



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:04 PM UTC

PDB ID : 2AJT / pdb_00002ajt
Title : Crystal structure of L-Arabinose Isomerase from E.coli
Authors : Manjasetty, B.A.; Fedorov, E.V.; Almo, S.C.; Chance, M.R.; Burley, S.K.;
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

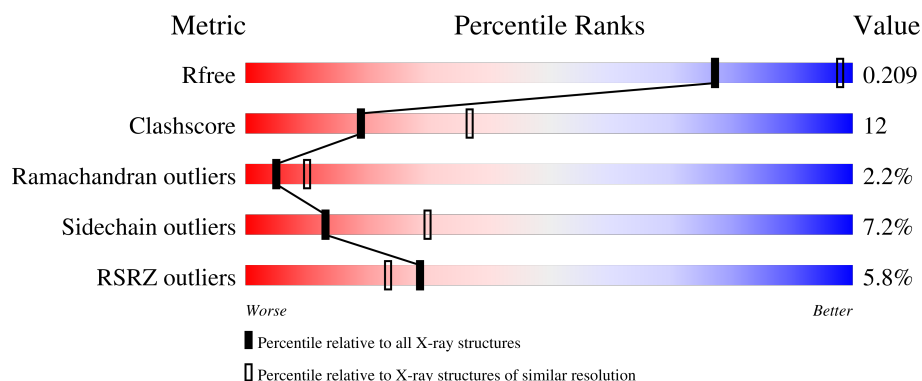
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	2% 71% 24% .
1	B	500	2% 75% 19% ..
1	C	500	13% 78% 19% .

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

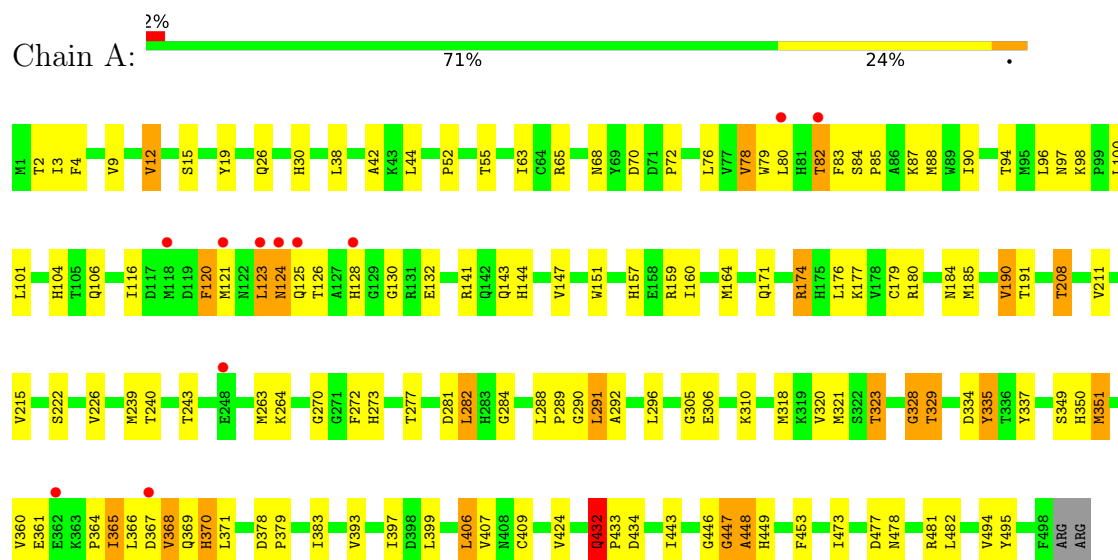
- Molecule 2 is water.

