



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:07 AM GMT

PDB ID : 2ZIH  
Title : Crystal Structure of Yeast Vps74  
Authors : Schmitz, K.R.; Li, S.; Setty, T.G.; Ferguson, K.M.  
Deposited on : 2008-02-18  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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  
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

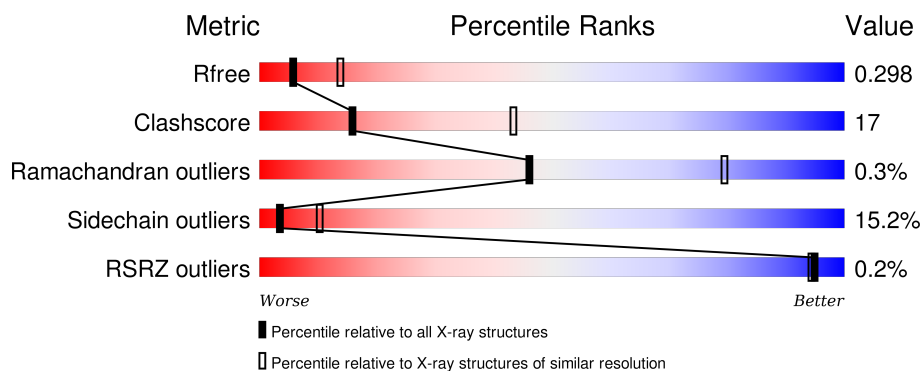
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	347	<div> <div>55%</div> <div>22%</div> <div>•</div> <div>19%</div> </div>
1	B	347	<div> <div>54%</div> <div>23%</div> <div>•</div> <div>19%</div> </div>
1	C	347	<div> <div>55%</div> <div>20%</div> <div>5% •</div> <div>20%</div> </div>
1	D	347	<div> <div>51%</div> <div>24%</div> <div>6%</div> <div>18%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8541 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 Vacuolar protein sorting-associated protein 74.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2135	1354	362	407	12			
1	B	281	Total	C	N	O	S	0	0	0
			2104	1333	360	400	11			
1	C	279	Total	C	N	O	S	0	0	0
			2115	1347	357	400	11			
1	D	283	Total	C	N	O	S	0	0	0
			2182	1391	369	410	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q06385
A	0	SER	-	EXPRESSION TAG	UNP Q06385
B	-1	GLY	-	EXPRESSION TAG	UNP Q06385
B	0	SER	-	EXPRESSION TAG	UNP Q06385
C	-1	GLY	-	EXPRESSION TAG	UNP Q06385
C	0	SER	-	EXPRESSION TAG	UNP Q06385
D	-1	GLY	-	EXPRESSION TAG	UNP Q06385
D	0	SER	-	EXPRESSION TAG	UNP Q06385

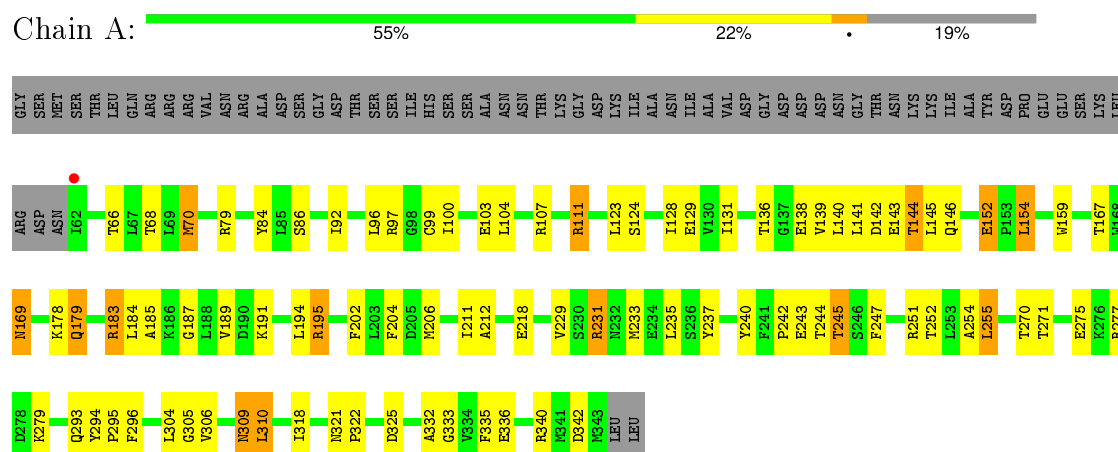
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		

