Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 05:16 PM JST

PDB ID	:	7D1I
Title	:	Crystal structure of acinetobacter baumannii MurG
Authors	:	Park, H.H.; Jeong, k.H.
Deposited on	:	2020-09-14
Resolution	:	3.49 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:

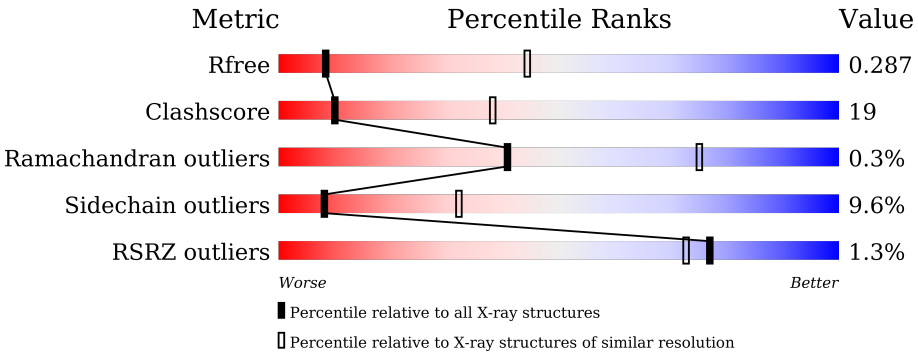
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 <=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	365	64% 26% • • 5%
1	B	365	58% 28% • 9%
1	C	365	59% 32% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7702 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 UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase.

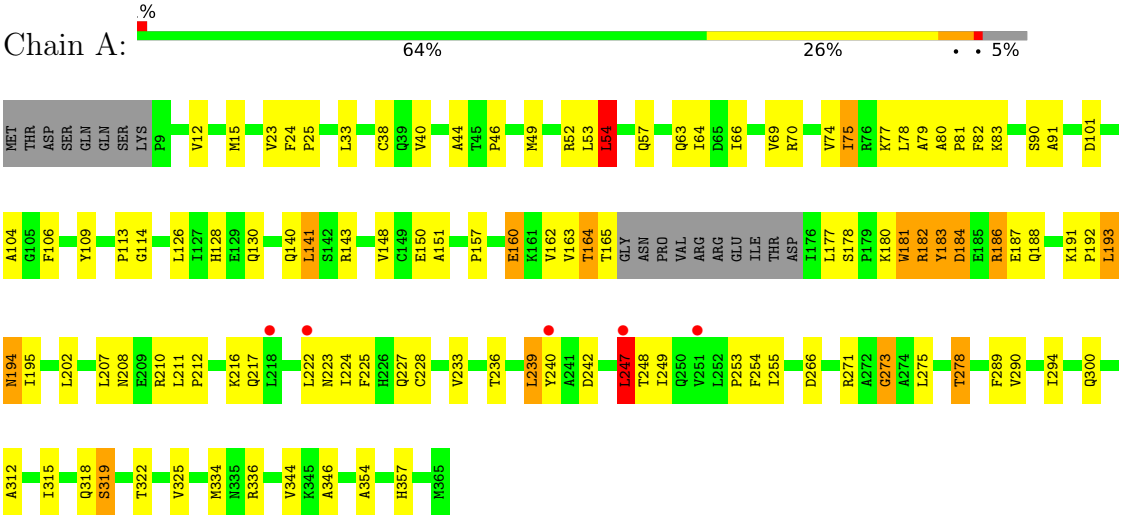
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2624	1673	460	475	16			
1	B	332	Total	C	N	O	S	0	0	0
			2489	1587	435	451	16			
1	C	343	Total	C	N	O	S	0	0	0
			2589	1650	456	467	16			

3 Residue-property plots (i)

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.

