



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:36 PM GMT

PDB ID : 2AJT
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.;
New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2005-08-02
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

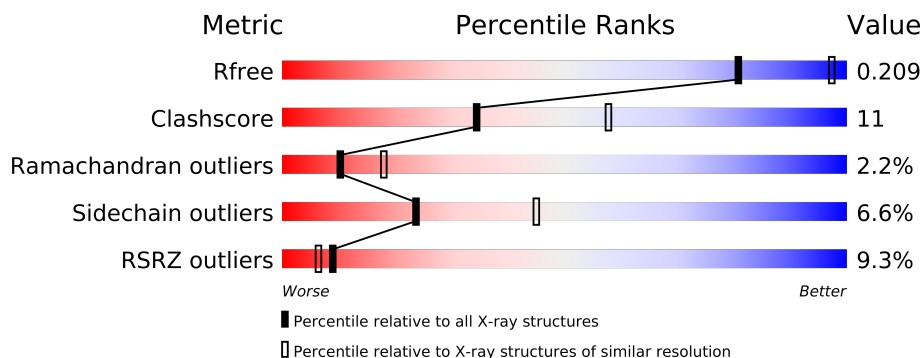
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	
1	C	500	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11483 atoms, of which 0 are hydrogen and 0 are deuterium.

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

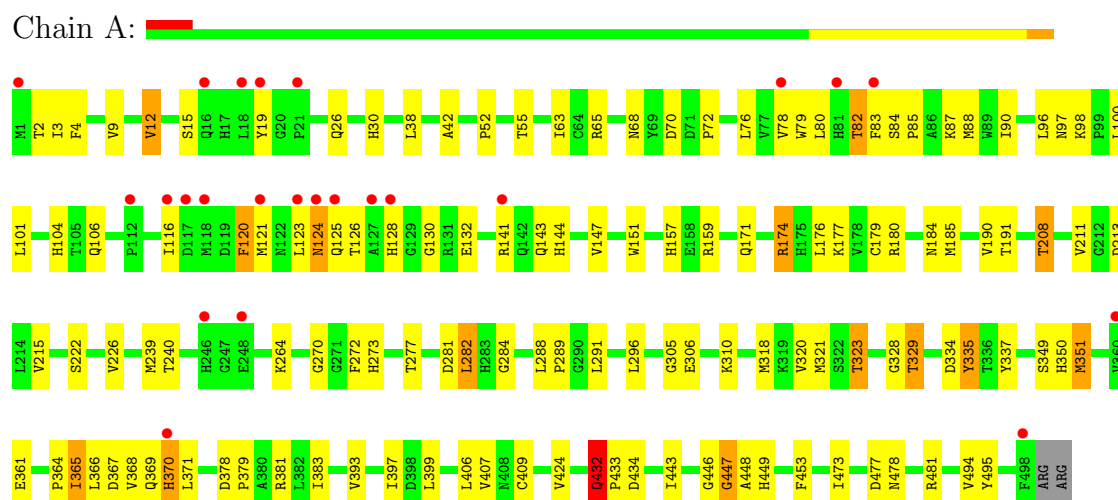
- Molecule 2 is water.

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		

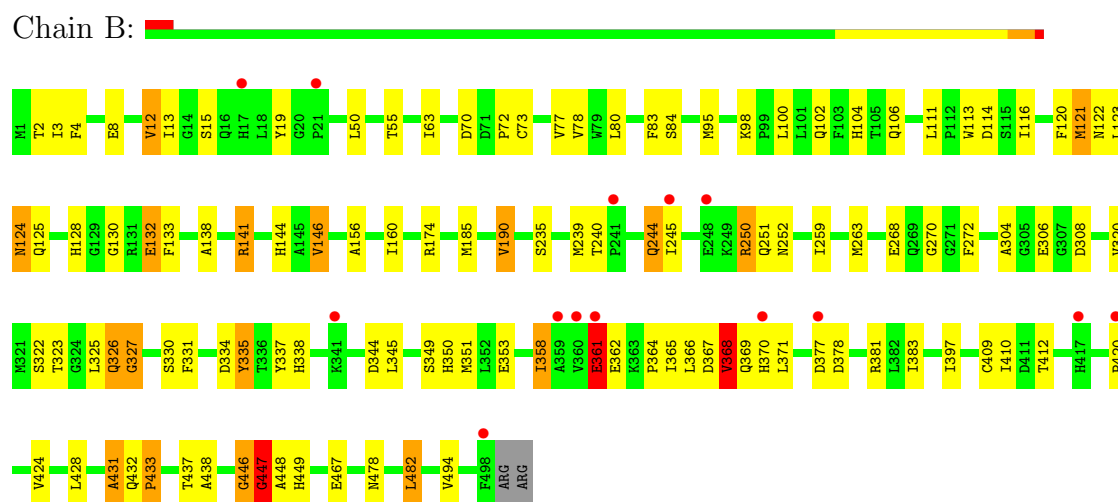
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