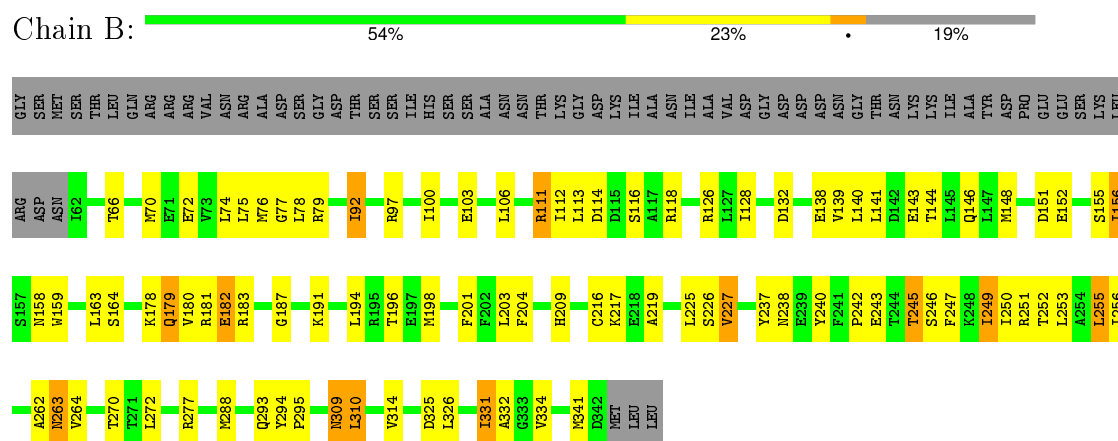
### 3 Residue-property plots

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

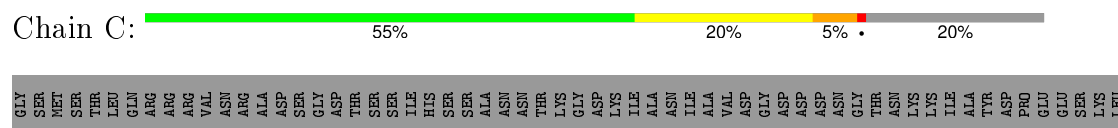
- Molecule 1: Vacuolar protein sorting-associated protein 74

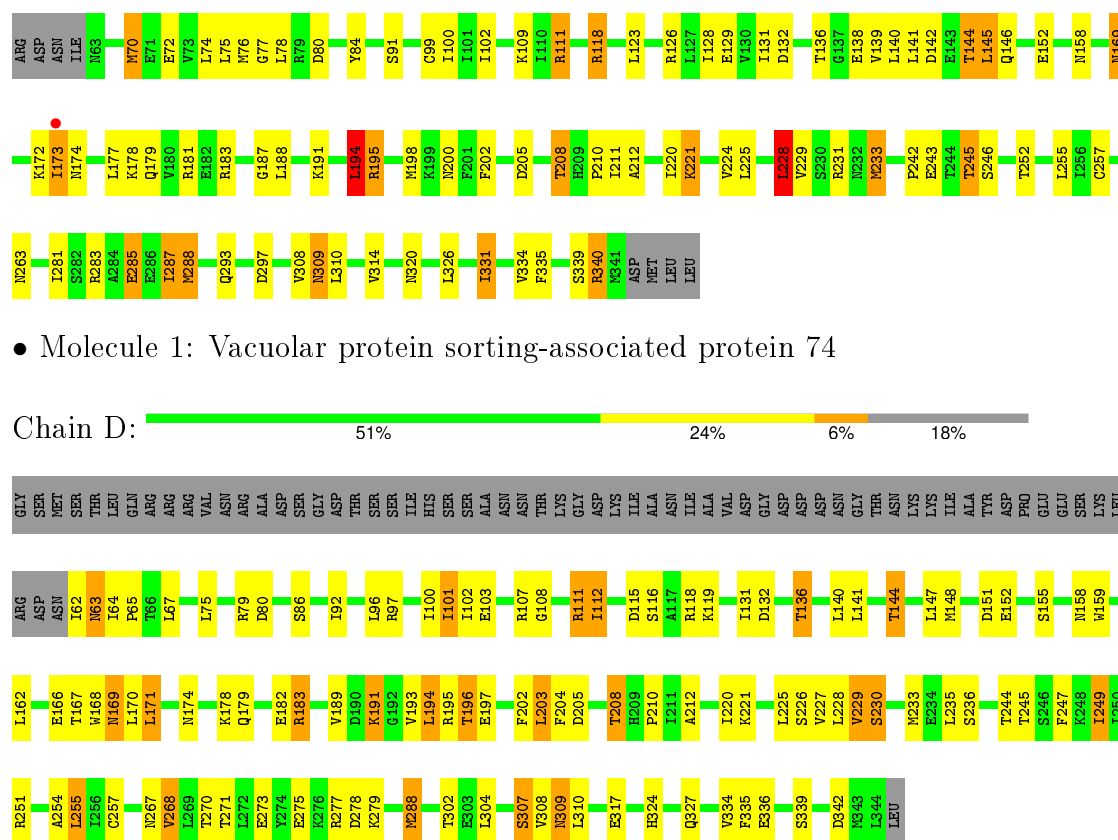


- Molecule 1: Vacuolar protein sorting-associated protein 74



- Molecule 1: Vacuolar protein sorting-associated protein 74





- Molecule 1: Vacuolar protein sorting-associated protein 74

Chain D: 51% 24% 6% 18%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.69Å 102.69Å 292.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.99 – 2.80 37.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.6 (37.99-2.80) 97.2 (37.99-2.81)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.233 , 0.302 0.234 , 0.298	Depositor DCC
$R_{free}$ test set	2198 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.4	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 43510 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.10 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1442e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [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	0.64	0/2164	0.77	0/2939
1	B	0.57	0/2135	0.71	0/2905
1	C	0.62	0/2146	0.74	2/2917 (0.1%)
1	D	0.64	0/2214	0.73	0/3003
All	All	0.62	0/8659	0.74	2/11764 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	LEU	CA-CB-CG	6.70	130.72	115.30
1	C	194	LEU	CA-CB-CG	5.21	127.28	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	2135	0	2068	69	0
1	B	2104	0	1994	61	0
1	C	2115	0	2044	77	0
1	D	2182	0	2149	95	0
2	A	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8541	0	8255	285	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 17.

