



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:50 am GMT

PDB ID : 2AJT  
Title : Crystal structure of L-Arabinose Isomerase from E.coli  
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Deposited on : 2005-08-02  
Resolution : 2.60 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

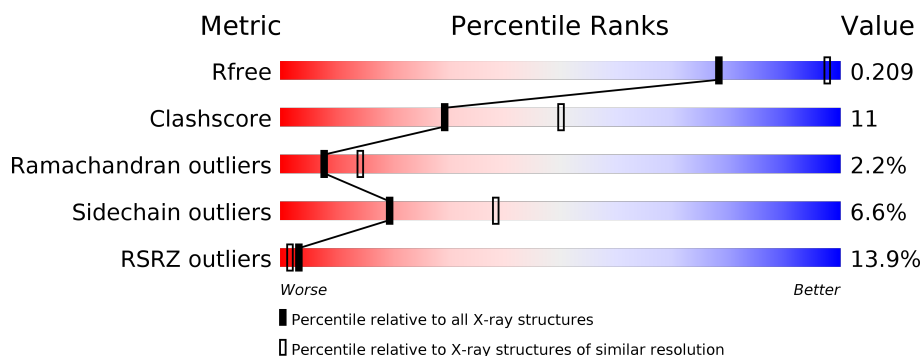
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	500	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	500	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	500	<div> <div>25%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11483 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3833	2434	663	712	24			
1	B	498	Total	C	N	O	S	0	1	0
			3875	2461	670	719	25			
1	C	498	Total	C	N	O	S	0	0	0
			3687	2335	635	693	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	PRO	ARG	SEE REMARK 999	UNP P08202
B	72	PRO	ARG	SEE REMARK 999	UNP P08202
C	72	PRO	ARG	SEE REMARK 999	UNP P08202

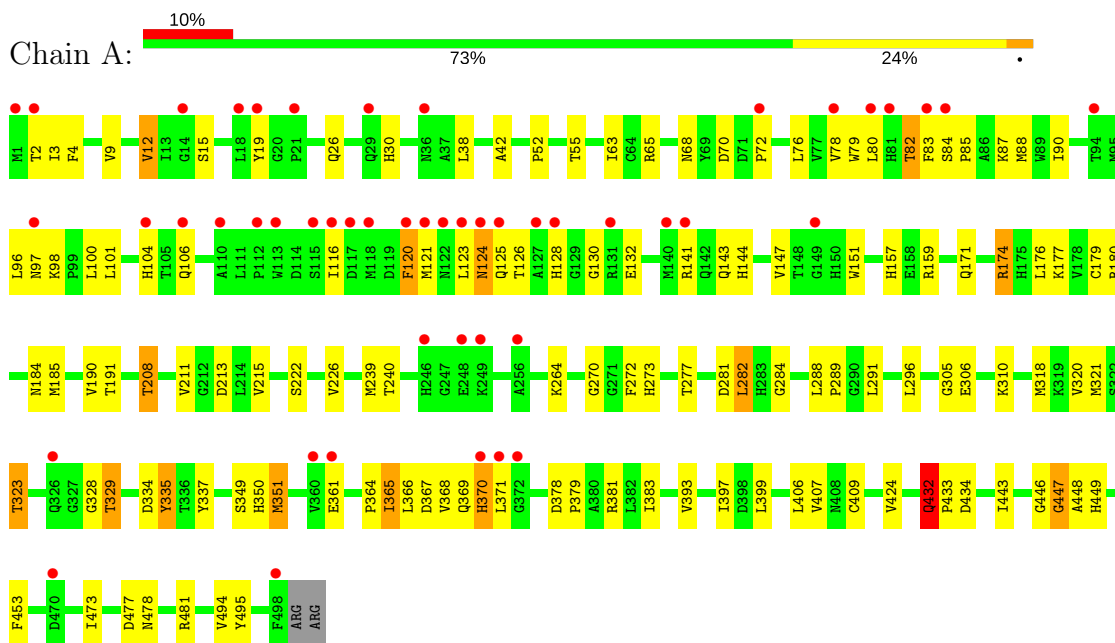
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	33	Total	O	0	0
			33	33		
2	C	15	Total	O	0	0
			15	15		

