



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:08 pm GMT

PDB ID : 3VGO  
Title : Crystal structure of the N-terminal fragment of Cbl-b  
Authors : Kobashigawa, Y.; Noda, N.N.; Inagaki, F.  
Deposited on : 2011-08-18  
Resolution : 3.10 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.

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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

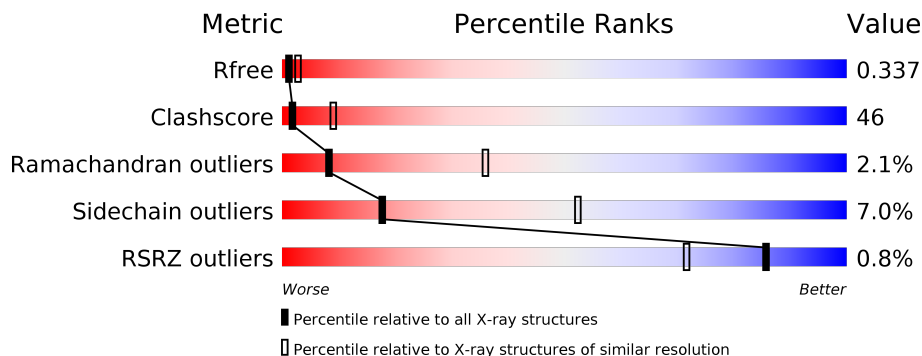
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	394	<div> <div>27%</div> <div>40%</div> <div>6%</div> <div>27%</div> </div>
1	B	394	<div> <div>27%</div> <div>45%</div> <div>•</div> <div>25%</div> </div>
1	C	394	<div> <div>2%</div> <div>31%</div> <div>39%</div> <div>•</div> <div>26%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6668 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 E3 ubiquitin-protein ligase CBL-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2196	1430	371	385	10			
1	B	294	Total	C	N	O	S	0	0	0
			2252	1465	384	393	10			
1	C	292	Total	C	N	O	S	0	0	0
			2220	1450	370	391	9			

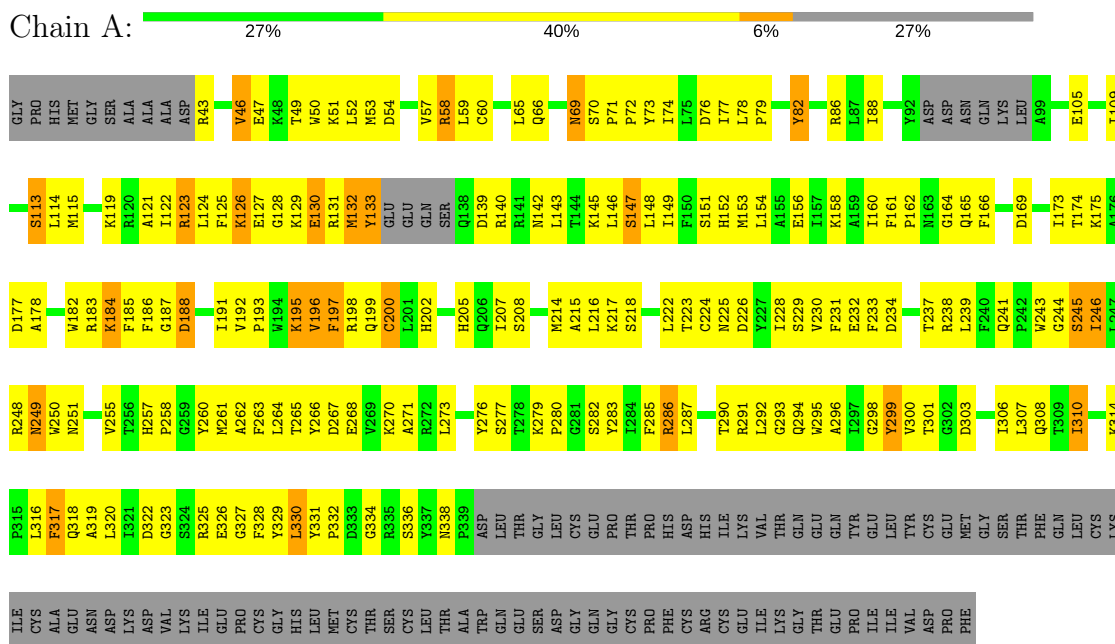
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	EXPRESSION TAG	UNP Q13191
A	34	PRO	-	EXPRESSION TAG	UNP Q13191
A	35	HIS	-	EXPRESSION TAG	UNP Q13191
A	36	MET	-	EXPRESSION TAG	UNP Q13191
A	37	GLY	-	EXPRESSION TAG	UNP Q13191
A	38	SER	-	EXPRESSION TAG	UNP Q13191
B	33	GLY	-	EXPRESSION TAG	UNP Q13191
B	34	PRO	-	EXPRESSION TAG	UNP Q13191
B	35	HIS	-	EXPRESSION TAG	UNP Q13191
B	36	MET	-	EXPRESSION TAG	UNP Q13191
B	37	GLY	-	EXPRESSION TAG	UNP Q13191
B	38	SER	-	EXPRESSION TAG	UNP Q13191
C	33	GLY	-	EXPRESSION TAG	UNP Q13191
C	34	PRO	-	EXPRESSION TAG	UNP Q13191
C	35	HIS	-	EXPRESSION TAG	UNP Q13191
C	36	MET	-	EXPRESSION TAG	UNP Q13191
C	37	GLY	-	EXPRESSION TAG	UNP Q13191
C	38	SER	-	EXPRESSION TAG	UNP Q13191

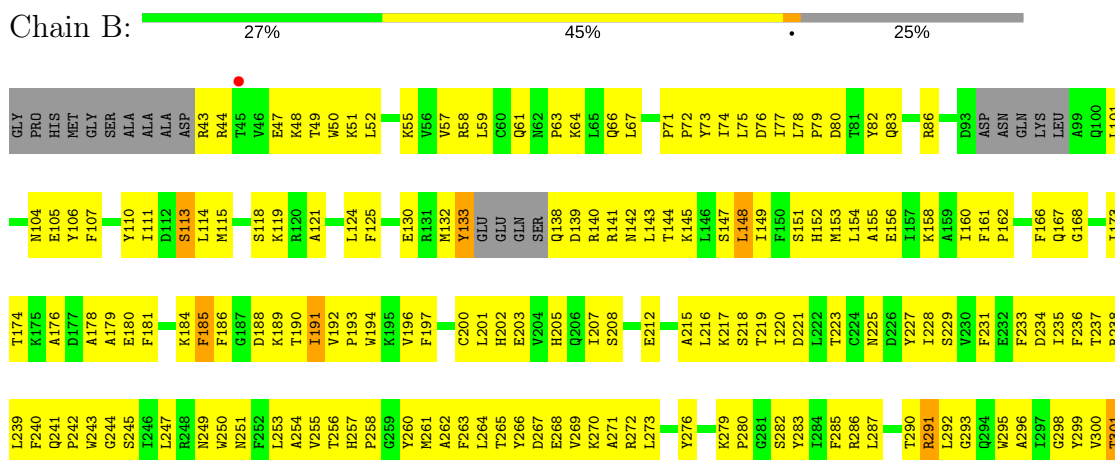
### 3 Residue-property plots

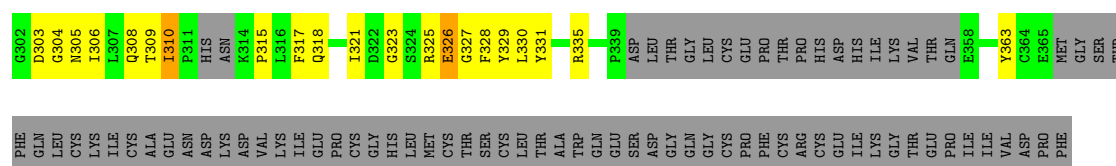
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: E3 ubiquitin-protein ligase CBL-B

