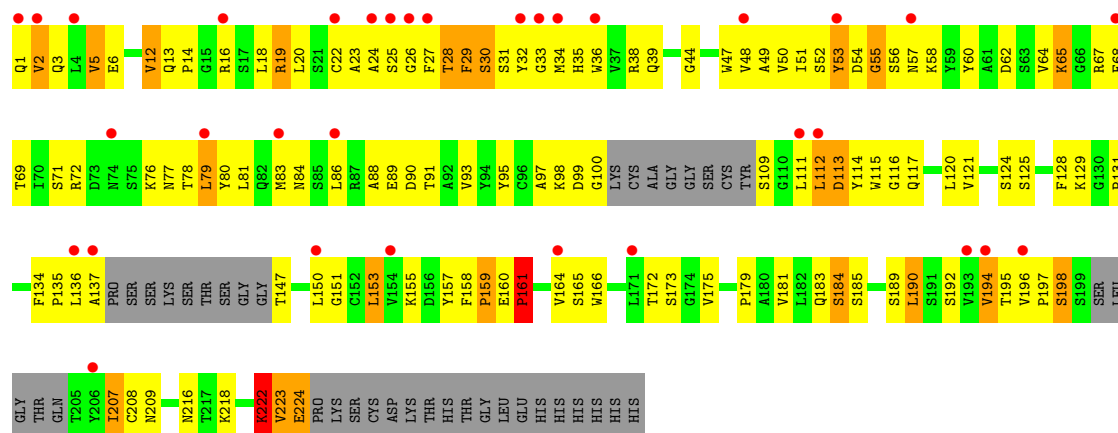


#### • Molecule 2: 8f9 Fab





### • Molecule 2: 8f9 Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.86Å 87.86Å 241.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.95 47.34 – 2.93	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 93.0 (47.34-2.93)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.65 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.300 , 0.320 0.304 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	6303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/1668	0.79	0/2270
1	C	0.50	0/1680	0.84	0/2285
2	B	0.47	0/1541	0.84	2/2091 (0.1%)
2	D	0.51	0/1557	0.89	2/2115 (0.1%)
All	All	0.49	0/6446	0.84	4/8761 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	55	GLY	N-CA-C	6.86	130.24	113.10
2	B	77	ASN	N-CA-C	5.65	126.25	111.00
2	B	66	GLY	N-CA-C	-5.40	99.59	113.10
2	D	44	GLY	N-CA-C	5.27	126.27	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	53	TYR	Sidechain



## 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	1630	0	1580	107	8
1	C	1642	0	1585	141	8
2	B	1508	0	1472	126	0
2	D	1523	0	1484	167	0
All	All	6303	0	6121	489	8

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 39.

All (489) 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)
2:B:218:LYS:HB2	2:D:16:ARG:HH21	1.09	1.09
2:D:12:VAL:HG22	2:D:16:ARG:HD3	1.23	1.09
1:A:61:ARG:NH1	1:A:79:GLU:HG3	1.75	1.02
2:D:135:PRO:HB3	2:D:223:VAL:HG22	1.42	1.01
1:C:110:THR:O	1:C:141:TYR:HB3	1.57	1.01
1:C:97:TRP:HE1	2:D:35:HIS:CE1	1.77	1.01
1:C:193:TYR:O	1:C:209:SER:HB2	1.62	0.99
2:D:71:SER:HB3	2:D:80:TYR:HB2	1.46	0.96
2:B:160:GLU:HG2	2:B:161:PRO:HA	1.44	0.96
2:B:218:LYS:HE3	2:D:16:ARG:HE	1.27	0.96
2:D:55:GLY:HA2	2:D:72:ARG:HD3	1.50	0.92
1:A:18:ARG:HG3	1:A:76:SER:HA	1.53	0.91
1:C:38:GLN:NE2	2:D:39:GLN:HE22	1.68	0.91
2:B:4:LEU:HG	2:B:98:LYS:HZ3	1.32	0.90
2:D:135:PRO:HB3	2:D:223:VAL:CG2	2.03	0.89
2:D:29:PHE:O	2:D:53:TYR:HD1	1.54	0.89
2:B:218:LYS:HB2	2:D:16:ARG:NH2	1.86	0.89
2:D:34:MET:HB2	2:D:53:TYR:CE2	2.12	0.84
1:A:94:TRP:HB2	1:A:97:TRP:CZ3	2.13	0.84
1:A:171:ASP:O	1:A:172:SER:HB3	1.75	0.83
2:B:34:MET:HE3	2:B:98:LYS:HA	1.58	0.83
2:D:5:VAL:HG23	2:D:23:ALA:HB3	1.61	0.82
2:B:4:LEU:HD11	2:B:98:LYS:HG3	1.62	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLU:OE2	2:D:95:TYR:HA	1.79	0.82
2:D:13:GLN:H	2:D:16:ARG:HD2	1.45	0.81
2:D:109:SER:OG	2:D:111:LEU:HB3	1.80	0.81
1:C:97:TRP:HE1	2:D:35:HIS:HE1	1.24	0.81
2:B:17:SER:HB2	2:B:83:MET:O	1.81	0.80
1:C:108:LYS:HA	1:C:169:SER:HA	1.62	0.80
1:C:38:GLN:HE22	2:D:39:GLN:HE22	1.26	0.80
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.62	0.80
2:D:13:GLN:N	2:D:16:ARG:HD2	1.98	0.79
2:D:53:TYR:HA	2:D:72:ARG:NH1	1.99	0.78
2:B:4:LEU:HG	2:B:98:LYS:NZ	1.97	0.78
2:D:53:TYR:CD2	2:D:72:ARG:NH1	2.50	0.77
1:C:56:THR:O	1:C:58:ILE:N	2.18	0.77
1:C:116:VAL:O	1:C:208:LYS:HD2	1.85	0.77
2:D:93:VAL:HG22	2:D:120:LEU:CD1	2.14	0.77
2:B:41:PRO:HD3	2:B:92:ALA:HA	1.66	0.76
2:D:12:VAL:HG22	2:D:16:ARG:CD	2.12	0.75
1:C:8:PRO:O	1:C:103:THR:HG23	1.86	0.75
2:D:19:ARG:HH11	2:D:19:ARG:HG3	1.49	0.75
2:D:52:SER:H	2:D:57:ASN:HB2	1.50	0.74
2:D:14:PRO:HD3	2:D:124:SER:O	1.87	0.74
1:A:30:SER:OG	1:A:31:SER:N	2.21	0.74
2:B:34:MET:CE	2:B:98:LYS:HA	2.16	0.74
2:D:52:SER:HB3	2:D:57:ASN:CG	2.08	0.74
1:A:39:LYS:HB2	1:A:42:GLN:NE2	2.03	0.73
1:A:85:VAL:HG22	1:A:104:LYS:HG2	1.67	0.73
1:A:39:LYS:HB2	1:A:42:GLN:HE21	1.54	0.73
2:B:97:ALA:HB1	2:B:112:LEU:HB3	1.71	0.73
1:C:50:ASP:HB2	1:C:53:ASN:HD22	1.54	0.72
2:B:218:LYS:CE	2:D:16:ARG:HE	2.02	0.72
2:B:62:ASP:O	2:B:64:VAL:N	2.23	0.72
1:C:56:THR:O	1:C:58:ILE:HG12	1.91	0.71
