



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:29 PM GMT

PDB ID : 1FT8  
Title : CRYSTAL STRUCTURE OF THE RNA-BINDING DOMAIN OF THE  
MRNA EXPORT FACTOR TAP  
Authors : Liker, E.; Fernandez, E.; Izaurralde, E.; Conti, E.  
Deposited on : 2000-09-12  
Resolution : 3.15 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  
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

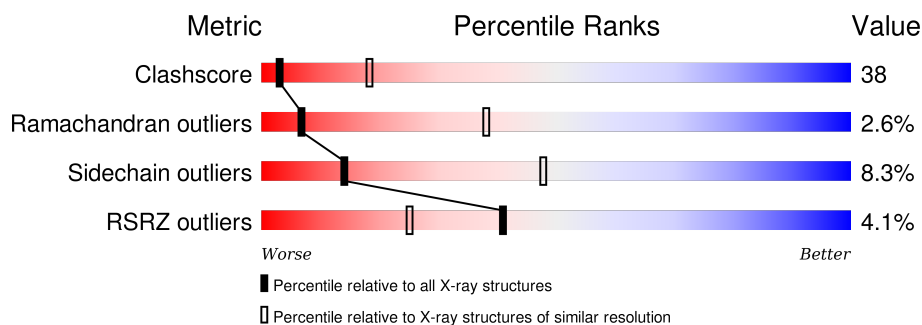
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	271	<div> <div>3%</div> <div>42% 38% 8% 11%</div> </div>
1	B	271	<div> <div>2%</div> <div>32% 25% 39%</div> </div>
1	C	271	<div> <div>2%</div> <div>49% 34% 6% 10%</div> </div>
1	D	271	<div> <div>3%</div> <div>28% 27% 5% 40%</div> </div>
1	E	271	<div> <div>3%</div> <div>6% 8% 84%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6913 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 TIP ASSOCIATING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1961	1245	343	366	7			
1	B	165	Total	C	N	O	S	0	0	0
			1323	831	232	255	5			
1	C	244	Total	C	N	O	S	0	0	0
			1973	1253	346	367	7			
1	D	162	Total	C	N	O	S	0	0	0
			1302	818	229	250	5			
1	E	44	Total	C	N	O	S	0	0	0
			354	236	54	62	2			

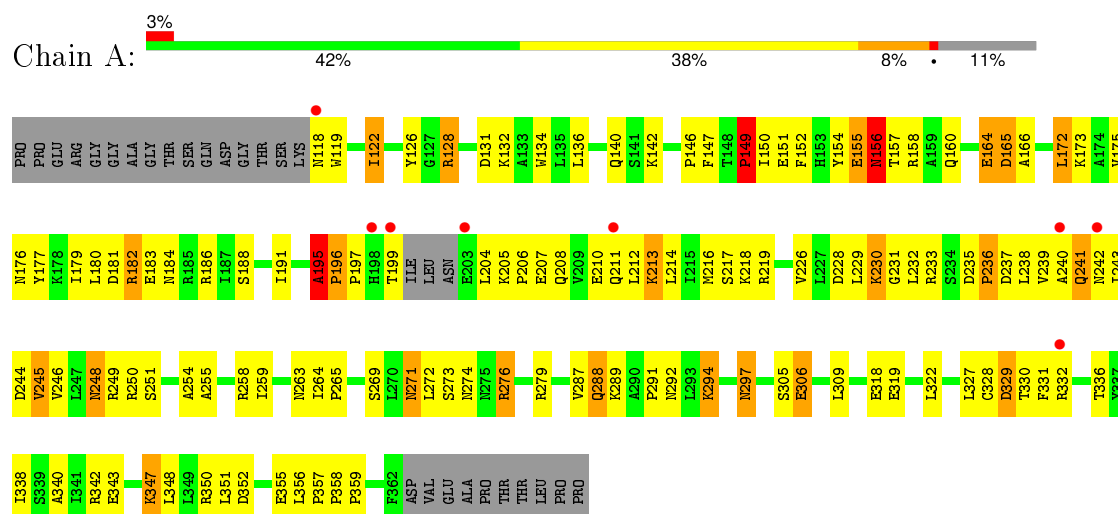
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
A	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
B	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
B	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
C	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
C	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
D	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
D	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
E	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
E	226	VAL	ALA	ENGINEERED	UNP Q9UBU9

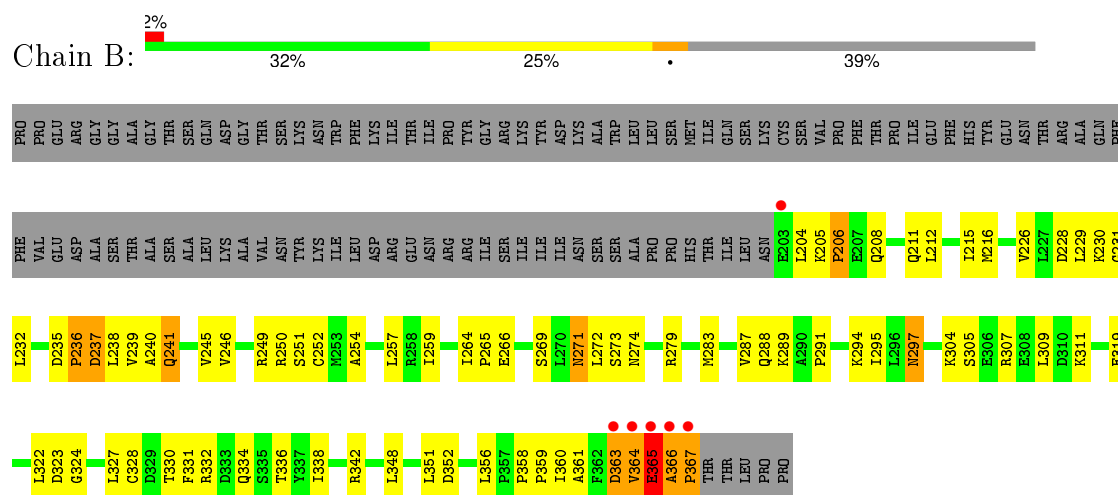
### 3 Residue-property plots

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.

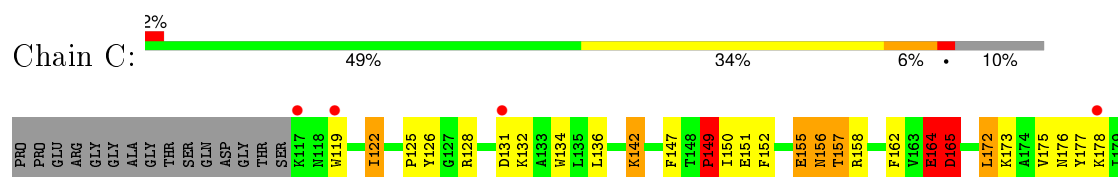
#### • Molecule 1: TIP ASSOCIATING PROTEIN