All (285) 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:173:ILE:HA	1:C:174:ASN:ND2	1.39	1.33
1:A:231:ARG:HH21	1:A:231:ARG:HB3	1.15	1.05
1:D:221:LYS:HG3	1:D:268:VAL:HG22	1.34	1.02
1:D:168:TRP:CZ3	1:D:170:LEU:HD11	1.97	0.99
1:D:101:ILE:HD11	1:D:334:VAL:CG2	1.92	0.99
1:C:173:ILE:HA	1:C:174:ASN:HD22	1.17	0.98
1:D:111:ARG:HG2	1:D:131:ILE:HD11	1.45	0.97
1:C:169:ASN:ND2	1:C:172:LYS:H	1.63	0.97
1:C:173:ILE:CA	1:C:174:ASN:ND2	2.30	0.93
1:C:136:THR:HG22	1:C:142:ASP:OD1	1.68	0.92
1:D:65:PRO:HD3	1:D:245:THR:HG23	1.50	0.91
1:A:231:ARG:HH21	1:A:231:ARG:CB	1.82	0.91
1:A:242:PRO:O	1:A:245:THR:HG23	1.70	0.90
1:A:231:ARG:HB3	1:A:231:ARG:NH2	1.85	0.89
1:C:309:ASN:HD22	1:C:309:ASN:H	1.20	0.89
1:D:225:LEU:O	1:D:229:VAL:HG23	1.72	0.88
1:A:136:THR:HG22	1:A:142:ASP:OD1	1.73	0.87
1:B:114:ASP:HA	1:B:118:ARG:HH22	1.41	0.86
1:B:242:PRO:O	1:B:245:THR:HG23	1.76	0.85
1:D:101:ILE:HD11	1:D:334:VAL:HG22	1.58	0.84
1:D:65:PRO:HD3	1:D:245:THR:CG2	2.07	0.84
1:D:171:LEU:N	1:D:171:LEU:CD1	2.41	0.83
1:A:136:THR:HG21	1:A:141:LEU:HB2	1.61	0.81
1:D:221:LYS:HG3	1:D:268:VAL:CG2	2.10	0.80
1:C:80:ASP:O	1:C:211:ILE:HG12	1.81	0.80
1:C:136:THR:HG23	1:C:138:GLU:H	1.46	0.79
1:D:140:LEU:O	1:D:144:THR:HG22	1.83	0.79
1:D:171:LEU:HD13	1:D:171:LEU:H	1.48	0.79
1:C:242:PRO:HD2	1:C:245:THR:CG2	2.14	0.78
1:A:309:ASN:H	1:A:309:ASN:HD22	1.30	0.78
1:D:225:LEU:HD22	1:D:229:VAL:HG21	1.64	0.77
1:D:79:ARG:HG3	1:D:86:SER:OG	1.87	0.75
1:A:271:THR:HB	1:D:271:THR:HB	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:TRP:CH2	1:D:170:LEU:HD21	2.22	0.74
1:D:111:ARG:HG2	1:D:131:ILE:CD1	2.16	0.74
1:D:225:LEU:CD2	1:D:229:VAL:HG21	2.17	0.74
1:C:169:ASN:HD22	1:C:172:LYS:H	1.37	0.73
1:B:72:GLU:O	1:B:76:MET:HG2	1.90	0.72
1:A:70:MET:H	1:A:70:MET:HE2	1.53	0.72
1:A:111:ARG:HD2	1:A:131:ILE:HG21	1.71	0.72
1:D:178:LYS:O	1:D:183:ARG:NH1	2.23	0.71
1:B:201:PHE:HD1	1:B:204:PHE:CE1	2.09	0.71
1:D:162:LEU:HD23	1:D:167:THR:CG2	2.21	0.70
1:A:233:MET:H	1:A:309:ASN:HD21	1.37	0.70
1:D:64:ILE:HG23	1:D:65:PRO:HD2	1.73	0.70
1:A:202:PHE:O	1:B:181:ARG:HD2	1.92	0.69
1:A:279:LYS:HE3	1:A:304:LEU:O	1.92	0.69
1:A:143:GLU:OE2	1:A:183:ARG:NH2	2.25	0.69
1:C:100:ILE:HG21	1:C:144:THR:HG21	1.75	0.68
1:B:201:PHE:CD1	1:B:204:PHE:CE1	2.82	0.68
1:D:309:ASN:HD22	1:D:309:ASN:H	1.41	0.68
1:B:179:GLN:HB3	1:B:182:GLU:HG2	1.75	0.68
1:D:64:ILE:CG2	1:D:65:PRO:HD2	2.26	0.66
1:D:171:LEU:N	1:D:171:LEU:HD12	2.10	0.66
1:C:224:VAL:O	1:C:228:LEU:HD22	1.96	0.66
1:C:310:LEU:O	1:C:314:VAL:HG23	1.95	0.66
1:B:143:GLU:O	1:B:146:GLN:HB2	1.95	0.65
1:D:100:ILE:HG21	1:D:144:THR:HG21	1.78	0.65
1:B:148:MET:HG2	1:B:159:TRP:CZ2	2.32	0.65
1:C:111:ARG:HG3	1:C:326:LEU:HB3	1.80	0.64
1:C:140:LEU:O	1:C:144:THR:HG22	1.97	0.64
1:D:162:LEU:HD23	1:D:167:THR:HG21	1.79	0.63
1:A:70:MET:CE	1:A:70:MET:H	2.12	0.63
1:C:198:MET:CE	1:C:205:ASP:HB3	2.28	0.63
1:B:187:GLY:O	1:B:191:LYS:HG2	1.99	0.63
1:D:171:LEU:HD13	1:D:171:LEU:N	2.10	0.62
1:C:178:LYS:O	1:C:183:ARG:NH1	2.32	0.62
1:C:293:GLN:HE22	1:C:297:ASP:HB2	1.63	0.62
1:C:118:ARG:HB2	1:C:126:ARG:HG2	1.81	0.62
1:B:310:LEU:O	1:B:314:VAL:HG23	1.99	0.62
1:A:100:ILE:HG21	1:A:144:THR:HG21	1.80	0.62
1:A:233:MET:N	1:A:309:ASN:HD21	1.98	0.61