2:D:13:GLN:H	2:D:16:ARG:CD	2.02	0.71
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.26	0.71
1:C:108:LYS:HA	1:C:169:SER:CA	2.21	0.70
2:D:13:GLN:H	2:D:16:ARG:HH11	1.37	0.70
1:C:43:ALA:HB2	2:D:116:GLY:O	1.91	0.70
2:D:53:TYR:HA	2:D:72:ARG:CZ	2.20	0.70
1:A:49:TYR:O	1:A:50:ASP:HB2	1.90	0.69
1:C:27:GLN:O	1:C:29:VAL:HG13	1.92	0.69
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.57	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:SER:HA	2:B:79:LEU:O	1.92	0.69
1:A:32:TYR:HD1	1:A:91:ARG:HE	1.39	0.69
1:C:191:LYS:O	1:C:211:ASN:HA	1.93	0.69
2:B:54:ASP:HA	2:B:74:ASN:ND2	2.07	0.68
2:D:1:GLN:O	2:D:26:GLY:HA3	1.93	0.68
2:D:47:TRP:HZ2	2:D:50:VAL:HB	1.58	0.68
1:C:43:ALA:HB2	2:D:117:GLN:HA	1.76	0.68
2:D:32:TYR:O	2:D:53:TYR:CG	2.46	0.68
1:C:13:LEU:HD21	1:C:18:ARG:O	1.94	0.68
2:B:160:GLU:CG	2:B:161:PRO:HA	2.20	0.67
2:B:218:LYS:HE3	2:D:16:ARG:NE	2.06	0.67
2:D:222:LYS:O	2:D:223:VAL:HB	1.94	0.67
1:C:43:ALA:H	2:D:117:GLN:HA	1.59	0.67
2:B:4:LEU:CD1	2:B:98:LYS:HG3	2.24	0.67
1:C:94:TRP:HB2	1:C:97:TRP:CE3	2.29	0.67
1:C:125:GLN:HE22	1:C:132:SER:HB2	1.60	0.67
1:C:79:GLU:O	1:C:82:ASP:HB2	1.95	0.66
1:A:61:ARG:HH11	1:A:79:GLU:HG3	1.53	0.66
1:A:97:TRP:NE1	2:B:47:TRP:CE2	2.63	0.66
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.76	0.66
1:A:50:ASP:O	1:A:51:ALA:CB	2.43	0.66
1:C:169:SER:O	1:C:170:LYS:HG3	1.95	0.66
1:A:91:ARG:O	1:A:91:ARG:HG3	1.95	0.66
2:D:19:ARG:NH1	2:D:19:ARG:HG3	2.08	0.66
2:D:93:VAL:HG22	2:D:120:LEU:HD12	1.77	0.66
1:A:49:TYR:O	1:A:53:ASN:HB2	1.96	0.65
2:B:4:LEU:HD11	2:B:98:LYS:CG	2.26	0.65
2:B:165:SER:HB2	2:B:209:ASN:HB2	1.77	0.65
2:B:112:LEU:HD13	2:B:112:LEU:N	2.12	0.65
2:B:180:ALA:HB2	2:B:190:LEU:HB3	1.79	0.65
1:C:108:LYS:HG3	1:C:108:LYS:O	1.95	0.64
2:D:14:PRO:HD3	2:D:124:SER:C	2.18	0.64
2:B:12:VAL:HG11	2:B:86:LEU:CD1	2.28	0.64
2:D:12:VAL:CG2	2:D:16:ARG:HD3	2.15	0.64
2:D:13:GLN:H	2:D:16:ARG:NH1	1.96	0.64
2:D:135:PRO:CB	2:D:223:VAL:HG22	2.25	0.63
1:C:164:VAL:HG22	1:C:176:LEU:HD12	1.80	0.63
1:C:125:GLN:C	1:C:127:LYS:H	2.02	0.63
1:C:95:PRO:HB3	1:C:97:TRP:CZ3	2.33	0.63
2:D:55:GLY:HA2	2:D:72:ARG:CD	2.27	0.63
1:A:113:ALA:HB2	1:A:201:GLY:O	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ASP:HB2	1:C:53:ASN:ND2	2.13	0.63
2:D:164:VAL:HG11	2:D:192:SER:CB	2.29	0.63
1:C:38:GLN:HE22	2:D:39:GLN:NE2	1.96	0.62
2:B:172:THR:O	2:B:175:VAL:HG23	1.99	0.62
1:A:50:ASP:O	1:A:51:ALA:HB3	1.98	0.62
2:D:24:ALA:HB1	2:D:27:PHE:HE1	1.63	0.62
2:B:84:ASN:O	2:B:85:SER:HB3	1.99	0.62
1:C:143:ARG:HB2	1:C:174:TYR:CE2	2.35	0.62
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.33	0.62
2:B:4:LEU:HD13	2:B:96:CYS:O	1.99	0.62
1:C:104:LYS:HD3	1:C:106:GLU:CG	2.30	0.62
1:A:167:GLN:HB2	1:A:174:TYR:CZ	2.34	0.61
2:B:211:ASN:HD21	2:B:213:LYS:HG3	1.66	0.61
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.83	0.61
2:B:12:VAL:HG22	2:B:16:ARG:HB2	1.82	0.61
2:B:2:VAL:HB	2:B:98:LYS:HE3	1.81	0.61
1:C:14:SER:HB2	1:C:17:GLU:OE1	2.01	0.61
1:A:163:SER:OG	2:B:179:PRO:O	2.11	0.61
2:D:111:LEU:HD12	2:D:111:LEU:O	2.02	0.60
1:A:97:TRP:CD1	2:B:47:TRP:CG	2.90	0.60
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.36	0.60
1:C:90:GLN:HG2	1:C:91:ARG:N	2.17	0.60
1:C:66:GLY:HA3	1:C:71:PHE:CD1	2.37	0.59
2:D:19:ARG:HH11	2:D:19:ARG:CG	2.16	0.59
2:B:29:PHE:O	2:B:72:ARG:NH2	2.34	0.59
1:C:104:LYS:HD3	1:C:106:GLU:HG3	1.83	0.59
2:B:98:LYS:HD2	2:B:114:TYR:HB2	1.84	0.59
2:D:91:THR:HG23	2:D:91:THR:O	2.02	0.59
1:C:168:ASP:OD1	1:C:171:ASP:HB2	2.02	0.59
2:D:207:ILE:HD13	2:D:222:LYS:HA	1.84	0.59
1:C:171:ASP:HB3	1:C:173:THR:HG23	1.84	0.59
2:D:13:GLN:N	2:D:16:ARG:HH11	2.00	0.59
1:C:138:ASN:ND2	1:C:175:SER:OG	2.36	0.59