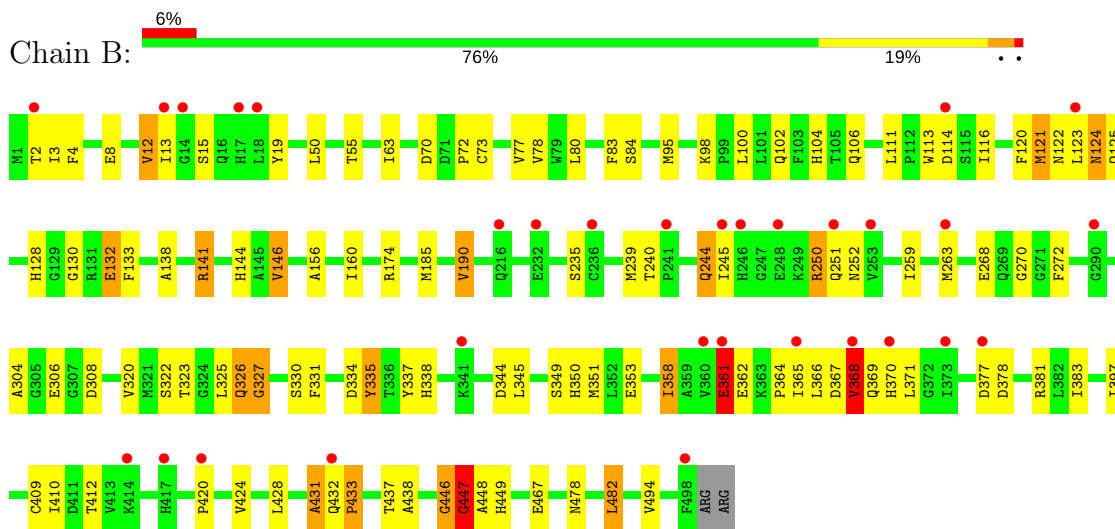
### 3 Residue-property plots

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.

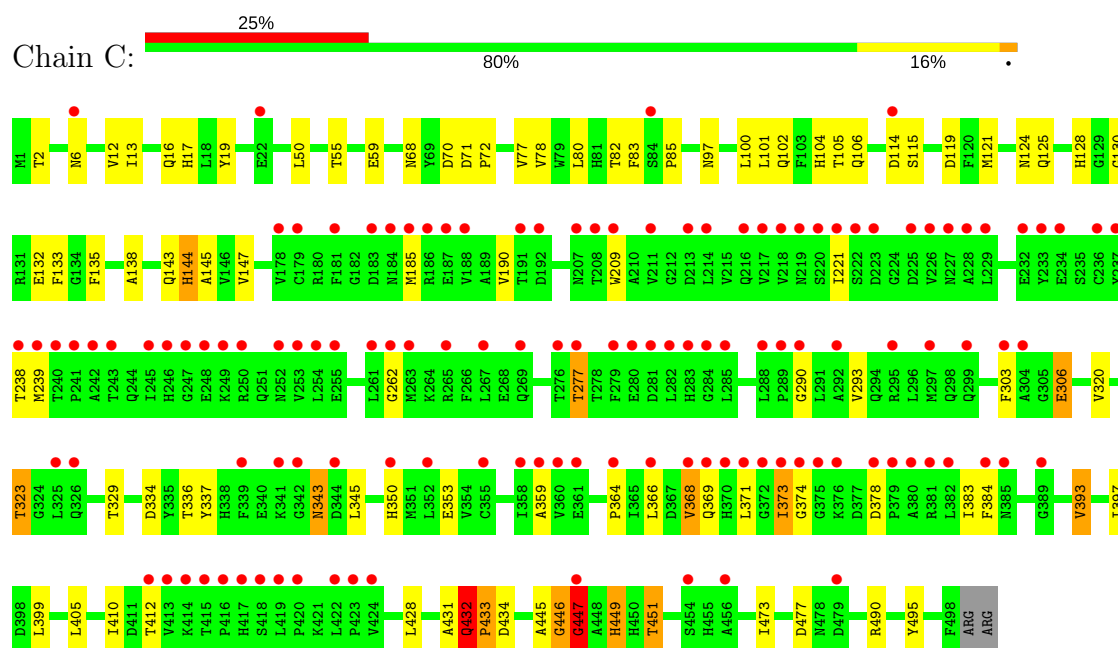
- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.54Å 116.54Å 214.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 2.60 19.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.5 (19.84-2.60) 84.5 (19.84-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	71.36 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217 , 0.278 0.224 , 0.209	Depositor DCC
$R_{free}$ test set	2204 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 67.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.49	0/3927	0.66	1/5351 (0.0%)
1	B	0.49	1/3976 (0.0%)	0.65	0/5411
1	C	0.44	0/3776	0.60	1/5157 (0.0%)
All	All	0.47	1/11679 (0.0%)	0.64	2/15919 (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	B	0	6
1	C	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	GLU	CB-CG	5.09	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	GLN	C-N-CD	7.85	144.88	128.40
1	C	447	GLY	N-CA-C	7.12	130.89	113.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	361	GLU	Peptide
1	B	362	GLU	Peptide
1	B	368	VAL	Peptide
1	B	431	ALA	Peptide
1	B	446	GLY	Peptide
1	B	447	GLY	Peptide
1	C	432	GLN	Peptide
1	C	447	GLY	Peptide

## 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	3833	0	3662	100	0
1	B	3875	0	3727	93	0
1	C	3687	0	3407	70	0
2	A	40	0	0	0	0
2	B	33	0	0	0	0
2	C	15	0	0	1	0
All	All	11483	0	10796	240	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 11.

