



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:07 am BST

PDB ID : 3UU2  
Title : Salmonella typhi osmoporin(OmpC):an Outer Membrane Protein  
Authors : Prasanth, P.; Putcha, B.K.; Arockiasamy, A.; Krishnaswamy, S.  
Deposited on : 2011-11-27  
Resolution : 3.59 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

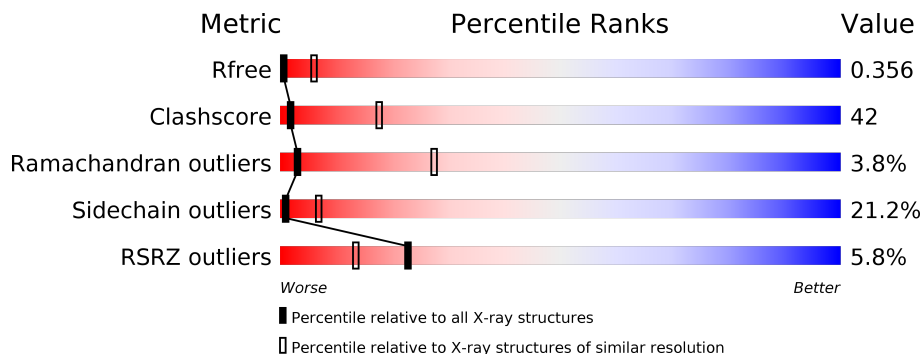
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	357	 4% 31% 38% 14% 17%
1	B	357	 4% 31% 43% 10% 17%
1	C	357	 7% 33% 40% 10% 17%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6988 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.

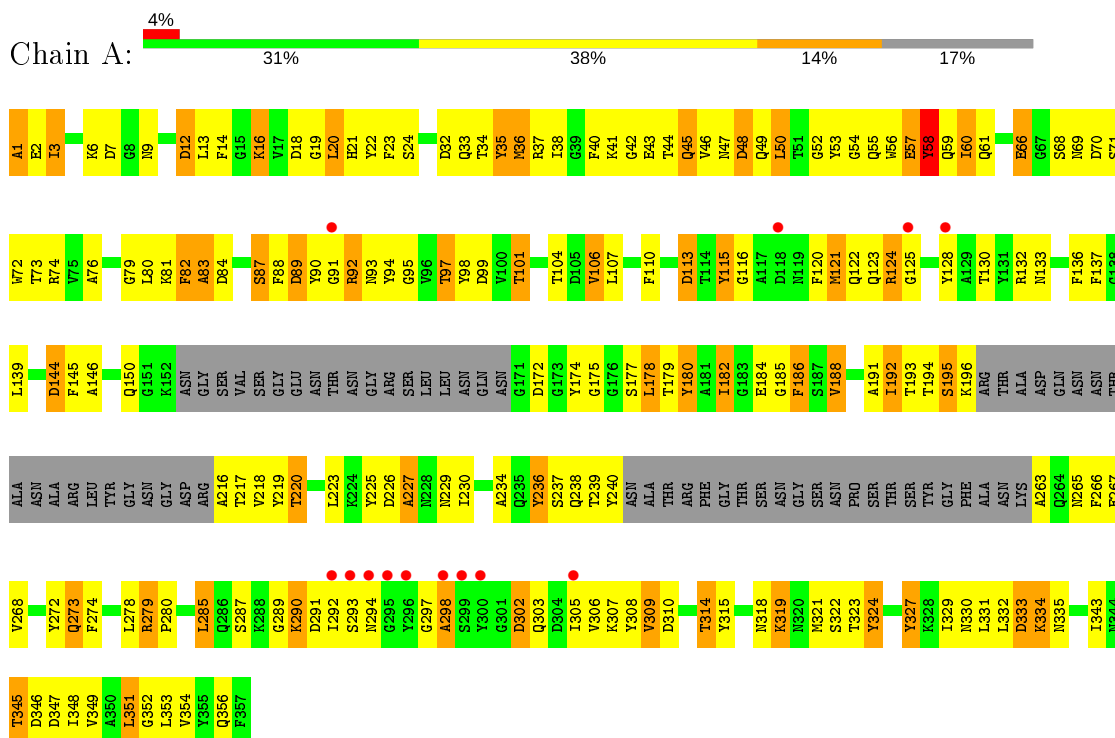
- Molecule 1 is a protein called Outer membrane protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	Total 2328	C 1476	N 374	O 475	S 3	0	0	0
1	B	298	Total 2333	C 1480	N 375	O 475	S 3	0	0	0
1	C	298	Total 2327	C 1476	N 373	O 475	S 3	0	0	0

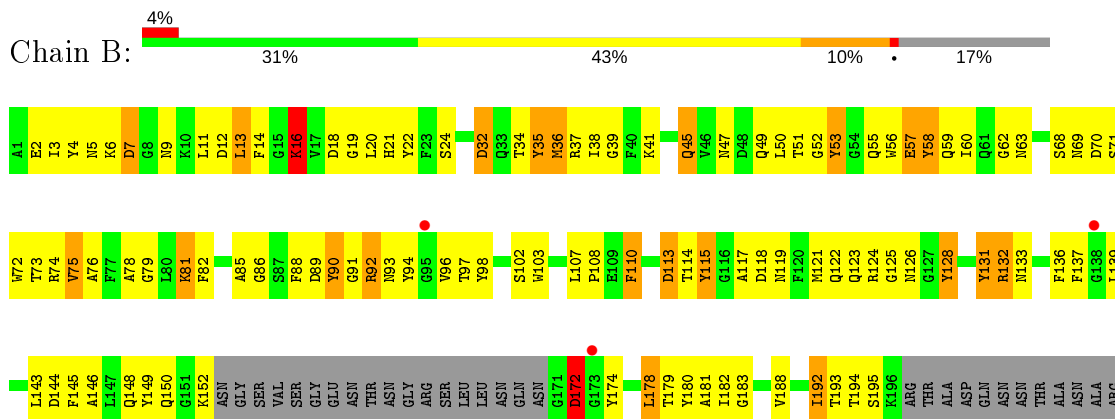
### 3 Residue-property plots i

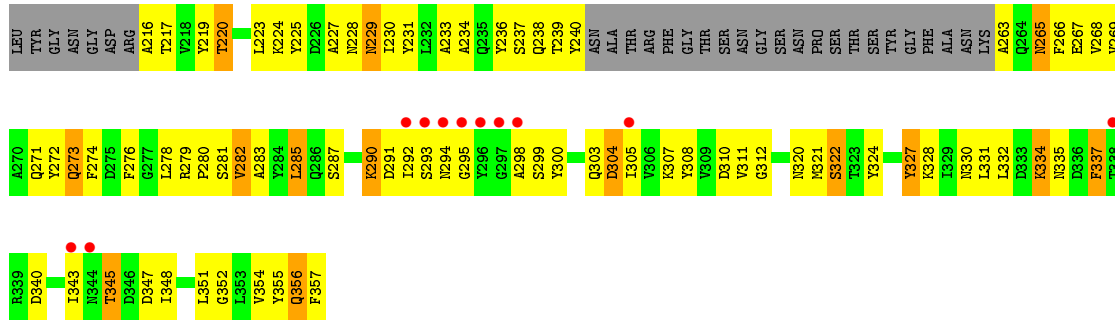
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Outer membrane protein C