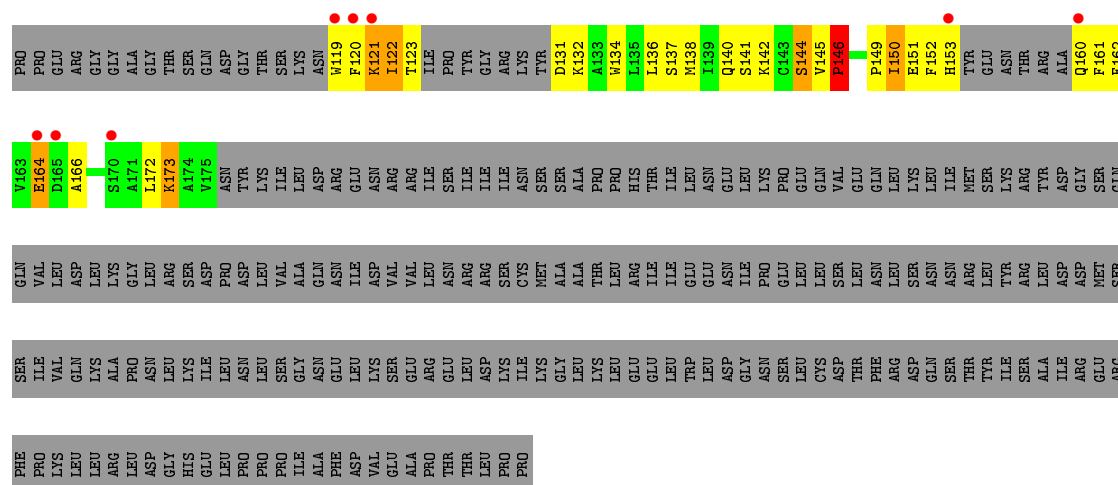


#### • Molecule 1: TIP ASSOCIATING PROTEIN



#### • Molecule 1: TIP ASSOCIATING PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.92Å 139.92Å 206.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 29.94 – 3.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.15) 99.6 (29.94-3.16)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.10 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.303 , 0.303 0.301 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35832 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	6913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.73	4/1996 (0.2%)	0.91	10/2696 (0.4%)
1	B	0.60	1/1340 (0.1%)	0.79	2/1808 (0.1%)
1	C	0.75	7/2008 (0.3%)	0.98	8/2711 (0.3%)
1	D	0.61	1/1318 (0.1%)	0.92	8/1777 (0.5%)
1	E	0.72	0/363	0.95	2/489 (0.4%)
All	All	0.69	13/7025 (0.2%)	0.92	30/9481 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	ASP	CB-CG	-11.57	1.27	1.51
1	C	228	ASP	CB-CG	-10.18	1.30	1.51
1	A	164	GLU	CB-CG	-10.11	1.32	1.52
1	C	165	ASP	CB-CG	-9.04	1.32	1.51
1	C	164	GLU	CB-CG	-7.82	1.37	1.52
1	A	164	GLU	CG-CD	-6.55	1.42	1.51
1	C	242	ASN	CA-CB	6.28	1.69	1.53
1	D	228	ASP	CB-CG	-6.16	1.38	1.51
1	C	155	GLU	CD-OE2	-5.90	1.19	1.25
1	C	242	ASN	CA-C	-5.64	1.38	1.52
1	B	228	ASP	CB-CG	-5.63	1.40	1.51
1	A	228	ASP	CB-CG	-5.55	1.40	1.51
1	C	164	GLU	CG-CD	-5.40	1.43	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	ASP	CB-CG-OD1	-19.55	100.71	118.30
1	A	165	ASP	CB-CG-OD2	-18.87	101.32	118.30
1	C	165	ASP	CB-CG-OD2	-18.30	101.83	118.30
1	C	155	GLU	OE1-CD-OE2	-8.83	112.70	123.30
1	C	165	ASP	CB-CG-OD1	8.22	125.70	118.30
1	C	228	ASP	OD1-CG-OD2	7.78	138.09	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	ASP	CA-C-N	-7.59	100.51	117.20
1	A	155	GLU	OE1-CD-OE2	-7.46	114.35	123.30
1	D	228	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	E	144	SER	C-N-CA	-7.23	103.62	121.70
1	A	195	ALA	C-N-CD	-7.16	104.84	120.60
1	A	165	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	228	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	D	237	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	196	PRO	C-N-CD	-6.65	105.98	120.60
1	A	228	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	C	236	PRO	N-CA-C	6.01	127.73	112.10
1	B	366	ALA	C-N-CD	-5.95	107.50	120.60
1	D	237	ASP	CB-CA-C	5.84	122.09	110.40
1	C	228	ASP	N-CA-CB	5.84	121.11	110.60
1	A	165	ASP	OD1-CG-OD2	5.69	134.11	123.30
1	D	241	GLN	CA-C-N	-5.57	104.94	117.20
1	C	241	GLN	O-C-N	5.57	131.60	122.70
1	A	164	GLU	N-CA-CB	-5.48	100.73	110.60
1	D	237	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	165	ASP	N-CA-CB	-5.33	101.00	110.60
1	E	146	PRO	N-CA-C	5.30	125.87	112.10
1	A	236	PRO	N-CA-C	-5.13	98.77	112.10
1	D	237	ASP	O-C-N	5.06	130.80	122.70
1	D	289	LYS	CD-CE-NZ	5.00	123.21	111.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1961	0	2003	171	0
1	B	1323	0	1363	107	0
1	C	1973	0	2013	135	0
1	D	1302	0	1345	113	0
1	E	354	0	349	50	1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6913	0	7073	536	1

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 38.