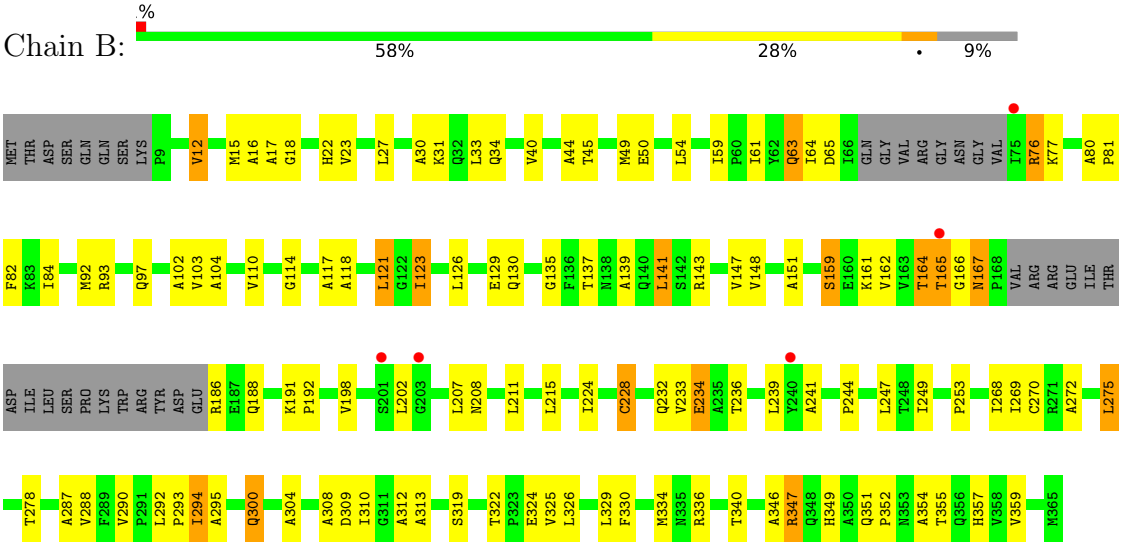
• Molecule 1: UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase

Chain A:



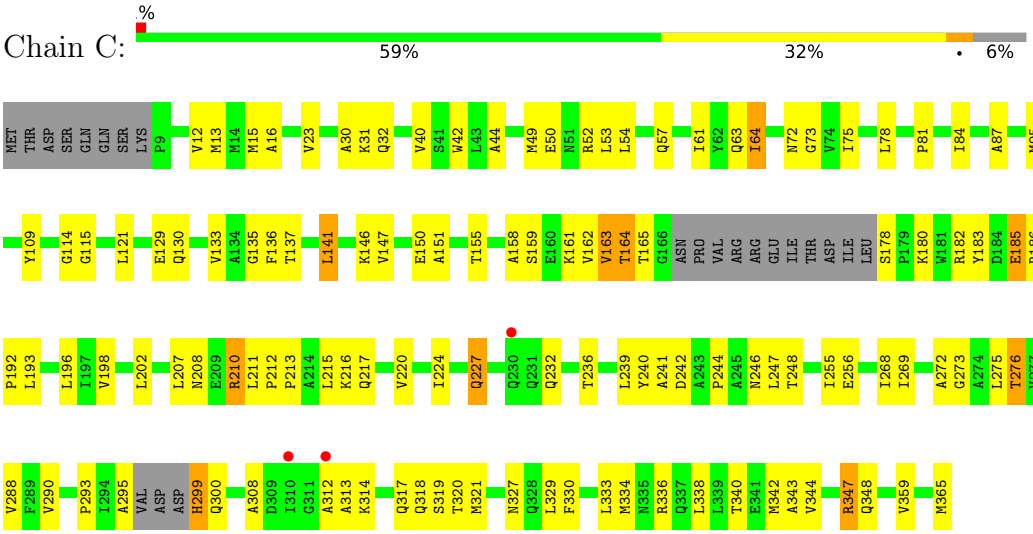
• Molecule 1: UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase

Chain B:



• Molecule 1: UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase

Chain C:


%
59%
32%
6%
MET THR ASP SER GLN GLN SER LYS P9 V12 M13 M14 M15 A16 V23 A30 K31 Q32 V40 S41 W42 L43 A44 M49 E50 N51 R52 L53 L54 Q57 I61 Y62 Q63 I64 N72 G73 V74 I75 L78 P81 I84 A87 M95 V103 F106
Y109 G114 G115 L121 E129 Q130 V133 A134 G135 F136 T137 L141 K146 V147 E150 A151 T155 A158 S159 E160 K161 V162 V163 T164 T165 G166 ASN PRO VAL ARG ARG GLU ILE THR ASP ILE LEU S178 P179 K180 W181 R182 Y183 D184 E185 R186 E187 Q188 K191
P192 L193 L196 I197 V198 L202 L207 N208 E209 R210 L211 P212 P213 A214 L215 K216 Q217 V220 I224 Q227 Q230 Q231 Q232 T236 L239 Y240 A241 D242 A243 P244 A245 N246 L247 T248 I255 E256 I268 I269 A272 G273 A274 L275 T276 V277 T278 G284
V288 F289 V290 P293 I294 A295 VAL ASP ASP H299 Q300 A308 D309 I310 G311 A312 A313 K314 Q317 Q318 S319 T320 M321 N327 Q328 L329 F330 L333 M334 N335 R336 Q337 L338 L339 T340 E341 M342 A343 V344 R347 Q348 V359 M365

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	182.91Å 182.91Å 156.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 3.49 48.26 – 3.49	Depositor EDS
% Data completeness (in resolution range)	90.6 (48.26-3.49) 90.7 (48.26-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.261 , 0.298 0.252 , 0.287	Depositor DCC
R_{free} test set	1511 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7702	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.48	0/2671	0.72	3/3628 (0.1%)
1	B	0.50	0/2532	0.73	3/3441 (0.1%)
1	C	0.53	2/2635 (0.1%)	0.76	1/3576 (0.0%)
All	All	0.51	2/7838 (0.0%)	0.74	7/10645 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	GLU	CG-CD	5.92	1.60	1.51
1	C	187	GLU	CB-CG	5.27	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	GLY	N-CA-C	6.99	130.58	113.10
1	C	239	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	247	LEU	CA-CB-CG	5.51	127.96	115.30
1	A	54	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	159	SER	N-CA-C	5.39	125.55	111.00
1	B	347	ARG	CA-CB-CG	5.14	124.71	113.40
1	A	157	PRO	N-CA-C	5.03	125.18	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	295	ALA	Peptide

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	2624	0	2706	111	0
1	B	2489	0	2563	94	0
1	C	2589	0	2669	104	0
All	All	7702	0	7938	297	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 19.