All (240) 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:190:VAL:HG11	1:B:448:ALA:HB2	1.38	1.04
1:A:190:VAL:HG11	1:A:448:ALA:HB2	1.41	1.02
1:B:337:TYR:H	1:C:106:GLN:HE22	1.10	0.98
1:A:432:GLN:O	1:A:433:PRO:C	2.04	0.88
1:B:364:PRO:HD2	1:B:383:ILE:O	1.75	0.87
1:B:397:ILE:HG21	1:B:447:GLY:HA2	1.57	0.86
1:A:369:GLN:O	1:A:370:HIS:C	2.13	0.82
1:B:70:ASP:OD1	1:B:72:PRO:HD2	1.81	0.80
1:A:369:GLN:CB	1:A:379:PRO:HD2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLN:HE21	1:A:478:ASN:CG	1.85	0.80
1:A:80:LEU:O	1:A:126:THR:HG22	1.81	0.79
1:A:449:HIS:HB2	1:B:128:HIS:HB2	1.63	0.79
1:B:369:GLN:CB	1:B:378:ASP:HB3	2.13	0.79
1:C:70:ASP:OD1	1:C:72:PRO:HD2	1.83	0.78
1:A:432:GLN:HE21	1:A:478:ASN:ND2	1.82	0.77
1:B:368:VAL:HG12	1:B:368:VAL:O	1.85	0.76
1:B:367:ASP:O	1:B:368:VAL:C	2.23	0.76
1:B:239:MET:SD	1:B:365:ILE:HG21	2.26	0.75
1:A:397:ILE:HG21	1:A:447:GLY:HA2	1.68	0.75
1:A:369:GLN:O	1:A:371:LEU:N	2.21	0.73
1:B:369:GLN:O	1:B:370:HIS:C	2.27	0.72
1:C:433:PRO:HD3	1:C:477:ASP:O	1.90	0.72
1:C:78:VAL:HG13	1:C:100:LEU:HD11	1.71	0.71
1:B:12:VAL:HG23	1:B:78:VAL:HG12	1.73	0.70
1:B:2:THR:HG23	1:B:323:THR:HG21	1.73	0.70
1:C:366:LEU:CB	1:C:368:VAL:HG23	2.21	0.70
1:A:409:CYS:O	1:A:432:GLN:HB2	1.91	0.70
1:B:73:CYS:O	1:B:98:LYS:HE2	1.92	0.69
1:B:2:THR:HG22	1:B:4:PHE:H	1.57	0.69
1:A:368:VAL:HG12	1:A:368:VAL:O	1.92	0.68
1:B:78:VAL:HG13	1:B:100:LEU:CD1	2.24	0.68
1:C:433:PRO:HD3	1:C:477:ASP:C	2.14	0.68
1:C:80:LEU:HD12	1:C:130:GLY:HA2	1.75	0.67
1:A:337:TYR:H	1:B:106:GLN:HE22	1.41	0.67
1:B:80:LEU:HD12	1:B:130:GLY:HA2	1.76	0.66
1:C:393:VAL:HG22	1:C:451:THR:OG1	1.95	0.66
1:A:19:TYR:CE1	1:A:82:THR:HB	2.32	0.65
1:B:367:ASP:O	1:B:369:GLN:CA	2.44	0.65
1:B:494:VAL:HG21	1:C:495:TYR:HA	1.79	0.65
1:A:82:THR:O	1:A:125:GLN:CG	2.46	0.64
1:A:432:GLN:O	1:A:433:PRO:O	2.16	0.64
1:B:330:SER:CB	1:B:358:ILE:HD11	2.27	0.64
1:C:373:ILE:HG22	1:C:374:GLY:H	1.62	0.63
1:A:180:ARG:HD3	1:A:208:THR:HG22	1.80	0.63
1:A:70:ASP:OD1	1:A:72:PRO:HD2	1.98	0.62
1:C:397:ILE:HG21	1:C:447:GLY:HA2	1.81	0.62
1:A:368:VAL:CG1	1:A:368:VAL:O	2.46	0.62
1:B:19:TYR:OH	1:B:125:GLN:NE2	2.27	0.62
1:B:78:VAL:HG13	1:B:100:LEU:HD11	1.81	0.62
1:A:190:VAL:HG23	1:B:132:GLU:OE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:VAL:HG13	1:C:135:PHE:CG	2.36	0.61
1:B:125:GLN:HB2	1:B:128:HIS:CE1	2.36	0.61
1:B:369:GLN:O	1:B:371:LEU:N	2.34	0.61
1:A:19:TYR:HE1	1:A:82:THR:HB	1.64	0.60
1:C:71:ASP:OD1	1:C:72:PRO:HD3	2.01	0.60
1:B:12:VAL:CG2	1:B:78:VAL:HG12	2.31	0.60
1:B:100:LEU:HD23	1:B:144:HIS:CD2	2.37	0.60
1:B:335:TYR:CE1	1:C:121:MET:HG2	2.37	0.60
1:C:71:ASP:CG	1:C:72:PRO:HD3	2.21	0.59
1:B:239:MET:SD	1:B:365:ILE:CG2	2.90	0.59
1:C:68:ASN:HD21	1:C:97:ASN:H	1.50	0.59
1:B:83:PHE:H	1:B:125:GLN:HE21	1.49	0.59
1:C:125:GLN:HB2	1:C:128:HIS:NE2	2.17	0.58
1:C:221:ILE:HD11	1:C:262:GLY:HA2	1.84	0.58
1:B:2:THR:CG2	1:B:323:THR:HG21	2.32	0.58
1:B:368:VAL:CG1	1:B:368:VAL:O	2.49	0.58
1:B:330:SER:HB3	1:B:358:ILE:HD11	1.84	0.58
1:A:443:ILE:HG21	1:B:146:VAL:HG11	1.86	0.57
1:A:55:THR:O	1:A:88:MET:SD	2.62	0.57
1:A:367:ASP:O	1:A:368:VAL:C	2.43	0.57
1:B:156:ALA:O	1:B:160:ILE:HG12	2.05	0.56
1:B:111:LEU:HD23	1:B:113:TRP:CZ3	2.40	0.56
1:B:367:ASP:O	1:B:369:GLN:N	2.39	0.56
1:B:409:CYS:O	1:B:432:GLN:HB2	2.06	0.56
1:A:82:THR:O	1:A:125:GLN:HG3	2.05	0.56
1:A:15:SER:CB	1:A:82:THR:HG1	2.18	0.55
1:A:239:MET:SD	1:A:365:ILE:HG21	2.47	0.55
1:B:326:GLN:O	1:B:327:GLY:O	2.25	0.55
1:C:102:GLN:NE2	1:C:104:HIS:HD2	2.05	0.55
1:A:432:GLN:HG3	1:A:478:ASN:ND2	2.22	0.54
1:B:410:ILE:HG22	1:B:431:ALA:HA	1.90	0.54