All (536) 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:A:230:LYS:HD2	1:A:273:SER:OG	1.29	1.32
1:B:323:ASP:HB2	1:C:177:TYR:CE2	1.78	1.19
1:C:119:TRP:HZ3	1:C:150:ILE:CD1	1.56	1.19
1:E:144:SER:O	1:E:145:VAL:HG23	1.39	1.19
1:E:145:VAL:HG22	1:E:146:PRO:CD	1.73	1.17
1:C:119:TRP:CZ3	1:C:150:ILE:HD11	1.81	1.15
1:A:238:LEU:HD12	1:A:241:GLN:CB	1.78	1.12
1:A:238:LEU:CD1	1:A:241:GLN:HB3	1.82	1.10
1:E:145:VAL:HG22	1:E:146:PRO:HD3	1.21	1.10
1:E:145:VAL:CG1	1:E:146:PRO:HD2	1.81	1.09
1:E:145:VAL:HG13	1:E:146:PRO:HD2	1.16	1.09
1:A:238:LEU:HD12	1:A:241:GLN:HB2	1.35	1.09
1:A:230:LYS:HA	1:A:230:LYS:HE3	1.34	1.08
1:A:230:LYS:HE2	1:A:273:SER:N	1.65	1.07
1:C:119:TRP:HZ3	1:C:150:ILE:HD11	0.92	1.07
1:A:230:LYS:CE	1:A:230:LYS:HA	1.84	1.05
1:B:323:ASP:CB	1:C:177:TYR:HE2	1.68	1.05
1:B:204:LEU:HA	1:B:208:GLN:NE2	1.71	1.05
1:B:323:ASP:HB2	1:C:177:TYR:HE2	0.96	1.04
1:E:144:SER:O	1:E:145:VAL:CG2	2.07	1.03
1:B:366:ALA:HB3	1:B:367:PRO:HD3	1.32	1.02
1:A:238:LEU:HD21	1:A:243:ILE:O	1.61	1.00
1:A:119:TRP:HZ3	1:A:150:ILE:HD11	1.26	1.00
1:B:238:LEU:HD21	1:B:245:VAL:HG21	1.41	1.00
1:E:145:VAL:HG13	1:E:146:PRO:CD	1.91	0.99
1:D:235:ASP:HB3	1:D:236:PRO:HD3	1.45	0.99
1:C:237:ASP:O	1:C:240:ALA:N	1.96	0.98
1:A:126:TYR:HA	1:A:157:THR:HG22	1.44	0.98
1:B:215:ILE:HG13	1:B:238:LEU:HD13	1.41	0.97
1:A:230:LYS:CD	1:A:273:SER:OG	2.11	0.97
1:A:238:LEU:HD11	1:A:241:GLN:HB3	1.44	0.96
1:A:230:LYS:NZ	1:A:271:ASN:O	1.99	0.96
1:C:165:ASP:OD2	1:C:165:ASP:N	1.87	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ASP:O	1:C:239:VAL:N	2.00	0.94
1:E:145:VAL:CG2	1:E:146:PRO:CD	2.47	0.92
1:B:366:ALA:CB	1:B:367:PRO:HD3	1.99	0.92
1:B:366:ALA:HB3	1:B:367:PRO:CD	1.99	0.92
1:B:364:VAL:HG22	1:B:367:PRO:HB2	1.50	0.92
1:C:142:LYS:HD3	1:C:178:LYS:HG2	1.51	0.91
1:A:238:LEU:CD1	1:A:241:GLN:CB	2.44	0.91
1:E:145:VAL:CG2	1:E:146:PRO:HD3	2.00	0.91
1:D:235:ASP:O	1:D:237:ASP:N	2.04	0.89
1:C:126:TYR:HA	1:C:157:THR:HG22	1.54	0.89
1:C:119:TRP:CZ3	1:C:150:ILE:CD1	2.47	0.88
1:C:164:GLU:OE2	1:C:164:GLU:O	1.92	0.88
1:A:230:LYS:HE2	1:A:273:SER:H	1.35	0.87
1:A:119:TRP:CZ3	1:A:150:ILE:HD11	2.10	0.87
1:A:232:LEU:HD23	1:A:245:VAL:HG11	1.55	0.87
1:A:230:LYS:HZ2	1:A:230:LYS:N	1.72	0.86
1:B:361:ALA:HB1	1:B:364:VAL:HB	1.57	0.86
1:D:347:LYS:HE3	1:D:347:LYS:H	1.38	0.86
1:A:119:TRP:HZ3	1:A:150:ILE:CD1	1.89	0.86
1:A:195:ALA:HB1	1:A:196:PRO:HD2	1.58	0.85
1:A:213:LYS:HD2	1:D:360:ILE:HD12	1.57	0.85
1:E:145:VAL:HG22	1:E:146:PRO:HD2	1.59	0.84
1:D:235:ASP:O	1:D:237:ASP:CG	2.16	0.84
1:E:144:SER:O	1:E:145:VAL:CB	2.22	0.83
1:E:132:LYS:HD3	1:E:152:PHE:CE2	2.13	0.83
1:B:216:MET:HE1	1:B:259:ILE:HD12	1.59	0.83
1:A:236:PRO:HA	1:A:239:VAL:HG23	1.59	0.83
1:A:195:ALA:CB	1:A:196:PRO:HD2	2.10	0.82
1:C:156:ASN:O	1:C:158:ARG:N	2.12	0.82
1:A:232:LEU:CD2	1:A:245:VAL:HG11	2.10	0.81
1:D:204:LEU:HA	1:D:208:GLN:NE2	1.95	0.81
1:E:122:ILE:HG12	1:E:161:PHE:CZ	2.15	0.81
1:B:364:VAL:C	1:B:366:ALA:H	1.85	0.80
1:A:164:GLU:OE2	1:A:164:GLU:O	1.99	0.80
1:E:145:VAL:CB	1:E:146:PRO:CD	2.59	0.80
1:B:336:THR:HG21	1:D:307:ARG:HH11	1.46	0.80
1:E:145:VAL:CG2	1:E:146:PRO:HD2	2.10	0.79
1:B:204:LEU:HA	1:B:208:GLN:HE21	1.44	0.79
1:A:177:TYR:CE1	1:A:186:ARG:HG3	2.18	0.79
1:A:276:ARG:HB3	1:A:276:ARG:HH21	1.48	0.78
1:D:235:ASP:C	1:D:237:ASP:H	1.85	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:MET:HE1	1:D:259:ILE:HD12	1.63	0.78
1:A:230:LYS:CE	1:A:230:LYS:CA	2.61	0.78
1:A:230:LYS:CE	1:A:273:SER:N	2.46	0.76
1:E:145:VAL:CB	1:E:146:PRO:HD2	2.13	0.76
1:A:230:LYS:HZ3	1:A:271:ASN:CG	1.89	0.76
1:A:240:ALA:C	1:A:242:ASN:H	1.89	0.76
1:C:238:LEU:CD2	1:C:238:LEU:H	1.97	0.76
1:D:235:ASP:HB3	1:D:236:PRO:CD	2.17	0.75
1:D:212:LEU:HG	1:D:216:MET:CE	2.16	0.75
1:B:204:LEU:HA	1:B:208:GLN:HE22	1.52	0.75
1:C:212:LEU:HG	1:C:216:MET:CE	2.17	0.75
1:B:238:LEU:CD2	1:B:245:VAL:HG21	2.17	0.74
1:C:158:ARG:NH2	1:C:207:GLU:OE2	2.19	0.74
1:C:158:ARG:HH22	1:C:207:GLU:CD	1.89	0.74
1:A:204:LEU:HD22	1:A:208:GLN:NE2	2.02	0.74
1:B:327:LEU:O	1:B:330:THR:HB	1.87	0.74
1:A:230:LYS:HE2	1:A:272:LEU:C	2.08	0.74
1:D:219:ARG:NH2	1:D:235:ASP:OD2	2.20	0.74
1:D:235:ASP:O	1:D:237:ASP:OD1	2.06	0.74
1:A:288:GLN:HE22	1:B:287:VAL:HB	1.53	0.73
1:C:238:LEU:H	1:C:238:LEU:HD23	1.51	0.73
1:A:248:ASN:H	1:A:248:ASN:ND2	1.87	0.73
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.54	0.73
1:A:240:ALA:O	1:A:242:ASN:N	2.21	0.72
1:C:327:LEU:O	1:C:330:THR:HB	1.89	0.72
1:E:122:ILE:HG12	1:E:161:PHE:CE2	2.25	0.72
1:A:327:LEU:O	1:A:330:THR:HB	1.89	0.71
1:A:158:ARG:NH1	1:A:160:GLN:OE1	2.19	0.71
1:A:216:MET:HE1	1:A:259:ILE:HD12	1.71	0.71
1:A:235:ASP:OD1	1:A:236:PRO:O	2.08	0.71
1:B:212:LEU:HG	1:B:216:MET:CE	2.20	0.71
1:B:216:MET:CE	1:B:259:ILE:HD12	2.20	0.71
1:B:366:ALA:CB	1:B:367:PRO:CD	2.62	0.71
1:D:258:ARG:HH21	1:D:258:ARG:HG3	1.55	0.71
1:D:327:LEU:O	1:D:330:THR:HB	1.91	0.71
1:A:236:PRO:O	1:A:237:ASP:HB2	1.89	0.70
1:D:235:ASP:CB	1:D:236:PRO:HD3	2.21	0.70
1:C:307:ARG:O	1:C:309:LEU:N	2.25	0.70
1:A:212:LEU:HG	1:A:216:MET:CE	2.22	0.70
1:A:230:LYS:HZ3	1:A:271:ASN:CB	2.03	0.70
1:B:205:LYS:HG2	1:B:208:GLN:CD	2.12	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLU:OE1	1:B:365:GLU:HA	1.92	0.70
1:C:216:MET:HE1	1:C:259:ILE:HD12	1.74	0.70
1:E:120:PHE:CE1	1:E:166:ALA:HA	2.26	0.70
1:C:304:LYS:HD3	1:C:326:SER:OG	1.92	0.69
1:A:230:LYS:NZ	1:A:271:ASN:C	2.45	0.69
1:C:319:GLU:HG3	1:C:350:ARG:HB2	1.74	0.69
1:D:347:LYS:CE	1:D:347:LYS:H	2.06	0.69
1:A:126:TYR:HA	1:A:157:THR:CG2	2.20	0.69
1:D:216:MET:CE	1:D:259:ILE:HD12	2.23	0.69
1:E:121:LYS:HB2	1:E:121:LYS:NZ	2.08	0.69
1:D:349:LEU:HD13	1:E:132:LYS:HE3	1.73	0.68
1:C:147:PHE:CE1	1:C:149:PRO:HD3	2.29	0.68
1:A:230:LYS:HE2	1:A:272:LEU:CA	2.24	0.68
1:E:121:LYS:HG3	1:E:121:LYS:O	1.93	0.68
1:D:318:GLU:HB2	1:D:319:GLU:OE1	1.93	0.68
1:D:204:LEU:HD11	1:D:252:CYS:HA	1.76	0.67
1:A:249:ARG:HE	1:A:249:ARG:HA	1.59	0.67
1:A:306:GLU:CD	1:A:306:GLU:H	1.97	0.67