All (297) 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:158:ALA:CB	1:C:161:LYS:HE2	1.01	1.49
1:C:158:ALA:HB3	1:C:161:LYS:CE	0.98	1.45
1:A:70:ARG:HG2	1:A:77:LYS:HG3	1.32	1.09
1:A:193:LEU:HD13	1:A:334:MET:HE3	1.32	1.08
1:A:195:ILE:HD11	1:A:224:ILE:HG12	1.33	1.07
1:C:158:ALA:CB	1:C:161:LYS:CE	1.77	1.06
1:A:195:ILE:HD11	1:A:224:ILE:CG1	1.87	1.05
1:C:284:GLY:O	1:C:343:ALA:HB1	1.56	1.05
1:A:195:ILE:CD1	1:A:224:ILE:HA	1.87	1.04
1:A:69:VAL:O	1:A:70:ARG:HG3	1.61	1.01
1:B:207:LEU:HD21	1:B:290:VAL:HG11	1.43	1.00
1:A:191:LYS:HD2	1:A:192:PRO:HD2	1.43	0.98
1:C:158:ALA:HB2	1:C:161:LYS:CE	1.95	0.96
1:A:195:ILE:HD11	1:A:224:ILE:HA	1.45	0.94
1:C:158:ALA:HB3	1:C:161:LYS:HE3	1.48	0.94
1:C:158:ALA:CB	1:C:161:LYS:HE3	1.98	0.91
1:A:212:PRO:HB3	1:A:240:TYR:CD1	2.06	0.90
1:A:207:LEU:HD21	1:A:290:VAL:HG11	1.52	0.88
1:A:193:LEU:HD13	1:A:334:MET:CE	2.06	0.85
1:A:195:ILE:HD11	1:A:224:ILE:CA	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HD11	1:A:224:ILE:CB	2.07	0.84
1:A:195:ILE:CD1	1:A:224:ILE:HG12	2.06	0.84
1:A:69:VAL:C	1:A:70:ARG:HG3	1.94	0.83
1:A:212:PRO:HB3	1:A:240:TYR:CE1	2.15	0.82
1:C:295:ALA:HB1	1:C:299:HIS:HD1	1.44	0.82
1:C:158:ALA:HB3	1:C:161:LYS:CD	2.09	0.82
1:A:23:VAL:HG11	1:A:53:LEU:HD12	1.62	0.81
1:C:158:ALA:CB	1:C:161:LYS:NZ	2.43	0.81
1:A:182:ARG:O	1:A:186:ARG:HB2	1.81	0.81
1:A:240:TYR:CD2	1:A:249:ILE:HG21	2.16	0.81
1:A:195:ILE:O	1:A:195:ILE:HD12	1.81	0.81
1:B:292:LEU:H	1:B:300:GLN:HG2	1.45	0.81
1:C:158:ALA:H	1:C:161:LYS:HE3	1.46	0.81
1:A:69:VAL:O	1:A:70:ARG:CG	2.29	0.81
1:A:195:ILE:HD12	1:A:224:ILE:HA	1.63	0.80
1:B:151:ALA:HA	1:B:164:THR:O	1.83	0.79
1:B:165:THR:H	1:B:354:ALA:HB2	1.45	0.79
1:C:312:ALA:HB3	1:C:342:MET:HA	1.66	0.78
1:A:225:PHE:HE2	1:A:255:ILE:HD12	1.50	0.77
1:A:143:ARG:NH1	1:B:319:SER:O	2.16	0.77
1:B:208:ASN:HB3	1:B:236:THR:HG21	1.65	0.77
1:C:158:ALA:HB1	1:C:161:LYS:HE2	1.56	0.76
1:C:158:ALA:HB2	1:C:161:LYS:NZ	2.01	0.74
1:A:183:TYR:O	1:A:187:GLU:HG2	1.87	0.74
1:B:16:ALA:O	1:B:50:GLU:HG2	1.87	0.73
1:C:182:ARG:HE	1:C:186:ARG:HB2	1.55	0.71
1:A:273:GLY:N	1:A:300:GLN:OE1	2.20	0.71
1:C:31:LYS:NZ	1:C:57:GLN:O	2.24	0.71
1:A:148:VAL:O	1:A:160:GLU:HB2	1.91	0.70
1:C:49:MET:SD	1:C:52:ARG:NH2	2.63	0.70
1:B:228:CYS:SG	1:B:236:THR:OG1	2.50	0.69
1:C:216:LYS:HD2	1:C:242:ASP:O	1.92	0.68
1:A:188:GLN:HB2	1:A:336:ARG:HH12	1.58	0.68