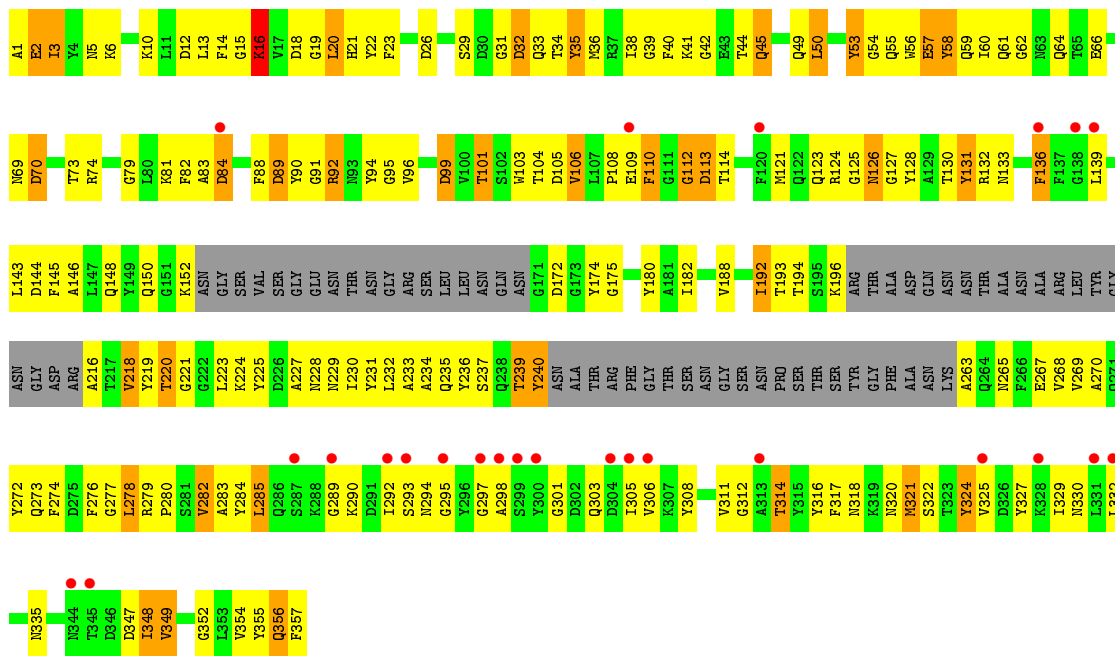


- Molecule 1: Outer membrane protein C





● Molecule 1: Outer membrane protein C



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.20Å 108.57Å 113.39Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	50.00 – 3.59 49.65 – 3.34	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.59) 95.5 (49.65-3.34)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 3.33Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.302 , 0.358 0.302 , 0.356	Depositor DCC
$R_{free}$ test set	1383 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.5	Xtrriage
Anisotropy	0.653	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 141.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	226.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% 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	0.70	3/2380 (0.1%)	0.79	2/3217 (0.1%)
1	B	0.68	2/2385 (0.1%)	0.74	0/3223
1	C	0.61	1/2379 (0.0%)	0.68	0/3217
All	All	0.66	6/7144 (0.1%)	0.74	2/9657 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	LYS	CE-NZ	10.89	1.76	1.49
1	C	105	ASP	CB-CG	7.33	1.67	1.51
1	A	1	ALA	CA-CB	6.27	1.65	1.52
1	B	57	GLU	CG-CD	5.96	1.60	1.51
1	A	12	ASP	CB-CG	5.77	1.63	1.51
1	A	58	TYR	CE1-CZ	5.31	1.45	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	351	LEU	CA-CB-CG	5.09	127.01	115.30