1:B:232:LEU:HD23	1:B:245:VAL:HG11	1.76	0.67
1:D:219:ARG:HH11	1:D:232:LEU:CD1	2.07	0.67
1:A:240:ALA:C	1:A:242:ASN:N	2.45	0.67
1:A:216:MET:CE	1:A:259:ILE:HD12	2.25	0.66
1:B:365:GLU:OE1	1:B:365:GLU:CA	2.43	0.66
1:A:165:ASP:OD2	1:A:165:ASP:C	2.21	0.66
1:D:327:LEU:HD12	1:D:327:LEU:C	2.16	0.66
1:D:205:LYS:H	1:D:208:GLN:CD	1.99	0.66
1:B:361:ALA:CB	1:B:364:VAL:HB	2.25	0.65
1:B:212:LEU:HG	1:B:216:MET:HE2	1.77	0.65
1:B:364:VAL:C	1:B:366:ALA:N	2.46	0.65
1:A:205:LYS:HG2	1:A:208:GLN:OE1	1.96	0.65
1:B:305:SER:OG	1:B:307:ARG:HG2	1.96	0.65
1:B:204:LEU:HD11	1:B:252:CYS:SG	2.36	0.65
1:B:241:GLN:N	1:B:241:GLN:HE21	1.95	0.65
1:D:212:LEU:HG	1:D:216:MET:HE2	1.79	0.65
1:E:119:TRP:CZ3	1:E:150:ILE:HG21	2.31	0.65
1:B:334:GLN:HG3	1:C:125:PRO:HB3	1.79	0.65
1:A:327:LEU:C	1:A:327:LEU:HD12	2.16	0.64
1:C:119:TRP:CD2	1:C:164:GLU:HB3	2.32	0.64
1:C:237:ASP:O	1:C:238:LEU:C	2.35	0.64
1:A:230:LYS:NZ	1:A:230:LYS:N	2.45	0.64
1:C:176:ASN:CG	1:C:177:TYR:HD1	2.00	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PHE:HD2	1:C:336:THR:HG22	1.63	0.64
1:C:288:GLN:HE21	1:D:287:VAL:HB	1.63	0.64
1:A:231:GLY:HA2	1:A:274:ASN:O	1.98	0.64
1:C:237:ASP:HA	1:C:240:ALA:HB3	1.79	0.63
1:A:276:ARG:NH2	1:A:276:ARG:HB3	2.12	0.63
1:B:235:ASP:O	1:B:239:VAL:HG23	1.98	0.63
1:D:204:LEU:HA	1:D:208:GLN:HE22	1.61	0.63
1:C:147:PHE:CD1	1:C:149:PRO:HD3	2.34	0.63
1:D:245:VAL:O	1:D:245:VAL:HG12	1.99	0.62
1:D:273:SER:HB3	1:D:297:ASN:ND2	2.14	0.62
1:D:279:ARG:CB	1:D:279:ARG:HH11	2.12	0.62
1:B:205:LYS:H	1:B:208:GLN:NE2	1.97	0.62
1:D:205:LYS:HB2	1:D:208:GLN:HG3	1.82	0.62
1:A:294:LYS:HD3	1:A:318:GLU:OE1	1.99	0.62
1:D:232:LEU:O	1:D:236:PRO:HD2	2.00	0.62
1:C:215:ILE:HD13	1:C:238:LEU:HD22	1.82	0.62
1:C:211:GLN:O	1:C:215:ILE:HG13	2.00	0.62
1:A:195:ALA:HB1	1:A:196:PRO:CD	2.28	0.62
1:B:327:LEU:HD12	1:B:327:LEU:C	2.20	0.61
1:B:365:GLU:OE1	1:B:365:GLU:O	2.19	0.61
1:E:150:ILE:HG23	1:E:162:PHE:HB2	1.81	0.61
1:A:238:LEU:O	1:A:238:LEU:HG	2.00	0.61
1:C:122:ILE:N	1:C:122:ILE:HD13	2.16	0.61
1:C:215:ILE:O	1:C:219:ARG:HG3	2.00	0.61
1:E:121:LYS:HB2	1:E:121:LYS:HZ2	1.65	0.61
1:A:273:SER:HB3	1:A:297:ASN:ND2	2.16	0.61
1:B:204:LEU:CA	1:B:208:GLN:NE2	2.58	0.61
1:E:153:HIS:NE2	1:E:160:GLN:NE2	2.49	0.61
1:A:142:LYS:HG3	1:A:179:ILE:HD11	1.82	0.61
1:D:236:PRO:HB2	1:D:242:ASN:CG	2.20	0.61
1:A:236:PRO:HA	1:A:239:VAL:CG2	2.30	0.61
1:A:147:PHE:CE1	1:A:149:PRO:HD3	2.35	0.61
1:D:347:LYS:HE3	1:D:347:LYS:N	2.13	0.61
1:C:327:LEU:HD12	1:C:327:LEU:C	2.20	0.60
1:A:119:TRP:CZ3	1:A:150:ILE:CD1	2.76	0.60
1:E:122:ILE:HD12	1:E:123:THR:O	2.00	0.60
1:C:241:GLN:NE2	1:C:243:ILE:O	2.31	0.60
1:A:217:SER:HA	1:D:362:PHE:CD2	2.36	0.60
1:D:215:ILE:O	1:D:218:LYS:HG2	2.00	0.60
1:C:311:LYS:HE2	1:D:258:ARG:NH1	2.17	0.60
1:C:288:GLN:NE2	1:D:287:VAL:HB	2.17	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ILE:HB	1:C:213:LYS:HE2	1.82	0.60
1:D:231:GLY:HA2	1:D:274:ASN:O	2.02	0.60
1:C:237:ASP:C	1:C:239:VAL:N	2.55	0.60
1:A:122:ILE:CD1	1:A:122:ILE:N	2.65	0.60
1:A:331:PHE:HD2	1:A:336:THR:HG22	1.66	0.60
1:C:273:SER:HB3	1:C:297:ASN:ND2	2.17	0.59
1:E:145:VAL:CG1	1:E:146:PRO:CD	2.59	0.59
1:C:292:ASN:O	1:C:294:LYS:HG3	2.02	0.59
1:C:271:ASN:ND2	1:C:273:SER:H	2.01	0.59
1:C:142:LYS:HA	1:C:142:LYS:HZ3	1.66	0.59
1:C:238:LEU:N	1:C:238:LEU:HD23	2.18	0.59
1:C:126:TYR:HA	1:C:157:THR:CG2	2.31	0.58
1:A:250:ARG:HG2	1:B:250:ARG:HD3	1.85	0.58
1:A:230:LYS:HG2	1:A:271:ASN:OD1	2.03	0.58
1:A:232:LEU:HD23	1:A:245:VAL:CG1	2.29	0.58
1:A:173:LYS:HB2	1:A:191:ILE:HD12	1.84	0.58
1:A:249:ARG:NE	1:A:249:ARG:HA	2.18	0.58
1:C:287:VAL:HB	1:D:288:GLN:OE1	2.03	0.58
1:A:230:LYS:HD3	1:A:273:SER:O	2.02	0.58
1:B:237:ASP:HA	1:B:240:ALA:HB3	1.86	0.58
1:D:271:ASN:ND2	1:D:273:SER:H	2.01	0.58
1:D:240:ALA:O	1:D:241:GLN:HG3	2.04	0.58
1:E:173:LYS:HE3	1:E:173:LYS:HA	1.86	0.58
1:A:230:LYS:CE	1:A:273:SER:H	2.11	0.58
1:C:234:SER:HA	1:C:239:VAL:CG2	2.33	0.58
1:E:120:PHE:CZ	1:E:166:ALA:HA	2.39	0.58
1:C:343:GLU:OE2	1:C:344:ARG:HD2	2.04	0.58
1:E:132:LYS:HG3	1:E:136:LEU:HG	1.86	0.57
1:C:212:LEU:HG	1:C:216:MET:HE2	1.85	0.57
1:A:205:LYS:N	1:A:208:GLN:OE1	2.30	0.57
1:D:279:ARG:HH11	1:D:279:ARG:HB3	1.67	0.57
1:B:271:ASN:ND2	1:B:273:SER:H	2.01	0.57
1:D:279:ARG:NH1	1:D:279:ARG:HB3	2.19	0.57
1:A:230:LYS:HD2	1:A:273:SER:CB	2.32	0.57
1:D:331:PHE:HD2	1:D:336:THR:HG22	1.68	0.57
1:C:122:ILE:HD12	1:C:191:ILE:HG12	1.87	0.57
1:B:273:SER:HB3	1:B:297:ASN:ND2	2.20	0.57
1:A:230:LYS:HD2	1:A:271:ASN:HD21	1.70	0.57
1:B:366:ALA:H	1:B:367:PRO:HD2	1.70	0.56
1:C:142:LYS:HB3	1:C:175:VAL:HG13	1.87	0.56
1:A:147:PHE:CD1	1:A:149:PRO:HD3	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PRO:HD3	1:E:149:PRO:HD3	1.87	0.56
1:A:205:LYS:H	1:A:208:GLN:CD	2.07	0.56
1:C:216:MET:CE	1:C:259:ILE:HD12	2.35	0.56
1:A:230:LYS:HD2	1:A:271:ASN:ND2	2.20	0.56
1:C:119:TRP:CE3	1:C:164:GLU:HB3	2.40	0.56
1:B:342:ARG:NH1	1:B:348:LEU:O	2.39	0.56
1:B:332:ARG:NH1	1:D:304:LYS:HE3	2.22	0.55
1:B:304:LYS:HE2	1:D:332:ARG:NH1	2.21	0.55
1:C:313:LYS:HD2	1:C:313:LYS:O	2.06	0.55
1:A:211:GLN:HE21	1:E:145:VAL:HG11	1.71	0.55
1:C:331:PHE:CD2	1:C:336:THR:HG22	2.41	0.55
1:A:294:LYS:HE3	1:A:294:LYS:HA	1.87	0.55
1:A:212:LEU:HG	1:A:216:MET:HE2	1.89	0.55
1:C:261:GLU:OE2	1:C:289:LYS:HE3	2.07	0.55
1:A:156:ASN:OD1	1:A:207:GLU:OE2	2.25	0.54
1:B:364:VAL:O	1:B:366:ALA:N	2.39	0.54
1:D:219:ARG:NH1	1:D:232:LEU:CD1	2.70	0.54
1:C:158:ARG:CZ	1:C:207:GLU:OE2	2.55	0.54
1:A:207:GLU:O	1:A:211:GLN:HG3	2.07	0.54
1:C:173:LYS:HB2	1:C:191:ILE:HD12	1.87	0.54
1:C:176:ASN:CG	1:C:177:TYR:CD1	2.79	0.54
1:C:158:ARG:NH1	1:C:207:GLU:OE2	2.41	0.54
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.07	0.54
1:A:244:ASP:O	1:A:246:VAL:HG23	2.07	0.54
1:C:212:LEU:HG	1:C:216:MET:HE3	1.90	0.54
1:A:238:LEU:CD2	1:A:243:ILE:O	2.47	0.54
1:C:142:LYS:HD3	1:C:178:LYS:CG	2.32	0.54
1:E:122:ILE:HG21	1:E:172:LEU:HD13	1.90	0.54
1:C:173:LYS:NZ	1:C:191:ILE:HB	2.23	0.54
1:A:319:GLU:HG3	1:A:350:ARG:HB2	1.90	0.54