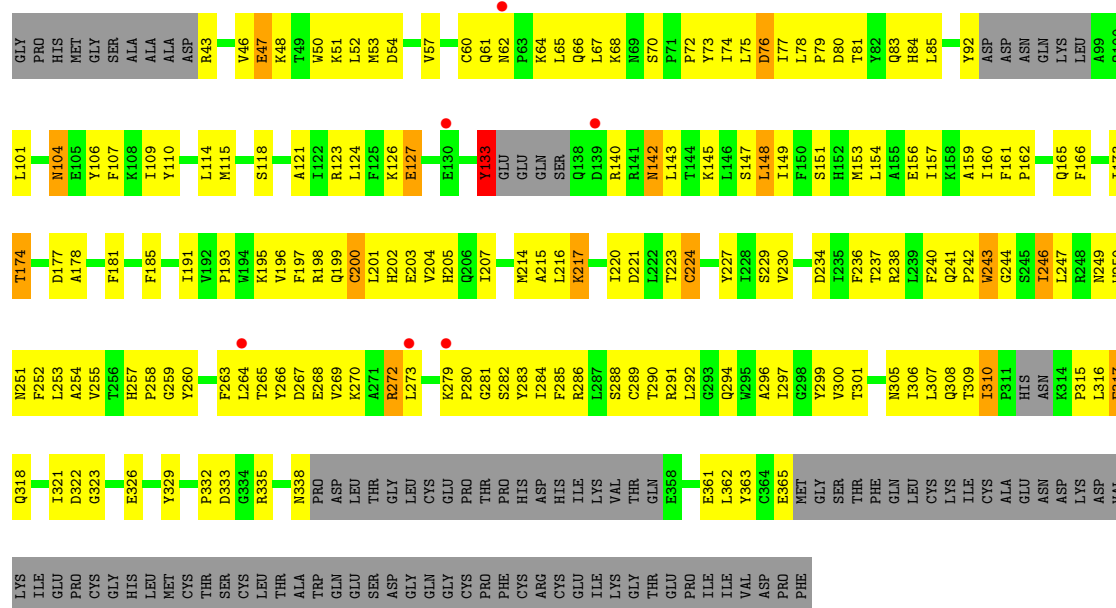


#### • Molecule 1: E3 ubiquitin-protein ligase CBL-B





• Molecule 1: E3 ubiquitin-protein ligase CBL-B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.88Å 98.88Å 105.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.82 – 3.10 44.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.82-3.10) 96.4 (44.81-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.73 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.270 , 0.328 0.272 , 0.337	Depositor DCC
$R_{free}$ test set	1909 reflections (10.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.074 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for h+k, -k, -l	Depositor
Outliers	0 of 23046 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.36% 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

### 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	0.69	0/2253	0.88	2/3063 (0.1%)
1	B	0.68	0/2308	0.84	0/3133
1	C	0.61	0/2275	0.80	0/3091
All	All	0.66	0/6836	0.84	2/9287 (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
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	SER	N-CA-C	-7.75	90.07	111.00
1	A	314	LYS	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	TYR	Sidechain
1	C	133	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	2196	0	2035	200	0
1	B	2252	0	2084	221	0
1	C	2220	0	2045	174	0
All	All	6668	0	6164	595	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 46.