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	A	2328	0	2118	221	0
1	B	2333	0	2133	212	0
1	C	2327	0	2115	169	0
All	All	6988	0	6366	564	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 (564) 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:B:334:LYS:NZ	1:B:334:LYS:CE	1.76	1.47
1:A:123:GLN:HG3	1:A:124:ARG:H	1.07	1.14
1:B:58:TYR:HB2	1:B:73:THR:HA	1.18	1.11
1:A:19:GLY:HA2	1:A:34:THR:HG22	1.16	1.05
1:C:236:TYR:HB2	1:C:265:ASN:O	1.57	1.04
1:B:22:TYR:HE1	1:B:110:PHE:CE1	1.76	1.03
1:B:263:ALA:HB2	1:B:290:LYS:HD2	1.42	1.02
1:B:22:TYR:CE1	1:B:110:PHE:HE1	1.78	1.01
1:B:123:GLN:HG2	1:B:124:ARG:H	1.27	0.99
1:A:22:TYR:HD2	1:A:33:GLN:OE1	1.41	0.99
1:A:334:LYS:HG3	1:A:345:THR:HG21	1.43	0.96
1:B:123:GLN:CG	1:B:124:ARG:H	1.78	0.96
1:A:324:TYR:HE2	1:A:352:GLY:HA3	1.31	0.96
1:A:123:GLN:CG	1:A:124:ARG:H	1.80	0.95
1:B:3:ILE:HD11	1:B:13:LEU:HD22	1.46	0.94
1:B:271:GLN:OE1	1:B:281:SER:HB3	1.66	0.94
1:A:123:GLN:HG3	1:A:124:ARG:N	1.81	0.94
1:C:322:SER:HB2	1:C:354:VAL:HG22	1.47	0.94
1:A:19:GLY:CA	1:A:34:THR:HG22	1.98	0.94
1:C:18:ASP:HB3	1:C:35:TYR:HE1	1.30	0.93
1:A:234:ALA:HB2	1:A:268:VAL:HG23	1.49	0.92
1:A:19:GLY:HA2	1:A:34:THR:CG2	1.99	0.92
1:C:23:PHE:HB2	1:C:349:VAL:HG13	1.52	0.92
1:B:16:LYS:HD2	1:B:37:ARG:HD2	1.52	0.91
1:C:59:GLN:O	1:C:60:ILE:HG13	1.72	0.89
1:B:92:ARG:HD2	1:B:125:GLY:O	1.72	0.88
1:C:322:SER:HB2	1:C:354:VAL:CG2	2.04	0.88
1:A:18:ASP:HB3	1:A:35:TYR:HE1	1.38	0.88
1:B:303:GLN:HE22	1:B:335:ASN:HD21	1.21	0.87
1:C:18:ASP:HB3	1:C:35:TYR:CE1	2.08	0.87
1:A:16:LYS:HB2	1:A:16:LYS:NZ	1.89	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLU:OE2	1:B:74:ARG:NH2	2.06	0.87
1:C:53:TYR:OH	1:C:89:ASP:OD2	1.92	0.87
1:B:34:THR:HG21	1:C:91:GLY:HA2	1.56	0.86
1:A:267:GLU:HB3	1:A:285:LEU:HB3	1.58	0.85
1:A:303:GLN:HE22	1:A:335:ASN:HD21	1.23	0.85
1:C:277:GLY:O	1:C:278:LEU:HB2	1.78	0.83
1:A:22:TYR:HE1	1:A:110:PHE:HE1	1.23	0.83
1:A:128:TYR:CE1	1:A:150:GLN:HG2	2.14	0.83
1:A:324:TYR:CE2	1:A:352:GLY:HA3	2.14	0.83
1:B:58:TYR:CB	1:B:73:THR:HA	2.05	0.82
1:A:309:VAL:HG13	1:A:329:ILE:HB	1.62	0.82
1:A:145:PHE:HB2	1:A:178:LEU:HD23	1.60	0.82
1:C:19:GLY:HA2	1:C:34:THR:HG22	1.62	0.81
1:C:267:GLU:HB3	1:C:285:LEU:HB3	1.63	0.81
1:B:263:ALA:HB2	1:B:290:LYS:CD	2.11	0.81
1:B:45:GLN:HA	1:B:51:THR:HG22	1.63	0.81
1:A:216:ALA:HA	1:A:240:TYR:HB3	1.61	0.80
1:C:92:ARG:HH12	1:C:124:ARG:HB3	1.45	0.80
1:A:240:TYR:HD1	1:A:240:TYR:O	1.65	0.80
1:A:18:ASP:HB3	1:A:35:TYR:CE1	2.17	0.79
1:C:273:GLN:HG2	1:C:279:ARG:HD3	1.62	0.79
1:A:182:ILE:HD11	1:A:188:VAL:HB	1.65	0.79
1:C:132:ARG:HG3	1:C:146:ALA:HB2	1.65	0.78
1:B:303:GLN:HE22	1:B:335:ASN:ND2	1.81	0.78
1:A:229:ASN:HB2	1:A:272:TYR:CE1	2.19	0.78
1:C:19:GLY:CA	1:C:34:THR:HG22	2.13	0.78
1:B:303:GLN:NE2	1:B:335:ASN:HD21	1.81	0.78
1:A:20:LEU:HD23	1:A:20:LEU:O	1.84	0.77
1:A:47:ASN:O	1:A:49:GLN:N	2.17	0.77
1:B:97:THR:OG1	1:B:193:THR:HG21	1.86	0.76
1:A:46:VAL:HG11	1:C:317:PHE:HB3	1.66	0.76
1:A:132:ARG:HG3	1:A:146:ALA:HB2	1.67	0.76
1:B:117:ALA:O	1:B:118:ASP:HB2	1.85	0.76
1:B:121:MET:SD	1:B:150:GLN:OE1	2.45	0.75
1:C:239:THR:HG23	1:C:263:ALA:HB1	1.69	0.75
1:A:236:TYR:HB2	1:A:266:PHE:HA	1.67	0.75
1:B:19:GLY:O	1:B:352:GLY:HA3	1.87	0.74
1:A:128:TYR:HE1	1:A:150:GLN:HG2	1.52	0.73
1:C:56:TRP:CZ2	1:C:58:TYR:HD2	2.06	0.73
1:B:263:ALA:CB	1:B:290:LYS:HD2	2.17	0.73
1:B:272:TYR:O	1:B:280:PRO:HD2	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:PHE:HE2	1:C:41:LYS:HG3	1.53	0.72
1:B:267:GLU:HB3	1:B:285:LEU:HB3	1.71	0.72
1:A:194:THR:HB	1:A:217:THR:HG22	1.72	0.72
1:B:107:LEU:HD23	1:B:310:ASP:OD1	1.88	0.72
1:A:218:VAL:HG22	1:A:219:TYR:O	1.90	0.71
1:A:92:ARG:HD2	1:A:125:GLY:O	1.90	0.71
1:C:121:MET:HG3	1:C:128:TYR:HE1	1.55	0.71
1:A:91:GLY:HA2	1:C:34:THR:HG21	1.73	0.71
1:B:103:TRP:CD2	1:B:224:LYS:HD2	2.26	0.71
1:B:219:TYR:O	1:B:237:SER:CB	2.39	0.71
1:B:229:ASN:HB2	1:B:272:TYR:CE1	2.25	0.71
1:A:22:TYR:CE1	1:A:110:PHE:HE1	2.07	0.71
1:A:16:LYS:HZ1	1:A:18:ASP:HB2	1.57	0.70
1:A:50:LEU:HA	1:A:81:LYS:O	1.91	0.70
1:C:20:LEU:HD23	1:C:33:GLN:O	1.90	0.70
1:B:123:GLN:CG	1:B:124:ARG:N	2.49	0.70
1:B:19:GLY:HA2	1:B:34:THR:HG22	1.72	0.70
1:B:266:PHE:CZ	1:B:268:VAL:HB	2.26	0.70
1:B:3:ILE:CD1	1:B:13:LEU:HD22	2.21	0.70
1:A:22:TYR:CD2	1:A:33:GLN:OE1	2.34	0.70
1:B:56:TRP:HA	1:B:75:VAL:O	1.92	0.70
1:C:18:ASP:CG	1:C:354:VAL:HG12	2.12	0.70
1:A:240:TYR:O	1:A:240:TYR:CD1	2.46	0.69
1:A:66:GLU:HG3	1:B:72:TRP:CD1	2.28	0.69
1:C:16:LYS:HB3	1:C:356:GLN:HB3	1.75	0.69
1:A:16:LYS:HZ2	1:A:16:LYS:HB2	1.56	0.69
1:B:14:PHE:CE1	1:B:57:GLU:HB3	2.26	0.68
1:C:193:THR:OG1	1:C:218:VAL:HG13	1.93	0.68
1:A:79:GLY:HA3	1:A:89:ASP:HB3	1.73	0.68
1:A:36:MET:HE2	1:A:38:ILE:HD11	1.76	0.68
1:C:56:TRP:HZ2	1:C:58:TYR:CD2	2.11	0.68
1:B:2:GLU:HA	1:B:12:ASP:HA	1.76	0.67
1:B:194:THR:HG22	1:B:217:THR:CG2	2.25	0.67
1:C:56:TRP:CZ2	1:C:58:TYR:CD2	2.83	0.67
1:B:273:GLN:NE2	1:B:279:ARG:HB2	2.09	0.67
1:A:194:THR:HA	1:A:217:THR:HA	1.76	0.67
1:B:145:PHE:HB3	1:B:178:LEU:HD13	1.75	0.67
1:C:88:PHE:HA	1:C:130:THR:O	1.95	0.67
1:A:36:MET:HE2	1:A:38:ILE:CD1	2.26	0.66
1:A:82:PHE:CD2	1:A:83:ALA:N	2.63	0.66
1:B:57:GLU:CD	1:B:74:ARG:HH21	1.97	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:O	1:A:80:LEU:HD23	1.95	0.66
1:A:16:LYS:HB3	1:A:356:GLN:HA	1.76	0.66
1:C:121:MET:HA	1:C:128:TYR:OH	1.96	0.66
1:B:180:TYR:CE2	1:B:182:ILE:HA	2.31	0.66
1:C:50:LEU:HA	1:C:81:LYS:O	1.96	0.66
1:C:58:TYR:CB	1:C:73:THR:HA	2.26	0.65
1:A:21:HIS:HB2	1:B:90:TYR:OH	1.96	0.65
1:A:36:MET:HE1	1:A:38:ILE:HG13	1.78	0.65
1:A:82:PHE:HD2	1:A:83:ALA:N	1.94	0.65
1:C:35:TYR:C	1:C:35:TYR:CD1	2.68	0.65
1:C:303:GLN:HE22	1:C:335:ASN:HD21	1.44	0.65
1:A:3:ILE:HD11	1:B:3:ILE:HG21	1.78	0.64
1:C:182:ILE:HD11	1:C:188:VAL:HB	1.80	0.64
1:C:308:TYR:HB2	1:C:329:ILE:O	1.97	0.64
1:B:50:LEU:HA	1:B:81:LYS:O	1.97	0.64
1:B:92:ARG:HD3	1:B:126:ASN:OD1	1.97	0.64
1:B:355:TYR:CE2	1:C:42:GLY:HA3	2.33	0.64
1:A:145:PHE:CB	1:A:178:LEU:HD23	2.27	0.64
1:C:136:PHE:O	1:C:139:LEU:HD23	1.98	0.64
1:A:132:ARG:CG	1:A:146:ALA:HB2	2.28	0.64
1:A:273:GLN:NE2	1:A:279:ARG:HB2	2.13	0.63
1:A:95:GLY:HA3	1:A:121:MET:O	1.98	0.63
1:A:46:VAL:HG13	1:C:318:ASN:HD22	1.64	0.63
1:B:32:ASP:OD2	1:C:126:ASN:HB3	1.99	0.63
1:A:294:ASN:H	1:A:298:ALA:HB3	1.63	0.63
1:B:14:PHE:HE2	1:B:41:LYS:HG3	1.63	0.63
1:B:117:ALA:HB2	1:B:123:GLN:HE21	1.63	0.63
1:B:276:PHE:CE2	1:B:278:LEU:HB2	2.34	0.63
1:B:74:ARG:HG2	1:B:124:ARG:NH2	2.14	0.62
1:A:121:MET:HE3	1:A:150:GLN:HG3	1.81	0.62
1:A:107:LEU:HD23	1:A:310:ASP:OD1	1.99	0.62
1:A:16:LYS:HZ3	1:A:16:LYS:HB2	1.61	0.62
1:A:59:GLN:NE2	1:A:72:TRP:CZ2	2.68	0.62
1:C:269:VAL:HG23	1:C:283:ALA:HB2	1.82	0.62
1:A:273:GLN:HE21	1:A:279:ARG:HD3	1.63	0.62
1:B:216:ALA:HA	1:B:240:TYR:C	2.20	0.62
1:B:14:PHE:HE1	1:B:57:GLU:HB3	1.64	0.61
1:A:273:GLN:NE2	1:A:279:ARG:HD3	2.14	0.61
1:B:231:TYR:HB3	1:B:271:GLN:HB2	1.83	0.61
1:B:19:GLY:CA	1:B:34:THR:HG22	2.31	0.61
1:A:174:TYR:CD1	1:A:175:GLY:N	2.68	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:C	1:A:35:TYR:CD1	2.73	0.61
1:C:1:ALA:N	1:C:357:PHE:OXT	2.33	0.61
1:A:306:VAL:HA	1:A:332:LEU:HD11	1.81	0.61
1:A:133:ASN:HB3	1:A:145:PHE:CE2	2.36	0.61
1:A:267:GLU:CB	1:A:285:LEU:HB3	2.28	0.61
1:C:58:TYR:HB2	1:C:73:THR:HA	1.83	0.60
1:B:82:PHE:HB3	1:B:85:ALA:HB3	1.82	0.60
1:C:16:LYS:NZ	1:C:18:ASP:HB2	2.16	0.60
1:A:52:GLY:HA3	1:C:321:MET:SD	2.41	0.60
1:A:16:LYS:HD2	1:A:37:ARG:HD2	1.84	0.60
1:B:121:MET:SD	1:B:193:THR:HB	2.41	0.60
1:B:334:LYS:CD	1:B:334:LYS:NZ	2.63	0.60
1:B:16:LYS:HB3	1:B:356:GLN:HB3	1.84	0.60
1:A:236:TYR:HB2	1:A:265:ASN:O	2.02	0.60
1:C:74:ARG:HG2	1:C:124:ARG:HH21	1.67	0.60
1:A:35:TYR:HD1	1:A:35:TYR:C	2.04	0.60
1:C:64:GLN:HG3	1:C:70:ASP:HB2	1.84	0.60
1:A:121:MET:HE3	1:A:150:GLN:CG	2.31	0.59
1:A:18:ASP:CG	1:A:354:VAL:HG12	2.23	0.59
1:B:94:TYR:HE1	1:B:98:TYR:CE2	2.21	0.59
1:C:49:GLN:HB3	1:C:82:PHE:CE1	2.37	0.59
1:A:2:GLU:HA	1:A:12:ASP:HA	1.85	0.59
1:A:23:PHE:HB2	1:A:349:VAL:HG13	1.84	0.59
1:A:36:MET:HE1	1:A:37:ARG:C	2.23	0.59
1:A:180:TYR:HB3	1:A:188:VAL:HG12	1.85	0.58
1:B:273:GLN:HG2	1:B:279:ARG:HD3	1.85	0.58
1:B:97:THR:HB	1:B:122:GLN:HA	1.85	0.58
1:A:278:LEU:HD23	1:A:280:PRO:HD3	1.86	0.58
1:B:294:ASN:H	1:B:298:ALA:CB	2.17	0.58
1:B:3:ILE:HG22	1:B:3:ILE:O	2.03	0.58
1:A:123:GLN:CG	1:A:124:ARG:N	2.52	0.58