1:A:136:LEU:HD22	1:A:149:PRO:HG2	1.90	0.54
1:B:271:ASN:C	1:B:271:ASN:HD22	2.10	0.54
1:B:238:LEU:HG	1:B:245:VAL:HG23	1.90	0.53
1:D:258:ARG:HG3	1:D:258:ARG:NH2	2.17	0.53
1:D:306:GLU:HG2	1:D:344:ARG:NH2	2.23	0.53
1:A:331:PHE:CD2	1:A:336:THR:HG22	2.43	0.53
1:B:205:LYS:N	1:B:208:GLN:NE2	2.55	0.53
1:C:142:LYS:HA	1:C:142:LYS:NZ	2.22	0.53
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.19	0.53
1:D:205:LYS:HD3	1:D:208:GLN:OE1	2.09	0.53
1:D:349:LEU:CD1	1:E:132:LYS:HE3	2.37	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LEU:O	1:D:236:PRO:CD	2.57	0.53
1:C:241:GLN:HG3	1:C:243:ILE:H	1.73	0.53
1:C:319:GLU:OE1	1:C:350:ARG:NH1	2.41	0.53
1:D:305:SER:OG	1:D:307:ARG:HG2	2.09	0.53
1:C:271:ASN:C	1:C:271:ASN:HD22	2.12	0.52
1:C:271:ASN:HD22	1:C:272:LEU:N	2.06	0.52
1:B:331:PHE:HD2	1:B:336:THR:HG22	1.74	0.52
1:C:311:LYS:HE2	1:D:258:ARG:HH11	1.73	0.52
1:D:219:ARG:NH1	1:D:232:LEU:HD12	2.24	0.52
1:C:278:TYR:OH	1:C:279:ARG:NH1	2.42	0.52
1:B:323:ASP:CB	1:C:177:TYR:CE2	2.60	0.52
1:D:219:ARG:CZ	1:D:235:ASP:OD2	2.58	0.52
1:B:215:ILE:HD11	1:B:237:ASP:HB2	1.91	0.52
1:E:132:LYS:HD3	1:E:152:PHE:CD2	2.44	0.52
1:C:136:LEU:HD22	1:C:149:PRO:HG2	1.90	0.52
1:B:271:ASN:HD22	1:B:272:LEU:N	2.06	0.52
1:B:236:PRO:O	1:B:239:VAL:N	2.42	0.52
1:E:131:ASP:HB3	1:E:134:TRP:HB3	1.92	0.52
1:B:324:GLY:CA	1:C:186:ARG:NH1	2.73	0.52
1:C:164:GLU:OE2	1:C:164:GLU:C	2.48	0.52
1:B:205:LYS:HG2	1:B:208:GLN:CG	2.40	0.51
1:D:342:ARG:NH1	1:D:348:LEU:O	2.44	0.51
1:A:347:LYS:HB3	1:A:347:LYS:NZ	2.25	0.51
1:A:248:ASN:H	1:A:248:ASN:HD22	1.57	0.51
1:D:242:ASN:C	1:D:243:ILE:O	2.42	0.51
1:A:338:ILE:HD13	1:A:356:LEU:HD22	1.93	0.51
1:D:243:ILE:HG22	1:D:244:ASP:N	2.26	0.51
1:D:331:PHE:CD2	1:D:336:THR:HG22	2.45	0.51
1:A:328:CYS:C	1:A:330:THR:H	2.14	0.51
1:A:271:ASN:HD22	1:A:272:LEU:N	2.09	0.51
1:B:231:GLY:HA2	1:B:274:ASN:O	2.11	0.51
1:A:172:LEU:HB3	1:A:191:ILE:HD11	1.92	0.50
1:C:340:ALA:O	1:C:343:GLU:HB3	2.10	0.50
1:C:311:LYS:HE3	1:D:258:ARG:CZ	2.42	0.50
1:A:142:LYS:HG3	1:A:179:ILE:CD1	2.40	0.50
1:B:205:LYS:HG2	1:B:208:GLN:HG3	1.92	0.50
1:A:230:LYS:HZ2	1:A:230:LYS:CA	2.23	0.50
1:B:232:LEU:CD2	1:B:245:VAL:HG11	2.41	0.50
1:A:165:ASP:OD2	1:A:166:ALA:N	2.45	0.50
1:E:145:VAL:HG13	1:E:146:PRO:N	2.26	0.50
1:A:218:LYS:HB3	1:A:218:LYS:NZ	2.27	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:O	1:C:241:GLN:HG2	2.11	0.50
1:C:231:GLY:HA2	1:C:274:ASN:O	2.11	0.50
1:C:156:ASN:HD22	1:C:157:THR:H	1.60	0.50
1:D:338:ILE:HD13	1:D:356:LEU:HD22	1.93	0.50
1:B:238:LEU:CD2	1:B:245:VAL:CG2	2.87	0.50
1:D:213:LYS:HB2	1:D:213:LYS:NZ	2.27	0.50
1:A:271:ASN:ND2	1:A:273:SER:H	2.10	0.49
1:C:176:ASN:ND2	1:C:177:TYR:CD1	2.80	0.49
1:D:219:ARG:HH11	1:D:232:LEU:HD12	1.74	0.49
1:A:219:ARG:NH1	1:A:232:LEU:HD12	2.26	0.49
1:B:230:LYS:HB3	1:B:230:LYS:NZ	2.26	0.49
1:C:132:LYS:HE3	1:C:152:PHE:CD2	2.47	0.49
1:A:235:ASP:OD1	1:A:236:PRO:N	2.45	0.49
1:A:342:ARG:NH1	1:A:348:LEU:O	2.44	0.49
1:D:294:LYS:HG3	1:D:316:LYS:O	2.12	0.49
1:A:230:LYS:HZ3	1:A:271:ASN:HB3	1.76	0.49
1:B:295:ILE:HG12	1:B:319:GLU:HB3	1.94	0.49
1:D:271:ASN:HD22	1:D:272:LEU:N	2.09	0.49
1:D:293:LEU:O	1:D:294:LYS:HD2	2.12	0.49
1:B:323:ASP:CA	1:C:177:TYR:HE2	2.23	0.49
1:A:196:PRO:HB2	1:A:199:THR:OG1	2.12	0.49
1:A:204:LEU:CD2	1:A:208:GLN:NE2	2.74	0.49
1:B:331:PHE:CD2	1:B:336:THR:HG22	2.48	0.49
1:E:151:GLU:HG3	1:E:153:HIS:HD1	1.77	0.49
1:C:338:ILE:HD13	1:C:356:LEU:HD22	1.95	0.49
1:A:210:GLU:HG3	1:D:360:ILE:HD11	1.95	0.49
1:D:212:LEU:HG	1:D:216:MET:HE3	1.95	0.49
1:B:241:GLN:N	1:B:241:GLN:NE2	2.61	0.49
1:C:311:LYS:CE	1:D:258:ARG:NH1	2.76	0.49
1:A:243:ILE:N	1:A:243:ILE:HD12	2.28	0.48
1:D:351:LEU:O	1:D:352:ASP:HB2	2.13	0.48
1:B:266:GLU:H	1:B:266:GLU:CD	2.16	0.48
1:C:225:GLN:HG2	1:C:266:GLU:OE2	2.14	0.48
1:D:207:GLU:OE2	1:D:208:GLN:HG3	2.13	0.48
1:B:364:VAL:HG22	1:B:367:PRO:CB	2.34	0.48
1:D:235:ASP:CB	1:D:236:PRO:CD	2.83	0.48
1:B:294:LYS:HG3	1:B:295:ILE:HG13	1.94	0.48
1:C:258:ARG:CZ	1:D:311:LYS:HE3	2.43	0.48
1:B:215:ILE:CG1	1:B:238:LEU:HD13	2.28	0.48
1:E:122:ILE:HD12	1:E:123:THR:N	2.29	0.48
1:A:248:ASN:N	1:A:248:ASN:ND2	2.57	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HB2	1:A:175:VAL:HG13	1.96	0.48
1:A:358:PRO:HA	1:A:359:PRO:HD3	1.82	0.48
1:C:176:ASN:OD1	1:C:177:TYR:CD1	2.67	0.47
1:D:327:LEU:HD12	1:D:328:CYS:N	2.29	0.47
1:D:205:LYS:HB2	1:D:208:GLN:CG	2.44	0.47
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.67	0.47
1:D:204:LEU:HD23	1:D:208:GLN:NE2	2.29	0.47
1:A:140:GLN:OE1	1:A:146:PRO:HA	2.14	0.47
1:C:119:TRP:CD1	1:C:196:PRO:HG3	2.49	0.47
1:D:271:ASN:C	1:D:271:ASN:HD22	2.18	0.47
1:B:324:GLY:HA3	1:C:186:ARG:NH1	2.28	0.47
1:C:156:ASN:ND2	1:C:157:THR:N	2.63	0.47
1:D:358:PRO:HA	1:D:359:PRO:HD3	1.82	0.47
1:A:263:ASN:HB3	1:D:362:PHE:CD1	2.49	0.47
1:B:226:VAL:HG13	1:B:269:SER:HB3	1.96	0.47
1:E:140:GLN:O	1:E:141:SER:C	2.51	0.47
1:A:132:LYS:HE3	1:A:152:PHE:CD2	2.49	0.47
1:A:230:LYS:CD	1:A:271:ASN:ND2	2.78	0.47
1:E:134:TRP:O	1:E:138:MET:HB2	2.14	0.47
1:C:342:ARG:NH1	1:C:348:LEU:O	2.48	0.47
1:B:365:GLU:OE1	1:B:365:GLU:C	2.53	0.47
1:A:250:ARG:HD3	1:B:250:ARG:HG2	1.97	0.47
1:C:258:ARG:NE	1:D:311:LYS:HE3	2.30	0.47
1:C:232:LEU:CD2	1:C:245:VAL:HG11	2.44	0.47
1:D:204:LEU:HD23	1:D:208:GLN:HE21	1.80	0.47
1:A:249:ARG:HH11	1:A:279:ARG:NH2	2.12	0.47
1:A:271:ASN:C	1:A:271:ASN:HD22	2.19	0.47
1:B:236:PRO:HB2	1:B:237:ASP:OD1	2.13	0.46
1:B:364:VAL:HA	1:B:367:PRO:HD2	1.97	0.46
1:A:180:LEU:HD21	1:A:184:ASN:OD1	2.14	0.46
1:D:219:ARG:HH11	1:D:232:LEU:HD13	1.77	0.46
1:A:236:PRO:O	1:A:237:ASP:CB	2.60	0.46
1:A:305:SER:OG	1:A:306:GLU:N	2.48	0.46
1:A:118:ASN:OD1	1:A:118:ASN:N	2.48	0.46
1:C:122:ILE:CD1	1:C:122:ILE:N	2.78	0.46
1:A:122:ILE:HD13	1:A:122:ILE:N	2.31	0.46
1:A:164:GLU:CD	1:A:164:GLU:O	2.53	0.46
1:D:244:ASP:HB3	1:D:246:VAL:HG23	1.97	0.46
1:E:137:SER:O	1:E:141:SER:N	2.40	0.46
1:B:336:THR:HG21	1:D:307:ARG:NH1	2.25	0.46