1:A:12:VAL:HG21	1:A:33:LEU:HD13	1.76	0.67
1:C:208:ASN:HD22	1:C:232:GLN:HG2	1.59	0.67
1:A:212:PRO:CB	1:A:240:TYR:CE1	2.78	0.67
1:A:78:LEU:HD23	1:A:83:LYS:HD2	1.77	0.66
1:C:227:GLN:HG3	1:C:255:ILE:HG13	1.76	0.66
1:B:18:GLY:N	1:B:50:GLU:HG3	2.10	0.66
1:C:72:ASN:OD1	1:C:73:GLY:N	2.28	0.66
1:C:269:ILE:HG23	1:C:288:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ASN:HB2	1:B:275:LEU:HD11	1.77	0.65
1:B:129:GLU:OE1	1:B:135:GLY:N	2.26	0.65
1:C:312:ALA:HB1	1:C:342:MET:HG2	1.79	0.65
1:B:268:ILE:CG2	1:B:287:ALA:HB2	2.26	0.65
1:B:236:THR:HA	1:B:239:LEU:HD12	1.79	0.64
1:B:215:LEU:HD21	1:B:224:ILE:HD11	1.80	0.64
1:C:295:ALA:O	1:C:299:HIS:HB3	1.98	0.63
1:B:312:ALA:HB1	1:B:346:ALA:HB2	1.80	0.63
1:A:191:LYS:CD	1:A:192:PRO:HD2	2.26	0.63
1:C:220:VAL:O	1:C:246:ASN:ND2	2.31	0.63
1:A:187:GLU:O	1:A:188:GLN:NE2	2.32	0.62
1:C:106:PHE:O	1:C:130:GLN:NE2	2.33	0.62
1:B:93:ARG:O	1:B:97:GLN:HG2	2.00	0.62
1:A:183:TYR:O	1:A:183:TYR:HD1	1.82	0.62
1:B:247:LEU:HD11	1:B:249:ILE:HD11	1.82	0.61
1:B:310:ILE:HD13	1:B:349:HIS:ND1	2.14	0.61
1:C:308:ALA:HA	1:C:313:ALA:O	2.00	0.61
1:B:15:MET:HE2	1:B:114:GLY:HA3	1.81	0.61
1:C:165:THR:HG21	1:C:278:THR:HG21	1.82	0.61
1:B:233:VAL:HG21	1:B:253:PRO:HG3	1.83	0.61
1:C:158:ALA:N	1:C:161:LYS:HE3	2.15	0.61
1:C:188:GLN:HB2	1:C:336:ARG:HH12	1.66	0.61
1:C:150:GLU:HG2	1:C:162:VAL:O	2.01	0.60
1:A:49:MET:HE2	1:A:52:ARG:NH2	2.17	0.60
1:A:312:ALA:HB1	1:A:346:ALA:HB2	1.82	0.60
1:B:76:ARG:HH11	1:B:77:LYS:H	1.49	0.60
1:C:182:ARG:HD3	1:C:284:GLY:O	2.01	0.60
1:A:182:ARG:HD2	1:A:183:TYR:H	1.66	0.60
1:A:319:SER:O	1:B:143:ARG:NH2	2.35	0.60
1:B:12:VAL:HG21	1:B:33:LEU:HD13	1.84	0.60
1:B:165:THR:N	1:B:354:ALA:HB2	2.16	0.59
1:B:268:ILE:HG22	1:B:287:ALA:HB2	1.83	0.59
1:A:319:SER:HB2	1:B:139:ALA:HB1	1.83	0.59
1:B:308:ALA:HA	1:B:313:ALA:O	2.02	0.59
1:A:194:ASN:HD21	1:A:223:ASN:ND2	2.00	0.59
1:A:182:ARG:HG2	1:A:344:VAL:HA	1.84	0.59
1:C:288:VAL:HG21	1:C:329:LEU:HD21	1.84	0.59
1:A:208:ASN:HB3	1:A:236:THR:CG2	2.32	0.58
1:B:322:THR:HG22	1:B:325:VAL:HG13	1.86	0.58
1:C:295:ALA:HB1	1:C:299:HIS:ND1	2.15	0.58
1:A:227:GLN:HB2	1:A:255:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LYS:HG2	1:C:192:PRO:HD2	1.85	0.57
1:C:207:LEU:HD11	1:C:290:VAL:HG11	1.87	0.57
1:A:182:ARG:HD3	1:A:344:VAL:HG22	1.87	0.57
1:B:34:GLN:OE1	1:B:59:ILE:HG22	2.05	0.57
1:C:163:VAL:O	1:C:164:THR:HG23	2.04	0.57