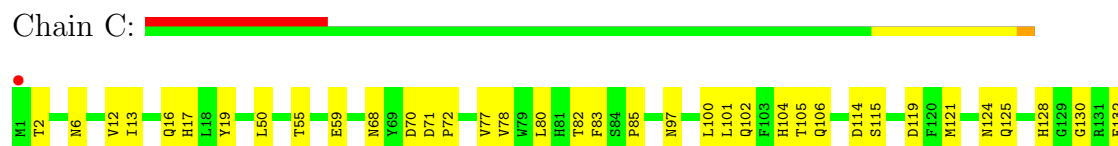
- Molecule 1: L-arabinose isomerase

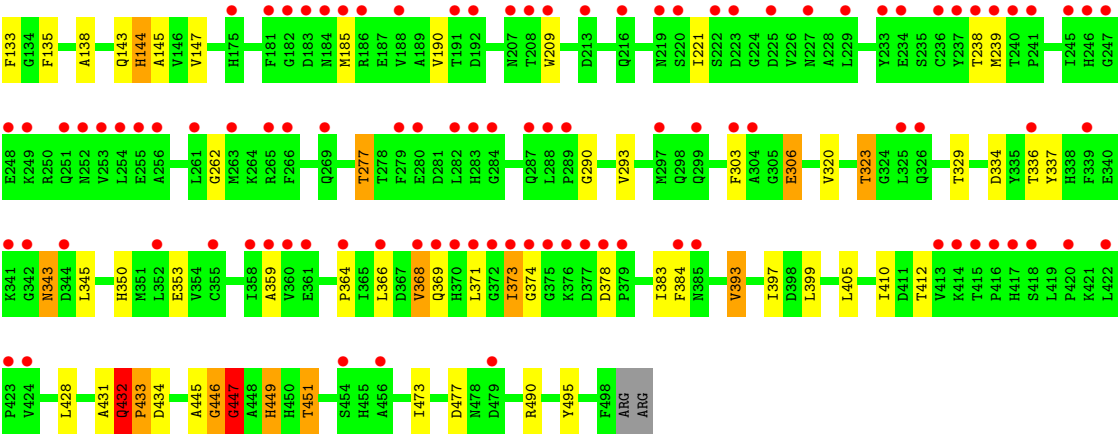


- Molecule 1: L-arabinose isomerase



- 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) 84.5 (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 0.223 , 0.209	Depositor DCC
R_{free} test set	2205 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.6	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44290 reflections	Xtriage
F_o, F_c correlation	0.93	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (240) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:432:GLN:HE21	1:A:478:ASN:CG	1.85	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:C:433:PRO:HD3	1:C:477:ASP:C	2.14	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: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
1:B:190:VAL:HG13	1:C:135:PHE:CG	2.36	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:102:GLN:NE2	1:C:104:HIS:HD2	2.05	0.55
1:B:326:GLN:O	1:B:327:GLY:O	2.25	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:B:337:TYR:OH	1:C:104:HIS:HE1	1.92	0.53
1:A:432:GLN:NE2	1:A:478:ASN:OD1	2.41	0.53
1:A:399:LEU:O	1:B:141:ARG:NH2	2.42	0.53
1:A:239:MET:SD	1:A:365:ILE:CG2	2.98	0.52
1:B:190:VAL:HG22	1:C:132:GLU:OE2	2.09	0.52
1:B:111:LEU:HD11	1:B:116:ILE:HD12	1.91	0.52
1:A:184:ASN:HD21	1:A:191:THR:C	2.13	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:B:80:LEU:CD1	1:B:130:GLY:HA2	2.40	0.51
1:A:2:THR:HG22	1:A:4:PHE:H	1.75	0.51
1:B:369:GLN:CB	1:B:378:ASP:CB	2.87	0.51
1:B:80:LEU:HD11	1:B:133:PHE:CB	2.40	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:B:446:GLY:HA2	1:C:138:ALA:HB3	1.93	0.51
1:A:320:VAL:O	1:A:323:THR:OG1	2.28	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:68:ASN:HD21	1:C:97:ASN:N	2.09	0.50
1:C:17:HIS:HB3	1:C:55:THR:HG22	1.94	0.50
1:C:68:ASN:ND2	1:C:97:ASN:H	2.10	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: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:C:80:LEU:HD11	1:C:133:PHE:CB	2.42	0.49
1:A:449:HIS:CB	1:B:128:HIS:HB2	2.37	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:318:MET:HA	1:A:321:MET:HE3	1.96	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:343:ASN:HD21	1:C:345:LEU:HD11	1.79	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:432:GLN:NE2	1:A:478:ASN:CG	2.63	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:B:367:ASP:O	1:B:369:GLN:HA	2.15	0.45
1:A:12:VAL:O	1:A:78:VAL: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:240:THR:HG21	1:A:366:LEU:HD13	1.99	0.45
1:A:120:PHE:HE2	1:A:124:ASN:HB2	1.80	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:C:397:ILE:HG21	1:C:447:GLY:CA	2.46	0.45