1:B:240:THR:HG21	1:B:366:LEU:HD13	1.89	0.54
1:B:433:PRO:HD2	1:B:438:ALA:HB2	1.90	0.54
1:A:270:GLY:HA3	1:A:272:PHE:CE2	2.42	0.53
1:B:102:GLN:NE2	1:B:104:HIS:HD2	2.07	0.53
1:B:397:ILE:HG21	1:B:447:GLY:CA	2.34	0.53
1:A:399:LEU:O	1:B:141:ARG:NH2	2.42	0.53
1:A:432:GLN:NE2	1:A:478:ASN:OD1	2.41	0.53
1:B:337:TYR:OH	1:C:104:HIS:HE1	1.92	0.53
1:A:239:MET:SD	1:A:365:ILE:CG2	2.98	0.52
1:B:111:LEU:HD11	1:B:116:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:VAL:HG22	1:C:132:GLU:OE2	2.09	0.52
1:A:184:ASN:HD21	1:A:191:THR:C	2.13	0.52
1:B:270:GLY:HA3	1:B:272:PHE:CE2	2.44	0.52
1:B:446:GLY:HA2	1:C:138:ALA:CB	2.39	0.52
1:A:120:PHE:C	1:A:120:PHE:CD2	2.82	0.52
1:B:437:THR:HG23	1:B:482:LEU:HD12	1.92	0.52
1:B:349:SER:OG	1:B:350:HIS:N	2.44	0.51
1:A:495:TYR:CZ	1:C:490:ARG:HG2	2.46	0.51
1:A:2:THR:HG22	1:A:4:PHE:H	1.75	0.51
1:B:80:LEU:CD1	1:B:130:GLY:HA2	2.40	0.51
1:B:80:LEU:HD11	1:B:133:PHE:CB	2.40	0.51
1:B:369:GLN:CB	1:B:378:ASP:CB	2.87	0.51
1:C:143:GLN:O	1:C:144:HIS:C	2.48	0.51
1:A:82:THR:O	1:A:125:GLN:HG2	2.11	0.51
1:A:320:VAL:O	1:A:323:THR:OG1	2.28	0.51
1:B:446:GLY:HA2	1:C:138:ALA:HB3	1.93	0.51
1:C:102:GLN:NE2	1:C:104:HIS:CD2	2.78	0.51
1:A:19:TYR:HE1	1:A:82:THR:CB	2.24	0.50
1:A:432:GLN:HB3	1:A:477:ASP:HA	1.93	0.50
1:B:432:GLN:O	1:B:478:ASN:ND2	2.45	0.50
1:C:55:THR:HB	1:C:59:GLU:OE1	2.10	0.50
1:B:366:LEU:HD21	1:B:368:VAL:HB	1.93	0.50
1:C:17:HIS:HB3	1:C:55:THR:HG22	1.94	0.50
1:C:68:ASN:HD21	1:C:97:ASN:N	2.09	0.50
1:A:78:VAL:HG12	1:A:100:LEU:HD11	1.94	0.50
1:B:3:ILE:HD11	1:B:320:VAL:HG13	1.93	0.50
1:C:68:ASN:ND2	1:C:97:ASN:H	2.10	0.50
1:A:116:ILE:HG22	1:A:120:PHE:CD1	2.47	0.49
1:A:335:TYR:HE1	1:A:350:HIS:HA	1.77	0.49
1:C:405:LEU:HD23	1:C:473:ILE:CD1	2.42	0.49
1:A:329:THR:HA	1:A:453:PHE:O	2.12	0.49
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.95	0.49
1:A:449:HIS:CB	1:B:128:HIS:HB2	2.37	0.49
1:C:80:LEU:HD11	1:C:133:PHE:CB	2.42	0.49
1:B:367:ASP:O	1:B:369:GLN:CB	2.61	0.49
1:B:185:MET:HB2	1:B:306:GLU:HB3	1.94	0.49
1:C:373:ILE:HG22	1:C:374:GLY:N	2.28	0.48
1:A:369:GLN:CB	1:A:378:ASP:HB3	2.44	0.48
1:A:120:PHE:O	1:A:123:LEU:N	2.41	0.48
1:A:185:MET:HB2	1:A:306:GLU:HB3	1.96	0.48
1:A:318:MET:HA	1:A:321:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:HD2	1:A:88:MET:CE	2.44	0.47
1:A:335:TYR:CD2	1:B:121:MET:HG3	2.50	0.47
1:C:19:TYR:CE1	1:C:82:THR:HG21	2.49	0.47
1:A:367:ASP:O	1:A:369:GLN:N	2.47	0.47
1:C:343:ASN:HD21	1:C:345:LEU:HD11	1.79	0.47
1:A:80:LEU:HD13	1:A:130:GLY:HA2	1.96	0.47
1:C:238:THR:O	1:C:364:PRO:HA	2.15	0.47
1:B:100:LEU:HD23	1:B:144:HIS:NE2	2.30	0.47
1:A:15:SER:HB2	1:A:82:THR:OG1	2.15	0.47
1:A:104:HIS:CD2	1:A:130:GLY:HA3	2.50	0.46
1:A:38:LEU:O	1:A:42:ALA:HB3	2.15	0.46
1:A:68:ASN:HD21	1:A:96:LEU:HD12	1.80	0.46
1:A:12:VAL:HG11	1:A:63:ILE:HG21	1.96	0.46
1:C:185:MET:HB2	1:C:306:GLU:HB3	1.98	0.46
1:A:264:LYS:HG3	1:A:296:LEU:HD21	1.98	0.46
1:A:128:HIS:HB2	1:C:449:HIS:CB	2.46	0.46
1:A:432:GLN:NE2	1:A:478:ASN:CG	2.63	0.46
1:A:151:TRP:O	1:A:157:HIS:NE2	2.45	0.46
1:A:12:VAL:O	1:A:78:VAL:HA	2.15	0.45
1:B:367:ASP:O	1:B:369:GLN:HA	2.15	0.45
1:C:101:LEU:HD12	1:C:145:ALA:CB	2.47	0.45
1:C:336:THR:HG22	1:C:337:TYR:N	2.30	0.45
1:C:277:THR:HG22	1:C:303:PHE:HE1	1.81	0.45
1:A:120:PHE:HE2	1:A:124:ASN:HB2	1.80	0.45
1:A:240:THR:HG21	1:A:366:LEU:HD13	1.99	0.45
1:B:13:ILE:N	1:B:13:ILE:HD12	2.31	0.45
1:B:420:PRO:HD2	1:C:114:ASP:HA	1.99	0.45
1:A:349:SER:OG	1:A:350:HIS:N	2.50	0.45
1:C:397:ILE:HG21	1:C:447:GLY:CA	2.46	0.45
1:A:101:LEU:HD11	1:A:147:VAL:HG23	1.98	0.45
1:B:114:ASP:OD1	1:B:114:ASP:N	2.49	0.45