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		

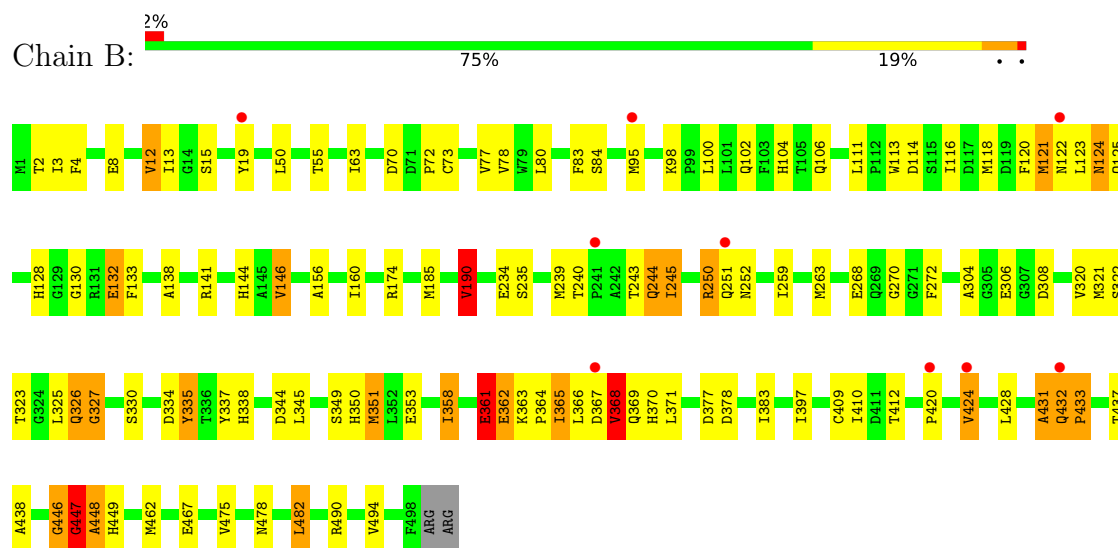
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

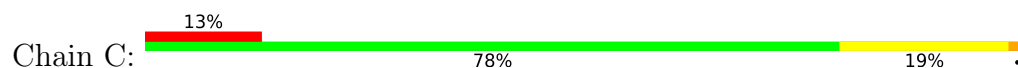
• Molecule 1: L-arabinose isomerase

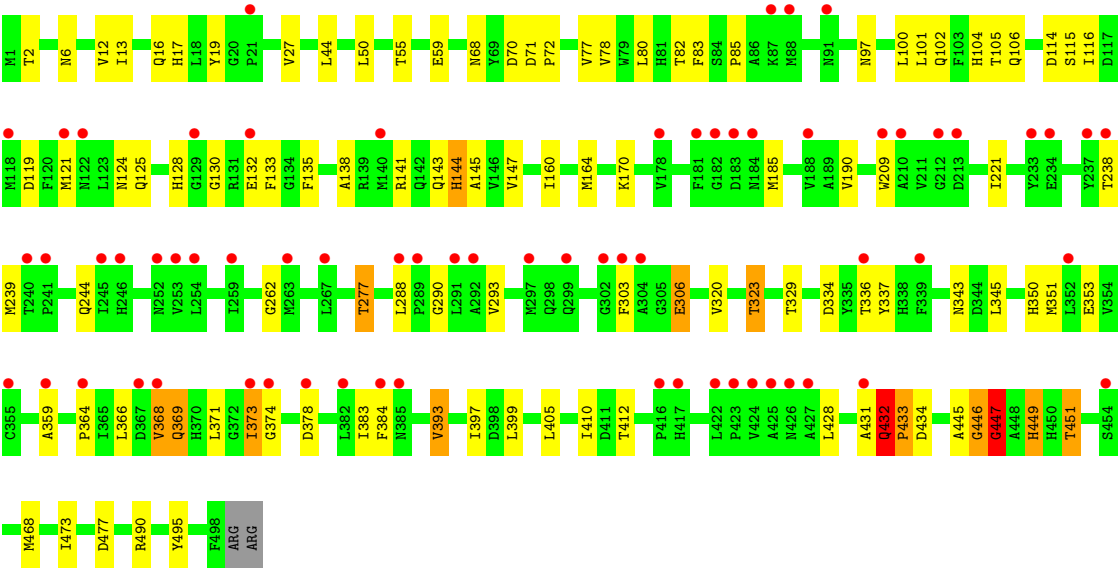


• Molecule 1: L-arabinose isomerase



• 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, α , β , γ	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) 84.3 (19.84-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.65	0/3927	0.92	7/5351 (0.1%)
1	B	0.63	0/3976	0.89	8/5411 (0.1%)
1	C	0.60	0/3776	0.84	3/5157 (0.1%)
All	All	0.63	0/11679	0.89	18/15919 (0.1%)

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	GLN	CA-C-N	-14.95	101.15	119.84
1	A	432	GLN	C-N-CA	-14.95	101.15	119.84
1	B	432	GLN	CA-C-N	-10.07	107.25	119.84
1	B	432	GLN	C-N-CA	-10.07	107.25	119.84
1	C	369	GLN	N-CA-C	7.86	120.85	109.14
1	A	360	VAL	CB-CA-C	-7.49	104.47	111.06
1	C	447	GLY	N-CA-C	7.47	130.89	113.18
1	B	448	ALA	N-CA-C	7.25	120.38	109.95
1	B	190	VAL	CB-CA-C	-7.11	102.54	112.14
1	A	448	ALA	N-CA-C	6.27	119.36	110.14
1	B	432	GLN	N-CA-C	6.21	123.54	109.81
1	B	245	ILE	N-CA-C	5.96	116.43	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	GLY	N-CA-C	5.79	115.48	110.21
1	B	363	LYS	N-CA-C	5.56	117.96	110.29
1	C	449	HIS	N-CA-C	5.38	117.84	111.33
1	A	482	LEU	CA-C-N	-5.06	113.71	118.97
1	A	482	LEU	C-N-CA	-5.06	113.71	118.97
1	B	190	VAL	N-CA-C	5.06	115.78	110.62

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	GLY	Peptide
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	112	0
1	B	3875	0	3727	98	0
1	C	3687	0	3407	76	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	262	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 12.