1:A:349:SER:OG	1:A:350:HIS:N	2.50	0.45
1:B:114:ASP:OD1	1:B:114:ASP:N	2.49	0.45
1:A:101:LEU:HD11	1:A:147:VAL:HG23	1.98	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:B:102:GLN:NE2	1:B:104:HIS:CD2	2.85	0.44
1:A:87:LYS:HA	1:A:90:ILE:HG12	1.99	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:B:330:SER:OG	1:B:331:PHE:O	2.34	0.44
1:A:121:MET:SD	1:A:125:GLN:OE1	2.76	0.44
1:C:125:GLN:HB2	1:C:128:HIS:CE1	2.53	0.44
1:B:120:PHE:O	1:B:123:LEU:O	2.35	0.44
1:C:410:ILE:HG22	1:C:431:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:82:THR:HG22	1:C:83:PHE:O	2.18	0.43
1:A:446:GLY:HA2	1:B:138:ALA:HB3	1.99	0.43
1:A:177:LYS:H	1:A:273:HIS:HD2	1.66	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:366:LEU:CD2	1:A:368:VAL:HB	2.49	0.42
1:A:176:LEU:HD23	1:A:176:LEU:C	2.39	0.42
1:C:320:VAL:O	1:C:323:THR:OG1	2.35	0.42
1:C:102:GLN:HE22	1:C:130:GLY:HA3	1.84	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: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:12:VAL:HG11	1:B:63:ILE:HG21	2.01	0.42
1:A:222:SER:O	1:A:226:VAL:HG23	2.20	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: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: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: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:B:494:VAL:HG23	1:C:495:TYR:HD1	1.85	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
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:B:244:GLN:O	1:B:250:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:215:VAL:HG21	1:A:284:GLY:HA3	2.02	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:C:101:LEU:HD12	1:C:145:ALA:HB3	2.03	0.41
1:A:106:GLN:HE22	1:C:336:THR:HG23	1.86	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:C:102:GLN:HE22	1:C:130:GLY:CA	2.33	0.41
1:A:76:LEU:HB2	1:A:100:LEU:HD12	2.02	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:B:239:MET:HE3	1:B:365:ILE:HD13	2.03	0.40
1:A:282:LEU:HD21	1:A:288:LEU:HD13	2.04	0.40
1:C:80:LEU:CD1	1:C:133:PHE:CB	2.99	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

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	496/500 (99%)	456 (92%)	30 (6%)	10 (2%)	11	21
1	B	497/500 (99%)	465 (94%)	22 (4%)	10 (2%)	11	21
1	C	496/500 (99%)	467 (94%)	17 (3%)	12 (2%)	9	16
All	All	1489/1500 (99%)	1388 (93%)	69 (5%)	32 (2%)	10	19

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%)	19 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	406/419 (97%)	378 (93%)	28 (7%)	22	42
1	C	363/419 (87%)	343 (94%)	20 (6%)	30	56
All	All	1165/1257 (93%)	1087 (93%)	78 (7%)	24	44