1:C:173:ILE:HA	1:C:174:ASN:CG	2.15	0.61
1:A:103:GLU:OE2	1:A:251:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASN:ND2	1:C:205:ASP:OD1	2.34	0.60
1:C:188:LEU:HB3	1:C:194:LEU:HD22	1.82	0.60
1:A:68:THR:HB	1:A:70:MET:CE	2.31	0.60
1:B:309:ASN:HD22	1:B:309:ASN:H	1.49	0.60
1:C:80:ASP:O	1:C:211:ILE:CG1	2.50	0.60
1:A:111:ARG:NH1	1:A:129:GLU:OE1	2.34	0.60
1:A:70:MET:HG3	1:A:184:LEU:HD21	1.82	0.60
1:A:68:THR:HB	1:A:70:MET:HE2	1.84	0.60
1:C:111:ARG:NH1	1:C:129:GLU:OE1	2.31	0.60
1:C:70:MET:HG3	1:C:99:CYS:HB2	1.83	0.60
1:D:101:ILE:CD1	1:D:334:VAL:CG2	2.76	0.59
1:B:219:ALA:CB	1:B:238:ASN:HD22	2.16	0.59
1:C:293:GLN:NE2	1:C:297:ASP:HB2	2.18	0.59
1:A:140:LEU:O	1:A:144:THR:HG22	2.03	0.58
1:D:204:PHE:C	1:D:204:PHE:CD2	2.73	0.58
1:B:97:ARG:HG3	1:B:164:SER:HB3	1.85	0.58
1:C:257:CYS:SG	1:C:288:MET:HG2	2.43	0.58
1:D:170:LEU:H	1:D:170:LEU:HD12	1.68	0.58
1:C:309:ASN:H	1:C:309:ASN:ND2	1.98	0.58
1:B:246:SER:O	1:B:247:PHE:HB2	2.03	0.58
1:C:136:THR:HG21	1:C:141:LEU:HB2	1.86	0.58
1:C:242:PRO:HD2	1:C:245:THR:HG22	1.85	0.58
1:D:336:GLU:O	1:D:339:SER:HB2	2.04	0.58
1:D:227:VAL:O	1:D:307:SER:HB3	2.04	0.58
1:B:249:ILE:HD11	1:B:314:VAL:HA	1.86	0.57
1:A:79:ARG:HG3	1:A:86:SER:OG	2.04	0.57
1:D:171:LEU:CD1	1:D:171:LEU:H	2.07	0.56
1:A:140:LEU:O	1:A:144:THR:CG2	2.53	0.56
1:C:187:GLY:O	1:C:191:LYS:HG2	2.04	0.56
1:B:151:ASP:OD1	1:B:152:GLU:N	2.39	0.56
1:B:144:THR:HG22	1:B:163:LEU:HD22	1.87	0.56
1:B:178:LYS:O	1:B:183:ARG:NH1	2.38	0.56
1:A:84:TYR:O	1:B:201:PHE:HB3	2.06	0.56
1:D:108:GLY:HA2	1:D:327:GLN:NE2	2.21	0.56
1:A:103:GLU:HG3	1:A:107:ARG:HE	1.71	0.55
1:C:181:ARG:NH2	1:D:205:ASP:OD1	2.37	0.55
1:C:140:LEU:O	1:C:144:THR:CG2	2.55	0.55
1:C:320:ASN:HD22	1:C:320:ASN:N	2.04	0.55
1:A:218:GLU:OE1	1:D:273:GLU:HA	2.07	0.55
1:B:118:ARG:HD2	1:B:126:ARG:HD3	1.89	0.55
1:B:112:ILE:CD1	1:B:326:LEU:HD22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:HG2	1:B:141:LEU:HD11	1.90	0.54
1:A:178:LYS:O	1:A:183:ARG:NH1	2.41	0.54
1:D:189:VAL:C	1:D:191:LYS:H	2.11	0.53
1:C:181:ARG:HD2	1:D:202:PHE:O	2.09	0.53
1:A:136:THR:HG23	1:A:138:GLU:H	1.72	0.53
1:A:97:ARG:HA	1:A:100:ILE:HD12	1.91	0.53
1:C:169:ASN:ND2	1:C:172:LYS:N	2.46	0.53
1:A:321:ASN:N	1:A:322:PRO:HD3	2.24	0.52
1:A:123:LEU:HB3	1:A:333:GLY:HA2	1.92	0.52
1:D:107:ARG:HD3	1:D:136:THR:HG21	1.91	0.52
1:C:140:LEU:HD22	1:C:177:LEU:HD13	1.92	0.52
1:C:340:ARG:HH11	1:C:340:ARG:HG2	1.74	0.52
1:B:128:ILE:HD13	1:B:156:ILE:HG22	1.91	0.52
1:B:74:LEU:C	1:B:74:LEU:HD23	2.30	0.52
1:A:247:PHE:O	1:A:251:ARG:HG3	2.09	0.52
1:D:225:LEU:C	1:D:229:VAL:HG23	2.30	0.52
1:D:169:ASN:OD1	1:D:169:ASN:C	2.48	0.52
1:C:72:GLU:O	1:C:76:MET:HG2	2.09	0.52
1:D:225:LEU:CA	1:D:229:VAL:HG23	2.39	0.51
1:B:79:ARG:HH21	1:D:166:GLU:HG2	1.75	0.51
1:B:294:TYR:CD1	1:B:295:PRO:HA	2.45	0.51
1:A:231:ARG:HH21	1:A:231:ARG:CG	2.22	0.51
1:D:148:MET:HG2	1:D:159:TRP:CZ2	2.45	0.51
1:D:168:TRP:HZ3	1:D:170:LEU:HD11	1.68	0.51
1:B:219:ALA:CB	1:B:238:ASN:ND2	2.73	0.51
1:D:257:CYS:SG	1:D:288:MET:HG2	2.51	0.51
1:A:136:THR:HG22	1:A:142:ASP:CG	2.30	0.51
1:B:139:VAL:O	1:B:143:GLU:HG3	2.11	0.51
1:D:204:PHE:C	1:D:204:PHE:HD2	2.14	0.51
1:D:233:MET:N	1:D:309:ASN:HD21	2.09	0.51
1:C:84:TYR:CG	1:D:202:PHE:HB2	2.46	0.50
1:D:62:ILE:O	1:D:63:ASN:CB	2.58	0.50