1:D:204:LEU:CD1	1:D:252:CYS:HA	2.44	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HG	1:A:216:MET:HE3	1.96	0.45
1:B:246:VAL:O	1:B:249:ARG:HB2	2.16	0.45
1:D:234:SER:O	1:D:235:ASP:C	2.54	0.45
1:D:273:SER:HB3	1:D:297:ASN:HD22	1.80	0.45
1:D:264:ILE:N	1:D:265:PRO:HD3	2.32	0.45
1:A:258:ARG:CZ	1:B:311:LYS:HE3	2.46	0.45
1:D:309:LEU:HD11	1:D:322:LEU:HD11	1.98	0.45
1:C:232:LEU:HD23	1:C:245:VAL:HG11	1.99	0.45
1:C:156:ASN:HD22	1:C:157:THR:N	2.14	0.45
1:A:233:ARG:HG2	1:A:244:ASP:OD1	2.16	0.45
1:A:176:ASN:OD1	1:A:188:SER:HA	2.16	0.45
1:B:204:LEU:HD12	1:B:204:LEU:N	2.32	0.45
1:A:288:GLN:HG2	1:A:288:GLN:H	1.52	0.45
1:A:327:LEU:HD12	1:A:328:CYS:N	2.32	0.45
1:E:144:SER:O	1:E:145:VAL:HB	2.14	0.45
1:B:309:LEU:HD11	1:B:322:LEU:HD11	1.98	0.45
1:B:257:LEU:HD11	1:B:283:MET:HA	1.99	0.45
1:C:219:ARG:NH1	1:C:232:LEU:HD12	2.32	0.44
1:A:155:GLU:OE2	1:A:205:LYS:CE	2.66	0.44
1:C:264:ILE:N	1:C:265:PRO:HD3	2.32	0.44
1:C:207:GLU:OE1	1:C:207:GLU:N	2.50	0.44
1:D:205:LYS:HB2	1:D:208:GLN:OE1	2.18	0.44
1:B:324:GLY:CA	1:C:186:ARG:HH12	2.30	0.44
1:E:121:LYS:HZ1	1:E:160:GLN:HG2	1.83	0.44
1:B:251:SER:O	1:B:254:ALA:HB3	2.17	0.44
1:A:182:ARG:HG2	1:A:183:GLU:N	2.32	0.44
1:C:176:ASN:OD1	1:C:188:SER:HA	2.18	0.44
1:E:153:HIS:HE1	1:E:162:PHE:HE1	1.64	0.44
1:A:230:LYS:HE2	1:A:272:LEU:N	2.32	0.44
1:B:289:LYS:C	1:B:291:PRO:HD3	2.38	0.44
1:D:239:VAL:C	1:D:241:GLN:N	2.71	0.44
1:C:289:LYS:C	1:C:291:PRO:HD3	2.39	0.44
1:C:176:ASN:ND2	1:C:177:TYR:HD1	2.14	0.43
1:B:246:VAL:HB	1:B:249:ARG:HH11	1.83	0.43
1:B:289:LYS:O	1:B:291:PRO:HD3	2.17	0.43
1:A:230:LYS:CA	1:A:230:LYS:NZ	2.80	0.43
1:C:309:LEU:HD11	1:C:322:LEU:HD11	2.00	0.43
1:B:351:LEU:O	1:B:352:ASP:HB2	2.17	0.43
1:A:204:LEU:HD12	1:A:255:ALA:CB	2.49	0.43
1:D:294:LYS:HE3	1:D:316:LYS:HB2	2.00	0.43
1:D:251:SER:O	1:D:254:ALA:HB3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HD23	1:E:146:PRO:HD3	2.00	0.43
1:D:242:ASN:O	1:D:243:ILE:C	2.56	0.43
1:A:332:ARG:HB2	1:A:332:ARG:NH2	2.33	0.43
1:C:197:PRO:C	1:C:198:HIS:CG	2.92	0.43
1:B:366:ALA:N	1:B:367:PRO:HD2	2.33	0.43
1:A:128:ARG:CG	1:A:128:ARG:NH1	2.81	0.43
1:D:266:GLU:CD	1:D:266:GLU:H	2.22	0.43
1:B:271:ASN:C	1:B:271:ASN:ND2	2.71	0.43
1:D:340:ALA:O	1:D:343:GLU:HB3	2.19	0.43
1:C:327:LEU:HD12	1:C:328:CYS:N	2.33	0.43
1:A:158:ARG:HD2	1:A:160:GLN:OE1	2.19	0.43
1:A:292:ASN:C	1:A:294:LYS:HZ2	2.21	0.43
1:B:264:ILE:N	1:B:265:PRO:HD3	2.34	0.43
1:A:329:ASP:OD2	1:A:329:ASP:N	2.51	0.43
1:A:351:LEU:O	1:A:352:ASP:HB2	2.19	0.43
1:C:155:GLU:O	1:C:156:ASN:HB3	2.19	0.43
1:E:172:LEU:HA	1:E:172:LEU:HD23	1.89	0.43
1:A:264:ILE:N	1:A:265:PRO:HD3	2.34	0.42
1:A:128:ARG:NH1	1:A:154:TYR:CD1	2.86	0.42
1:A:331:PHE:HD2	1:A:336:THR:CG2	2.32	0.42
1:A:340:ALA:O	1:A:343:GLU:HB3	2.20	0.42
1:E:136:LEU:HD13	1:E:149:PRO:HG2	1.99	0.42
1:A:273:SER:HB3	1:A:297:ASN:HD22	1.84	0.42
1:C:156:ASN:ND2	1:C:157:THR:H	2.17	0.42
1:A:279:ARG:O	1:A:279:ARG:HG3	2.18	0.42
1:C:214:LEU:HG	1:C:218:LYS:HE3	2.01	0.42
1:C:131:ASP:HB3	1:C:134:TRP:HB3	2.01	0.42
1:A:230:LYS:CE	1:A:271:ASN:ND2	2.82	0.42
1:A:150:ILE:O	1:A:150:ILE:HG13	2.20	0.42
1:B:232:LEU:HD23	1:B:245:VAL:CG1	2.48	0.42
1:D:317:LEU:N	1:D:347:LYS:NZ	2.67	0.42
1:D:215:ILE:HA	1:D:218:LYS:HE3	2.02	0.42
1:C:128:ARG:O	1:C:128:ARG:HG3	2.19	0.42
1:A:230:LYS:HG2	1:A:271:ASN:CG	2.40	0.42
1:D:219:ARG:NH1	1:D:232:LEU:HD13	2.34	0.42
1:B:327:LEU:HD12	1:B:328:CYS:N	2.34	0.42
1:C:180:LEU:HD21	1:C:184:ASN:OD1	2.19	0.42
1:B:279:ARG:O	1:B:279:ARG:HG3	2.19	0.42
1:B:338:ILE:HD13	1:B:356:LEU:HD22	2.00	0.42
1:A:216:MET:HG2	1:A:229:LEU:HD21	2.01	0.42
1:C:331:PHE:HD2	1:C:336:THR:CG2	2.29	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LEU:O	1:C:293:LEU:HD12	2.20	0.42
1:A:175:VAL:HG12	1:A:175:VAL:O	2.20	0.42
1:D:224:GLN:OE1	1:D:224:GLN:HA	2.20	0.42
1:D:238:LEU:HD13	1:D:238:LEU:C	2.39	0.42
1:B:323:ASP:CA	1:C:177:TYR:CE2	3.02	0.42
1:C:150:ILE:HG13	1:C:150:ILE:O	2.19	0.42
1:C:307:ARG:O	1:C:308:GLU:C	2.57	0.42
1:B:204:LEU:CA	1:B:208:GLN:HE21	2.23	0.41
1:A:288:GLN:NE2	1:B:287:VAL:HB	2.29	0.41
1:C:289:LYS:O	1:C:291:PRO:HD3	2.20	0.41
1:A:289:LYS:O	1:A:291:PRO:HD3	2.20	0.41
1:B:364:VAL:O	1:B:364:VAL:HG13	2.20	0.41
1:A:292:ASN:O	1:A:294:LYS:HG2	2.20	0.41
1:B:216:MET:HG2	1:B:229:LEU:HD21	2.03	0.41
1:D:239:VAL:O	1:D:241:GLN:N	2.54	0.41
1:A:182:ARG:HG2	1:A:183:GLU:H	1.85	0.41
1:C:271:ASN:C	1:C:271:ASN:ND2	2.72	0.41
1:C:235:ASP:HB3	1:C:236:PRO:HD2	2.02	0.41
1:B:236:PRO:O	1:B:239:VAL:HB	2.20	0.41
1:C:273:SER:HB3	1:C:297:ASN:HD22	1.86	0.41
1:B:246:VAL:HB	1:B:249:ARG:NH1	2.35	0.41
1:D:355:GLU:N	1:D:355:GLU:OE1	2.53	0.41
1:C:175:VAL:HG12	1:C:175:VAL:O	2.20	0.41
1:D:347:LYS:H	1:D:347:LYS:CD	2.34	0.41
1:E:119:TRP:CE2	1:E:164:GLU:HB2	2.56	0.41
1:A:289:LYS:C	1:A:291:PRO:HD3	2.41	0.41
1:C:257:LEU:HD11	1:C:283:MET:HA	2.03	0.41
1:D:232:LEU:CD2	1:D:245:VAL:HG11	2.50	0.41
1:A:356:LEU:HA	1:A:357:PRO:HD3	1.93	0.41
1:B:358:PRO:HA	1:B:359:PRO:HD3	1.79	0.41
1:A:309:LEU:HD11	1:A:322:LEU:HD11	2.03	0.41
1:C:151:GLU:HB3	1:C:162:PHE:HD1	1.86	0.41
1:A:287:VAL:HB	1:B:288:GLN:NE2	2.36	0.41
1:A:131:ASP:HB3	1:A:134:TRP:HB3	2.03	0.41
1:D:289:LYS:C	1:D:291:PRO:HD3	2.40	0.41
1:C:337:TYR:CE2	1:C:351:LEU:HD21	2.56	0.41
1:A:251:SER:O	1:A:254:ALA:HB3	2.21	0.41
1:C:355:GLU:OE1	1:C:355:GLU:N	2.53	0.41
1:E:132:LYS:HD3	1:E:152:PHE:CZ	2.54	0.40
1:C:279:ARG:O	1:C:279:ARG:HG2	2.20	0.40
1:D:289:LYS:O	1:D:291:PRO:HD3	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLN:HG3	1:C:243:ILE:N	2.36	0.40
1:A:155:GLU:OE2	1:A:205:LYS:HE3	2.21	0.40
1:D:213:LYS:HZ2	1:D:213:LYS:HB2	1.87	0.40
1:A:226:VAL:HG13	1:A:269:SER:HB3	2.03	0.40
1:C:176:ASN:O	1:C:177:TYR:HB2	2.21	0.40
1:D:216:MET:HG2	1:D:229:LEU:HD21	2.04	0.40
1:A:204:LEU:HD12	1:A:255:ALA:HB2	2.03	0.40
1:B:324:GLY:HA3	1:C:186:ARG:HH12	1.86	0.40
1:A:236:PRO:CA	1:A:239:VAL:HG23	2.42	0.40
1:B:363:ASP:C	1:B:365:GLU:N	2.74	0.40
1:D:257:LEU:HD11	1:D:283:MET:HA	2.03	0.40