1:A:406:LEU:HD12	1:A:406:LEU:N	2.31	0.45
1:B:345:LEU:HD13	1:B:428:LEU:HD21	1.99	0.45
1:A:80:LEU:CD1	1:A:130:GLY:HA2	2.47	0.44
1:A:87:LYS:HA	1:A:90:ILE:HG12	1.99	0.44
1:B:102:GLN:NE2	1:B:104:HIS:CD2	2.85	0.44
1:B:259:ILE:O	1:B:263:MET:HG3	2.17	0.44
1:A:328:GLY:O	1:A:329:THR:CB	2.65	0.44
1:A:79:TRP:HE1	1:A:126:THR:HG21	1.82	0.44
1:C:359:ALA:HB2	1:C:384:PHE:CD1	2.52	0.44
1:B:330:SER:OG	1:B:331:PHE:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:MET:SD	1:A:125:GLN:OE1	2.76	0.44
1:B:120:PHE:O	1:B:123:LEU:O	2.35	0.44
1:C:125:GLN:HB2	1:C:128:HIS:CE1	2.53	0.44
1:C:410:ILE:HG22	1:C:431:ALA:HA	1.98	0.44
1:A:211:VAL:HG21	1:A:281:ASP:O	2.17	0.44
1:A:15:SER:OG	1:A:19:TYR:CE1	2.70	0.44
1:B:245:ILE:O	1:B:250:ARG:HG3	2.17	0.44
1:C:101:LEU:HD11	1:C:147:VAL:HG23	1.99	0.44
1:C:432:GLN:O	1:C:434:ASP:N	2.51	0.44
1:B:350:HIS:O	1:B:424:VAL:HG11	2.18	0.43
1:C:13:ILE:CD1	1:C:50:LEU:HD11	2.48	0.43
1:A:177:LYS:H	1:A:273:HIS:HD2	1.66	0.43
1:A:446:GLY:HA2	1:B:138:ALA:HB3	1.99	0.43
1:C:82:THR:HG22	1:C:83:PHE:O	2.18	0.43
1:A:350:HIS:O	1:A:351:MET:C	2.55	0.43
1:B:304:ALA:HB3	1:B:308:ASP:O	2.18	0.43
1:B:322:SER:HA	1:B:325:LEU:HD12	2.01	0.43
1:A:104:HIS:NE2	1:A:126:THR:O	2.49	0.43
1:A:171:GLN:O	1:A:174:ARG:HB2	2.19	0.43
1:C:431:ALA:C	1:C:432:GLN:O	2.57	0.43
1:B:252:ASN:HB2	1:B:367:ASP:OD2	2.18	0.43
1:A:176:LEU:HD23	1:A:176:LEU:C	2.39	0.42
1:A:366:LEU:CD2	1:A:368:VAL:HB	2.49	0.42
1:C:320:VAL:O	1:C:323:THR:OG1	2.35	0.42
1:A:30:HIS:CE1	1:A:124:ASN:HD21	2.38	0.42
1:A:85:PRO:HD2	1:A:88:MET:HE2	2.01	0.42
1:C:102:GLN:HE22	1:C:130:GLY:HA3	1.84	0.42
1:A:222:SER:O	1:A:226:VAL:HG23	2.20	0.42
1:B:12:VAL:HG11	1:B:63:ILE:HG21	2.01	0.42
1:C:105:THR:OG1	1:C:106:GLN:N	2.51	0.42
1:C:12:VAL:O	1:C:78:VAL:HA	2.19	0.42
1:B:80:LEU:CD1	1:B:133:PHE:CB	2.97	0.42
1:B:13:ILE:HD13	1:B:50:LEU:HD11	2.02	0.42
1:B:338:HIS:O	1:B:344:ASP:HA	2.19	0.42
1:B:15:SER:O	1:B:84:SER:HB2	2.20	0.42
1:C:78:VAL:CG1	1:C:100:LEU:HD11	2.45	0.42
1:B:449:HIS:HB2	1:C:128:HIS:CB	2.50	0.42
1:A:179:CYS:HB2	1:A:272:PHE:CD1	2.55	0.42
1:A:120:PHE:O	1:A:121:MET:C	2.58	0.41
1:A:68:ASN:ND2	1:A:96:LEU:HD12	2.35	0.41
1:C:2:THR:HG23	1:C:323:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:VAL:HG23	1:C:495:TYR:HD1	1.85	0.41
1:A:478:ASN:HA	1:A:478:ASN:HD22	1.72	0.41
1:A:364:PRO:HD2	1:A:383:ILE:O	2.20	0.41
1:A:179:CYS:HB2	1:A:272:PHE:CE1	2.55	0.41
1:A:215:VAL:HG21	1:A:284:GLY:HA3	2.02	0.41
1:B:244:GLN:O	1:B:250:ARG:HG2	2.21	0.41
1:C:350:HIS:ND1	1:C:353:GLU:OE1	2.53	0.41
1:B:80:LEU:HD11	1:B:133:PHE:CG	2.56	0.41
1:A:106:GLN:HE22	1:C:336:THR:HG23	1.86	0.41
1:C:101:LEU:HD12	1:C:145:ALA:HB3	2.03	0.41
1:C:431:ALA:O	1:C:432:GLN:O	2.38	0.41
1:A:367:ASP:O	1:A:369:GLN:CA	2.69	0.41
1:C:16:GLN:NE2	1:C:85:PRO:HG2	2.36	0.41
1:A:76:LEU:HB2	1:A:100:LEU:HD12	2.02	0.41
1:C:102:GLN:HE22	1:C:130:GLY:CA	2.33	0.41
1:C:383:ILE:HG23	2:C:504:HOH:O	2.21	0.41
1:C:19:TYR:CE1	1:C:82:THR:CG2	3.04	0.40
1:A:190:VAL:O	1:A:310:LYS:NZ	2.54	0.40
1:B:330:SER:HB2	1:B:358:ILE:HD11	2.02	0.40
1:C:445:ALA:O	1:C:446:GLY:C	2.59	0.40
1:B:190:VAL:HG13	1:C:135:PHE:CB	2.51	0.40
1:A:282:LEU:HD21	1:A:288:LEU:HD13	2.04	0.40
1:B:239:MET:HE3	1:B:365:ILE:HD13	2.03	0.40
1:A:350:HIS:O	1:A:424:VAL:HG11	2.21	0.40
1:A:15:SER:HA	1:A:84:SER:HB3	2.02	0.40
1:C:80:LEU:CD1	1:C:133:PHE:CB	2.99	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	496/500 (99%)	456 (92%)	30 (6%)	10 (2%)	9	17
1	B	497/500 (99%)	465 (94%)	22 (4%)	10 (2%)	9	17
1	C	496/500 (99%)	467 (94%)	17 (3%)	12 (2%)	7	12
All	All	1489/1500 (99%)	1388 (93%)	69 (5%)	32 (2%)	8	15