1:A:114:PRO:HD2	1:A:202:LEU:HD11	1.85	0.58
1:C:49:TYR:HB2	2:D:111:LEU:CD1	2.33	0.58
2:B:54:ASP:HA	2:B:74:ASN:HD21	1.67	0.58
2:D:150:LEU:HD11	2:D:196:VAL:HG21	1.85	0.58
2:D:24:ALA:HB3	2:D:29:PHE:HD1	1.69	0.58
1:A:199:HIS:HB3	1:A:202:LEU:HD12	1.84	0.58
1:A:55:ALA:O	1:A:58:ILE:HG12	2.04	0.58
1:A:111:VAL:O	1:A:111:VAL:HG13	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TRP:HD1	1:A:94:TRP:O	1.86	0.58
2:D:57:ASN:O	2:D:58:LYS:HG3	2.03	0.58
1:A:48:ILE:HA	1:A:53:ASN:O	2.03	0.58
2:D:100:GLY:HA2	2:D:113:ASP:OD1	2.03	0.58
2:D:53:TYR:CG	2:D:72:ARG:NH2	2.68	0.57
2:B:4:LEU:HD21	2:B:34:MET:HE2	1.86	0.57
2:D:222:LYS:HD3	2:D:224:GLU:HG2	1.85	0.57
2:D:34:MET:SD	2:D:53:TYR:CZ	2.98	0.57
1:A:21:LEU:HD23	1:A:21:LEU:N	2.19	0.57
1:C:54:ARG:HG3	1:C:54:ARG:HH11	1.69	0.57
1:A:171:ASP:HB2	1:A:173:THR:OG1	2.04	0.57
1:A:97:TRP:CZ2	2:B:35:HIS:HE1	2.22	0.57
2:D:13:GLN:CA	2:D:16:ARG:HD2	2.34	0.57
1:C:143:ARG:HG2	1:C:143:ARG:O	2.05	0.57
2:D:5:VAL:CG2	2:D:23:ALA:HB3	2.33	0.57
1:A:23:CYS:SG	1:A:33:LEU:HD21	2.45	0.57
2:B:174:GLY:O	2:B:194:VAL:HA	2.05	0.57
2:B:207:ILE:HG12	2:B:222:LYS:HA	1.87	0.57
1:C:107:ILE:O	1:C:108:LYS:HG2	2.05	0.57
1:A:207:THR:CG2	1:A:208:LYS:N	2.67	0.57
1:A:113:ALA:HB1	1:A:202:LEU:HG	1.87	0.56
1:A:152:ASP:OD2	1:A:191:LYS:HD2	2.04	0.56
1:C:186:ASP:N	1:C:186:ASP:OD1	2.37	0.56
1:C:21:LEU:N	1:C:21:LEU:HD23	2.20	0.56
1:C:168:ASP:O	1:C:169:SER:HB3	2.05	0.56
2:D:29:PHE:O	2:D:53:TYR:CD1	2.46	0.56
2:D:20:LEU:HD22	2:D:81:LEU:HD23	1.87	0.56
1:A:116:VAL:HG12	1:A:208:LYS:HG3	1.87	0.56
2:B:206:TYR:O	2:B:223:VAL:HG23	2.04	0.56
1:C:85:VAL:HG22	1:C:104:LYS:HG2	1.87	0.56
1:A:148:GLN:OE1	1:A:155:LEU:HD22	2.05	0.56
2:D:25:SER:O	2:D:27:PHE:HD1	1.88	0.56
1:C:49:TYR:CB	2:D:111:LEU:HD11	2.35	0.56
2:B:166:TRP:CZ2	2:B:208:CYS:HB3	2.40	0.56
1:A:111:VAL:O	1:A:111:VAL:CG1	2.52	0.56
1:A:94:TRP:CD1	1:A:94:TRP:O	2.58	0.56
2:D:28:THR:O	2:D:29:PHE:C	2.44	0.56
1:A:141:TYR:CD1	1:A:142:PRO:HA	2.41	0.56
2:B:20:LEU:O	2:B:21:SER:HB3	2.06	0.56
1:A:31:SER:O	1:A:50:ASP:O	2.23	0.55
1:A:20:THR:C	1:A:21:LEU:HD23	2.27	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HB2	1:A:45:ARG:HH11	1.70	0.55
1:C:148:GLN:HB2	1:C:196:GLU:HB3	1.88	0.55
2:D:222:LYS:O	2:D:223:VAL:CB	2.54	0.55
1:A:188:GLU:HA	1:A:212:ARG:NH1	2.21	0.55
1:C:38:GLN:HG3	1:C:38:GLN:O	2.05	0.55
1:A:207:THR:HG22	1:A:208:LYS:N	2.21	0.55
2:B:62:ASP:C	2:B:64:VAL:H	2.10	0.55
1:C:97:TRP:CE3	1:C:97:TRP:N	2.74	0.55
2:D:34:MET:SD	2:D:53:TYR:OH	2.65	0.55
1:C:121:PRO:O	1:C:122:SER:O	2.25	0.55
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.89	0.54
2:B:97:ALA:CB	2:B:112:LEU:HB3	2.36	0.54
2:D:175:VAL:HA	2:D:194:VAL:HG23	1.88	0.54
1:A:49:TYR:CD2	2:B:111:LEU:HD21	2.42	0.54
1:C:108:LYS:CA	1:C:169:SER:HA	2.35	0.54
1:C:21:LEU:HG	1:C:73:LEU:HD23	1.90	0.54
1:C:148:GLN:OE1	1:C:155:LEU:HD11	2.08	0.54
2:D:190:LEU:HD12	2:D:190:LEU:C	2.28	0.54
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.89	0.54
1:C:107:ILE:HG23	1:C:108:LYS:N	2.23	0.54
2:D:34:MET:HG2	2:D:98:LYS:HA	1.90	0.54
1:C:120:PRO:HG3	1:C:210:PHE:CE1	2.42	0.54
1:A:97:TRP:CD1	2:B:47:TRP:CD2	2.97	0.53
1:A:94:TRP:HB2	1:A:97:TRP:HZ3	1.69	0.53
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.56	0.53
2:B:87:ARG:C	2:B:123:VAL:HG11	2.28	0.53
1:A:49:TYR:CE1	1:A:53:ASN:HB3	2.44	0.53
2:D:13:GLN:HB2	2:D:16:ARG:CZ	2.38	0.53
1:A:39:LYS:CB	1:A:42:GLN:HE21	2.21	0.53
2:B:4:LEU:HD22	2:B:22:CYS:SG	2.49	0.53
2:D:29:PHE:CD2	2:D:53:TYR:CE1	2.96	0.53
1:C:125:GLN:C	1:C:127:LYS:N	2.62	0.53
2:D:136:LEU:O	2:D:137:ALA:HB2	2.09	0.53
1:C:94:TRP:CD1	1:C:97:TRP:CZ3	2.96	0.53
1:A:164:VAL:HG13	1:A:175:SER:O	2.09	0.53