All (1) 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:E:142:LYS:NZ	1:E:142:LYS:NZ[8_665]	1.44	0.76

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/271 (88%)	213 (90%)	20 (8%)	5 (2%)	9	44
1	B	163/271 (60%)	149 (91%)	10 (6%)	4 (2%)	7	39
1	C	240/271 (89%)	216 (90%)	17 (7%)	7 (3%)	6	35
1	D	160/271 (59%)	139 (87%)	16 (10%)	5 (3%)	5	32
1	E	38/271 (14%)	35 (92%)	2 (5%)	1 (3%)	7	38
All	All	839/1355 (62%)	752 (90%)	65 (8%)	22 (3%)	7	38

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	PRO
1	C	157	THR
1	C	236	PRO
1	C	238	LEU
1	C	308	GLU
1	D	236	PRO
1	D	238	LEU
1	A	241	GLN
1	A	245	VAL
1	D	235	ASP
1	E	146	PRO
1	B	363	ASP
1	B	365	GLU
1	C	237	ASP
1	C	242	ASN
1	A	156	ASN
1	B	206	PRO
1	D	206	PRO
1	D	231	GLY
1	C	149	PRO
1	A	149	PRO
1	A	195	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/245 (91%)	201 (90%)	21 (10%)	11	38
1	B	152/245 (62%)	143 (94%)	9 (6%)	24	63
1	C	222/245 (91%)	205 (92%)	17 (8%)	16	52
1	D	150/245 (61%)	137 (91%)	13 (9%)	13	44
1	E	39/245 (16%)	34 (87%)	5 (13%)	5	24
All	All	785/1225 (64%)	720 (92%)	65 (8%)	14	48