1:A:107:LEU:HD22	1:A:110:PHE:O	2.05	0.57
1:A:175:GLY:HA2	1:A:193:THR:HA	1.85	0.57
1:B:290:LYS:HG2	1:B:291:ASP:N	2.19	0.57
1:B:265:ASN:N	1:B:265:ASN:OD1	2.36	0.57
1:B:278:LEU:O	1:B:280:PRO:HD3	2.05	0.57
1:B:108:PRO:HD3	1:B:281:SER:OG	2.04	0.57
1:B:143:LEU:HD13	1:B:180:TYR:HD1	1.69	0.57
1:B:194:THR:HG22	1:B:217:THR:HG22	1.85	0.57
1:A:18:ASP:CB	1:A:35:TYR:HE1	2.16	0.57
1:B:145:PHE:HB3	1:B:178:LEU:CD1	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:TYR:HE2	1:C:352:GLY:HA3	1.70	0.57
1:A:58:TYR:HE1	1:A:71:SER:HB2	1.69	0.56
1:B:304:ASP:HB2	1:B:332:LEU:HD21	1.86	0.56
1:B:36:MET:CE	1:B:38:ILE:HG13	2.35	0.56
1:A:193:THR:OG1	1:A:218:VAL:HG12	2.04	0.56
1:B:6:LYS:HB3	1:B:7:ASP:OD1	2.06	0.56
1:C:45:GLN:O	1:C:45:GLN:HG3	2.04	0.56
1:A:226:ASP:O	1:A:227:ALA:HB2	2.05	0.56
1:A:266:PHE:CZ	1:A:268:VAL:HB	2.40	0.56
1:B:94:TYR:CD1	1:B:98:TYR:CD2	2.93	0.56
1:B:132:ARG:HG3	1:B:146:ALA:HB2	1.87	0.56
1:C:234:ALA:HB2	1:C:268:VAL:HG23	1.88	0.56
1:B:322:SER:HB2	1:B:354:VAL:HG22	1.88	0.56
1:A:324:TYR:CE2	1:A:352:GLY:CA	2.89	0.56
1:B:294:ASN:H	1:B:298:ALA:HB3	1.71	0.56
1:C:306:VAL:HA	1:C:332:LEU:HD11	1.87	0.56
1:A:353:LEU:HD23	1:B:78:ALA:O	2.06	0.56
1:A:16:LYS:HB3	1:A:356:GLN:CB	2.37	0.55
1:C:272:TYR:O	1:C:280:PRO:HD2	2.06	0.55
1:B:276:PHE:HE2	1:B:278:LEU:HB2	1.69	0.55
1:C:230:ILE:CD1	1:C:272:TYR:HD1	2.20	0.55
1:C:14:PHE:CE2	1:C:41:LYS:HG3	2.38	0.55
1:B:58:TYR:HD1	1:B:72:TRP:C	2.10	0.55
1:C:219:TYR:O	1:C:237:SER:OG	2.23	0.55
1:A:16:LYS:NZ	1:A:18:ASP:HB2	2.21	0.55
1:A:46:VAL:HB	1:A:50:LEU:HD21	1.89	0.55
1:A:319:LYS:CD	1:A:319:LYS:H	2.19	0.55
1:B:148:GLN:HG2	1:B:149:TYR:N	2.21	0.55
1:C:227:ALA:O	1:C:229:ASN:N	2.40	0.55
1:A:263:ALA:N	1:A:289:GLY:HA2	2.21	0.55
1:A:36:MET:CE	1:A:38:ILE:CD1	2.85	0.55
1:B:114:THR:HB	1:B:265:ASN:HD22	1.71	0.55
1:A:128:TYR:HE1	1:A:150:GLN:CG	2.19	0.54
1:A:321:MET:SD	1:B:52:GLY:HA3	2.48	0.54
1:B:285:LEU:HD11	1:B:308:TYR:CE1	2.43	0.54
1:A:3:ILE:CD1	1:B:3:ILE:HG21	2.37	0.54
1:A:334:LYS:HE2	1:A:345:THR:HG21	1.89	0.54
1:B:34:THR:O	1:B:62:GLY:N	2.41	0.54
1:C:293:SER:HA	1:C:298:ALA:O	2.08	0.54
1:B:266:PHE:HZ	1:B:268:VAL:HB	1.68	0.54
1:B:308:TYR:HA	1:B:331:LEU:HG	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:MET:HE1	1:B:38:ILE:HG13	1.90	0.54
1:A:220:THR:HA	1:A:237:SER:HB2	1.90	0.54
1:A:278:LEU:CD2	1:A:280:PRO:HD3	2.38	0.54
1:C:126:ASN:N	1:C:126:ASN:HD22	2.06	0.54
1:A:16:LYS:HB3	1:A:356:GLN:CA	2.38	0.53
1:B:269:VAL:HG23	1:B:283:ALA:HB2	1.89	0.53
1:B:233:ALA:O	1:B:268:VAL:HG23	2.09	0.53
1:B:79:GLY:HA3	1:B:88:PHE:O	2.07	0.53
1:C:16:LYS:HZ1	1:C:18:ASP:HB2	1.71	0.53
1:C:61:GLN:HG3	1:C:70:ASP:HB3	1.90	0.53
1:A:36:MET:HG2	1:B:56:TRP:CD1	2.43	0.53
1:A:3:ILE:CG1	1:B:3:ILE:HG21	2.38	0.53
1:B:58:TYR:HB2	1:B:73:THR:CA	2.13	0.53
1:C:92:ARG:HD2	1:C:125:GLY:O	2.08	0.53
1:A:16:LYS:HB3	1:A:356:GLN:HB3	1.90	0.53
1:C:174:TYR:CG	1:C:175:GLY:N	2.77	0.53
1:B:357:PHE:HE1	1:C:40:PHE:CZ	2.26	0.53
1:A:237:SER:OG	1:A:238:GLN:N	2.41	0.53
1:C:16:LYS:HB2	1:C:16:LYS:NZ	2.23	0.53
1:C:3:ILE:CG2	1:C:3:ILE:O	2.56	0.53
1:C:90:TYR:HA	1:C:128:TYR:O	2.09	0.53
1:B:311:VAL:HG12	1:B:327:TYR:HB3	1.90	0.53
1:C:311:VAL:HG12	1:C:327:TYR:HB3	1.91	0.53
1:C:39:GLY:HA2	1:C:56:TRP:CE3	2.44	0.53
1:B:96:VAL:HB	1:B:148:GLN:OE1	2.09	0.53
1:C:131:TYR:HD2	1:C:131:TYR:C	2.12	0.53
1:B:57:GLU:HG3	1:B:57:GLU:O	2.09	0.52
1:B:321:MET:HB2	1:C:44:THR:HG21	1.91	0.52
1:C:133:ASN:HB3	1:C:145:PHE:CE2	2.43	0.52
1:A:334:LYS:HE2	1:A:345:THR:CG2	2.40	0.52
1:C:194:THR:O	1:C:196:LYS:NZ	2.25	0.52
1:C:324:TYR:HE2	1:C:352:GLY:CA	2.21	0.52
1:C:38:ILE:HG22	1:C:39:GLY:H	1.75	0.52
1:B:143:LEU:HD12	1:B:179:THR:O	2.08	0.52
1:A:14:PHE:HE2	1:A:41:LYS:HG3	1.73	0.52
1:A:58:TYR:CE1	1:A:71:SER:HB2	2.44	0.52
1:A:97:THR:O	1:A:101:THR:OG1	2.24	0.52
1:C:131:TYR:CD2	1:C:131:TYR:C	2.83	0.52
1:A:24:SER:OG	1:A:348:ILE:HG22	2.09	0.52
1:B:14:PHE:HE1	1:B:57:GLU:CB	2.23	0.52
1:B:234:ALA:HB2	1:B:268:VAL:HG23	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:CB	1:A:266:PHE:HA	2.36	0.51
1:C:16:LYS:HA	1:C:355:TYR:O	2.10	0.51
1:C:18:ASP:OD2	1:C:354:VAL:HG12	2.10	0.51
1:B:94:TYR:CE1	1:B:98:TYR:CE2	2.98	0.51
1:C:240:TYR:C	1:C:240:TYR:CD1	2.84	0.51
1:A:1:ALA:N	1:A:12:ASP:OD1	2.40	0.51
1:A:36:MET:C	1:A:36:MET:HE3	2.30	0.51
1:A:54:GLY:HA3	1:C:355:TYR:CD2	2.46	0.51
1:B:94:TYR:HD1	1:B:98:TYR:CD2	2.28	0.51
1:C:53:TYR:H	1:C:53:TYR:HD1	1.57	0.51
1:A:266:PHE:HZ	1:A:268:VAL:HB	1.75	0.51
1:A:293:SER:HA	1:A:298:ALA:O	2.10	0.51
1:B:62:GLY:O	1:C:126:ASN:OD1	2.28	0.51
1:C:223:LEU:O	1:C:233:ALA:HA	2.10	0.51
1:C:294:ASN:H	1:C:298:ALA:HB3	1.75	0.51
1:C:83:ALA:O	1:C:84:ASP:HB2	2.10	0.51
1:A:57:GLU:HG2	1:A:74:ARG:HB2	1.92	0.51
1:B:121:MET:HB3	1:B:150:GLN:NE2	2.26	0.51
1:C:103:TRP:CD2	1:C:224:LYS:HD2	2.45	0.51
1:A:185:GLY:HA3	1:A:226:ASP:O	2.11	0.51
1:A:22:TYR:CE1	1:A:110:PHE:CE1	2.95	0.51
1:C:42:GLY:N	1:C:54:GLY:O	2.44	0.51
1:B:282:VAL:HA	1:B:310:ASP:O	2.10	0.51
1:A:346:ASP:O	1:A:348:ILE:HG23	2.10	0.50
1:A:66:GLU:OE2	1:B:92:ARG:NH2	2.43	0.50
1:A:92:ARG:HH22	1:C:66:GLU:HB2	1.76	0.50
1:C:231:TYR:O	1:C:232:LEU:HD23	2.10	0.50
1:B:107:LEU:HD21	1:B:283:ALA:HB3	1.93	0.50
1:B:18:ASP:HB3	1:B:35:TYR:HE1	1.75	0.50
1:C:3:ILE:HD12	1:C:13:LEU:HB3	1.92	0.50
1:A:71:SER:O	1:A:72:TRP:HE3	1.95	0.50
1:B:292:ILE:HB	1:B:300:TYR:HB2	1.94	0.50
1:C:239:THR:OG1	1:C:240:TYR:N	2.44	0.50
1:C:39:GLY:HA3	1:C:57:GLU:HB2	1.93	0.50
1:A:18:ASP:HA	1:A:354:VAL:HA	1.94	0.50
1:B:103:TRP:CG	1:B:224:LYS:HD2	2.47	0.50
1:B:22:TYR:CE1	1:B:110:PHE:CE1	2.68	0.50
1:B:115:TYR:CD2	1:B:115:TYR:N	2.80	0.50
1:B:49:GLN:HB3	1:B:82:PHE:CE1	2.47	0.50
1:C:3:ILE:O	1:C:3:ILE:HG23	2.10	0.50
1:B:128:TYR:CD1	1:B:148:GLN:NE2	2.80	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLY:O	1:C:278:LEU:CB	2.53	0.50
1:A:182:ILE:HD12	1:A:186:PHE:HB3	1.94	0.49
1:A:20:LEU:H	1:A:34:THR:HG22	1.76	0.49
1:C:121:MET:HG3	1:C:128:TYR:CE1	2.41	0.49
1:C:294:ASN:N	1:C:297:GLY:O	2.45	0.49
1:A:47:ASN:C	1:A:49:GLN:N	2.65	0.49
1:B:3:ILE:HD11	1:B:13:LEU:CD2	2.32	0.49
1:B:36:MET:SD	1:C:56:TRP:NE1	2.85	0.49
1:B:278:LEU:O	1:B:280:PRO:CD	2.60	0.49
1:C:16:LYS:NZ	1:C:354:VAL:HB	2.27	0.49
1:A:47:ASN:C	1:A:49:GLN:H	2.14	0.49
1:C:104:THR:HG21	1:C:235:GLN:HB3	1.93	0.49
1:C:132:ARG:CG	1:C:146:ALA:HB2	2.41	0.49
1:C:36:MET:C	1:C:36:MET:SD	2.90	0.49
1:A:333:ASP:OD1	1:A:333:ASP:N	2.45	0.49
1:B:225:TYR:OH	1:B:227:ALA:HB3	2.12	0.49
1:B:357:PHE:CE1	1:C:40:PHE:CZ	3.01	0.49
1:C:220:THR:HG22	1:C:235:GLN:HE21	1.78	0.49
1:A:266:PHE:CG	1:A:267:GLU:N	2.81	0.49
1:B:18:ASP:C	1:B:18:ASP:OD1	2.51	0.49
1:B:266:PHE:CG	1:B:267:GLU:N	2.81	0.49
1:B:148:GLN:HG2	1:B:149:TYR:H	1.77	0.49
1:C:192:ILE:N	1:C:192:ILE:HD13	2.28	0.49
1:C:292:ILE:HG22	1:C:293:SER:N	2.28	0.49
1:A:22:TYR:CD1	1:A:348:ILE:HD12	2.48	0.48
1:B:125:GLY:HA3	1:B:128:TYR:CZ	2.49	0.48
1:C:126:ASN:N	1:C:126:ASN:ND2	2.60	0.48
1:C:216:ALA:HA	1:C:240:TYR:HB3	1.96	0.48
1:A:66:GLU:OE1	1:B:124:ARG:NH2	2.45	0.48
1:C:180:TYR:CE2	1:C:182:ILE:HA	2.48	0.48
1:A:291:ASP:O	1:A:292:ILE:HG13	2.13	0.48
1:B:180:TYR:CD2	1:B:182:ILE:HA	2.48	0.48
1:A:192:ILE:H	1:A:192:ILE:HD13	1.78	0.48
1:B:53:TYR:HE2	1:B:81:LYS:NZ	2.12	0.48
1:A:36:MET:HE2	1:A:60:ILE:CG2	2.44	0.48
1:B:334:LYS:HG2	1:B:345:THR:OG1	2.13	0.48
1:A:184:GLU:OE1	1:A:225:TYR:HE1	1.96	0.48
1:C:2:GLU:HA	1:C:12:ASP:HA	1.95	0.48
1:C:18:ASP:HA	1:C:354:VAL:HA	1.95	0.48
1:C:6:LYS:HE2	1:C:6:LYS:HB3	1.58	0.48
1:C:110:PHE:CE1	1:C:348:ILE:HD11	2.49	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:PHE:CZ	1:B:57:GLU:HB3	2.48	0.47
1:C:61:GLN:CG	1:C:70:ASP:HB3	2.44	0.47
1:C:99:ASP:N	1:C:99:ASP:OD1	2.43	0.47
1:B:237:SER:OG	1:B:238:GLN:N	2.47	0.47
1:A:3:ILE:CG1	1:B:3:ILE:CG2	2.92	0.47
1:B:53:TYR:CE2	1:B:81:LYS:NZ	2.82	0.47
1:A:60:ILE:HD11	1:B:73:THR:OG1	2.15	0.47
1:C:74:ARG:HG2	1:C:124:ARG:NH2	2.29	0.47
1:A:125:GLY:CA	1:A:128:TYR:HE2	2.28	0.47
1:A:121:MET:HB2	1:A:150:GLN:OE1	2.15	0.47
1:C:123:GLN:NE2	1:C:124:ARG:HD3	2.29	0.47
1:C:103:TRP:CG	1:C:224:LYS:HD2	2.50	0.47
1:B:355:TYR:CD2	1:C:54:GLY:HA3	2.50	0.47
1:C:38:ILE:HG22	1:C:39:GLY:N	2.29	0.47
1:B:36:MET:HE3	1:B:36:MET:HB2	1.64	0.47
1:C:18:ASP:CB	1:C:35:TYR:HE1	2.13	0.47
1:C:89:ASP:OD1	1:C:130:THR:HB	2.14	0.47
1:C:143:LEU:HD13	1:C:180:TYR:HD1	1.80	0.47