All (595) 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:C:77:ILE:HG23	1:C:154:LEU:HD22	1.22	1.14
1:C:174:THR:HG21	1:C:238:ARG:HD3	1.29	1.10
1:A:263:PHE:O	1:A:264:LEU:HD12	1.49	1.10
1:B:193:PRO:HG2	1:B:196:VAL:HB	1.40	1.03
1:A:52:LEU:HD21	1:A:119:LYS:HG2	1.41	1.01
1:B:156:GLU:O	1:B:160:ILE:HG12	1.60	1.01
1:A:290:THR:O	1:A:291:ARG:HG3	1.61	1.01
1:C:263:PHE:O	1:C:264:LEU:HD12	1.59	1.00
1:A:174:THR:HG21	1:A:238:ARG:HD3	1.44	0.99
1:B:142:ASN:O	1:B:145:LYS:HB3	1.62	0.98
1:B:173:ILE:HB	1:B:179:ALA:HB2	1.48	0.96
1:A:49:THR:HA	1:A:115:MET:SD	2.07	0.94
1:B:265:THR:HG22	1:B:267:ASP:H	1.28	0.94
1:C:201:LEU:O	1:C:205:HIS:N	2.03	0.92
1:A:280:PRO:HB3	1:A:301:THR:O	1.71	0.90
1:B:282:SER:HA	1:B:331:TYR:O	1.71	0.90
1:B:72:PRO:HB2	1:B:77:ILE:HD11	1.54	0.89
1:B:48:LYS:O	1:B:52:LEU:HD13	1.73	0.87
1:A:60:CYS:SG	1:A:74:ILE:HD13	2.15	0.86
1:B:295:TRP:O	1:B:310:ILE:HG22	1.74	0.86
1:A:318:GLN:HG3	1:A:322:ASP:OD2	1.74	0.86
1:C:153:MET:HG2	1:C:223:THR:HG22	1.55	0.86
1:B:263:PHE:O	1:B:264:LEU:HD12	1.75	0.86
1:C:241:GLN:HG3	1:C:315:PRO:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:CE1	1:A:307:LEU:HB2	2.11	0.85
1:A:121:ALA:O	1:A:124:LEU:HB3	1.78	0.84
1:C:269:VAL:HG21	1:C:286:ARG:HE	1.43	0.84
1:B:245:SER:O	1:B:249:ASN:ND2	2.10	0.84
1:C:174:THR:CG2	1:C:238:ARG:HD3	2.09	0.83
1:B:315:PRO:HG3	1:B:317:PHE:CE1	2.14	0.83
1:A:52:LEU:HD21	1:A:119:LYS:CG	2.09	0.82
1:A:49:THR:CA	1:A:115:MET:SD	2.69	0.81
1:A:185:PHE:CD1	1:A:200:CYS:HB3	2.16	0.80
1:A:156:GLU:O	1:A:160:ILE:HG12	1.81	0.80
1:A:332:PRO:HD3	1:A:338:ASN:HD22	1.47	0.80
1:B:138:GLN:OE1	1:B:141:ARG:HD2	1.83	0.79
1:A:285:PHE:CE1	1:A:316:LEU:HD21	2.18	0.79
1:C:156:GLU:O	1:C:160:ILE:HG12	1.84	0.78
1:A:195:LYS:HD2	1:A:196:VAL:N	1.99	0.78
1:C:205:HIS:HE1	1:C:244:GLY:O	1.66	0.77
1:A:76:ASP:C	1:A:79:PRO:HD2	2.05	0.77
1:A:49:THR:CB	1:A:115:MET:SD	2.72	0.77
1:B:296:ALA:HB1	1:B:308:GLN:HE21	1.49	0.77
1:B:101:LEU:HD11	1:B:107:PHE:CE1	2.20	0.77
1:A:299:TYR:OH	1:A:307:LEU:HD12	1.85	0.77
1:C:77:ILE:HD13	1:C:151:SER:HA	1.67	0.77
1:B:286:ARG:HH21	1:B:308:GLN:HE22	1.30	0.76
1:B:185:PHE:CD1	1:B:200:CYS:HB3	2.20	0.76
1:B:193:PRO:HG2	1:B:196:VAL:CB	2.14	0.76
1:C:72:PRO:HG2	1:C:147:SER:HB3	1.68	0.76
1:A:192:VAL:HG22	1:A:228:ILE:O	1.86	0.76
1:B:162:PRO:CG	1:B:167:GLN:HG3	2.17	0.75
1:A:185:PHE:CE1	1:A:200:CYS:HB3	2.22	0.75
1:C:250:TRP:O	1:C:255:VAL:HG23	1.87	0.75
1:C:299:TYR:CE1	1:C:307:LEU:HB2	2.21	0.75
1:A:174:THR:HG22	1:A:175:LYS:HD2	1.67	0.75
1:C:280:PRO:HB3	1:C:301:THR:O	1.87	0.75
1:A:178:ALA:HB2	1:A:237:THR:HG21	1.70	0.74
1:B:191:ILE:HA	1:B:229:SER:HA	1.70	0.74
1:C:142:ASN:ND2	1:C:145:LYS:HD2	2.02	0.74
1:A:175:LYS:O	1:A:178:ALA:HB3	1.87	0.74
1:C:109:ILE:HG21	1:C:191:ILE:HD13	1.70	0.74
1:B:72:PRO:HB2	1:B:77:ILE:CD1	2.18	0.74
1:A:76:ASP:O	1:A:79:PRO:HD2	1.87	0.73
1:A:258:PRO:HG2	1:A:332:PRO:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:HD2	1:A:165:GLN:O	1.89	0.73
1:A:273:LEU:O	1:A:306:ILE:HD11	1.88	0.73
1:C:60:CYS:HB3	1:C:75:LEU:HD21	1.71	0.73
1:B:132:MET:HB2	1:B:133:TYR:CE1	2.23	0.73
1:B:160:ILE:HD11	1:B:231:PHE:HB2	1.71	0.73
1:B:286:ARG:NH2	1:B:308:GLN:HE22	1.87	0.72
1:A:261:MET:O	1:A:264:LEU:HD13	1.88	0.72
1:A:178:ALA:CB	1:A:237:THR:HG21	2.19	0.72
1:B:205:HIS:HE1	1:B:244:GLY:O	1.72	0.72
1:B:335:ARG:HH11	1:B:335:ARG:HG3	1.54	0.72
1:A:260:TYR:CZ	1:A:262:ALA:HA	2.25	0.72
1:B:145:LYS:O	1:B:149:ILE:HG13	1.89	0.71
1:B:234:ASP:O	1:B:238:ARG:HG3	1.89	0.71
1:A:43:ARG:O	1:A:47:GLU:HG2	1.90	0.71
1:B:296:ALA:HA	1:B:310:ILE:CG2	2.20	0.71
1:A:160:ILE:HG22	1:A:166:PHE:CE1	2.26	0.71
1:B:296:ALA:HB1	1:B:308:GLN:NE2	2.04	0.71
1:C:332:PRO:HD3	1:C:338:ASN:HD22	1.56	0.71
1:A:152:HIS:CD2	1:A:292:LEU:HD21	2.26	0.70
1:B:300:VAL:HA	1:B:305:ASN:O	1.91	0.70
1:C:216:LEU:HD11	1:C:220:ILE:HD11	1.73	0.70
1:A:123:ARG:O	1:A:127:GLU:HG2	1.90	0.70
1:B:242:PRO:HD3	1:B:317:PHE:HE1	1.55	0.70
1:B:326:GLU:HA	1:B:326:GLU:OE1	1.90	0.70
1:C:191:ILE:HG12	1:C:227:TYR:HD2	1.57	0.70
1:A:325:ARG:C	1:A:327:GLY:H	1.94	0.69
1:B:72:PRO:HG2	1:B:147:SER:HB3	1.73	0.69
1:B:216:LEU:HD11	1:B:236:PHE:CZ	2.28	0.68
1:A:327:GLY:HA2	1:A:330:LEU:HD21	1.73	0.68
1:A:285:PHE:CZ	1:A:316:LEU:HD21	2.29	0.68
1:B:104:ASN:HB3	1:B:107:PHE:HB2	1.76	0.68
1:B:202:HIS:CD2	1:B:207:ILE:H	2.12	0.68
1:B:217:LYS:NZ	1:B:221:ASP:OD2	2.27	0.67
1:B:43:ARG:O	1:B:47:GLU:HG2	1.94	0.67
1:C:193:PRO:HG2	1:C:196:VAL:HB	1.74	0.67
1:B:64:LYS:O	1:B:66:GLN:HG3	1.94	0.67
1:B:301:THR:O	1:B:304:GLY:N	2.23	0.67
1:B:326:GLU:HB3	1:B:328:PHE:CE2	2.30	0.67
1:B:194:TRP:HE3	1:B:228:ILE:HD11	1.60	0.67
1:A:316:LEU:HG	1:A:320:LEU:HD11	1.75	0.67
1:C:161:PHE:HA	1:C:165:GLN:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:HIS:HD2	1:B:207:ILE:H	1.43	0.66
1:C:43:ARG:O	1:C:47:GLU:HG2	1.96	0.66
1:C:288:SER:O	1:C:292:LEU:HD23	1.95	0.66
1:C:332:PRO:HD3	1:C:338:ASN:HB2	1.77	0.66
1:A:113:SER:OG	1:A:225:ASN:HB3	1.95	0.66
1:A:148:LEU:O	1:A:151:SER:HB3	1.95	0.66
1:C:361:GLU:HG3	1:C:362:LEU:N	2.10	0.66
1:B:181:PHE:CG	1:B:243:TRP:CH2	2.84	0.66
1:A:54:ASP:O	1:A:58:ARG:HB2	1.96	0.66
1:A:257:HIS:CD2	1:A:258:PRO:HD2	2.31	0.65
1:B:57:VAL:HG13	1:B:75:LEU:CD2	2.27	0.65
1:B:242:PRO:HD3	1:B:317:PHE:CE1	2.31	0.65
1:C:43:ARG:O	1:C:46:VAL:HG22	1.97	0.65
1:C:332:PRO:CD	1:C:338:ASN:HB2	2.27	0.65
1:A:151:SER:O	1:A:154:LEU:HB3	1.97	0.65
1:C:289:CYS:HA	1:C:292:LEU:CD2	2.26	0.65
1:B:261:MET:O	1:B:262:ALA:HB3	1.95	0.65
1:A:145:LYS:O	1:A:149:ILE:HG13	1.96	0.65
1:B:315:PRO:CG	1:B:317:PHE:CE1	2.79	0.65
1:C:148:LEU:O	1:C:151:SER:HB3	1.97	0.65
1:C:280:PRO:HA	1:C:300:VAL:HB	1.80	0.64
1:B:241:GLN:CG	1:B:315:PRO:HB3	2.27	0.64
1:C:283:TYR:OH	1:C:338:ASN:ND2	2.30	0.64
1:A:301:THR:C	1:A:303:ASP:H	1.99	0.64
1:C:301:THR:OG1	1:C:305:ASN:HB2	1.97	0.64
1:B:130:GLU:HA	1:B:133:TYR:CE2	2.33	0.64
1:B:216:LEU:HD11	1:B:236:PHE:HZ	1.62	0.64
1:B:265:THR:HG22	1:B:267:ASP:N	2.09	0.63
1:C:253:LEU:HD22	1:C:316:LEU:HD23	1.79	0.63
1:A:160:ILE:HG22	1:A:166:PHE:HE1	1.61	0.63
1:B:161:PHE:CZ	1:B:166:PHE:HD1	2.17	0.63
1:B:173:ILE:HB	1:B:179:ALA:CB	2.26	0.63
1:A:332:PRO:HD3	1:A:338:ASN:HB2	1.79	0.62
1:B:101:LEU:HD11	1:B:107:PHE:CD1	2.34	0.62
1:B:49:THR:CB	1:B:115:MET:SD	2.87	0.62
1:A:265:THR:HG22	1:A:267:ASP:H	1.63	0.62
1:A:323:GLY:HA3	1:A:329:TYR:CE2	2.35	0.62
1:C:202:HIS:HD2	1:C:207:ILE:H	1.48	0.62
1:B:296:ALA:HA	1:B:310:ILE:HG22	1.81	0.62
1:B:57:VAL:O	1:B:61:GLN:HG3	1.99	0.62