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ILE
1	A	128	ARG
1	A	149	PRO
1	A	156	ASN
1	A	172	LEU
1	A	181	ASP
1	A	182	ARG
1	A	197	PRO
1	A	206	PRO
1	A	213	LYS
1	A	230	LYS
1	A	248	ASN
1	A	271	ASN
1	A	276	ARG
1	A	288	GLN
1	A	294	LYS
1	A	297	ASN
1	A	306	GLU
1	A	329	ASP
1	A	347	LYS
1	A	355	GLU
1	B	206	PRO
1	B	211	GLN
1	B	237	ASP
1	B	241	GLN
1	B	271	ASN
1	B	297	ASN
1	B	364	VAL
1	B	365	GLU
1	B	367	PRO
1	C	122	ILE
1	C	142	LYS
1	C	149	PRO
1	C	156	ASN
1	C	164	GLU
1	C	165	ASP
1	C	172	LEU
1	C	181	ASP
1	C	228	ASP
1	C	236	PRO
1	C	238	LEU
1	C	266	GLU
1	C	271	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	297	ASN
1	C	306	GLU
1	C	346	PRO
1	C	355	GLU
1	D	207	GLU
1	D	210	GLU
1	D	235	ASP
1	D	236	PRO
1	D	258	ARG
1	D	266	GLU
1	D	271	ASN
1	D	297	ASN
1	D	306	GLU
1	D	329	ASP
1	D	347	LYS
1	D	355	GLU
1	D	363	ASP
1	E	121	LYS
1	E	122	ILE
1	E	150	ILE
1	E	164	GLU
1	E	173	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	156	ASN
1	A	248	ASN
1	A	263	ASN
1	A	271	ASN
1	A	288	GLN
1	A	297	ASN
1	B	208	GLN
1	B	211	GLN
1	B	241	GLN
1	B	263	ASN
1	B	271	ASN
1	B	297	ASN
1	C	156	ASN
1	C	263	ASN
1	C	271	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	297	ASN
1	D	208	GLN
1	D	211	GLN
1	D	263	ASN
1	D	271	ASN
1	D	297	ASN
1	E	160	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	242/271 (89%)	0.02	8 (3%)	50	33	55, 66, 89, 109	0
1	B	165/271 (60%)	0.03	6 (3%)	46	29	49, 63, 82, 97	0
1	C	244/271 (90%)	0.18	6 (2%)	61	45	55, 74, 106, 106	0
1	D	162/271 (59%)	0.14	7 (4%)	39	23	52, 65, 85, 100	0
1	E	44/271 (16%)	1.01	8 (18%)	2	1	89, 94, 94, 94	0
All	All	857/1355 (63%)	0.14	35 (4%)	41	25	49, 68, 106, 109	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	239	VAL	4.3
1	E	164	GLU	4.1
1	B	367	PRO	3.4
1	A	242	ASN	3.2
1	D	365	GLU	3.2
1	E	160	GLN	3.0
1	A	118	ASN	3.0
1	D	238	LEU	2.9
1	C	242	ASN	2.8
1	E	170	SER	2.8
1	A	211	GLN	2.8
1	D	363	ASP	2.8
1	A	198	HIS	2.6
1	A	240	ALA	2.5
1	B	203	GLU	2.5
1	D	244	ASP	2.4
1	E	119	TRP	2.4
1	E	121	LYS	2.4
1	D	364	VAL	2.3
1	C	178	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	117	LYS	2.3
1	B	364	VAL	2.2
1	C	329	ASP	2.2
1	A	199	THR	2.2
1	E	120	PHE	2.2
1	B	363	ASP	2.2
1	B	366	ALA	2.1
1	E	165	ASP	2.1
1	B	365	GLU	2.1
1	E	153	HIS	2.1
1	D	319	GLU	2.1
1	A	332	ARG	2.1
1	C	119	TRP	2.1
1	C	131	ASP	2.1
1	A	203	GLU	2.1

## 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.