2:B:166:TRP:O	2:B:167:ASN:HB2	2.08	0.53
2:B:197:PRO:O	2:B:198:SER:O	2.27	0.53
1:C:199:HIS:CG	1:C:200:GLN:H	2.26	0.53
1:C:48:ILE:HG21	1:C:51:ALA:O	2.08	0.53
2:D:24:ALA:HB3	2:D:29:PHE:CD1	2.44	0.53
2:D:34:MET:HB2	2:D:53:TYR:HE2	1.70	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:HB2	1:A:87:TYR:HB2	1.91	0.52
2:B:20:LEU:O	2:B:21:SER:CB	2.57	0.52
2:B:34:MET:HE1	2:B:98:LYS:HG2	1.91	0.52
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.24	0.52
2:D:97:ALA:CB	2:D:112:LEU:HD22	2.40	0.52
1:C:171:ASP:O	1:C:172:SER:HB3	2.09	0.52
1:C:108:LYS:HA	1:C:169:SER:CB	2.39	0.52
2:B:113:ASP:OD2	2:B:114:TYR:CD2	2.63	0.52
2:B:91:THR:O	2:B:91:THR:HG23	2.10	0.52
2:D:166:TRP:CH2	2:D:208:CYS:SG	3.01	0.52
2:B:72:ARG:NE	2:B:74:ASN:OD1	2.38	0.52
1:C:10:THR:HA	1:C:104:LYS:O	2.09	0.52
1:C:194:ALA:HA	1:C:209:SER:HB3	1.91	0.52
1:C:94:TRP:HB2	1:C:97:TRP:CZ3	2.44	0.52
2:B:52:SER:O	2:B:72:ARG:NH1	2.43	0.52
1:C:113:ALA:HB1	1:C:202:LEU:CD2	2.40	0.52
2:B:112:LEU:CD1	2:B:112:LEU:N	2.73	0.52
2:B:25:SER:O	2:B:27:PHE:HD1	1.93	0.52
1:A:151:VAL:HG22	1:A:193:TYR:CE1	2.45	0.51
1:C:166:GLU:O	1:C:167:GLN:C	2.48	0.51
1:A:94:TRP:HB2	1:A:97:TRP:CE3	2.45	0.51
1:C:89:GLN:HG2	1:C:98:THR:O	2.11	0.51
1:C:38:GLN:O	1:C:84:ALA:HB1	2.10	0.51
2:D:111:LEU:CG	2:D:111:LEU:O	2.59	0.51
1:A:91:ARG:HD2	2:B:109:SER:O	2.11	0.51
1:C:147:VAL:O	1:C:147:VAL:HG12	2.10	0.51
1:C:80:PRO:O	1:C:83:PHE:HD2	1.93	0.51
1:A:97:TRP:HD1	2:B:47:TRP:CG	2.29	0.51
2:D:52:SER:O	2:D:72:ARG:NH1	2.44	0.51
2:B:6:GLU:OE1	2:B:6:GLU:N	2.42	0.51
1:C:59:PRO:HG2	1:C:62:PHE:CD2	2.46	0.51
2:D:13:GLN:N	2:D:16:ARG:NH1	2.58	0.51
2:D:48:VAL:HG13	2:D:64:VAL:HG11	1.92	0.51
2:B:6:GLU:HG3	2:B:96:CYS:SG	2.51	0.50
2:B:213:LYS:N	2:B:214:PRO:CD	2.73	0.50
1:C:9:ALA:O	1:C:103:THR:HA	2.12	0.50
1:C:6:GLN:HG2	1:C:23:CYS:SG	2.52	0.50
2:D:194:VAL:HG13	2:D:196:VAL:HG13	1.92	0.50
2:D:131:PRO:HB3	2:D:157:TYR:HB3	1.94	0.50
2:D:183:GLN:O	2:D:185:SER:N	2.45	0.50
1:A:135:CYS:HB2	1:A:149:TRP:CZ2	2.46	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HD11	2:B:79:LEU:HD21	1.93	0.50
2:B:50:VAL:HG22	2:B:51:ILE:N	2.26	0.50
2:B:62:ASP:O	2:B:64:VAL:HG22	2.11	0.50
2:D:29:PHE:CG	2:D:53:TYR:HE1	2.29	0.50
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.47	0.50
2:B:37:VAL:HG13	2:B:47:TRP:HA	1.94	0.49
1:C:204:SER:O	1:C:205:PRO:C	2.48	0.49
2:B:98:LYS:O	2:B:112:LEU:HA	2.12	0.49
2:D:33:GLY:O	2:D:99:ASP:CB	2.60	0.49
1:C:107:ILE:HG23	1:C:108:LYS:H	1.77	0.49
1:C:49:TYR:HB2	2:D:111:LEU:HD13	1.94	0.49
1:A:61:ARG:NH1	1:A:79:GLU:CG	2.63	0.49
1:A:97:TRP:CE2	2:B:35:HIS:HE1	2.31	0.49
1:C:120:PRO:HG3	1:C:210:PHE:CD1	2.48	0.49
1:C:43:ALA:CB	2:D:117:GLN:HA	2.43	0.49
1:C:49:TYR:HB2	2:D:111:LEU:HD11	1.93	0.49
1:A:152:ASP:N	1:A:152:ASP:OD1	2.46	0.49
2:B:64:VAL:HG23	2:B:65:LYS:N	2.28	0.49
1:C:171:ASP:O	1:C:172:SER:CB	2.61	0.49
1:C:171:ASP:HB3	1:C:173:THR:H	1.78	0.49
2:B:61:ALA:O	2:B:62:ASP:O	2.31	0.48
2:D:28:THR:OG1	2:D:28:THR:O	2.24	0.48
1:C:97:TRP:NE1	2:D:35:HIS:HE1	2.02	0.48
1:A:188:GLU:HA	1:A:212:ARG:CZ	2.43	0.48
2:D:20:LEU:HB3	2:D:36:TRP:CH2	2.49	0.48
2:B:97:ALA:HB3	2:B:112:LEU:HG	1.93	0.48
1:A:11:LEU:HD23	1:A:21:LEU:HD22	1.95	0.48
2:D:29:PHE:O	2:D:31:SER:N	2.46	0.48
1:C:135:CYS:HB2	1:C:149:TRP:CZ2	2.48	0.48
1:C:43:ALA:N	2:D:117:GLN:HA	2.27	0.48
2:D:124:SER:HB3	2:D:158:PHE:CZ	2.48	0.48
2:B:65:LYS:C	2:B:67:ARG:N	2.64	0.48
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.46	0.48
1:C:94:TRP:CD1	1:C:97:TRP:CH2	3.02	0.48
2:B:24:ALA:HB1	2:B:27:PHE:CE1	2.49	0.48
2:D:88:ALA:O	2:D:91:THR:HG22	2.14	0.48
1:C:184:LYS:O	1:C:188:GLU:HG3	2.14	0.47
2:B:218:LYS:NZ	2:D:16:ARG:HG2	2.29	0.47