1:A:208:ASN:HB3	1:A:236:THR:HG21	1.86	0.57
1:A:46:PRO:HA	1:A:63:GLN:OE1	2.06	0.56
1:A:195:ILE:CD1	1:A:224:ILE:HG23	2.36	0.56
1:C:15:MET:HE2	1:C:114:GLY:HA3	1.88	0.56
1:B:22:HIS:HA	1:B:130:GLN:HE22	1.70	0.56
1:A:188:GLN:HB2	1:A:336:ARG:NH1	2.21	0.56
1:C:208:ASN:HB3	1:C:236:THR:HG21	1.88	0.56
1:B:148:VAL:O	1:B:161:LYS:HA	2.06	0.56
1:C:146:LYS:HD3	1:C:365:MET:HG2	1.88	0.55
1:B:310:ILE:HD13	1:B:349:HIS:CE1	2.42	0.55
1:C:208:ASN:HB3	1:C:236:THR:CG2	2.36	0.55
1:A:212:PRO:HG3	1:A:240:TYR:CE1	2.43	0.54
1:C:16:ALA:O	1:C:50:GLU:HG2	2.07	0.54
1:A:233:VAL:HG21	1:A:253:PRO:HG3	1.90	0.54
1:B:292:LEU:N	1:B:300:GLN:HG2	2.19	0.54
1:A:106:PHE:O	1:A:130:GLN:NE2	2.41	0.54
1:A:182:ARG:CD	1:A:182:ARG:H	2.21	0.54
1:B:322:THR:HG22	1:B:325:VAL:HG22	1.90	0.53
1:A:33:LEU:O	1:A:38:CYS:HB2	2.08	0.53
1:B:186:ARG:HD2	1:B:340:THR:OG1	2.08	0.53
1:A:271:ARG:NH2	1:A:318:GLN:OE1	2.42	0.53
1:C:23:VAL:HG11	1:C:53:LEU:HD12	1.91	0.53
1:A:322:THR:H	1:A:325:VAL:HG22	1.74	0.53
1:C:150:GLU:HB2	1:C:155:THR:OG1	2.09	0.53
1:B:84:ILE:HD11	1:C:81:PRO:HB3	1.92	0.52
1:C:284:GLY:HA3	1:C:347:ARG:HB2	1.91	0.52
1:A:182:ARG:CD	1:A:182:ARG:N	2.73	0.52
1:A:289:PHE:HB2	1:A:315:ILE:HG22	1.90	0.52
1:B:30:ALA:HB1	1:B:40:VAL:HG11	1.91	0.52
1:B:355:THR:O	1:B:359:VAL:HG23	2.08	0.52
1:B:82:PHE:HB3	1:C:136:PHE:CD2	2.43	0.52
1:C:16:ALA:HB3	1:C:42:TRP:HE1	1.75	0.52
1:A:15:MET:HE2	1:A:114:GLY:HA3	1.91	0.52
1:C:150:GLU:HG3	1:C:163:VAL:HG13	1.91	0.52
1:A:150:GLU:HG3	1:A:162:VAL:HG13	1.90	0.52
1:A:193:LEU:O	1:A:266:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:HA	1:A:223:ASN:O	2.10	0.51
1:A:294:ILE:HG13	1:C:75:ILE:HG12	1.92	0.51
1:B:186:ARG:HG3	1:B:186:ARG:O	2.09	0.51
1:C:158:ALA:CA	1:C:161:LYS:CE	2.77	0.51
1:B:81:PRO:HB2	1:C:109:TYR:HD1	1.75	0.51
1:C:188:GLN:HB2	1:C:336:ARG:NH1	2.26	0.51
1:A:44:ALA:O	1:A:63:GLN:HA	2.11	0.51
1:A:184:ASP:N	1:A:184:ASP:OD1	2.44	0.51
1:B:93:ARG:HG3	1:B:97:GLN:HE21	1.75	0.50
1:A:163:VAL:HG11	1:A:357:HIS:CD2	2.47	0.50
1:A:211:LEU:HB3	1:A:212:PRO:HD3	1.92	0.50
1:B:191:LYS:HB3	1:B:336:ARG:HH22	1.76	0.50
1:B:12:VAL:HA	1:B:102:ALA:O	2.12	0.50
1:B:324:GLU:OE1	1:B:324:GLU:N	2.45	0.50
1:A:25:PRO:HG3	1:A:275:LEU:HD21	1.93	0.49
1:B:44:ALA:O	1:B:63:GLN:HA	2.12	0.49
1:B:188:GLN:HA	1:B:336:ARG:NH1	2.27	0.49
1:C:338:LEU:O	1:C:342:MET:HG3	2.11	0.49
1:A:54:LEU:HA	1:A:57:GLN:HG3	1.95	0.49