1:C:267:ASP:OD1	1:C:270:LYS:NZ	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HG23	1:A:154:LEU:HD22	1.82	0.62
1:C:288:SER:HB3	1:C:291:ARG:O	2.00	0.61
1:B:72:PRO:CB	1:B:77:ILE:HD11	2.28	0.61
1:A:77:ILE:HG21	1:A:151:SER:HA	1.82	0.61
1:B:241:GLN:HB2	1:B:242:PRO:HA	1.83	0.61
1:C:205:HIS:CE1	1:C:244:GLY:O	2.51	0.61
1:B:280:PRO:HB3	1:B:301:THR:O	2.00	0.61
1:B:83:GLN:O	1:B:86:ARG:HB2	2.00	0.61
1:C:142:ASN:HD22	1:C:145:LYS:HD2	1.64	0.60
1:C:299:TYR:OH	1:C:307:LEU:HD12	2.01	0.60
1:B:153:MET:HG2	1:B:223:THR:HG22	1.82	0.60
1:B:215:ALA:O	1:B:218:SER:HB3	2.02	0.60
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.37	0.60
1:C:257:HIS:HD2	1:C:259:GLY:H	1.49	0.60
1:B:241:GLN:HG3	1:B:315:PRO:HB3	1.83	0.60
1:C:115:MET:O	1:C:118:SER:HB2	2.01	0.60
1:B:113:SER:OG	1:B:225:ASN:HB3	2.02	0.60
1:C:234:ASP:O	1:C:237:THR:OG1	2.19	0.60
1:A:160:ILE:CG2	1:A:166:PHE:HE1	2.15	0.60
1:A:196:VAL:O	1:A:199:GLN:HB2	2.01	0.60
1:A:128:GLY:O	1:A:131:ARG:HB2	2.02	0.59
1:B:138:GLN:CD	1:B:141:ARG:HD2	2.22	0.59
1:A:174:THR:CG2	1:A:238:ARG:HD3	2.24	0.59
1:C:323:GLY:HA3	1:C:329:TYR:CD2	2.37	0.59
1:A:216:LEU:HB2	1:A:250:TRP:CH2	2.38	0.59
1:B:263:PHE:O	1:B:264:LEU:CD1	2.47	0.59
1:A:132:MET:HB2	1:A:133:TYR:CE1	2.37	0.59
1:C:145:LYS:O	1:C:149:ILE:HG13	2.02	0.59
1:C:65:LEU:HD23	1:C:133:TYR:CD1	2.38	0.59
1:A:332:PRO:HD3	1:A:338:ASN:ND2	2.16	0.58
1:A:143:LEU:O	1:A:146:LEU:HB2	2.03	0.58
1:C:243:TRP:O	1:C:246:ILE:N	2.34	0.58
1:A:268:GLU:O	1:A:271:ALA:HB3	2.02	0.58
1:A:69:ASN:CB	1:A:73:TYR:HD2	2.16	0.58
1:B:166:PHE:CZ	1:B:168:GLY:HA3	2.39	0.58
1:B:77:ILE:HG23	1:B:154:LEU:HD22	1.84	0.58
1:C:65:LEU:HD23	1:C:133:TYR:CE1	2.39	0.58
1:B:111:ILE:O	1:B:115:MET:HG2	2.03	0.58
1:A:322:ASP:O	1:A:325:ARG:N	2.37	0.58
1:B:220:ILE:HG12	1:B:236:PHE:CD1	2.39	0.58
1:B:270:LYS:HG2	1:B:306:ILE:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:TYR:O	1:B:76:ASP:N	2.32	0.58
1:A:140:ARG:O	1:A:143:LEU:HB3	2.04	0.57
1:C:290:THR:O	1:C:291:ARG:HG3	2.04	0.57
1:C:253:LEU:HD22	1:C:316:LEU:CD2	2.34	0.57
1:A:149:ILE:HD13	1:A:224:CYS:SG	2.44	0.57
1:B:270:LYS:HA	1:B:306:ILE:HD13	1.86	0.57
1:C:251:ASN:HA	1:C:255:VAL:HB	1.86	0.57
1:C:43:ARG:HA	1:C:46:VAL:HG22	1.85	0.57
1:C:252:PHE:O	1:C:257:HIS:HB2	2.04	0.57
1:C:269:VAL:HG21	1:C:286:ARG:NE	2.17	0.57
1:B:57:VAL:O	1:B:61:GLN:CG	2.52	0.57
1:C:74:ILE:HG12	1:C:74:ILE:O	2.03	0.57
1:A:245:SER:O	1:A:249:ASN:OD1	2.22	0.56
1:B:106:TYR:OH	1:B:156:GLU:HG2	2.05	0.56
1:A:47:GLU:O	1:A:51:LYS:HB2	2.05	0.56
1:C:257:HIS:CD2	1:C:258:PRO:HD2	2.40	0.56
1:A:146:LEU:C	1:A:148:LEU:N	2.56	0.56
1:A:177:ASP:HB3	1:A:243:TRP:CD1	2.41	0.56
1:B:240:PHE:CE1	1:B:254:ALA:HB2	2.41	0.56
1:B:335:ARG:NH1	1:B:335:ARG:HG3	2.16	0.56
1:B:262:ALA:O	1:B:287:LEU:N	2.38	0.56
1:B:235:ILE:HG23	1:B:293:GLY:HA2	1.87	0.56
1:C:60:CYS:O	1:C:65:LEU:HD12	2.05	0.56
1:C:266:TYR:CD2	1:C:270:LYS:NZ	2.74	0.56
1:A:146:LEU:O	1:A:148:LEU:N	2.38	0.56
1:B:110:TYR:O	1:B:114:LEU:N	2.36	0.56
1:B:133:TYR:N	1:B:133:TYR:CD1	2.73	0.56
1:B:261:MET:N	1:B:285:PHE:O	2.39	0.56
1:B:296:ALA:HA	1:B:310:ILE:HG23	1.87	0.56
1:B:243:TRP:CD1	1:B:243:TRP:C	2.79	0.56
1:A:266:TYR:O	1:A:270:LYS:HG3	2.06	0.56
1:A:60:CYS:O	1:A:65:LEU:HD12	2.06	0.55
1:B:52:LEU:O	1:B:55:LYS:HB2	2.06	0.55
1:B:72:PRO:CG	1:B:147:SER:HB3	2.36	0.55
1:C:197:PHE:O	1:C:200:CYS:HB2	2.06	0.55
1:A:191:ILE:HA	1:A:229:SER:HA	1.88	0.55
1:B:44:ARG:O	1:B:47:GLU:HB2	2.05	0.55
1:B:233:PHE:CE2	1:B:237:THR:HG21	2.41	0.55
1:B:57:VAL:HG13	1:B:75:LEU:HD22	1.87	0.55
1:B:240:PHE:HE1	1:B:254:ALA:HB2	1.71	0.55
1:C:142:ASN:O	1:C:145:LYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG12	1:B:236:PHE:CE1	2.41	0.55
1:C:217:LYS:O	1:C:221:ASP:HB2	2.07	0.55
1:B:101:LEU:HD21	1:B:107:PHE:CZ	2.42	0.55
1:C:92:TYR:CB	1:C:101:LEU:HD22	2.36	0.55
1:B:176:ALA:O	1:B:180:GLU:N	2.32	0.55
1:B:76:ASP:O	1:B:80:ASP:OD2	2.23	0.55
1:C:317:PHE:O	1:C:321:ILE:HG13	2.07	0.55
1:A:215:ALA:O	1:A:218:SER:HB3	2.08	0.54
1:B:273:LEU:HB2	1:B:306:ILE:CD1	2.37	0.54
1:B:323:GLY:HA3	1:B:329:TYR:CD2	2.42	0.54
1:C:142:ASN:O	1:C:145:LYS:HB2	2.08	0.54
1:C:214:MET:HA	1:C:217:LYS:HB3	1.89	0.54
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.22	0.54
1:A:105:GLU:O	1:A:109:ILE:HG13	2.07	0.54
1:B:205:HIS:CE1	1:B:244:GLY:O	2.58	0.54
1:C:318:GLN:HA	1:C:318:GLN:HE21	1.71	0.54
1:B:82:TYR:O	1:B:86:ARG:HG2	2.08	0.54
1:A:140:ARG:O	1:A:143:LEU:N	2.40	0.54
1:B:104:ASN:HB3	1:B:107:PHE:CB	2.38	0.54
1:B:266:TYR:CE2	1:B:270:LYS:HD3	2.42	0.54
1:C:191:ILE:HG12	1:C:227:TYR:CD2	2.41	0.54
1:A:332:PRO:HD3	1:A:338:ASN:CB	2.38	0.54
1:C:121:ALA:O	1:C:124:LEU:HB3	2.08	0.54
1:C:62:ASN:O	1:C:65:LEU:HG	2.07	0.54
1:B:201:LEU:O	1:B:205:HIS:N	2.36	0.54
1:B:283:TYR:CE1	1:B:329:TYR:HB3	2.43	0.54
1:C:251:ASN:HA	1:C:255:VAL:CG2	2.38	0.53
1:A:265:THR:HG22	1:A:266:TYR:N	2.22	0.53
1:A:282:SER:OG	1:A:334:GLY:HA2	2.08	0.53
1:B:161:PHE:CE1	1:B:166:PHE:HD1	2.27	0.53
1:B:291:ARG:NH1	1:B:291:ARG:HB3	2.22	0.53
1:B:235:ILE:HD13	1:B:292:LEU:HB3	1.91	0.53
1:B:318:GLN:O	1:B:321:ILE:N	2.42	0.53
1:A:74:ILE:HB	1:A:147:SER:OG	2.08	0.53
1:B:253:LEU:O	1:B:260:TYR:HB2	2.08	0.53
1:C:273:LEU:HB2	1:C:306:ILE:HD13	1.89	0.53
1:A:161:PHE:HA	1:A:165:GLN:O	2.07	0.53
1:B:144:THR:HA	1:B:147:SER:HB2	1.91	0.53
1:A:325:ARG:C	1:A:327:GLY:N	2.60	0.53
1:B:52:LEU:HD21	1:B:119:LYS:CE	2.39	0.53
1:B:156:GLU:HA	1:B:231:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:O	1:A:126:LYS:HB3	2.09	0.53
1:B:193:PRO:HG2	1:B:196:VAL:CG2	2.38	0.53
1:A:264:LEU:O	1:A:286:ARG:NH1	2.40	0.52
1:C:198:ARG:HG3	1:C:207:ILE:CD1	2.39	0.52
1:A:109:ILE:HD12	1:A:191:ILE:HD13	1.91	0.52
1:B:73:TYR:HB2	1:B:76:ASP:HB2	1.91	0.52
1:A:77:ILE:HD12	1:A:154:LEU:HD23	1.91	0.52
1:B:162:PRO:CD	1:B:167:GLN:HG3	2.39	0.52
1:B:270:LYS:HG2	1:B:306:ILE:CG2	2.39	0.52
1:B:216:LEU:HA	1:B:250:TRP:CZ2	2.44	0.52
1:B:272:ARG:HG3	1:B:272:ARG:HH11	1.73	0.52
1:A:316:LEU:HG	1:A:320:LEU:CD1	2.38	0.52
1:B:161:PHE:CZ	1:B:166:PHE:CD1	2.98	0.52
1:A:82:TYR:O	1:A:86:ARG:HG2	2.09	0.52
1:B:118:SER:O	1:B:121:ALA:HB3	2.10	0.52
1:B:260:TYR:HA	1:B:285:PHE:CE1	2.45	0.52
1:B:49:THR:HA	1:B:115:MET:SD	2.50	0.52
1:A:326:GLU:HB2	1:A:328:PHE:CE2	2.45	0.52
1:B:260:TYR:HA	1:B:285:PHE:CD1	2.45	0.52
1:B:205:HIS:HB3	1:B:247:LEU:CD1	2.39	0.52
1:A:263:PHE:O	1:A:264:LEU:CD1	2.41	0.51
1:A:276:TYR:O	1:A:277:SER:C	2.48	0.51
1:A:202:HIS:HD2	1:A:207:ILE:H	1.58	0.51
1:C:333:ASP:O	1:C:333:ASP:OD2	2.28	0.51
1:C:264:LEU:CB	1:C:286:ARG:HD3	2.40	0.51