1:A:128:TYR:CD1	1:A:150:GLN:HG2	2.50	0.47
1:A:90:TYR:HA	1:A:128:TYR:O	2.15	0.47
1:B:192:ILE:HD13	1:B:192:ILE:H	1.80	0.47
1:C:15:GLY:HA3	1:C:357:PHE:CZ	2.49	0.47
1:C:263:ALA:N	1:C:289:GLY:HA2	2.30	0.47
1:A:45:GLN:HG3	1:A:45:GLN:O	2.14	0.46
1:B:18:ASP:CG	1:B:354:VAL:HG12	2.36	0.46
1:A:16:LYS:CE	1:A:18:ASP:HB2	2.45	0.46
1:C:32:ASP:OD1	1:C:34:THR:HG23	2.14	0.46
1:A:20:LEU:HD23	1:A:20:LEU:C	2.35	0.46
1:A:193:THR:OG1	1:A:218:VAL:CG1	2.63	0.46
1:B:354:VAL:O	1:B:354:VAL:HG23	2.15	0.46
1:A:3:ILE:HG12	1:B:3:ILE:HG21	1.98	0.46
1:A:22:TYR:HE1	1:A:110:PHE:CE1	2.15	0.46
1:A:59:GLN:NE2	1:A:61:GLN:OE1	2.49	0.46
1:B:194:THR:HG22	1:B:217:THR:HB	1.97	0.46
1:B:172:ASP:O	1:B:195:SER:HB2	2.16	0.46
1:C:96:VAL:HB	1:C:148:GLN:HB2	1.98	0.46
1:A:20:LEU:N	1:A:34:THR:HG22	2.31	0.46
1:B:267:GLU:CB	1:B:285:LEU:HB3	2.41	0.46
1:B:320:ASN:N	1:B:320:ASN:HD22	2.14	0.46
1:B:133:ASN:HB3	1:B:145:PHE:CE2	2.50	0.46
1:B:192:ILE:O	1:B:193:THR:CG2	2.64	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:OE1	1:A:225:TYR:CE1	2.69	0.46
1:C:16:LYS:HB3	1:C:356:GLN:CB	2.45	0.46
1:A:115:TYR:N	1:A:115:TYR:CD2	2.84	0.45
1:A:303:GLN:HE22	1:A:335:ASN:ND2	2.01	0.45
1:A:36:MET:CE	1:A:60:ILE:CG2	2.94	0.45
1:B:228:ASN:C	1:B:230:ILE:N	2.69	0.45
1:C:35:TYR:C	1:C:35:TYR:HD1	2.15	0.45
1:A:272:TYR:HD2	1:A:274:PHE:HD2	1.63	0.45
1:B:35:TYR:CE2	1:B:59:GLN:OE1	2.68	0.45
1:A:308:TYR:HA	1:A:331:LEU:HG	1.98	0.45
1:A:36:MET:HE3	1:A:36:MET:O	2.17	0.45
1:B:355:TYR:CZ	1:C:42:GLY:HA3	2.51	0.45
1:B:47:ASN:HB3	1:B:49:GLN:H	1.80	0.45
1:C:55:GLN:HG2	1:C:56:TRP:H	1.82	0.45
1:A:3:ILE:HG12	1:B:3:ILE:CG2	2.47	0.45
1:A:88:PHE:HA	1:A:130:THR:O	2.17	0.45
1:B:45:GLN:HG3	1:B:45:GLN:O	2.17	0.45
1:C:121:MET:SD	1:C:150:GLN:HG3	2.55	0.45
1:A:1:ALA:C	1:A:12:ASP:OD1	2.54	0.45
1:B:128:TYR:N	1:B:128:TYR:HD2	2.14	0.45
1:B:263:ALA:HB2	1:B:290:LYS:CE	2.46	0.45
1:B:98:TYR:O	1:B:102:SER:OG	2.27	0.45
1:C:180:TYR:HE2	1:C:182:ILE:HA	1.81	0.45
1:B:228:ASN:C	1:B:230:ILE:H	2.19	0.45
1:A:225:TYR:HE2	1:A:230:ILE:HB	1.81	0.45
1:A:80:LEU:O	1:A:87:SER:HB2	2.17	0.45
1:A:94:TYR:CD1	1:A:98:TYR:CD2	3.05	0.45
1:C:58:TYR:HB3	1:C:73:THR:HA	1.97	0.45
1:A:236:TYR:HB2	1:A:266:PHE:CA	2.43	0.45
1:A:294:ASN:N	1:A:297:GLY:O	2.50	0.45
1:A:240:TYR:C	1:A:240:TYR:CD1	2.90	0.45
1:A:93:ASN:OD1	1:A:94:TYR:N	2.43	0.45
1:B:32:ASP:HB2	1:C:127:GLY:HA2	1.99	0.45
1:C:274:PHE:HD1	1:C:276:PHE:CE1	2.34	0.45
1:C:59:GLN:C	1:C:60:ILE:HG13	2.37	0.44
1:B:97:THR:HG23	1:B:220:THR:OG1	2.18	0.44
1:C:110:PHE:HE1	1:C:348:ILE:HD11	1.81	0.44
1:A:144:ASP:HB2	1:A:179:THR:OG1	2.17	0.44
1:A:40:PHE:O	1:A:40:PHE:CD2	2.70	0.44
1:B:290:LYS:HG2	1:B:291:ASP:H	1.79	0.44
1:B:59:GLN:O	1:B:60:ILE:HG13	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ARG:NH1	1:C:124:ARG:HB3	2.22	0.44
1:A:46:VAL:HB	1:A:50:LEU:CD2	2.46	0.44
1:C:35:TYR:HD1	1:C:35:TYR:O	2.01	0.44
1:A:14:PHE:CE2	1:A:41:LYS:HG3	2.53	0.44
1:A:125:GLY:HA3	1:A:128:TYR:HE2	1.83	0.44
1:A:236:TYR:HB3	1:A:266:PHE:HD1	1.81	0.44
1:A:330:ASN:H	1:A:347:ASP:HB3	1.83	0.44
1:A:1:ALA:HB1	1:B:4:TYR:CD2	2.52	0.44
1:A:52:GLY:CA	1:C:321:MET:SD	3.06	0.44
1:A:121:MET:SD	1:A:193:THR:HB	2.57	0.44
1:B:39:GLY:HA3	1:B:57:GLU:HA	2.00	0.44
1:C:314:THR:HB	1:C:316:TYR:CE1	2.53	0.44
1:A:297:GLY:O	1:A:298:ALA:HB3	2.18	0.44
1:A:314:THR:HG22	1:A:324:TYR:HB3	2.00	0.44
1:B:86:GLY:HA3	1:B:131:TYR:HE2	1.82	0.44
1:B:293:SER:HA	1:B:298:ALA:HB3	2.00	0.44
1:B:307:LYS:HG3	1:B:307:LYS:O	2.18	0.44
1:B:59:GLN:HE21	1:B:72:TRP:HZ2	1.65	0.44
1:C:23:PHE:O	1:C:348:ILE:HB	2.18	0.43
1:B:11:LEU:O	1:B:11:LEU:HG	2.18	0.43
1:B:49:GLN:HB3	1:B:82:PHE:CZ	2.53	0.43
1:A:60:ILE:HD13	1:B:56:TRP:HE1	1.83	0.43
1:A:42:GLY:HA3	1:C:355:TYR:CE2	2.53	0.43
1:A:92:ARG:HB2	1:C:62:GLY:O	2.18	0.43
1:A:21:HIS:CD2	1:A:21:HIS:C	2.92	0.43
1:B:115:TYR:HD2	1:B:115:TYR:N	2.16	0.43
1:B:91:GLY:O	1:B:93:ASN:N	2.50	0.43
1:A:195:SER:CA	1:A:196:LYS:HE2	2.48	0.43
1:A:285:LEU:HD11	1:A:308:TYR:CZ	2.53	0.43
1:B:194:THR:HG22	1:B:217:THR:CB	2.48	0.43
1:A:194:THR:CB	1:A:196:LYS:HZ1	2.30	0.43
1:B:128:TYR:N	1:B:128:TYR:CD2	2.86	0.43
1:C:95:GLY:HA3	1:C:121:MET:O	2.18	0.43
1:B:32:ASP:O	1:B:63:ASN:HB3	2.19	0.43
1:C:225:TYR:OH	1:C:227:ALA:HB3	2.19	0.43
1:A:116:GLY:O	1:A:123:GLN:HB3	2.19	0.43
1:A:226:ASP:O	1:A:227:ALA:CB	2.67	0.43
1:B:192:ILE:C	1:B:193:THR:HG23	2.39	0.43
1:C:240:TYR:HD1	1:C:240:TYR:C	2.21	0.43
1:C:94:TYR:CZ	1:C:124:ARG:HD2	2.53	0.43
1:A:56:TRP:HD1	1:A:76:ALA:HB2	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:HG21	1:A:267:GLU:HG3	2.01	0.42
1:A:291:ASP:C	1:A:292:ILE:HG13	2.39	0.42
1:A:307:LYS:HG3	1:A:331:LEU:HB2	2.00	0.42
1:B:21:HIS:HD2	1:B:22:TYR:O	2.01	0.42
1:B:14:PHE:CE2	1:B:41:LYS:HG3	2.49	0.42
1:C:330:ASN:H	1:C:347:ASP:HB3	1.83	0.42
1:A:174:TYR:CG	1:A:175:GLY:N	2.88	0.42
1:B:96:VAL:N	1:B:148:GLN:OE1	2.52	0.42
1:C:108:PRO:HG2	1:C:312:GLY:HA3	2.00	0.42
1:B:305:ILE:O	1:B:343:ILE:HG21	2.19	0.42
1:C:274:PHE:HB2	1:C:278:LEU:O	2.20	0.42
1:B:128:TYR:CE2	1:B:150:GLN:HG2	2.54	0.42
1:B:108:PRO:HG2	1:B:312:GLY:HA3	2.00	0.42
1:C:16:LYS:HZ1	1:C:354:VAL:HB	1.84	0.42
1:A:180:TYR:CE2	1:A:182:ILE:HA	2.54	0.42
1:A:219:TYR:O	1:A:237:SER:OG	2.35	0.42
1:B:123:GLN:HG3	1:B:124:ARG:N	2.33	0.42
1:B:24:SER:CB	1:B:348:ILE:HG22	2.50	0.42
1:B:94:TYR:CE1	1:B:98:TYR:CD2	3.08	0.42
1:A:9:ASN:ND2	1:C:320:ASN:ND2	2.67	0.42
1:A:234:ALA:HB2	1:A:268:VAL:CG2	2.36	0.42
1:B:180:TYR:HE2	1:B:182:ILE:HA	1.80	0.42
1:B:351:LEU:O	1:B:351:LEU:HD23	2.20	0.42
1:C:123:GLN:HE21	1:C:124:ARG:HD3	1.84	0.42
1:A:290:LYS:HA	1:A:302:ASP:OD2	2.20	0.41
1:A:20:LEU:H	1:A:34:THR:CG2	2.33	0.41
1:A:35:TYR:HD1	1:A:35:TYR:O	2.03	0.41
1:A:55:GLN:O	1:A:76:ALA:HA	2.20	0.41
1:B:229:ASN:O	1:B:272:TYR:HA	2.20	0.41
1:B:328:LYS:O	1:B:347:ASP:HB2	2.20	0.41
1:B:180:TYR:HB3	1:B:188:VAL:HG12	2.02	0.41
1:B:265:ASN:HB3	1:B:287:SER:HB3	2.02	0.41
1:C:21:HIS:CD2	1:C:31:GLY:O	2.73	0.41
1:C:348:ILE:HD12	1:C:349:VAL:N	2.35	0.41
1:A:47:ASN:O	1:A:48:ASP:C	2.58	0.41
1:A:16:LYS:HD2	1:A:37:ARG:CD	2.50	0.41
1:A:18:ASP:C	1:A:18:ASP:OD1	2.58	0.41
1:A:327:TYR:CD2	1:A:329:ILE:HD13	2.55	0.41
1:A:36:MET:CE	1:A:38:ILE:HD11	2.48	0.41
1:B:181:ALA:C	1:B:183:GLY:H	2.24	0.41
1:C:5:ASN:ND2	1:C:10:LYS:HG2	2.36	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:TYR:CG	1:C:285:LEU:N	2.88	0.41
1:C:79:GLY:HA3	1:C:89:ASP:HB3	2.02	0.41
1:A:84:ASP:O	1:A:137:PHE:HA	2.20	0.41
1:A:287:SER:OG	1:A:305:ILE:HB	2.20	0.41
1:B:45:GLN:HE21	1:B:45:GLN:HB2	1.60	0.41
1:B:58:TYR:CE1	1:B:71:SER:HB2	2.56	0.41
1:C:40:PHE:CD2	1:C:40:PHE:O	2.74	0.41
1:A:182:ILE:HG13	1:A:182:ILE:H	1.54	0.41
1:A:177:SER:HA	1:A:191:ALA:HA	2.02	0.41
1:A:58:TYR:HB2	1:A:73:THR:HA	2.03	0.41
1:B:148:GLN:CG	1:B:149:TYR:N	2.83	0.41
1:B:53:TYR:HE1	1:B:89:ASP:HB3	1.85	0.41
1:C:112:GLY:O	1:C:114:THR:N	2.51	0.41
1:C:41:LYS:HA	1:C:55:GLN:HG3	2.02	0.41
1:C:59:GLN:CG	1:C:60:ILE:H	2.34	0.41
1:B:5:ASN:C	1:B:5:ASN:OD1	2.58	0.41
1:A:353:LEU:HD21	1:B:79:GLY:HA2	2.03	0.41
1:A:315:TYR:HB3	1:A:323:THR:HG22	2.03	0.41
1:B:53:TYR:HE1	1:B:79:GLY:HA3	1.86	0.41
1:B:55:GLN:O	1:B:76:ALA:HA	2.21	0.41
1:C:230:ILE:HD11	1:C:272:TYR:HD1	1.85	0.41
1:C:26:ASP:HB3	1:C:29:SER:HB2	2.02	0.41
1:B:132:ARG:HE	1:B:132:ARG:HB2	1.75	0.41
1:B:18:ASP:HB3	1:B:35:TYR:CE1	2.55	0.41
1:B:303:GLN:HB2	1:B:337:PHE:CD1	2.55	0.41
1:C:56:TRP:O	1:C:57:GLU:HB3	2.21	0.41
1:A:318:ASN:HB2	1:A:319:LYS:HD2	2.03	0.41
1:B:274:PHE:HD1	1:B:276:PHE:CE1	2.40	0.41
1:B:219:TYR:O	1:B:237:SER:HB3	2.17	0.40
1:A:120:PHE:O	1:A:121:MET:HB3	2.21	0.40
1:A:97:THR:HB	1:A:122:GLN:HA	2.02	0.40
1:A:73:THR:HG21	1:A:76:ALA:HB2	2.03	0.40
1:A:94:TYR:CZ	1:A:124:ARG:HD2	2.56	0.40
1:C:231:TYR:O	1:C:270:ALA:HA	2.21	0.40
1:A:309:VAL:CG2	1:A:310:ASP:N	2.85	0.40
1:B:304:ASP:HB2	1:B:332:LEU:CD2	2.50	0.40
1:B:308:TYR:HB2	1:B:330:ASN:HA	2.03	0.40
1:B:36:MET:HE1	1:B:38:ILE:CG1	2.51	0.40
1:C:221:GLY:O	1:C:235:GLN:HA	2.22	0.40
1:C:270:ALA:O	1:C:282:VAL:HG23	2.20	0.40
1:B:35:TYR:C	1:B:35:TYR:CD1	2.95	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	A	290/357 (81%)	235 (81%)	44 (15%)	11 (4%)	3	27
1	B	290/357 (81%)	239 (82%)	42 (14%)	9 (3%)	4	32
1	C	290/357 (81%)	238 (82%)	39 (13%)	13 (4%)	2	23
All	All	870/1071 (81%)	712 (82%)	125 (14%)	33 (4%)	3	27