2:D:5:VAL:HG23	2:D:23:ALA:O	2.14	0.47
1:A:2:ILE:HG23	1:A:2:ILE:O	2.14	0.47
1:A:124:GLU:O	1:A:127:LYS:HE2	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:HB2	1:A:82:ASP:OD2	2.14	0.47
1:C:44:PRO:HG2	2:D:115:TRP:CD2	2.50	0.47
2:D:150:LEU:HD11	2:D:196:VAL:CG2	2.44	0.47
2:B:209:ASN:HD22	2:B:209:ASN:N	2.11	0.47
1:C:43:ALA:HB2	2:D:116:GLY:C	2.34	0.47
1:A:39:LYS:HD3	1:A:42:GLN:HE22	1.79	0.47
2:B:197:PRO:O	2:B:198:SER:C	2.51	0.47
1:C:186:ASP:O	1:C:189:LYS:HB3	2.15	0.47
2:D:53:TYR:CD2	2:D:72:ARG:NH2	2.82	0.47
2:B:2:VAL:CB	2:B:98:LYS:HE3	2.44	0.47
1:C:151:VAL:HG23	1:C:156:GLN:HG3	1.95	0.47
1:C:54:ARG:HB2	1:C:54:ARG:CZ	2.44	0.47
1:C:36:TYR:O	1:C:86:TYR:HA	2.15	0.47
1:C:97:TRP:HE3	1:C:97:TRP:N	2.13	0.47
1:A:126:LEU:HD23	1:A:184:LYS:HB2	1.96	0.47
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.24	0.47
1:C:146:LYS:HB3	1:C:198:THR:HB	1.95	0.47
1:C:152:ASP:CG	1:C:190:HIS:HB3	2.35	0.47
1:C:189:LYS:HB2	1:C:189:LYS:HE3	1.69	0.47
2:D:33:GLY:O	2:D:99:ASP:HB3	2.15	0.47
1:C:152:ASP:OD2	1:C:190:HIS:HB3	2.15	0.46
1:A:58:ILE:HA	1:A:59:PRO:HD3	1.84	0.46
1:A:5:THR:HG22	1:A:5:THR:O	2.15	0.46
1:C:206:VAL:CG1	1:C:207:THR:N	2.78	0.46
1:A:11:LEU:HD23	1:A:21:LEU:CD2	2.45	0.46
2:D:62:ASP:O	2:D:65:LYS:HB2	2.16	0.46
1:A:141:TYR:CG	1:A:142:PRO:HA	2.51	0.46
1:A:188:GLU:HA	1:A:212:ARG:NH2	2.31	0.46
1:C:123:ASP:C	1:C:125:GLN:H	2.18	0.46
1:C:147:VAL:O	1:C:147:VAL:CG1	2.63	0.46
2:B:218:LYS:HZ3	2:D:16:ARG:HG2	1.80	0.46
1:A:143:ARG:O	1:A:144:GLU:C	2.53	0.46
1:A:148:GLN:OE1	1:A:155:LEU:HD13	2.16	0.46
1:C:104:LYS:HD3	1:C:106:GLU:CD	2.36	0.46
1:C:123:ASP:N	1:C:123:ASP:OD2	2.48	0.46
1:C:123:ASP:C	1:C:125:GLN:N	2.69	0.46
2:B:166:TRP:HB3	2:B:171:LEU:HB3	1.98	0.46
1:C:125:GLN:O	1:C:127:LYS:N	2.49	0.46
2:D:29:PHE:CG	2:D:53:TYR:CE1	3.04	0.46
2:D:111:LEU:CD1	2:D:111:LEU:O	2.64	0.46
1:A:135:CYS:HB2	1:A:149:TRP:CH2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:CD1	1:C:86:TYR:HB2	2.46	0.46
1:A:44:PRO:HB2	2:B:115:TRP:CD2	2.51	0.45
2:B:128:PHE:HE1	2:B:214:PRO:O	1.99	0.45
1:C:107:ILE:O	1:C:108:LYS:CG	2.63	0.45
1:C:168:ASP:O	1:C:169:SER:CB	2.64	0.45
2:B:216:ASN:ND2	2:D:16:ARG:HH12	2.14	0.45
1:A:210:PHE:O	1:A:210:PHE:CD2	2.70	0.45
1:C:113:ALA:HB1	1:C:202:LEU:HD23	1.98	0.45
2:D:68:PHE:N	2:D:68:PHE:HD1	2.14	0.45
1:A:202:LEU:HD22	1:A:206:VAL:HG21	1.99	0.45
1:C:108:LYS:HA	1:C:169:SER:HB2	1.97	0.45
2:D:113:ASP:OD1	2:D:113:ASP:N	2.49	0.45
2:D:164:VAL:HG11	2:D:192:SER:HB3	1.95	0.45
1:A:27:GLN:O	1:A:69:THR:HG22	2.15	0.45
1:C:42:GLN:HB3	2:D:117:GLN:OE1	2.17	0.45
2:D:51:ILE:HG13	2:D:57:ASN:O	2.16	0.45
2:D:76:LYS:O	2:D:78:THR:HG23	2.16	0.45
1:A:162:GLU:HA	1:A:177:SER:O	2.15	0.45
2:B:34:MET:HG3	2:B:79:LEU:HD12	1.97	0.45
2:D:13:GLN:HB2	2:D:16:ARG:NE	2.32	0.45
1:A:130:THR:CG2	1:A:131:ALA:N	2.80	0.45
1:A:36:TYR:O	1:A:86:TYR:HA	2.17	0.45
2:B:112:LEU:HD13	2:B:112:LEU:H	1.82	0.45
2:B:24:ALA:HB1	2:B:27:PHE:HE1	1.81	0.45
1:C:54:ARG:CG	1:C:54:ARG:HH11	2.30	0.45
2:D:153:LEU:HD23	2:D:155:LYS:HB2	1.97	0.45
1:A:163:SER:HB3	2:B:178:PHE:HB3	1.98	0.45
1:C:59:PRO:HG2	1:C:62:PHE:CE2	2.52	0.45
2:D:111:LEU:HG	2:D:111:LEU:O	2.16	0.45
2:D:13:GLN:HG2	2:D:125:SER:HA	1.98	0.45
2:D:49:ALA:HB2	2:D:60:TYR:HD1	1.82	0.45
2:D:29:PHE:C	2:D:53:TYR:HD1	2.19	0.45
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.53	0.45
1:A:32:TYR:HE1	1:A:91:ARG:NH2	2.15	0.45
1:A:91:ARG:O	1:A:94:TRP:CZ3	2.70	0.45
2:B:50:VAL:HG22	2:B:51:ILE:H	1.81	0.45
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.31	0.45
1:C:36:TYR:OH	2:D:112:LEU:HB2	2.17	0.45
2:D:22:CYS:O	2:D:78:THR:HA	2.17	0.45
2:D:38:ARG:NH1	2:D:90:ASP:HA	2.31	0.45