1:A:195:LYS:O	1:A:199:GLN:HG3	2.11	0.51
1:B:72:PRO:HD3	1:B:148:LEU:CD1	2.41	0.51
1:C:216:LEU:HA	1:C:250:TRP:CZ2	2.45	0.51
1:A:323:GLY:O	1:A:328:PHE:HB2	2.10	0.51
1:B:178:ALA:O	1:B:181:PHE:HB3	2.11	0.51
1:B:272:ARG:HG3	1:B:272:ARG:NH1	2.26	0.51
1:A:52:LEU:CD2	1:A:119:LYS:CG	2.84	0.51
1:A:152:HIS:HD2	1:A:292:LEU:HD11	1.74	0.51
1:A:280:PRO:HB3	1:A:301:THR:C	2.31	0.51
1:A:251:ASN:HA	1:A:255:VAL:CG2	2.41	0.51
1:C:216:LEU:CD1	1:C:220:ILE:HD11	2.41	0.51
1:C:289:CYS:SG	1:C:290:THR:HG23	2.51	0.51
1:A:173:ILE:HG23	1:A:234:ASP:OD1	2.10	0.50
1:A:146:LEU:O	1:A:147:SER:C	2.49	0.50
1:A:77:ILE:HG23	1:A:154:LEU:CD2	2.41	0.50
1:C:64:LYS:O	1:C:133:TYR:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:HIS:O	1:C:85:LEU:C	2.49	0.50
1:C:283:TYR:CE1	1:C:338:ASN:ND2	2.80	0.50
1:C:65:LEU:O	1:C:66:GLN:CG	2.59	0.50
1:C:215:ALA:HB1	1:C:363:TYR:HD2	1.75	0.50
1:A:153:MET:HG2	1:A:223:THR:HG22	1.94	0.50
1:A:239:LEU:HD13	1:A:287:LEU:HD21	1.94	0.50
1:A:286:ARG:HD2	1:A:287:LEU:O	2.11	0.50
1:A:49:THR:O	1:A:53:MET:HG3	2.11	0.50
1:A:132:MET:C	1:A:133:TYR:CD1	2.85	0.50
1:C:203:GLU:OE1	1:C:203:GLU:HA	2.11	0.50
1:C:265:THR:HG22	1:C:267:ASP:H	1.77	0.50
1:C:60:CYS:HA	1:C:65:LEU:HD11	1.94	0.50
1:C:178:ALA:O	1:C:181:PHE:HB3	2.12	0.50
1:C:260:TYR:HA	1:C:285:PHE:CE1	2.47	0.50
1:B:52:LEU:HD12	1:B:52:LEU:N	2.26	0.49
1:C:76:ASP:O	1:C:79:PRO:HD2	2.12	0.49
1:B:52:LEU:HD21	1:B:119:LYS:HE2	1.94	0.49
1:C:335:ARG:HG3	1:C:335:ARG:HH11	1.78	0.49
1:B:291:ARG:CZ	1:B:291:ARG:CB	2.89	0.49
1:A:69:ASN:CB	1:A:73:TYR:CD2	2.95	0.49
1:B:166:PHE:CZ	1:B:190:THR:HG21	2.46	0.49
1:B:268:GLU:O	1:B:269:VAL:C	2.49	0.49
1:A:132:MET:CB	1:A:133:TYR:CE1	2.95	0.49
1:A:197:PHE:O	1:A:200:CYS:N	2.44	0.49
1:A:266:TYR:CD1	1:A:308:GLN:OE1	2.65	0.49
1:C:73:TYR:O	1:C:77:ILE:HG13	2.13	0.49
1:A:88:ILE:HA	1:A:164:GLY:O	2.13	0.49
1:B:47:GLU:O	1:B:50:TRP:HB2	2.13	0.49
1:B:67:LEU:HD23	1:B:140:ARG:HH22	1.78	0.49
1:A:295:TRP:O	1:A:310:ILE:HG22	2.13	0.49
1:C:289:CYS:HA	1:C:292:LEU:HD21	1.95	0.49
1:B:326:GLU:OE1	1:B:326:GLU:CA	2.61	0.49
1:C:297:ILE:HG21	1:C:329:TYR:CZ	2.47	0.49
1:C:68:LYS:C	1:C:70:SER:N	2.66	0.49
1:A:326:GLU:HB2	1:A:328:PHE:CD2	2.47	0.48
1:B:301:THR:C	1:B:303:ASP:N	2.64	0.48
1:C:165:GLN:HG2	1:C:166:PHE:N	2.27	0.48
1:A:152:HIS:NE2	1:A:292:LEU:HD21	2.27	0.48
1:B:268:GLU:HA	1:B:271:ALA:HB3	1.95	0.48
1:B:78:LEU:CB	1:B:79:PRO:HD3	2.43	0.48
1:B:143:LEU:O	1:B:144:THR:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:LYS:O	1:C:199:GLN:HG3	2.13	0.48
1:A:222:LEU:N	1:A:232:GLU:OE2	2.46	0.48
1:A:276:TYR:O	1:A:279:LYS:N	2.45	0.48
1:A:283:TYR:OH	1:A:338:ASN:ND2	2.43	0.48
1:B:111:ILE:O	1:B:114:LEU:N	2.46	0.48
1:B:67:LEU:HD23	1:B:140:ARG:NH2	2.28	0.48
1:C:281:GLY:O	1:C:282:SER:C	2.51	0.48
1:B:186:PHE:O	1:B:189:LYS:HD2	2.13	0.48
1:B:298:GLY:O	1:B:299:TYR:HB3	2.12	0.48
1:C:283:TYR:HE1	1:C:338:ASN:HD22	1.61	0.48
1:A:214:MET:O	1:A:217:LYS:HB3	2.14	0.48
1:C:264:LEU:HB2	1:C:286:ARG:HD3	1.96	0.48
1:A:65:LEU:HD11	1:A:125:PHE:CE1	2.49	0.48
1:B:144:THR:O	1:B:147:SER:N	2.47	0.48
1:B:268:GLU:O	1:B:272:ARG:N	2.34	0.48
1:C:60:CYS:C	1:C:62:ASN:H	2.17	0.48
1:A:71:PRO:HA	1:A:72:PRO:HA	1.59	0.48
1:C:362:LEU:O	1:C:365:GLU:HB2	2.14	0.47
1:A:258:PRO:HG2	1:A:332:PRO:CB	2.40	0.47
1:A:146:LEU:O	1:A:149:ILE:N	2.47	0.47
1:A:322:ASP:O	1:A:325:ARG:HB2	2.13	0.47
1:B:261:MET:HB2	1:B:286:ARG:HB3	1.96	0.47
1:C:173:ILE:HD11	1:C:230:VAL:HG23	1.96	0.47
1:B:279:LYS:HG2	1:B:279:LYS:O	2.13	0.47
1:B:325:ARG:O	1:B:327:GLY:N	2.47	0.47
1:C:279:LYS:HG2	1:C:279:LYS:O	2.14	0.47
1:A:301:THR:C	1:A:303:ASP:N	2.67	0.47
1:A:332:PRO:CD	1:A:338:ASN:HB2	2.45	0.47
1:C:205:HIS:HB3	1:C:247:LEU:HG	1.96	0.47
1:C:223:THR:O	1:C:224:CYS:HB2	2.14	0.47
1:A:46:VAL:HA	1:A:49:THR:CB	2.44	0.47
1:B:234:ASP:O	1:B:238:ARG:CG	2.61	0.47
1:B:52:LEU:N	1:B:52:LEU:CD1	2.78	0.47
1:A:283:TYR:HB2	1:A:298:GLY:O	2.14	0.47
1:A:306:ILE:HG22	1:A:306:ILE:O	2.14	0.47
1:C:202:HIS:CD2	1:C:207:ILE:H	2.30	0.47
1:B:114:LEU:HA	1:B:114:LEU:HD12	1.61	0.47
1:B:186:PHE:HB3	1:B:189:LYS:HD2	1.96	0.47
1:B:317:PHE:CD2	1:B:318:GLN:N	2.82	0.47
1:B:326:GLU:CB	1:B:328:PHE:CE2	2.97	0.47
1:C:265:THR:N	1:C:268:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:TYR:O	1:C:284:ILE:HG23	2.15	0.47
1:A:50:TRP:HH2	1:A:86:ARG:HH11	1.63	0.47
1:B:191:ILE:HG13	1:B:229:SER:HB3	1.96	0.47
1:C:178:ALA:HB1	1:C:237:THR:HG21	1.97	0.47
1:C:241:GLN:CG	1:C:315:PRO:HB3	2.38	0.47
1:A:183:ARG:O	1:A:187:GLY:CA	2.63	0.46
1:A:216:LEU:HA	1:A:250:TRP:CZ2	2.51	0.46
1:B:58:ARG:O	1:B:61:GLN:HB2	2.14	0.46
1:C:269:VAL:CG2	1:C:286:ARG:HE	2.23	0.46
1:C:53:MET:O	1:C:54:ASP:C	2.53	0.46
1:B:250:TRP:O	1:B:255:VAL:HG23	2.16	0.46
1:C:159:ALA:O	1:C:162:PRO:HD3	2.15	0.46
1:A:246:ILE:O	1:A:249:ASN:ND2	2.48	0.46
1:B:152:HIS:O	1:B:155:ALA:N	2.48	0.46
1:C:266:TYR:CD1	1:C:266:TYR:O	2.68	0.46
1:A:65:LEU:HD11	1:A:125:PHE:HE1	1.81	0.46
1:B:105:GLU:HG2	1:B:105:GLU:O	2.15	0.46
1:C:216:LEU:HB2	1:C:250:TRP:CH2	2.51	0.46
1:B:77:ILE:HG23	1:B:154:LEU:CD2	2.45	0.46
1:C:110:TYR:CE1	1:C:157:ILE:CB	2.98	0.46
1:C:60:CYS:C	1:C:62:ASN:N	2.69	0.46
1:A:145:LYS:O	1:A:148:LEU:HB3	2.16	0.46
1:C:77:ILE:HD13	1:C:151:SER:CA	2.43	0.46
1:A:318:GLN:OE1	1:A:322:ASP:OD1	2.35	0.46
1:B:124:LEU:HD21	1:B:139:ASP:O	2.16	0.46
1:C:123:ARG:O	1:C:126:LYS:HB3	2.16	0.46
1:C:60:CYS:HA	1:C:65:LEU:CD1	2.45	0.46
1:A:291:ARG:O	1:A:294:GLN:HB2	2.16	0.45
1:B:162:PRO:HD2	1:B:167:GLN:HG3	1.98	0.45
1:C:80:ASP:O	1:C:83:GLN:HB2	2.16	0.45
1:A:52:LEU:CD2	1:A:119:LYS:HG2	2.30	0.45
1:A:154:LEU:HD11	1:A:158:LYS:HE3	1.98	0.45
1:C:57:VAL:O	1:C:61:GLN:HG3	2.16	0.45
1:B:192:VAL:CG2	1:B:197:PHE:HB2	2.46	0.45
1:C:191:ILE:HA	1:C:229:SER:HA	1.98	0.45
1:A:183:ARG:O	1:A:187:GLY:N	2.50	0.45
1:B:71:PRO:HD3	1:B:73:TYR:OH	2.17	0.45
1:C:243:TRP:O	1:C:246:ILE:CB	2.65	0.45
1:C:240:PHE:O	1:C:249:ASN:ND2	2.49	0.45
1:A:202:HIS:CD2	1:A:207:ILE:H	2.34	0.45
1:B:52:LEU:HD23	1:B:119:LYS:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:HD13	1:C:316:LEU:HD23	1.99	0.45
1:A:78:LEU:CB	1:A:79:PRO:HD3	2.47	0.45
1:B:144:THR:O	1:B:145:LYS:C	2.55	0.45
1:B:205:HIS:HB3	1:B:247:LEU:HG	1.99	0.45
1:C:289:CYS:HA	1:C:292:LEU:HD23	1.99	0.45
1:C:322:ASP:O	1:C:326:GLU:CB	2.64	0.45
1:A:132:MET:HB2	1:A:133:TYR:CZ	2.51	0.45
1:B:233:PHE:O	1:B:237:THR:HG23	2.16	0.45
1:C:301:THR:N	1:C:305:ASN:O	2.47	0.45
1:B:57:VAL:HG23	1:B:78:LEU:HD23	1.98	0.45
1:C:297:ILE:O	1:C:308:GLN:HA	2.17	0.45