1:D:324:HIS:HD2	1:D:327:GLN:OE1	1.95	0.50
1:D:103:GLU:CG	1:D:141:LEU:HD11	2.42	0.50
1:A:187:GLY:O	1:A:191:LYS:HG3	2.11	0.50
1:D:225:LEU:HA	1:D:229:VAL:HG23	1.93	0.49
1:C:198:MET:HE1	1:C:205:ASP:HB3	1.93	0.49
1:D:169:ASN:OD1	1:D:169:ASN:O	2.30	0.49
1:B:216:CYS:HB2	1:B:240:TYR:CE1	2.48	0.49
1:D:103:GLU:HG2	1:D:141:LEU:HD11	1.94	0.49
1:A:96:LEU:O	1:A:99:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ARG:HG3	1:B:326:LEU:HB3	1.94	0.49
1:C:242:PRO:O	1:C:245:THR:HG23	2.13	0.49
1:C:281:ILE:O	1:C:285:GLU:HG2	2.13	0.49
1:A:111:ARG:HD2	1:A:131:ILE:CG2	2.40	0.49
1:B:179:GLN:O	1:B:183:ARG:HD3	2.12	0.48
1:A:128:ILE:HD11	1:A:159:TRP:CD1	2.47	0.48
1:D:169:ASN:CG	1:D:169:ASN:O	2.52	0.48
1:C:195:ARG:HG2	1:C:212:ALA:HB2	1.95	0.48
1:D:225:LEU:HA	1:D:229:VAL:CG2	2.44	0.48
1:D:67:LEU:HD23	1:D:191:LYS:HD3	1.95	0.48
1:A:254:ALA:HA	1:A:335:PHE:CZ	2.49	0.48
1:C:198:MET:HE3	1:C:205:ASP:HB3	1.96	0.47
1:D:226:SER:O	1:D:230:SER:HB2	2.14	0.47
1:B:144:THR:HG22	1:B:163:LEU:CD2	2.45	0.47
1:B:237:TYR:CD2	1:B:243:GLU:HA	2.50	0.47
1:B:76:MET:HB2	1:B:264:VAL:HG21	1.96	0.47
1:D:270:THR:HA	1:D:277:ARG:HD3	1.94	0.47
1:A:279:LYS:HD3	1:A:306:VAL:HG21	1.97	0.47
1:A:124:SER:HB3	1:A:336:GLU:HG2	1.97	0.47
1:C:169:ASN:HD22	1:C:169:ASN:C	2.18	0.47
1:D:111:ARG:CG	1:D:131:ILE:HD11	2.31	0.47
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.63	0.47
1:C:188:LEU:CB	1:C:194:LEU:HD22	2.45	0.47
1:D:108:GLY:HA2	1:D:327:GLN:HE21	1.79	0.47
1:A:202:PHE:CZ	1:B:77:GLY:HA3	2.50	0.46
1:D:193:VAL:HG12	1:D:194:LEU:HD13	1.97	0.46
1:C:283:ARG:O	1:C:287:ILE:HG23	2.13	0.46
1:A:242:PRO:HD2	1:A:245:THR:CG2	2.46	0.46
1:B:242:PRO:HD2	1:B:245:THR:CG2	2.46	0.46
1:C:78:LEU:CD2	1:D:202:PHE:CD2	2.98	0.46
1:D:254:ALA:HA	1:D:335:PHE:CE2	2.51	0.46
1:D:103:GLU:OE2	1:D:251:ARG:NH2	2.48	0.46
1:C:233:MET:H	1:C:309:ASN:HD21	1.62	0.46
1:C:123:LEU:HA	1:C:126:ARG:HD2	1.98	0.46
1:B:249:ILE:O	1:B:253:LEU:HG	2.16	0.46
1:C:288:MET:HE2	1:C:288:MET:HB3	1.91	0.46
1:C:208:THR:HG22	1:C:210:PRO:HD3	1.97	0.46
1:C:331:ILE:HD12	1:C:335:PHE:CE2	2.51	0.46
1:B:126:ARG:O	1:B:155:SER:HA	2.16	0.46
1:D:195:ARG:HG3	1:D:212:ALA:HB2	1.98	0.46
1:B:111:ARG:HG2	1:B:112:ILE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASP:OD1	1:D:152:GLU:N	2.48	0.45
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.77	0.45
1:A:237:TYR:CD2	1:A:243:GLU:HA	2.52	0.45
1:B:139:VAL:HG12	1:B:183:ARG:HH21	1.82	0.45
1:C:102:ILE:HG13	1:C:334:VAL:HG11	1.99	0.45
1:D:111:ARG:HG2	1:D:131:ILE:CG1	2.46	0.45
1:C:233:MET:HE1	1:C:310:LEU:HD12	1.99	0.45
1:D:208:THR:HG22	1:D:210:PRO:HD3	1.99	0.45
1:A:143:GLU:O	1:A:146:GLN:HB2	2.17	0.45
1:C:70:MET:H	1:C:70:MET:CE	2.29	0.45
1:A:185:ALA:O	1:A:189:VAL:HG23	2.17	0.45
1:A:179:GLN:O	1:A:183:ARG:HD3	2.17	0.45
1:A:277:ARG:HD2	1:D:80:ASP:OD2	2.17	0.45
1:B:272:LEU:O	1:B:277:ARG:NH2	2.50	0.45
1:B:143:GLU:OE2	1:B:183:ARG:NH2	2.50	0.45
1:D:155:SER:OG	1:D:158:ASN:HB2	2.17	0.45
1:C:179:GLN:O	1:C:183:ARG:HD3	2.17	0.44
1:B:97:ARG:HA	1:B:100:ILE:HD12	2.00	0.44
1:A:152:GLU:O	1:A:154:LEU:HD13	2.18	0.44
1:C:84:TYR:CD2	1:D:202:PHE:HB2	2.53	0.44
1:C:136:THR:HG22	1:C:142:ASP:CG	2.36	0.44
1:B:309:ASN:HD22	1:B:309:ASN:N	2.13	0.44