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	GLN
1	B	361	GLU
1	B	368	VAL
1	B	447	GLY
1	C	306	GLU
1	C	432	GLN
1	C	446	GLY
1	C	447	GLY
1	A	305	GLY
1	A	370	HIS
1	B	124	ASN
1	B	327	GLY
1	B	351	MET
1	B	353	GLU
1	C	373	ILE
1	A	143	GLN
1	A	144	HIS
1	A	329	THR
1	B	377	ASP
1	C	144	HIS
1	A	52	PRO
1	A	124	ASN
1	A	432	GLN
1	C	124	ASN
1	C	433	PRO
1	A	83	PHE
1	A	351	MET
1	C	329	THR
1	B	433	PRO
1	C	190	VAL
1	C	368	VAL
1	C	290	GLY

### 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	396/419 (94%)	366 (92%)	30 (8%)	15	30
1	B	406/419 (97%)	378 (93%)	28 (7%)	18	36
1	C	363/419 (87%)	343 (94%)	20 (6%)	25	49
All	All	1165/1257 (93%)	1087 (93%)	78 (7%)	19	38

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	9	VAL
1	A	12	VAL
1	A	26	GLN
1	A	65	ARG
1	A	82	THR
1	A	97	ASN
1	A	98	LYS
1	A	120	PHE
1	A	132	GLU
1	A	141	ARG
1	A	159	ARG
1	A	174	ARG
1	A	208	THR
1	A	213	ASP
1	A	277	THR
1	A	282	LEU
1	A	291	LEU
1	A	323	THR
1	A	334	ASP
1	A	335	TYR
1	A	361	GLU
1	A	365	ILE
1	A	381	ARG
1	A	393	VAL
1	A	407	VAL