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	C	287	GLN
1	C	298	GLN
1	C	343	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.02	24 (4%)	29 26	58, 66, 72, 81	0
1	B	498/500 (99%)	-0.08	14 (2%)	50 48	59, 66, 72, 82	0
1	C	498/500 (99%)	0.87	101 (20%)	1 1	58, 68, 71, 76	0
All	All	1494/1500 (99%)	0.27	139 (9%)	9 6	58, 67, 71, 82	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	237	TYR	12.8
1	C	246	HIS	12.0
1	C	245	ILE	9.6
1	C	238	THR	7.9
1	C	233	TYR	7.6
1	C	247	GLY	7.0
1	C	299	GLN	7.0
1	C	252	ASN	6.8
1	C	241	PRO	6.8
1	C	236	CYS	6.6
1	C	416	PRO	6.5
1	C	213	ASP	6.1
1	C	234	GLU	6.0
1	C	373	ILE	5.5
1	C	375	GLY	5.2
1	C	385	ASN	5.2
1	C	423	PRO	5.1
1	C	370	HIS	4.9
1	C	374	GLY	4.9
1	C	240	THR	4.9
1	C	209	TRP	4.8
1	C	248	GLU	4.8
1	C	253	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	417	HIS	4.7
1	C	372	GLY	4.6
1	C	360	VAL	4.5
1	A	128	HIS	4.4
1	B	248	GLU	4.4
1	C	219	ASN	4.3
1	C	420	PRO	4.2
1	C	229	LEU	4.1
1	C	342	GLY	4.0
1	C	184	ASN	4.0
1	B	360	VAL	3.9
1	A	248	GLU	3.9
1	A	18	LEU	3.9
1	C	288	LEU	3.9
1	C	216	GLN	3.9
1	A	123	LEU	3.8
1	C	188	VAL	3.8
1	C	185	MET	3.8
1	B	241	PRO	3.8
1	C	279	PHE	3.7
1	C	369	GLN	3.6
1	C	304	ALA	3.6
1	A	124	ASN	3.6
1	C	377	ASP	3.6
1	C	182	GLY	3.6
1	C	192	ASP	3.5
1	B	498	PHE	3.5
1	C	364	PRO	3.5
1	C	181	PHE	3.5
1	C	378	ASP	3.4
1	A	117	ASP	3.4
1	C	223	ASP	3.4
1	C	326	GLN	3.4
1	C	239	MET	3.3
1	C	191	THR	3.3
1	C	227	ASN	3.2
1	A	498	PHE	3.2
1	C	222	SER	3.2
1	C	256	ALA	3.2
1	C	371	LEU	3.2
1	C	283	HIS	3.2
1	C	454	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	422	LEU	3.1
1	C	359	ALA	3.1
1	C	376	LYS	3.1
1	A	83	PHE	3.1
1	A	1	MET	3.1
1	C	303	PHE	3.1
1	C	341	LYS	3.1
1	C	352	LEU	3.0
1	C	287	GLN	3.0
1	B	420	PRO	3.0
1	C	208	THR	2.9
1	A	125	GLN	2.9
1	A	112	PRO	2.9
1	C	183	ASP	2.9
1	C	368	VAL	2.9
1	C	269	GLN	2.9
1	A	19	TYR	2.9
1	B	370	HIS	2.9
1	C	251	GLN	2.9
1	C	220	SER	2.8
1	C	255	GLU	2.8
1	C	424	VAL	2.8
1	A	16	GLN	2.8
1	C	413	VAL	2.8
1	C	263	MET	2.8
1	C	254	LEU	2.7
1	C	418	SER	2.7
1	A	360	VAL	2.7
1	C	456	ALA	2.7
1	C	297	MET	2.7
1	C	261	LEU	2.7
1	C	186	ARG	2.7
1	A	118	MET	2.7
1	C	361	GLU	2.6
1	C	414	LYS	2.6
1	B	17	HIS	2.6
1	C	339	PHE	2.6
1	C	479	ASP	2.5
1	C	265	ARG	2.5
1	C	266	PHE	2.5
1	A	127	ALA	2.5
1	A	78	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	366	LEU	2.5
1	C	379	PRO	2.5
1	C	207	ASN	2.5
1	A	370	HIS	2.4
1	C	415	THR	2.4
1	C	336	THR	2.4
1	A	121	MET	2.4
1	B	377	ASP	2.3
1	C	325	LEU	2.3
1	A	246	HIS	2.3
1	A	116	ILE	2.3
1	A	141	ARG	2.3
1	B	245	ILE	2.3
1	C	384	PHE	2.3
1	C	249	LYS	2.3
1	C	225	ASP	2.3
1	C	289	PRO	2.2
1	C	284	GLY	2.2
1	C	280	GLU	2.2
1	B	361	GLU	2.1
1	C	358	ILE	2.1
1	A	81	HIS	2.1
1	B	417	HIS	2.1
1	C	344	ASP	2.1
1	B	21	PRO	2.0
1	B	359	ALA	2.0
1	C	1	MET	2.0
1	C	282	LEU	2.0
1	A	21	PRO	2.0
1	C	355	CYS	2.0
1	C	175	HIS	2.0
1	B	341	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.