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	92	ARG
1	B	113	ASP
1	B	136	PHE
1	B	172	ASP
1	C	113	ASP
1	C	228	ASN
1	C	278	LEU
1	A	113	ASP
1	A	136	PHE
1	A	227	ALA
1	B	128	TYR
1	B	137	PHE
1	C	92	ARG
1	C	101	THR
1	C	301	GLY
1	C	305	ILE
1	A	121	MET
1	C	84	ASP
1	C	295	GLY
1	A	186	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	229	ASN
1	B	295	GLY
1	C	16	LYS
1	C	112	GLY
1	C	136	PHE
1	A	6	LYS
1	A	99	ASP
1	A	83	ALA
1	A	298	ALA
1	B	16	LYS
1	C	106	VAL
1	A	106	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	233/282 (83%)	174 (75%)	59 (25%)	<b>0</b> <b>4</b>
1	B	234/282 (83%)	186 (80%)	48 (20%)	<b>1</b> <b>7</b>
1	C	232/282 (82%)	191 (82%)	41 (18%)	<b>2</b> <b>11</b>
All	All	699/846 (83%)	551 (79%)	148 (21%)	<b>1</b> <b>7</b>

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	7	ASP
1	A	13	LEU
1	A	16	LYS
1	A	20	LEU
1	A	32	ASP
1	A	35	TYR
1	A	36	MET
1	A	43	GLU
1	A	44	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	45	GLN
1	A	50	LEU
1	A	53	TYR
1	A	57	GLU
1	A	58	TYR
1	A	60	ILE
1	A	66	GLU
1	A	68	SER
1	A	69	ASN
1	A	70	ASP
1	A	82	PHE
1	A	87	SER
1	A	89	ASP
1	A	92	ARG
1	A	97	THR
1	A	101	THR
1	A	106	VAL
1	A	113	ASP
1	A	115	TYR
1	A	124	ARG
1	A	139	LEU
1	A	144	ASP
1	A	172	ASP
1	A	178	LEU
1	A	180	TYR
1	A	182	ILE
1	A	188	VAL
1	A	192	ILE
1	A	195	SER
1	A	220	THR
1	A	223	LEU
1	A	236	TYR
1	A	239	THR
1	A	273	GLN
1	A	279	ARG
1	A	285	LEU
1	A	290	LYS
1	A	302	ASP
1	A	309	VAL
1	A	314	THR
1	A	319	LYS
1	A	322	SER