1:A:261:MET:O	1:A:264:LEU:CD1	2.62	0.44
1:B:276:TYR:O	1:B:300:VAL:HG21	2.18	0.44
1:A:323:GLY:HA3	1:A:329:TYR:CD2	2.51	0.44
1:B:208:SER:N	1:B:212:GLU:OE1	2.47	0.44
1:B:194:TRP:CE3	1:B:228:ILE:HD11	2.45	0.44
1:B:253:LEU:O	1:B:257:HIS:HB3	2.18	0.44
1:B:57:VAL:HG13	1:B:75:LEU:HD23	1.95	0.44
1:A:182:TRP:CH2	1:A:230:VAL:HA	2.53	0.44
1:B:138:GLN:O	1:B:138:GLN:HG3	2.16	0.44
1:C:104:ASN:HB3	1:C:107:PHE:CB	2.47	0.44
1:A:126:LYS:O	1:A:129:LYS:HD3	2.17	0.44
1:B:265:THR:HB	1:B:268:GLU:OE1	2.18	0.44
1:C:74:ILE:CG1	1:C:74:ILE:O	2.66	0.44
1:A:231:PHE:O	1:A:232:GLU:C	2.56	0.44
1:A:265:THR:N	1:A:268:GLU:OE1	2.46	0.44
1:A:318:GLN:O	1:A:319:ALA:C	2.55	0.44
1:C:269:VAL:CG2	1:C:286:ARG:NE	2.80	0.44
1:A:260:TYR:OH	1:A:262:ALA:HA	2.17	0.44
1:A:285:PHE:CE2	1:A:320:LEU:CD1	3.01	0.44
1:B:148:LEU:O	1:B:151:SER:HB3	2.18	0.44
1:C:296:ALA:HA	1:C:310:ILE:HG22	1.99	0.44
1:C:300:VAL:HA	1:C:305:ASN:O	2.18	0.44
1:A:173:ILE:HG23	1:A:234:ASP:CB	2.47	0.44
1:B:227:TYR:O	1:B:228:ILE:HD13	2.16	0.44
1:A:237:THR:HG22	1:A:237:THR:O	2.18	0.43
1:A:331:TYR:O	1:A:332:PRO:C	2.54	0.43
1:C:196:VAL:O	1:C:200:CYS:SG	2.52	0.43
1:A:185:PHE:CE2	1:A:200:CYS:SG	3.11	0.43
1:B:268:GLU:O	1:B:271:ALA:N	2.52	0.43
1:B:71:PRO:HA	1:B:72:PRO:HA	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:C	1:A:306:ILE:HD11	2.37	0.43
1:B:185:PHE:CD2	1:B:185:PHE:O	2.72	0.43
1:B:190:THR:O	1:B:190:THR:HG22	2.18	0.43
1:B:251:ASN:HA	1:B:255:VAL:HG23	2.01	0.43
1:C:181:PHE:CG	1:C:243:TRP:CH2	3.06	0.43
1:A:60:CYS:HA	1:A:65:LEU:HD12	2.00	0.43
1:B:83:GLN:O	1:B:86:ARG:CB	2.67	0.43
1:C:68:LYS:C	1:C:70:SER:H	2.22	0.43
1:A:238:ARG:O	1:A:241:GLN:NE2	2.33	0.43
1:A:251:ASN:HA	1:A:255:VAL:HG21	2.00	0.43
1:B:192:VAL:HG23	1:B:197:PHE:HB2	2.01	0.43
1:B:291:ARG:HH11	1:B:291:ARG:CG	2.31	0.43
1:B:235:ILE:O	1:B:238:ARG:N	2.52	0.43
1:B:325:ARG:C	1:B:327:GLY:N	2.71	0.43
1:B:49:THR:CA	1:B:115:MET:SD	3.07	0.43
1:C:251:ASN:HA	1:C:255:VAL:CB	2.48	0.43
1:C:362:LEU:HA	1:C:365:GLU:HB2	2.01	0.43
1:A:65:LEU:HD23	1:A:133:TYR:HD1	1.84	0.43
1:A:182:TRP:O	1:A:186:PHE:N	2.52	0.43
1:A:193:PRO:HG2	1:A:196:VAL:CG2	2.48	0.43
1:A:245:SER:O	1:A:249:ASN:CG	2.57	0.43
1:B:290:THR:C	1:B:291:ARG:HG3	2.38	0.43
1:C:110:TYR:O	1:C:110:TYR:CD2	2.72	0.43
1:C:265:THR:O	1:C:268:GLU:HB2	2.19	0.43
1:C:272:ARG:HG3	1:C:272:ARG:NH1	2.33	0.43
1:A:122:ILE:O	1:A:125:PHE:N	2.52	0.43
1:A:198:ARG:O	1:A:202:HIS:HB2	2.19	0.43
1:B:161:PHE:CE1	1:B:166:PHE:CD1	3.06	0.42
1:B:216:LEU:HB2	1:B:250:TRP:CH2	2.54	0.42
1:C:217:LYS:O	1:C:221:ASP:CB	2.67	0.42
1:C:174:THR:CB	1:C:238:ARG:HD3	2.49	0.42
1:A:183:ARG:O	1:A:184:LYS:C	2.58	0.42
1:C:254:ALA:HA	1:C:260:TYR:CG	2.54	0.42
1:C:78:LEU:O	1:C:81:THR:HB	2.19	0.42
1:B:273:LEU:HB2	1:B:306:ILE:HD13	2.01	0.42
1:B:50:TRP:O	1:B:51:LYS:C	2.58	0.42
1:C:291:ARG:NH2	1:C:294:GLN:OE1	2.52	0.42
1:A:59:LEU:HD11	1:A:122:ILE:HG23	2.01	0.42
1:A:183:ARG:O	1:A:187:GLY:HA2	2.19	0.42
1:A:173:ILE:CG2	1:A:234:ASP:OD1	2.67	0.42
1:A:280:PRO:HA	1:A:300:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:CYS:O	1:B:203:GLU:N	2.48	0.42
1:B:257:HIS:HA	1:B:258:PRO:HD2	1.90	0.42
1:C:123:ARG:O	1:C:127:GLU:HG2	2.18	0.42
1:B:251:ASN:HA	1:B:255:VAL:CG2	2.50	0.42
1:B:301:THR:C	1:B:303:ASP:H	2.22	0.42
1:B:325:ARG:C	1:B:327:GLY:H	2.23	0.42
1:C:220:ILE:HG12	1:C:236:PHE:CD1	2.55	0.42
1:C:272:ARG:HD3	1:C:284:ILE:HD13	2.00	0.42
1:C:272:ARG:HG3	1:C:272:ARG:HH11	1.83	0.42
1:A:195:LYS:CD	1:A:196:VAL:N	2.76	0.42
1:A:261:MET:O	1:A:262:ALA:C	2.58	0.42
1:A:286:ARG:CD	1:A:287:LEU:O	2.68	0.42
1:A:285:PHE:CD1	1:A:316:LEU:HD21	2.55	0.42
1:A:57:VAL:HG12	1:A:57:VAL:O	2.20	0.42
1:C:114:LEU:HD12	1:C:114:LEU:HA	1.77	0.42
1:C:72:PRO:HG2	1:C:147:SER:CB	2.44	0.42
1:A:286:ARG:HE	1:A:296:ALA:HB3	1.84	0.41
1:A:60:CYS:HA	1:A:65:LEU:CD1	2.50	0.41
1:A:65:LEU:O	1:A:66:GLN:C	2.58	0.41
1:B:142:ASN:O	1:B:145:LYS:CB	2.51	0.41
1:B:154:LEU:O	1:B:158:LYS:HG3	2.20	0.41
1:C:161:PHE:CZ	1:C:166:PHE:CD1	3.07	0.41
1:C:202:HIS:C	1:C:204:VAL:N	2.71	0.41
1:A:257:HIS:HA	1:A:258:PRO:HD2	1.87	0.41
1:A:76:ASP:CA	1:A:79:PRO:HD2	2.50	0.41
1:B:261:MET:O	1:B:262:ALA:CB	2.64	0.41
1:B:74:ILE:O	1:B:78:LEU:HB2	2.21	0.41
1:C:64:LYS:HE3	1:C:133:TYR:CD2	2.55	0.41
1:C:72:PRO:CG	1:C:147:SER:HB3	2.46	0.41
1:C:332:PRO:HD2	1:C:338:ASN:HB2	2.01	0.41
1:A:230:VAL:O	1:A:233:PHE:HB3	2.20	0.41
1:A:178:ALA:HB1	1:A:237:THR:HG21	2.00	0.41
1:B:71:PRO:HG3	1:B:73:TYR:CE1	2.56	0.41
1:A:114:LEU:HA	1:A:114:LEU:HD12	1.83	0.41
1:B:264:LEU:CB	1:B:286:ARG:HD3	2.50	0.41
1:C:140:ARG:NH1	1:C:143:LEU:HD23	2.35	0.41
1:C:257:HIS:CD2	1:C:259:GLY:H	2.34	0.41
1:C:299:TYR:O	1:C:306:ILE:HA	2.20	0.41
1:A:130:GLU:HG3	1:A:130:GLU:H	1.39	0.41
1:A:160:ILE:CG2	1:A:166:PHE:CE1	2.96	0.41
1:B:215:ALA:HB1	1:B:363:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:O	1:B:79:PRO:HG2	2.19	0.41
1:A:205:HIS:HE1	1:A:244:GLY:O	2.03	0.41
1:B:235:ILE:HG23	1:B:293:GLY:CA	2.48	0.41
1:B:266:TYR:CD1	1:B:308:GLN:OE1	2.74	0.41
1:B:325:ARG:O	1:B:326:GLU:C	2.57	0.41
1:C:191:ILE:O	1:C:191:ILE:HG23	2.21	0.41
1:B:78:LEU:HB3	1:B:79:PRO:HD3	2.02	0.41
1:C:65:LEU:O	1:C:66:GLN:HG3	2.20	0.41
1:A:205:HIS:CE1	1:A:244:GLY:O	2.74	0.41
1:C:106:TYR:HA	1:C:109:ILE:HG22	2.03	0.41
1:C:241:GLN:HB2	1:C:242:PRO:HA	2.02	0.41
1:B:291:ARG:CB	1:B:291:ARG:NH1	2.84	0.41
1:C:140:ARG:O	1:C:143:LEU:HB3	2.20	0.41
1:A:139:ASP:O	1:A:142:ASN:HB2	2.21	0.41
1:B:238:ARG:HD2	1:B:238:ARG:HH11	1.73	0.41
1:C:177:ASP:HB3	1:C:243:TRP:CD1	2.56	0.41
1:C:283:TYR:CD1	1:C:329:TYR:HB3	2.56	0.41
1:A:188:ASP:N	1:A:188:ASP:OD1	2.49	0.41
1:A:231:PHE:C	1:A:233:PHE:N	2.73	0.41
1:A:239:LEU:HD21	1:A:293:GLY:C	2.41	0.41
1:B:235:ILE:HG22	1:B:239:LEU:HD12	2.03	0.41
1:B:256:THR:OG1	1:B:257:HIS:N	2.54	0.41
1:B:286:ARG:HH21	1:B:308:GLN:NE2	2.07	0.41
1:C:191:ILE:HD11	1:C:227:TYR:HB3	2.03	0.41
1:C:299:TYR:CE2	1:C:301:THR:CG2	3.04	0.41
1:A:146:LEU:C	1:A:148:LEU:H	2.22	0.40
1:A:162:PRO:O	1:A:162:PRO:HG2	2.21	0.40
1:A:217:LYS:NZ	1:A:226:ASP:HA	2.36	0.40
1:B:193:PRO:CG	1:B:196:VAL:CG2	3.00	0.40
1:B:59:LEU:HD22	1:B:125:PHE:CG	2.56	0.40
1:A:286:ARG:O	1:A:295:TRP:HA	2.21	0.40
1:C:48:LYS:HA	1:C:51:LYS:HE2	2.03	0.40
1:C:47:GLU:O	1:C:50:TRP:HB2	2.22	0.40
1:A:52:LEU:CD2	1:A:119:LYS:HG3	2.51	0.40
1:B:173:ILE:O	1:B:174:THR:C	2.59	0.40
1:A:113:SER:HG	1:A:225:ASN:HB3	1.86	0.40
1:A:316:LEU:O	1:A:317:PHE:C	2.59	0.40
1:B:327:GLY:HA2	1:B:330:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