1:A:194:ASN:HD21	1:A:223:ASN:HD22	1.60	0.49
1:A:216:LYS:HE2	1:A:239:LEU:O	2.13	0.49
1:B:22:HIS:HA	1:B:130:GLN:NE2	2.28	0.49
1:A:182:ARG:O	1:A:186:ARG:CB	2.58	0.49
1:C:165:THR:HG21	1:C:278:THR:CG2	2.43	0.49
1:B:23:VAL:O	1:B:27:LEU:N	2.34	0.48
1:B:137:THR:O	1:B:141:LEU:HB2	2.12	0.48
1:A:217:GLN:HG3	1:A:217:GLN:O	2.12	0.48
1:A:165:THR:O	1:A:278:THR:HG21	2.13	0.48
1:A:195:ILE:HD11	1:A:224:ILE:CG2	2.43	0.48
1:C:210:ARG:C	1:C:213:PRO:HD2	2.34	0.48
1:C:13:MET:CE	1:C:95:MET:HG2	2.44	0.48
1:C:30:ALA:HB1	1:C:40:VAL:HG11	1.94	0.48
1:B:130:GLN:HA	1:B:151:ALA:HB2	1.95	0.48
1:A:181:TRP:CD1	1:A:181:TRP:N	2.81	0.48
1:B:17:ALA:HA	1:B:50:GLU:OE2	2.14	0.48
1:B:268:ILE:CG2	1:B:287:ALA:CB	2.91	0.48
1:C:64:ILE:HG13	1:C:87:ALA:HB1	1.95	0.48
1:A:336:ARG:O	1:A:336:ARG:HG3	2.14	0.48
1:B:322:THR:H	1:B:325:VAL:HG22	1.77	0.48
1:C:151:ALA:HA	1:C:164:THR:O	2.14	0.47
1:A:194:ASN:ND2	1:A:223:ASN:ND2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:PRO:HG3	1:C:240:TYR:CZ	2.50	0.47
1:C:272:ALA:O	1:C:300:GLN:HG3	2.14	0.47
1:C:44:ALA:O	1:C:63:GLN:HA	2.14	0.47
1:A:128:HIS:CE1	1:A:130:GLN:HG3	2.49	0.47
1:A:240:TYR:CD2	1:A:249:ILE:CG2	2.95	0.47
1:C:186:ARG:HG2	1:C:340:THR:CG2	2.45	0.46
1:B:76:ARG:NH1	1:B:77:LYS:O	2.47	0.46
1:C:186:ARG:HG2	1:C:340:THR:HG23	1.98	0.46
1:C:224:ILE:HD12	1:C:247:LEU:HD23	1.98	0.46
1:B:330:PHE:O	1:B:334:MET:HG2	2.14	0.46
1:A:212:PRO:HA	1:A:240:TYR:HE1	1.81	0.46
1:B:92:MET:HE2	1:B:117:ALA:HA	1.97	0.46
1:B:198:VAL:HG22	1:B:270:CYS:HB3	1.97	0.46
1:C:198:VAL:O	1:C:198:VAL:HG23	2.16	0.45
1:A:64:ILE:HG21	1:A:91:ALA:HB2	1.98	0.45
1:A:194:ASN:ND2	1:A:223:ASN:HD22	2.13	0.45
1:B:81:PRO:HG3	1:C:84:ILE:HD11	1.98	0.45
1:C:115:GLY:HA3	1:C:141:LEU:HD21	1.98	0.45
1:A:224:ILE:HD12	1:A:249:ILE:HG12	1.98	0.45
1:B:207:LEU:O	1:B:211:LEU:HB2	2.16	0.45
1:C:344:VAL:O	1:C:348:GLN:HG2	2.15	0.45
1:B:272:ALA:CB	1:B:304:ALA:HB2	2.46	0.45
1:B:287:ALA:O	1:B:313:ALA:HB1	2.16	0.45
1:C:32:GLN:HG2	1:C:359:VAL:HG21	1.98	0.45
1:C:186:ARG:O	1:C:186:ARG:HG3	2.17	0.45
1:C:196:LEU:O	1:C:268:ILE:HA	2.17	0.45
1:A:163:VAL:HG11	1:A:357:HIS:CG	2.52	0.45
1:A:183:TYR:HD1	1:A:187:GLU:HG2	1.33	0.45
1:A:195:ILE:HD11	1:A:224:ILE:HG23	1.99	0.45
1:A:66:ILE:HD11	1:A:113:PRO:HG2	1.99	0.45
1:B:76:ARG:HD2	1:B:76:ARG:HA	1.69	0.45
1:A:182:ARG:HD2	1:A:183:TYR:N	2.31	0.45
1:A:104:ALA:HA	1:A:126:LEU:O	2.17	0.44