1:A:204:PHE:HE1	1:A:206:MET:HE2	1.82	0.44
1:A:169:ASN:C	1:A:169:ASN:HD22	2.21	0.44
1:A:296:PHE:HE2	1:A:332:ALA:HB2	1.82	0.44
1:B:194:LEU:HD13	1:B:209:HIS:HB3	1.98	0.44
1:D:115:ASP:O	1:D:118:ARG:HG2	2.17	0.44
1:B:155:SER:OG	1:B:158:ASN:HB2	2.18	0.44
1:A:242:PRO:HD2	1:A:245:THR:HG22	2.00	0.44
1:C:78:LEU:HD23	1:D:202:PHE:CD2	2.52	0.44
1:A:252:THR:O	1:A:255:LEU:HB3	2.18	0.44
1:D:102:ILE:HG13	1:D:334:VAL:HG11	1.99	0.44
1:C:136:THR:HG23	1:C:138:GLU:N	2.25	0.43
1:A:185:ALA:HB2	1:B:203:LEU:HD22	1.99	0.43
1:D:220:ILE:HG23	1:D:255:LEU:HD11	2.00	0.43
1:C:84:TYR:N	1:C:84:TYR:CD1	2.86	0.43
1:A:294:TYR:HA	1:A:295:PRO:C	2.37	0.43
1:D:275:GLU:O	1:D:279:LYS:HB2	2.19	0.43
1:C:309:ASN:N	1:C:309:ASN:ND2	2.64	0.43
1:B:249:ILE:O	1:B:250:ILE:C	2.57	0.43
1:C:221:LYS:O	1:C:225:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG21	1:A:141:LEU:CB	2.42	0.43
1:B:118:ARG:HB2	1:B:126:ARG:HG2	2.00	0.43
1:C:340:ARG:NH1	1:C:340:ARG:HG2	2.32	0.43
1:B:156:ILE:HD13	1:B:334:VAL:HG22	1.99	0.43
1:B:227:VAL:O	1:B:227:VAL:HG23	2.18	0.43
1:B:201:PHE:CD1	1:B:204:PHE:HE1	2.32	0.43
1:C:70:MET:H	1:C:70:MET:HE2	1.83	0.43
1:D:247:PHE:O	1:D:251:ARG:HG3	2.19	0.43
1:C:70:MET:HE2	1:C:99:CYS:HB3	1.99	0.43
1:C:145:LEU:HD23	1:C:145:LEU:HA	1.79	0.43
1:D:107:ARG:HH11	1:D:136:THR:HG21	1.83	0.43
1:D:309:ASN:N	1:D:309:ASN:HD22	2.12	0.43
1:C:78:LEU:HD21	1:D:202:PHE:HD2	1.83	0.43
1:D:249:ILE:HG12	1:D:317:GLU:OE2	2.19	0.43
1:A:195:ARG:HG2	1:A:212:ALA:HB2	2.00	0.43
1:D:111:ARG:HD2	1:D:112:ILE:O	2.18	0.42
1:B:331:ILE:HG13	1:B:332:ALA:N	2.34	0.42
1:A:309:ASN:H	1:A:309:ASN:ND2	2.07	0.42
1:A:104:LEU:HA	1:A:104:LEU:HD23	1.83	0.42
1:A:194:LEU:HD23	1:A:211:ILE:HA	2.00	0.42
1:B:262:ALA:O	1:B:263:ASN:HB2	2.19	0.42
1:A:231:ARG:HD2	1:A:305:GLY:O	2.19	0.42
1:A:242:PRO:O	1:A:245:THR:CG2	2.56	0.42
1:D:97:ARG:HD2	1:D:97:ARG:N	2.34	0.42
1:C:320:ASN:ND2	1:C:320:ASN:N	2.67	0.42
1:D:249:ILE:HG12	1:D:249:ILE:H	1.70	0.42
1:C:202:PHE:CG	1:D:86:SER:HB2	2.55	0.42
1:A:233:MET:CE	1:A:310:LEU:HD23	2.50	0.42
1:C:288:MET:HE2	1:C:339:SER:HB3	2.01	0.42
1:C:77:GLY:HA3	1:D:202:PHE:CZ	2.55	0.41
1:A:66:THR:OG1	1:A:240:TYR:HA	2.21	0.41
1:C:220:ILE:HG23	1:C:255:LEU:HD21	2.02	0.41
1:D:196:THR:HA	1:D:208:THR:O	2.21	0.41
1:C:132:ASP:OD1	1:C:132:ASP:C	2.58	0.41
1:B:140:LEU:HD11	1:B:180:VAL:HG13	2.02	0.41
1:B:112:ILE:HD11	1:B:326:LEU:HD22	2.02	0.41
1:B:294:TYR:HA	1:B:295:PRO:C	2.40	0.41
1:C:233:MET:HB3	1:C:233:MET:HE3	1.96	0.41
1:D:197:GLU:O	1:D:208:THR:HB	2.20	0.41
1:B:92:ILE:HG12	1:B:262:ALA:HB1	2.01	0.41
1:A:294:TYR:CG	1:A:295:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:HD2	1:B:251:ARG:HH11	1.75	0.41
1:D:179:GLN:HB2	1:D:183:ARG:HH11	1.85	0.40
1:D:92:ILE:O	1:D:96:LEU:HG	2.21	0.40
1:D:140:LEU:O	1:D:144:THR:CG2	2.62	0.40
1:D:225:LEU:HD23	1:D:229:VAL:HG21	2.01	0.40
1:B:252:THR:O	1:B:255:LEU:HB3	2.22	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	280/347 (81%)	260 (93%)	20 (7%)	0	100	100
1	B	279/347 (80%)	261 (94%)	17 (6%)	1 (0%)	39	74
1	C	277/347 (80%)	262 (95%)	15 (5%)	0	100	100
1	D	281/347 (81%)	259 (92%)	20 (7%)	2 (1%)	26	62
All	All	1117/1388 (80%)	1042 (93%)	72 (6%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	ASN
1	B	270	THR
1	D	307	SER