All (262) 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	0.93
1:A:369:GLN:O	1:A:370:HIS:C	2.13	0.87
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:432:GLN:HE21	1:A:478:ASN:CG	1.85	0.85
1:B:367:ASP:O	1:B:368:VAL:C	2.23	0.81
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
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:B:369:GLN:O	1:B:370:HIS:C	2.27	0.77
1:A:432:GLN:HE21	1:A:478:ASN:ND2	1.82	0.77
1:B:368:VAL:O	1:B:368:VAL:HG12	1.85	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:C:433:PRO:HD3	1:C:477:ASP:C	2.14	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: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:B:239:MET:HE3	1:B:243:THR:HG22	1.77	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:C:71:ASP:CG	1:C:72:PRO:HD3	2.21	0.64
1:A:82:THR:O	1:A:125:GLN:CG	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:116:ILE:HD11	1:C:121:MET:HE1	1.80	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:O	1:A:368:VAL:CG1	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
1:A:160:ILE:CG2	1:A:164:MET:HE3	2.30	0.62
1:A:367:ASP:O	1:A:368:VAL:C	2.43	0.61
1:A:160:ILE:HG22	1:A:164:MET:HE3	1.83	0.61
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: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:O	1:B:368:VAL:CG1	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:120:PHE:C	1:A:120:PHE:CD2	2.82	0.57
1:A:184:ASN:HD21	1:A:191:THR:C	2.13	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:C:143:GLN:O	1:C:144:HIS:C	2.48	0.56
1:A:82:THR:O	1:A:125:GLN:HG3	2.05	0.56
1:A:239:MET:HE3	1:A:243:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HD13	1:C:164:MET:HE1	1.87	0.55
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:A:424:VAL:HG23	1:B:118:MET:HE3	1.89	0.54
1:A:432:GLN:NE2	1:A:478:ASN:CG	2.63	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:185:MET:HE2	1:A:306:GLU:HG2	1.91	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
1:B:190:VAL:HG22	1:C:132:GLU:OE2	2.09	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:B:234:GLU:HG3	1:B:239:MET:HE2	1.90	0.52
1:B:437:THR:HG23	1:B:482:LEU:HD12	1.92	0.52
1:A:263:MET:HE2	1:A:292:ALA:HB1	1.92	0.52
1:A:495:TYR:CZ	1:C:490:ARG:HG2	2.46	0.51
1:B:349:SER:OG	1:B:350:HIS:N	2.44	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:A:320:VAL:O	1:A:323:THR:OG1	2.28	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:A:82:THR:O	1:A:125:GLN:HG2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:MET:HA	1:A:321:MET:HE3	1.95	0.49
1:C:160:ILE:HG22	1:C:164:MET:HE3	1.94	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:B:321:MET:SD	1:B:462:MET:HE1	2.53	0.48
1:C:373:ILE:HG22	1:C:374:GLY:N	2.28	0.48
1:A:350:HIS:O	1:A:351:MET:C	2.55	0.48
1:A:369:GLN:CB	1:A:378:ASP:HB3	2.44	0.48
1:C:116:ILE:CD1	1:C:121:MET:HE1	2.44	0.48
1:A:120:PHE:O	1:A:123:LEU:N	2.41	0.48
1:B:239:MET:HE3	1:B:243:THR:CG2	2.42	0.48
1:A:185:MET:HB2	1:A:306:GLU:HB3	1.96	0.48
1:A:85:PRO:HD2	1:A:88:MET:CE	2.44	0.47
1:B:121:MET:HE3	1:B:121:MET:HA	1.96	0.47
1:A:176:LEU:HD23	1:A:176:LEU:C	2.39	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:C:431:ALA:C	1:C:432:GLN:O	2.57	0.47
1:A:367:ASP:O	1:A:369:GLN:N	2.47	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:C:343:ASN:HD21	1:C:345:LEU:HD11	1.79	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:38:LEU:O	1:A:42:ALA:HB3	2.15	0.46
1:A:104:HIS:CD2	1:A:130:GLY:HA3	2.50	0.46
1:A:120:PHE:O	1:A:121:MET:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:O	1:A:94:THR:OG1	2.32	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: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:A:44:LEU:HD13	1:A:164:MET:HE1	1.98	0.45
1:C:277:THR:HG22	1:C:303:PHE:HE1	1.81	0.45
1:C:445:ALA:O	1:C:446:GLY:C	2.59	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:HD12	1:B:13:ILE:N	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:C:288:LEU:HD21	1:C:351:MET:HE3	1.99	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:79:TRP:HE1	1:A:126:THR:HG21	1.82	0.44
1:A:328:GLY:O	1:A:329:THR:CB	2.65	0.44
1:C:359:ALA:HB2	1:C:384:PHE:CD1	2.52	0.44
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:239:MET:HE3	1:A:243:THR:CG2	2.48	0.44
1:A:367:ASP:C	1:A:369:GLN:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:252:ASN:HB2	1:B:367:ASP:OD2	2.18	0.43
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:B:350:HIS:O	1:B:351:MET:C	2.62	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:12:VAL:O	1:C:78:VAL:HA	2.19	0.42
1:C:105:THR:OG1	1:C:106:GLN:N	2.51	0.42
1:C:170:LYS:HB2	1:C:468:MET:HE3	2.00	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:15:SER:O	1:B:84:SER:HB2	2.20	0.42
1:B:338:HIS:O	1:B:344:ASP:HA	2.19	0.42
1:B:449:HIS:HB2	1:C:128:HIS:CB	2.50	0.42
1:C:78:VAL:CG1	1:C:100:LEU:HD11	2.45	0.42
1:A:179:CYS:HB2	1:A:272:PHE:CD1	2.55	0.42
1:A:68:ASN:ND2	1:A:96:LEU:HD12	2.35	0.41
1:B:494:VAL:HG23	1:C:495:TYR:HD1	1.85	0.41
1:C:2:THR:HG23	1:C:323:THR:HG21	2.01	0.41
1:A:478:ASN:HD22	1:A:478:ASN:HA	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:A:121:MET:HE2	1:A:128:HIS:HE1	1.86	0.41
1:B:80:LEU:HD11	1:B:133:PHE:CG	2.56	0.41
1:A:85:PRO:HD2	1:A:88:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ALA:O	1:C:432:GLN:O	2.38	0.41
1:A:290:GLY:O	1:A:291:LEU:C	2.64	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: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:A:15:SER:HA	1:A:84:SER:HB3	2.02	0.40
1:A:350:HIS:O	1:A:424:VAL:HG11	2.21	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%)	6	12
1	B	497/500 (99%)	465 (94%)	22 (4%)	10 (2%)	6	12
1	C	496/500 (99%)	467 (94%)	17 (3%)	12 (2%)	4	9
All	All	1489/1500 (99%)	1388 (93%)	69 (5%)	32 (2%)	5	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	GLN
1	B	361	GLU