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Mol	Chain	Res	Type
1	A	434	ASP
1	A	473	ILE
1	A	481	ARG
1	A	494	VAL
1	B	8	GLU
1	B	12	VAL
1	B	55	THR
1	B	77	VAL
1	B	95[A]	MET
1	B	95[B]	MET
1	B	121	MET
1	B	122	ASN
1	B	124	ASN
1	B	132	GLU
1	B	141	ARG
1	B	146	VAL
1	B	174	ARG
1	B	190	VAL
1	B	235	SER
1	B	244	GLN
1	B	250	ARG
1	B	251	GLN
1	B	268	GLU
1	B	334	ASP
1	B	335	TYR
1	B	358	ILE
1	B	361	GLU
1	B	368	VAL
1	B	381	ARG
1	B	412	THR
1	B	467	GLU
1	B	482	LEU
1	C	6	ASN
1	C	77	VAL
1	C	115	SER
1	C	119	ASP
1	C	209	TRP
1	C	239	MET
1	C	277	THR
1	C	293	VAL
1	C	323	THR
1	C	334	ASP

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Mol	Chain	Res	Type
1	C	343	ASN
1	C	369	GLN
1	C	371	LEU
1	C	378	ASP
1	C	393	VAL
1	C	399	LEU
1	C	412	THR
1	C	428	LEU
1	C	449	HIS
1	C	451	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	68	ASN
1	A	81	HIS
1	A	102	GLN
1	A	106	GLN
1	A	122	ASN
1	A	184	ASN
1	A	273	HIS
1	A	287	GLN
1	A	343	ASN
1	A	408	ASN
1	A	432	GLN
1	A	478	ASN
1	B	29	GLN
1	B	102	GLN
1	B	104	HIS
1	B	106	GLN
1	B	125	GLN
1	B	128	HIS
1	B	142	GLN
1	B	252	ASN
1	B	269	GLN
1	B	287	GLN
1	B	343	ASN
1	B	417	HIS
1	B	455	HIS
1	B	460	ASN
1	B	464	GLN

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Mol	Chain	Res	Type
1	B	478	ASN
1	C	16	GLN
1	C	29	GLN
1	C	68	ASN
1	C	102	GLN
1	C	104	HIS
1	C	106	GLN
1	C	273	HIS
1	C	287	GLN
1	C	298	GLN
1	C	343	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	498/500 (99%)	0.47	49 (9%) 8 5	58, 66, 72, 81	0
1	B	498/500 (99%)	0.39	31 (6%) 21 16	59, 66, 72, 82	0
1	C	498/500 (99%)	1.44	127 (25%) 1 0	58, 68, 71, 76	0
All	All	1494/1500 (99%)	0.77	207 (13%) 3 2	58, 67, 71, 82	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	TYR	14.6
1	C	245	ILE	10.8
1	C	236	CYS	10.1
1	C	241	PRO	9.5
1	C	237	TYR	9.2
1	C	246	HIS	8.8
1	C	240	THR	7.8
1	C	378	ASP	7.5
1	C	416	PRO	7.4
1	C	253	VAL	7.3
1	C	360	VAL	7.3
1	C	213	ASP	7.3
1	C	423	PRO	7.0
1	C	229	LEU	7.0
1	C	252	ASN	7.0
1	C	417	HIS	7.0
1	C	379	PRO	6.9
1	C	376	LYS	6.9
1	C	370	HIS	6.9
1	A	123	LEU	6.7
1	C	185	MET	6.6
1	C	342	GLY	6.6
1	C	238	THR	6.5