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	324	TYR
1	A	327	TYR
1	A	333	ASP
1	A	334	LYS
1	A	343	ILE
1	A	345	THR
1	A	351	LEU
1	B	7	ASP
1	B	9	ASN
1	B	13	LEU
1	B	16	LYS
1	B	20	LEU
1	B	32	ASP
1	B	35	TYR
1	B	36	MET
1	B	45	GLN
1	B	53	TYR
1	B	58	TYR
1	B	68	SER
1	B	69	ASN
1	B	70	ASP
1	B	75	VAL
1	B	81	LYS
1	B	90	TYR
1	B	110	PHE
1	B	113	ASP
1	B	115	TYR
1	B	119	ASN
1	B	131	TYR
1	B	132	ARG
1	B	139	LEU
1	B	144	ASP
1	B	152	LYS
1	B	172	ASP
1	B	174	TYR
1	B	178	LEU
1	B	192	ILE
1	B	220	THR
1	B	223	LEU
1	B	236	TYR
1	B	239	THR
1	B	265	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	273	GLN
1	B	282	VAL
1	B	285	LEU
1	B	290	LYS
1	B	299	SER
1	B	304	ASP
1	B	322	SER
1	B	324	TYR
1	B	327	TYR
1	B	337	PHE
1	B	340	ASP
1	B	345	THR
1	B	356	GLN
1	C	2	GLU
1	C	3	ILE
1	C	16	LYS
1	C	20	LEU
1	C	22	TYR
1	C	32	ASP
1	C	35	TYR
1	C	45	GLN
1	C	50	LEU
1	C	53	TYR
1	C	57	GLU
1	C	58	TYR
1	C	69	ASN
1	C	70	ASP
1	C	89	ASP
1	C	99	ASP
1	C	101	THR
1	C	106	VAL
1	C	109	GLU
1	C	110	PHE
1	C	113	ASP
1	C	126	ASN
1	C	131	TYR
1	C	144	ASP
1	C	152	LYS
1	C	172	ASP
1	C	192	ILE
1	C	218	VAL
1	C	220	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	239	THR
1	C	240	TYR
1	C	282	VAL
1	C	285	LEU
1	C	290	LYS
1	C	314	THR
1	C	321	MET
1	C	324	TYR
1	C	325	VAL
1	C	348	ILE
1	C	349	VAL
1	C	356	GLN