## 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	281/394 (71%)	231 (82%)	41 (15%)	9 (3%)	5	25
1	B	284/394 (72%)	222 (78%)	59 (21%)	3 (1%)	17	54
1	C	282/394 (72%)	238 (84%)	38 (14%)	6 (2%)	8	36
All	All	847/1182 (72%)	691 (82%)	138 (16%)	18 (2%)	8	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ILE
1	C	200	CYS
1	C	246	ILE
1	A	147	SER
1	A	184	LYS
1	A	196	VAL
1	B	191	ILE
1	B	326	GLU
1	A	208	SER
1	C	174	THR
1	A	69	ASN
1	A	132	MET
1	A	197	PHE
1	A	336	SER
1	C	104	ASN
1	C	243	TRP
1	B	184	LYS
1	C	224	CYS

### 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	208/352 (59%)	189 (91%)	19 (9%)	11	39
1	B	212/352 (60%)	201 (95%)	11 (5%)	27	63
1	C	208/352 (59%)	194 (93%)	14 (7%)	19	54
All	All	628/1056 (60%)	584 (93%)	44 (7%)	18	52

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	VAL
1	A	58	ARG
1	A	113	SER
1	A	123	ARG
1	A	126	LYS
1	A	130	GLU
1	A	133	TYR
1	A	169	ASP
1	A	188	ASP
1	A	195	LYS
1	A	200	CYS
1	A	245	SER
1	A	248	ARG
1	A	249	ASN
1	A	286	ARG
1	A	299	TYR
1	A	310	ILE
1	A	317	PHE
1	A	330	LEU
1	B	63	PRO
1	B	113	SER
1	B	133	TYR
1	B	148	LEU
1	B	185	PHE
1	B	188	ASP
1	B	219	THR
1	B	291	ARG
1	B	301	THR
1	B	309	THR
1	B	310	ILE
1	C	47	GLU