### 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	222/310 (72%)	195 (88%)	27 (12%)	6	18
1	B	212/310 (68%)	180 (85%)	32 (15%)	3	10
1	C	218/310 (70%)	181 (83%)	37 (17%)	2	7
1	D	231/310 (74%)	193 (84%)	38 (16%)	3	8
All	All	883/1240 (71%)	749 (85%)	134 (15%)	3	10

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	MET
1	A	92	ILE
1	A	111	ARG
1	A	139	VAL
1	A	144	THR
1	A	152	GLU
1	A	154	LEU
1	A	167	THR
1	A	169	ASN
1	A	179	GLN
1	A	183	ARG
1	A	195	ARG
1	A	229	VAL
1	A	231	ARG
1	A	235	LEU
1	A	244	THR
1	A	245	THR
1	A	255	LEU
1	A	270	THR
1	A	275	GLU
1	A	293	GLN
1	A	309	ASN
1	A	310	LEU
1	A	318	ILE
1	A	325	ASP
1	A	340	ARG
1	A	342	ASP
1	B	66	THR
1	B	70	MET
1	B	75	LEU

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Mol	Chain	Res	Type
1	B	78	LEU
1	B	92	ILE
1	B	106	LEU
1	B	111	ARG
1	B	113	LEU
1	B	116	SER
1	B	132	ASP
1	B	138	GLU
1	B	156	ILE
1	B	179	GLN
1	B	182	GLU
1	B	196	THR
1	B	198	MET
1	B	217	LYS
1	B	225	LEU
1	B	226	SER
1	B	227	VAL
1	B	245	THR
1	B	249	ILE
1	B	255	LEU
1	B	256	ILE
1	B	263	ASN
1	B	288	MET
1	B	293	GLN
1	B	309	ASN
1	B	310	LEU
1	B	325	ASP
1	B	331	ILE
1	B	341	MET
1	C	70	MET
1	C	74	LEU
1	C	75	LEU
1	C	91	SER
1	C	109	LYS
1	C	111	ARG
1	C	118	ARG
1	C	128	ILE
1	C	131	ILE
1	C	139	VAL
1	C	144	THR
1	C	145	LEU
1	C	146	GLN