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Mol	Chain	Res	Type
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%)	363 (92%)	33 (8%)	10	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	406/419 (97%)	375 (92%)	31 (8%)	12	27
1	C	363/419 (87%)	342 (94%)	21 (6%)	18	39
All	All	1165/1257 (93%)	1080 (93%)	85 (7%)	13	29

All (85) 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	78	VAL
1	A	82	THR
1	A	97	ASN
1	A	98	LYS
1	A	120	PHE
1	A	123	LEU
1	A	132	GLU
1	A	141	ARG
1	A	159	ARG
1	A	174	ARG
1	A	190	VAL
1	A	208	THR
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	368	VAL
1	A	393	VAL
1	A	406	LEU
1	A	407	VAL
1	A	434	ASP
1	A	473	ILE
1	A	481	ARG
1	A	494	VAL
1	B	8	GLU

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Mol	Chain	Res	Type
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	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	362	GLU
1	B	365	ILE
1	B	368	VAL
1	B	412	THR
1	B	424	VAL
1	B	467	GLU
1	B	475	VAL
1	B	482	LEU
1	B	490	ARG
1	C	6	ASN
1	C	27	VAL
1	C	77	VAL
1	C	115	SER
1	C	119	ASP
1	C	141	ARG
1	C	209	TRP
1	C	239	MET
1	C	244	GLN
1	C	277	THR
1	C	293	VAL
1	C	323	THR