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Mol	Chain	Res	Type
1	C	52	LEU
1	C	67	LEU
1	C	76	ASP
1	C	127	GLU
1	C	133	TYR
1	C	142	ASN
1	C	148	LEU
1	C	185	PHE
1	C	217	LYS
1	C	272	ARG
1	C	309	THR
1	C	310	ILE
1	C	317	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	152	HIS
1	A	202	HIS
1	A	205	HIS
1	A	257	HIS
1	A	305	ASN
1	A	318	GLN
1	A	338	ASN
1	B	142	ASN
1	B	152	HIS
1	B	167	GLN
1	B	202	HIS
1	B	205	HIS
1	B	249	ASN
1	B	305	ASN
1	B	308	GLN
1	B	338	ASN
1	C	142	ASN
1	C	202	HIS
1	C	205	HIS
1	C	249	ASN
1	C	257	HIS
1	C	305	ASN
1	C	308	GLN
1	C	318	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	C	338	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	287/394 (72%)	-0.37	0 <span>100</span> <span>100</span>	43, 43, 46, 46	0
1	B	294/394 (74%)	-0.27	1 (0%) <span>93</span> <span>86</span>	40, 47, 55, 55	0
1	C	292/394 (74%)	-0.03	6 (2%) <span>64</span> <span>43</span>	47, 59, 101, 101	0
All	All	873/1182 (73%)	-0.22	7 (0%) <span>86</span> <span>71</span>	40, 47, 89, 101	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	GLU	3.8
1	C	62	ASN	3.1
1	C	273	LEU	2.5
1	B	45	THR	2.2
1	C	279	LYS	2.0
1	C	139	ASP	2.0
1	C	264	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.