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Mol	Chain	Res	Type	RSRZ
1	C	299	GLN	6.5
1	C	374	GLY	6.4
1	C	456	ALA	6.1
1	C	304	ALA	6.0
1	C	371	LEU	6.0
1	C	222	SER	6.0
1	C	382	LEU	5.9
1	C	247	GLY	5.9
1	C	209	TRP	5.7
1	C	361	GLU	5.6
1	C	239	MET	5.5
1	C	422	LEU	5.4
1	C	415	THR	5.4
1	A	128	HIS	5.3
1	C	281	ASP	5.3
1	C	375	GLY	5.0
1	C	243	THR	5.0
1	A	124	ASN	5.0
1	C	186	ARG	5.0
1	C	372	GLY	5.0
1	C	424	VAL	4.9
1	C	384	PHE	4.9
1	A	80	LEU	4.8
1	C	242	ALA	4.7
1	C	220	SER	4.7
1	A	83	PHE	4.7
1	C	234	GLU	4.7
1	C	188	VAL	4.6
1	C	267	LEU	4.4
1	C	303	PHE	4.4
1	C	288	LEU	4.4
1	C	385	ASN	4.3
1	B	417	HIS	4.2
1	C	352	LEU	4.2
1	C	369	GLN	4.2
1	C	227	ASN	4.2
1	C	228	ALA	4.2
1	B	17	HIS	4.1
1	A	121	MET	4.1
1	C	269	GLN	4.1
1	B	241	PRO	4.1
1	C	297	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLN	4.0
1	C	284	GLY	4.0
1	C	192	ASP	4.0
1	C	265	ARG	3.8
1	C	373	ILE	3.8
1	A	248	GLU	3.8
1	B	246	HIS	3.8
1	C	232	GLU	3.8
1	B	370	HIS	3.7
1	A	1	MET	3.7
1	C	254	LEU	3.7
1	C	279	PHE	3.7
1	B	420	PRO	3.7
1	C	181	PHE	3.7
1	B	13	ILE	3.7
1	C	419	LEU	3.7
1	C	225	ASP	3.7
1	C	216	GLN	3.6
1	C	208	THR	3.6
1	C	364	PRO	3.6
1	A	117	ASP	3.6
1	C	261	LEU	3.6
1	C	420	PRO	3.6
1	C	325	LEU	3.5
1	A	116	ILE	3.5
1	A	29	GLN	3.5
1	A	498	PHE	3.5
1	C	219	ASN	3.5
1	C	255	GLU	3.4
1	C	183	ASP	3.4
1	C	380	ALA	3.3
1	A	127	ALA	3.3
1	C	359	ALA	3.3
1	C	454	SER	3.3
1	A	113	TRP	3.2
1	A	370	HIS	3.2
1	B	498	PHE	3.2
1	A	112	PRO	3.2
1	C	479	ASP	3.1
1	C	184	ASN	3.1
1	A	81	HIS	3.1
1	A	115	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	19	TYR	3.1
1	C	263	MET	3.0
1	C	282	LEU	3.0
1	C	285	LEU	3.0
1	C	223	ASP	3.0
1	C	248	GLU	3.0
1	C	339	PHE	2.9
1	B	18	LEU	2.9
1	B	216	GLN	2.9
1	C	295	ARG	2.9
1	B	368	VAL	2.9
1	A	72	PRO	2.9
1	A	84	SER	2.8
1	B	245	ILE	2.8
1	C	358	ILE	2.8
1	A	360	VAL	2.8
1	C	341	LYS	2.8
1	C	114	ASP	2.8
1	C	366	LEU	2.8
1	C	179	CYS	2.8
1	C	187	GLU	2.7
1	B	373	ILE	2.7
1	A	2	THR	2.7
1	A	118	MET	2.7
1	A	141	ARG	2.7
1	A	14	GLY	2.6
1	C	207	ASN	2.6
1	B	251	GLN	2.6
1	B	14	GLY	2.6
1	B	2	THR	2.6
1	B	236	CYS	2.6
1	C	218	VAL	2.6
1	B	377	ASP	2.5
1	C	249	LYS	2.5
1	A	140	MET	2.5
1	C	389	GLY	2.5
1	C	280	GLU	2.5
1	A	470	ASP	2.5
1	C	262	GLY	2.5
1	C	290	GLY	2.5
1	C	355	CYS	2.5
1	C	447	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	214	LEU	2.4
1	C	191	THR	2.4
1	C	414	LYS	2.4
1	A	110	ALA	2.4
1	B	248	GLU	2.4
1	C	412	THR	2.4
1	C	418	SER	2.4
1	C	326	GLN	2.3
1	C	283	HIS	2.3
1	C	381	ARG	2.3
1	A	78	VAL	2.3
1	C	413	VAL	2.3
1	A	256	ALA	2.3
1	B	263	MET	2.3
1	C	344	ASP	2.3
1	B	290	GLY	2.3
1	A	18	LEU	2.3
1	A	36	ASN	2.3
1	A	106	GLN	2.3
1	C	250	ARG	2.3
1	A	361	GLU	2.3
1	A	249	LYS	2.3
1	C	211	VAL	2.3
1	A	122	ASN	2.2
1	C	217	VAL	2.2
1	C	22	GLU	2.2
1	B	253	VAL	2.2
1	B	360	VAL	2.2
1	C	84	SER	2.2
1	B	123	LEU	2.2
1	C	289	PRO	2.2
1	B	114	ASP	2.2
1	C	350	HIS	2.1
1	A	131	ARG	2.1
1	A	21	PRO	2.1
1	B	232	GLU	2.1
1	A	97	ASN	2.1
1	B	361	GLU	2.1
1	A	120	PHE	2.1
1	A	94	THR	2.1
1	A	246	HIS	2.1
1	C	178	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	221	ILE	2.1
1	C	368	VAL	2.1
1	C	277	THR	2.1
1	A	371	LEU	2.1
1	C	6	ASN	2.1
1	A	372	GLY	2.1
1	A	326	GLN	2.0
1	B	414	LYS	2.0
1	B	432	GLN	2.0
1	C	292	ALA	2.0
1	B	341	LYS	2.0
1	C	226	VAL	2.0
1	C	276	THR	2.0
1	B	365	ILE	2.0
1	A	149	GLY	2.0
1	A	104	HIS	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.