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Mol	Chain	Res	Type
1	C	334	ASP
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	451	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	30	HIS
1	A	68	ASN
1	A	81	HIS
1	A	97	ASN
1	A	102	GLN
1	A	106	GLN
1	A	122	ASN
1	A	128	HIS
1	A	166	GLN
1	A	184	ASN
1	A	244	GLN
1	A	251	GLN
1	A	273	HIS
1	A	287	GLN
1	A	298	GLN
1	A	343	ASN
1	A	385	ASN
1	A	408	ASN
1	A	426	ASN
1	A	432	GLN
1	A	478	ASN
1	B	91	ASN
1	B	97	ASN
1	B	102	GLN
1	B	104	HIS
1	B	106	GLN
1	B	125	GLN
1	B	128	HIS

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Mol	Chain	Res	Type
1	B	142	GLN
1	B	287	GLN
1	B	343	ASN
1	B	385	ASN
1	B	417	HIS
1	B	426	ASN
1	B	455	HIS
1	B	460	ASN
1	B	464	GLN
1	B	478	ASN
1	C	16	GLN
1	C	17	HIS
1	C	26	GLN
1	C	29	GLN
1	C	68	ASN
1	C	102	GLN
1	C	104	HIS
1	C	106	GLN
1	C	124	ASN
1	C	152	GLN
1	C	287	GLN
1	C	299	GLN
1	C	338	HIS
1	C	343	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th 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 ²)	Q<0.9
1	A	498/500 (99%)	0.20	11 (2%) 62 57	58, 66, 72, 81	0
1	B	498/500 (99%)	0.42	9 (1%) 67 63	48, 66, 72, 82	1 (0%)
1	C	498/500 (99%)	1.01	67 (13%) 7 5	58, 68, 71, 76	0
All	All	1494/1500 (99%)	0.54	87 (5%) 29 23	48, 67, 71, 82	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	237	TYR	5.0
1	C	213	ASP	4.3
1	C	233	TYR	4.3
1	C	289	PRO	3.9
1	C	288	LEU	3.9
1	C	304	ALA	3.9
1	C	423	PRO	3.7
1	C	181	PHE	3.7
1	A	128	HIS	3.6
1	C	382	LEU	3.6
1	C	374	GLY	3.5
1	C	240	THR	3.4
1	A	124	ASN	3.4
1	C	303	PHE	3.3
1	C	263	MET	3.2
1	C	234	GLU	3.2
1	C	183	ASP	3.1
1	A	367	ASP	3.1
1	C	267	LEU	3.1
1	C	246	HIS	3.1
1	C	299	GLN	3.1
1	C	238	THR	3.1
1	C	253	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	292	ALA	3.0
1	A	125	GLN	2.9
1	C	209	TRP	2.9
1	C	188	VAL	2.9
1	C	259	ILE	2.8
1	C	336	THR	2.8
1	C	373	ILE	2.8
1	C	417	HIS	2.8
1	C	364	PRO	2.7
1	C	416	PRO	2.7
1	C	122	ASN	2.7
1	C	241	PRO	2.7
1	C	87	LYS	2.7
1	B	241	PRO	2.6
1	A	123	LEU	2.6
1	C	291	LEU	2.6
1	C	121	MET	2.5
1	C	454	SER	2.4
1	A	121	MET	2.4
1	B	424	VAL	2.4
1	C	254	LEU	2.4
1	C	129	GLY	2.4
1	C	427	ALA	2.4
1	C	178	VAL	2.4
1	C	367	ASP	2.4
1	C	245	ILE	2.3
1	C	355	CYS	2.3
1	C	425	ALA	2.3
1	C	91	ASN	2.3
1	C	182	GLY	2.3
1	A	80	LEU	2.3
1	C	384	PHE	2.3
1	C	422	LEU	2.3
1	C	88	MET	2.3
1	B	19	TYR	2.3
1	C	21	PRO	2.3
1	C	424	VAL	2.3
1	C	184	ASN	2.2
1	B	367	ASP	2.2
1	C	297	MET	2.2
1	B	122	ASN	2.2
1	B	420	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	339	PHE	2.2
1	C	252	ASN	2.2
1	C	210	ALA	2.1
1	C	359	ALA	2.1
1	C	431	ALA	2.1
1	C	132	GLU	2.1
1	B	251	GLN	2.1
1	B	432	GLN	2.1
1	C	378	ASP	2.1
1	A	248	GLU	2.1
1	A	82	THR	2.1
1	C	118	MET	2.1
1	C	352	LEU	2.1
1	C	302	GLY	2.1
1	A	362	GLU	2.1
1	C	426	ASN	2.1
1	B	95[A]	MET	2.0
1	C	212	GLY	2.0
1	C	368	VAL	2.0
1	A	118	MET	2.0
1	C	140	MET	2.0
1	C	385	ASN	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 oligosaccharides 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.