1:A:11:LEU:HD13	1:A:11:LEU:HA	1.84	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ALA:O	1:A:155:LEU:C	2.54	0.44
1:A:2:ILE:H	1:A:98:THR:HG21	1.83	0.44
2:D:32:TYR:C	2:D:53:TYR:HB2	2.38	0.44
2:D:68:PHE:N	2:D:68:PHE:CD1	2.85	0.44
2:D:53:TYR:HD2	2:D:72:ARG:HH12	1.47	0.44
2:B:91:THR:O	2:B:91:THR:CG2	2.65	0.44
2:D:91:THR:CG2	2:D:91:THR:O	2.65	0.44
2:B:190:LEU:HD12	2:B:190:LEU:C	2.37	0.44
1:A:90:GLN:HE21	1:A:92:SER:H	1.65	0.44
2:B:61:ALA:C	2:B:62:ASP:O	2.55	0.44
2:B:66:GLY:O	2:B:67:ARG:HG3	2.18	0.44
1:C:46:LEU:HD22	2:D:112:LEU:O	2.18	0.44
1:A:107:ILE:HG12	1:A:108:LYS:N	2.32	0.44
2:B:182:LEU:HD11	2:B:186:GLY:HA2	2.00	0.44
2:B:215:SER:O	2:B:216:ASN:CB	2.65	0.44
1:C:118:ILE:HD12	1:C:210:PHE:HE1	1.83	0.44
1:C:193:TYR:O	1:C:209:SER:CB	2.50	0.44
2:B:62:ASP:C	2:B:64:VAL:N	2.69	0.44
2:D:67:ARG:O	2:D:84:ASN:HB2	2.18	0.44
2:D:67:ARG:HH22	2:D:90:ASP:CG	2.21	0.44
1:C:13:LEU:HB3	1:C:78:LEU:HD12	2.00	0.43
1:C:24:ARG:HH21	1:C:26:SER:HA	1.83	0.43
1:C:143:ARG:HB2	1:C:174:TYR:CZ	2.54	0.43
1:A:107:ILE:HG12	1:A:108:LYS:H	1.82	0.43
1:C:103:THR:O	1:C:103:THR:HG22	2.19	0.43
1:C:135:CYS:HB2	1:C:149:TRP:CH2	2.53	0.43
1:A:29:VAL:O	1:A:32:TYR:HB2	2.18	0.43
2:B:216:ASN:HD21	2:D:12:VAL:C	2.21	0.43
2:B:4:LEU:HD21	2:B:34:MET:CE	2.47	0.43
1:A:152:ASP:OD2	1:A:191:LYS:CD	2.66	0.43
1:A:39:LYS:CB	1:A:42:GLN:NE2	2.78	0.43
2:D:2:VAL:HG21	2:D:114:TYR:CZ	2.53	0.43
2:D:51:ILE:HG23	2:D:51:ILE:O	2.17	0.43
1:A:7:SER:HA	1:A:8:PRO:C	2.39	0.43
2:B:64:VAL:HB	2:B:68:PHE:HB2	2.00	0.43
2:B:64:VAL:O	2:B:65:LYS:O	2.36	0.43
1:C:134:VAL:HG12	1:C:135:CYS:N	2.32	0.43
1:A:137:LEU:HD11	1:A:197:VAL:CG2	2.48	0.43
2:D:197:PRO:O	2:D:198:SER:C	2.56	0.43
2:D:2:VAL:O	2:D:3:GLN:HG2	2.19	0.43
2:B:98:LYS:CD	2:B:114:TYR:HB2	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ALA:O	2:B:41:PRO:C	2.57	0.42
2:D:12:VAL:HA	2:D:16:ARG:HH11	1.84	0.42
1:A:171:ASP:HB3	1:A:173:THR:HG23	2.01	0.42
2:B:215:SER:HB2	2:D:128:PHE:HB2	2.00	0.42
1:C:108:LYS:CB	1:C:169:SER:HA	2.48	0.42
1:C:49:TYR:CB	2:D:111:LEU:CD1	2.97	0.42
2:B:160:GLU:CB	2:B:161:PRO:HA	2.49	0.42
2:B:194:VAL:HG13	2:B:196:VAL:HG13	2.02	0.42
2:B:4:LEU:HG	2:B:98:LYS:CE	2.49	0.42
2:B:9:GLY:HA3	2:B:119:THR:HG23	2.00	0.42
1:C:152:ASP:N	1:C:192:VAL:O	2.40	0.42
1:A:188:GLU:HA	1:A:212:ARG:HH12	1.85	0.42
2:D:13:GLN:HA	2:D:124:SER:O	2.20	0.42
1:C:43:ALA:HB1	1:C:44:PRO:HD2	2.00	0.42
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.54	0.42
2:D:151:GLY:HA2	2:D:166:TRP:CZ2	2.55	0.42
2:B:2:VAL:CG1	2:B:98:LYS:HE3	2.49	0.41
2:B:87:ARG:O	2:B:123:VAL:HG21	2.20	0.41
1:C:49:TYR:HB3	2:D:111:LEU:HD11	2.02	0.41
2:B:215:SER:HA	2:D:128:PHE:CD2	2.55	0.41
1:C:163:SER:OG	2:D:179:PRO:O	2.31	0.41
1:C:121:PRO:HA	1:C:132:SER:O	2.20	0.41
2:B:216:ASN:ND2	2:D:16:ARG:NH1	2.68	0.41
1:C:168:ASP:CB	1:C:171:ASP:HB2	2.51	0.41
1:C:143:ARG:HA	1:C:174:TYR:CD2	2.56	0.41
1:C:30:SER:OG	1:C:31:SER:N	2.50	0.41
1:A:145:ALA:HB2	1:A:199:HIS:HD2	1.86	0.41
1:C:124:GLU:HG3	2:D:134:PHE:CE1	2.55	0.41
2:D:20:LEU:HD23	2:D:36:TRP:CZ3	2.55	0.41
2:D:3:GLN:HB2	2:D:25:SER:HB2	2.02	0.41
2:B:218:LYS:NZ	2:D:16:ARG:CG	2.83	0.41
2:B:48:VAL:O	2:B:49:ALA:HB2	2.20	0.41
1:C:141:TYR:CD1	1:C:142:PRO:HA	2.56	0.41
1:C:152:ASP:C	1:C:154:ALA:H	2.23	0.41
2:D:50:VAL:HG22	2:D:51:ILE:N	2.36	0.41
1:C:54:ARG:H	1:C:54:ARG:NH1	2.19	0.41
2:B:166:TRP:CH2	2:B:208:CYS:HB3	2.56	0.41
2:D:160:GLU:HB3	2:D:161:PRO:HB3	2.02	0.41
1:A:138:ASN:HD21	2:B:176:HIS:CE1	2.39	0.41
1:A:108:LYS:HB3	1:A:169:SER:HB3	2.03	0.41
2:B:16:ARG:NH2	2:D:218:LYS:HB2	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:HB3	1:A:43:ALA:H	1.75	0.40
1:A:46:LEU:HD22	2:B:113:ASP:HA	2.02	0.40
2:B:70:ILE:HG12	2:B:71:SER:N	2.36	0.40