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	5	ASN
1	A	45	GLN
1	A	59	GLN
1	A	271	GLN
1	A	273	GLN
1	A	303	GLN
1	B	45	GLN
1	B	123	GLN
1	B	303	GLN
1	B	320	ASN
1	B	356	GLN
1	C	5	ASN
1	C	9	ASN
1	C	21	HIS
1	C	45	GLN
1	C	59	GLN
1	C	61	GLN
1	C	63	ASN
1	C	123	GLN
1	C	126	ASN
1	C	235	GLN
1	C	303	GLN
1	C	320	ASN
1	C	335	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 [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	298/357 (83%)	-0.06	13 (4%) 34 21	109, 199, 280, 322	0
1	B	298/357 (83%)	-0.03	14 (4%) 31 19	116, 235, 314, 335	0
1	C	298/357 (83%)	0.19	25 (8%) 11 7	136, 255, 343, 379	0
All	All	894/1071 (83%)	0.04	52 (5%) 23 13	109, 229, 322, 379	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	298	ALA	10.0
1	C	305	ILE	9.2
1	B	296	TYR	9.1
1	B	297	GLY	7.4
1	B	295	GLY	7.3
1	C	292	ILE	7.1
1	C	297	GLY	5.9
1	B	298	ALA	5.8
1	C	299	SER	5.2
1	A	292	ILE	4.2
1	C	293	SER	4.1
1	A	293	SER	4.1
1	C	344	ASN	4.0
1	A	299	SER	3.9
1	C	313	ALA	3.8
1	B	305	ILE	3.7
1	B	294	ASN	3.4
1	C	328	LYS	3.4
1	C	331	LEU	3.3
1	B	343	ILE	3.1
1	A	128	TYR	3.1
1	B	344	ASN	3.1
1	A	296	TYR	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	138	GLY	3.0
1	A	91	GLY	2.9
1	B	293	SER	2.9
1	A	305	ILE	2.8
1	A	125	GLY	2.8
1	A	298	ALA	2.8
1	C	345	THR	2.8
1	C	289	GLY	2.8
1	C	84	ASP	2.7
1	C	306	VAL	2.6
1	A	294	ASN	2.6
1	B	173	GLY	2.6
1	C	287	SER	2.6
1	C	120	PHE	2.6
1	C	109	GLU	2.6
1	C	332	LEU	2.6
1	C	139	LEU	2.5
1	A	118	ASP	2.5
1	C	304	ASP	2.5
1	B	292	ILE	2.4
1	C	325	VAL	2.4
1	A	295	GLY	2.4
1	A	300	TYR	2.4
1	C	295	GLY	2.3
1	B	138	GLY	2.3
1	B	338	THR	2.3
1	B	95	GLY	2.3
1	C	136	PHE	2.1
1	C	300	TYR	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

There are no such residues in this entry.