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Mol	Chain	Res	Type
1	C	152	GLU
1	C	158	ASN
1	C	169	ASN
1	C	173	ILE
1	C	194	LEU
1	C	195	ARG
1	C	208	THR
1	C	221	LYS
1	C	228	LEU
1	C	229	VAL
1	C	231	ARG
1	C	233	MET
1	C	243	GLU
1	C	245	THR
1	C	246	SER
1	C	252	THR
1	C	263	ASN
1	C	285	GLU
1	C	287	ILE
1	C	288	MET
1	C	308	VAL
1	C	309	ASN
1	C	331	ILE
1	C	340	ARG
1	D	75	LEU
1	D	101	ILE
1	D	111	ARG
1	D	112	ILE
1	D	116	SER
1	D	119	LYS
1	D	132	ASP
1	D	136	THR
1	D	144	THR
1	D	147	LEU
1	D	169	ASN
1	D	171	LEU
1	D	174	ASN
1	D	182	GLU
1	D	183	ARG
1	D	191	LYS
1	D	194	LEU
1	D	196	THR

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Mol	Chain	Res	Type
1	D	203	LEU
1	D	208	THR
1	D	228	LEU
1	D	229	VAL
1	D	230	SER
1	D	235	LEU
1	D	236	SER
1	D	244	THR
1	D	249	ILE
1	D	255	LEU
1	D	267	ASN
1	D	268	VAL
1	D	278	ASP
1	D	288	MET
1	D	302	THR
1	D	304	LEU
1	D	308	VAL
1	D	309	ASN
1	D	310	LEU
1	D	342	ASP

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	169	ASN
1	A	176	GLN
1	A	290	GLN
1	A	309	ASN
1	B	176	GLN
1	B	267	ASN
1	B	293	GLN
1	B	309	ASN
1	B	320	ASN
1	C	158	ASN
1	C	169	ASN
1	C	174	ASN
1	C	176	GLN
1	C	200	ASN
1	C	293	GLN
1	C	309	ASN
1	C	320	ASN
1	D	150	ASN

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Mol	Chain	Res	Type
1	D	176	GLN
1	D	179	GLN
1	D	209	HIS
1	D	309	ASN
1	D	324	HIS
1	D	327	GLN

### 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	282/347 (81%)	-0.49	1 (0%) 93 90	28, 43, 59, 66	0
1	B	281/347 (80%)	-0.41	0 100 100	29, 54, 65, 68	0
1	C	279/347 (80%)	-0.48	1 (0%) 93 90	33, 47, 60, 68	0
1	D	283/347 (81%)	-0.40	0 100 100	31, 46, 61, 68	0
All	All	1125/1388 (81%)	-0.45	2 (0%) 95 94	28, 47, 63, 68	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	ILE	5.9
1	A	62	ILE	3.5

### 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.