2:D:100:GLY:CA	2:D:113:ASP:OD1	2.67	0.40
2:D:128:PHE:O	2:D:129:LYS:HB2	2.22	0.40
2:D:207:ILE:CD1	2:D:222:LYS:HA	2.51	0.40
2:D:120:LEU:HG	2:D:121:VAL:N	2.36	0.40
2:D:20:LEU:HD13	2:D:83:MET:HE2	2.03	0.40
1:A:190:HIS:HB2	1:A:193:TYR:OH	2.21	0.40
2:B:183:GLN:HE21	2:B:183:GLN:HB2	1.70	0.40
1:C:37:GLN:O	1:C:37:GLN:CG	2.68	0.40
2:D:53:TYR:CE2	2:D:72:ARG:NH1	2.87	0.40
1:A:142:PRO:HG3	1:A:200:GLN:HE22	1.86	0.40
1:C:167:GLN:O	1:C:168:ASP:O	2.38	0.40
2:B:148:ALA:O	2:B:195:THR:HG22	2.22	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:CE	1:C:111:VAL:CG2[2_564]	0.27	1.93
1:A:108:LYS:NZ	1:C:111:VAL:CB[2_564]	0.69	1.51
1:A:108:LYS:CD	1:C:111:VAL:CG2[2_564]	1.26	0.94
1:A:108:LYS:NZ	1:C:111:VAL:CG1[2_564]	1.27	0.93
1:A:108:LYS:NZ	1:C:111:VAL:CA[2_564]	1.47	0.73
1:A:108:LYS:CE	1:C:111:VAL:CB[2_564]	1.50	0.70
1:A:108:LYS:NZ	1:C:111:VAL:CG2[2_564]	1.54	0.66
1:A:108:LYS:CD	1:C:111:VAL:CB[2_564]	2.04	0.16

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	207/216 (96%)	177 (86%)	23 (11%)	7 (3%)	4	21
1	C	209/216 (97%)	170 (81%)	27 (13%)	12 (6%)	2	10
2	B	189/242 (78%)	155 (82%)	20 (11%)	14 (7%)	1	5
2	D	194/242 (80%)	162 (84%)	22 (11%)	10 (5%)	2	11
All	All	799/916 (87%)	664 (83%)	92 (12%)	43 (5%)	2	11

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
1	A	126	LEU
1	A	139	ASN
2	B	21	SER
2	B	62	ASP
2	B	63	SER
2	B	198	SER
1	C	57	GLY
1	C	122	SER
1	C	165	THR
1	C	168	ASP
1	C	169	SER
2	D	30	SER
2	D	112	LEU
2	D	198	SER
2	D	222	LYS
2	B	16	ARG
2	B	65	LYS
2	B	74	ASN
1	C	56	THR
1	C	170	LYS
1	C	189	LYS
2	D	89	GLU
2	D	184	SER
2	D	223	VAL
1	A	122	SER
1	A	145	ALA
2	B	41	PRO
2	B	64	VAL
2	B	67	ARG
2	B	184	SER
2	D	29	PHE
1	A	15	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	126	LEU
1	C	172	SER
2	D	161	PRO
1	A	172	SER
1	C	153	ASN
2	B	29	PHE
2	B	156	ASP
1	C	59	PRO
2	B	159	PRO
2	D	159	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/188 (98%)	153 (83%)	31 (17%)	2	10
1	C	185/188 (98%)	147 (80%)	38 (20%)	1	6
2	B	167/202 (83%)	131 (78%)	36 (22%)	1	5
2	D	168/202 (83%)	136 (81%)	32 (19%)	2	8
All	All	704/780 (90%)	567 (80%)	137 (20%)	1	7

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	LEU
1	A	21	LEU
1	A	38	GLN
1	A	45	ARG
1	A	52	SER
1	A	61	ARG
1	A	65	SER
1	A	67	SER
1	A	72	THR
1	A	89	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	90	GLN
1	A	97	TRP
1	A	101	GLN
1	A	104	LYS
1	A	106	GLU
1	A	108	LYS
1	A	111	VAL
1	A	126	LEU
1	A	128	SER
1	A	132	SER
1	A	138	ASN
1	A	152	ASP
1	A	161	GLN
1	A	162	GLU
1	A	163	SER
1	A	170	LYS
1	A	184	LYS
1	A	191	LYS
1	A	198	THR
1	A	212	ARG
2	B	2	VAL
2	B	13	GLN
2	B	25	SER
2	B	27	PHE
2	B	28	THR
2	B	31	SER
2	B	34	MET
2	B	37	VAL
2	B	41	PRO
2	B	53	TYR
2	B	63	SER
2	B	69	THR
2	B	78	THR
2	B	79	LEU
2	B	87	ARG
2	B	112	LEU
2	B	117	GLN
2	B	119	THR
2	B	120	LEU
2	B	122	THR
2	B	128	PHE
2	B	147	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	155	LYS
2	B	161	PRO
2	B	162	VAL
2	B	163	THR
2	B	179	PRO
2	B	181	VAL
2	B	189	SER
2	B	190	LEU
2	B	191	SER
2	B	195	THR
2	B	207	ILE
2	B	216	ASN
2	B	223	VAL
2	B	224	GLU
1	C	4	LEU
1	C	10	THR
1	C	12	SER
1	C	14	SER
1	C	17	GLU
1	C	21	LEU
1	C	22	SER
1	C	33	LEU
1	C	37	GLN
1	C	38	GLN
1	C	42	GLN
1	C	69	THR
1	C	82	ASP
1	C	90	GLN
1	C	94	TRP
1	C	97	TRP
1	C	98	THR
1	C	101	GLN
1	C	104	LYS
1	C	118	ILE
1	C	123	ASP
1	C	127	LYS
1	C	138	ASN
1	C	146	LYS
1	C	147	VAL
1	C	152	ASP
1	C	161	GLN
1	C	163	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	165	THR
1	C	166	GLU
1	C	171	ASP
1	C	177	SER
1	C	181	THR
1	C	182	LEU
1	C	186	ASP
1	C	191	LYS
1	C	212	ARG
1	C	214	GLU
2	D	2	VAL
2	D	5	VAL
2	D	12	VAL
2	D	18	LEU
2	D	19	ARG
2	D	28	THR
2	D	30	SER
2	D	54	ASP
2	D	56	SER
2	D	65	LYS
2	D	69	THR
2	D	77	ASN
2	D	79	LEU
2	D	113	ASP
2	D	147	THR
2	D	153	LEU
2	D	159	PRO
2	D	161	PRO
2	D	165	SER
2	D	172	THR
2	D	173	SER
2	D	181	VAL
2	D	184	SER
2	D	189	SER
2	D	190	LEU
2	D	194	VAL
2	D	195	THR
2	D	207	ILE
2	D	209	ASN
2	D	216	ASN
2	D	222	LYS
2	D	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	42	GLN
1	A	89	GLN
1	A	138	ASN
1	A	139	ASN
1	A	161	GLN
1	A	200	GLN
2	B	13	GLN
2	B	35	HIS
2	B	77	ASN
2	B	117	GLN
2	B	176	HIS
2	B	183	GLN
2	B	209	ASN
2	B	211	ASN
2	B	216	ASN
1	C	38	GLN
1	C	53	ASN
1	C	138	ASN
1	C	161	GLN
1	C	211	ASN
2	D	77	ASN
2	D	176	HIS
2	D	216	ASN

### 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/216 (97%)	0.90	29 (13%) 3 2	49, 67, 85, 92	0
1	C	213/216 (98%)	1.15	46 (21%) 1 1	49, 69, 87, 96	0
2	B	199/242 (82%)	1.09	41 (20%) 1 1	49, 67, 88, 95	0
2	D	202/242 (83%)	0.93	33 (16%) 2 1	45, 63, 86, 111	0
All	All	825/916 (90%)	1.02	149 (18%) 1 1	45, 67, 87, 111	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	THR	12.2
2	B	54	ASP	7.5
2	B	98	LYS	7.4
2	B	23	ALA	6.8
1	A	110	THR	6.3
2	D	53	TYR	6.3
2	D	111	LEU	6.3
1	C	97	TRP	6.1
1	C	207	THR	5.5
2	D	32	TYR	5.4
2	B	4	LEU	5.1
1	C	213	GLY	5.1
2	D	79	LEU	4.9
2	B	68	PHE	4.7
2	D	2	VAL	4.6
1	C	159	ASN	4.6
2	B	53	TYR	4.4
1	C	116	VAL	4.4
1	A	33	LEU	4.3
2	B	35	HIS	4.3
1	A	97	TRP	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	193	TYR	4.2
1	A	49	TYR	4.2
1	C	190	HIS	4.1
2	B	70	ILE	4.1
1	A	78	LEU	4.1
2	D	24	ALA	4.0
2	B	24	ALA	4.0
2	B	29	PHE	4.0
1	C	192	VAL	3.9
1	A	128	SER	3.9
2	B	111	LEU	3.9
1	A	155	LEU	3.9
1	A	107	ILE	3.7
1	A	182	LEU	3.7
1	C	148	GLN	3.7
1	C	137	LEU	3.7
2	D	1	GLN	3.6
2	B	31	SER	3.6
2	B	58	LYS	3.5
2	B	77	ASN	3.5
1	C	35	TRP	3.5
2	B	150	LEU	3.5
1	C	129	GLY	3.4
2	D	4	LEU	3.4
1	C	49	TYR	3.4
1	A	47	LEU	3.4
1	A	193	TYR	3.4
2	B	97	ALA	3.3
1	A	99	PHE	3.3
2	D	57	ASN	3.3
1	C	206	VAL	3.3
2	D	33	GLY	3.3
1	A	32	TYR	3.2
2	B	219	VAL	3.2
2	B	48	VAL	3.2
1	C	42	GLN	3.2
1	A	62	PHE	3.1
1	C	82	ASP	3.0
1	A	132	SER	3.0
1	A	73	LEU	3.0
1	C	208	LYS	3.0
1	C	41	GLY	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	32	TYR	2.9
1	C	114	PRO	2.9
1	C	118	ILE	2.9
1	C	46	LEU	2.9
2	D	112	LEU	2.9
2	B	25	SER	2.9
1	C	150	LYS	2.8
2	D	171	LEU	2.8
2	B	36	TRP	2.8
2	B	206	TYR	2.8
1	C	211	ASN	2.8
1	A	58	ILE	2.7
2	B	112	LEU	2.7
1	C	11	LEU	2.7
1	A	145	ALA	2.7
2	D	164	VAL	2.7
1	A	176	LEU	2.7
1	C	73	LEU	2.7
2	B	121	VAL	2.7
2	D	154	VAL	2.7
1	C	187	TYR	2.6
1	C	182	LEU	2.6
2	D	150	LEU	2.6
1	C	119	PHE	2.6
2	B	74	ASN	2.6
1	C	62	PHE	2.5
2	B	60	TYR	2.5
1	C	158	GLY	2.5
2	B	27	PHE	2.5
2	B	80	TYR	2.5
1	C	26	SER	2.5
2	D	74	ASN	2.5
2	D	27	PHE	2.5
2	B	2	VAL	2.4
2	B	9	GLY	2.4
1	C	86	TYR	2.4
1	A	114	PRO	2.4
1	A	111	VAL	2.4
2	D	48	VAL	2.4
2	B	51	ILE	2.4
2	D	136	LEU	2.4
1	C	92	SER	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	196	VAL	2.4
2	B	34	MET	2.4
2	D	86	LEU	2.4
2	D	137	ALA	2.4
1	A	188	GLU	2.3
2	D	68	PHE	2.3
2	B	190	LEU	2.3
1	A	136	LEU	2.3
2	D	26	GLY	2.3
2	D	206	TYR	2.3
2	D	36	TRP	2.3
2	D	193	VAL	2.3
1	C	128	SER	2.3
1	C	47	LEU	2.2
2	D	194	VAL	2.2
2	D	83	MET	2.2
2	B	59	TYR	2.2
2	B	56	SER	2.2
1	C	43	ALA	2.2
2	B	94	TYR	2.2
1	C	78	LEU	2.2
2	B	50	VAL	2.2
2	B	115	TRP	2.1
1	A	148	GLN	2.1
1	C	126	LEU	2.1
1	C	48	ILE	2.1
1	A	46	LEU	2.1
1	C	210	PHE	2.1
2	B	178	PHE	2.1
1	A	187	TYR	2.1
1	C	180	LEU	2.1
1	A	191	LYS	2.1
1	A	124	GLU	2.1
2	B	153	LEU	2.1
2	B	75	SER	2.1
1	C	21	LEU	2.0
2	D	25	SER	2.0
1	C	33	LEU	2.0
2	D	22	CYS	2.0
2	D	34	MET	2.0
1	A	104	LYS	2.0
1	C	115	SER	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	16	ARG	2.0
1	C	155	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.