1:A:177:LEU:H	1:A:177:LEU:HG	1.64	0.44
1:B:80:ALA:HB3	1:B:81:PRO:HD3	1.99	0.44
1:B:322:THR:CG2	1:B:325:VAL:HG13	2.47	0.44
1:C:193:LEU:HD11	1:C:334:MET:O	2.17	0.44
1:B:294:ILE:O	1:B:294:ILE:HG22	2.17	0.44
1:C:207:LEU:O	1:C:211:LEU:HD23	2.17	0.44
1:C:273:GLY:HA3	1:C:276:THR:HG23	2.00	0.44
1:B:54:LEU:HB2	1:B:61:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLN:HA	1:B:352:PRO:HD2	1.81	0.44
1:C:54:LEU:HB2	1:C:61:ILE:HD11	2.00	0.44
1:B:18:GLY:HA3	1:B:49:MET:HB3	1.99	0.44
1:C:150:GLU:OE2	1:C:163:VAL:HG22	2.18	0.44
1:A:46:PRO:HD3	1:A:64:ILE:O	2.18	0.43
1:A:271:ARG:HD3	1:A:290:VAL:O	2.18	0.43
1:C:217:GLN:O	1:C:217:GLN:HG2	2.18	0.43
1:B:292:LEU:HD12	1:B:293:PRO:HD2	1.99	0.43
1:B:322:THR:HG23	1:B:324:GLU:H	1.84	0.43
1:C:72:ASN:HB3	1:C:75:ILE:HG22	2.00	0.43
1:A:182:ARG:H	1:A:182:ARG:NE	2.16	0.43
1:C:129:GLU:OE1	1:C:135:GLY:N	2.41	0.43
1:A:224:ILE:HD12	1:A:247:LEU:HD12	2.01	0.43
1:A:191:LYS:HD3	1:A:191:LYS:HA	1.69	0.43
1:B:82:PHE:CD1	1:C:136:PHE:HD2	2.37	0.43
1:B:121:LEU:HD12	1:B:121:LEU:HA	1.76	0.43
1:A:140:GLN:OE1	1:A:143:ARG:NH2	2.52	0.43
1:B:164:THR:HG21	1:B:357:HIS:HB3	2.00	0.43
1:C:182:ARG:HH21	1:C:186:ARG:HD3	1.84	0.43
1:A:195:ILE:HD12	1:A:195:ILE:C	2.39	0.43
1:A:322:THR:OG1	1:A:325:VAL:HG13	2.19	0.43
1:C:293:PRO:HG3	1:C:318:GLN:NE2	2.34	0.43
1:B:241:ALA:O	1:B:244:PRO:HD3	2.19	0.43
1:C:95:MET:HB2	1:C:121:LEU:CD1	2.49	0.43
1:C:31:LYS:HD3	1:C:31:LYS:HA	1.96	0.43
1:C:317:GLN:HB3	1:C:320:THR:HG22	2.01	0.43
1:A:207:LEU:O	1:A:211:LEU:HB2	2.19	0.42
1:B:82:PHE:CD1	1:C:136:PHE:HB3	2.54	0.42
1:C:64:ILE:HD13	1:C:64:ILE:HG21	1.77	0.42
1:A:75:ILE:O	1:A:75:ILE:HG22	2.18	0.42
1:B:82:PHE:HE1	1:C:137:THR:HG1	1.63	0.42
1:C:158:ALA:CA	1:C:161:LYS:HE3	2.49	0.42
1:C:330:PHE:O	1:C:334:MET:HG2	2.19	0.42
1:A:228:CYS:SG	1:A:233:VAL:HA	2.59	0.42
1:C:312:ALA:CB	1:C:342:MET:HG2	2.48	0.42
1:A:130:GLN:HA	1:A:151:ALA:HB2	2.00	0.42
1:B:272:ALA:HB3	1:B:300:GLN:HG3	2.00	0.42
1:A:24:PHE:CE1	1:A:53:LEU:HD13	2.55	0.42
1:A:164:THR:O	1:A:354:ALA:HB3	2.20	0.42
1:A:212:PRO:CG	1:A:240:TYR:CE1	3.03	0.42
1:A:227:GLN:NE2	1:A:254:PHE:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ALA:HA	1:B:126:LEU:O	2.20	0.42
1:C:182:ARG:HD3	1:C:343:ALA:HB1	2.02	0.42
1:B:82:PHE:CE1	1:C:136:PHE:HB3	2.55	0.42
1:B:288:VAL:HG21	1:B:329:LEU:HD21	2.01	0.42
1:C:78:LEU:HD12	1:C:78:LEU:HA	1.84	0.42
1:B:92:MET:HG3	1:B:121:LEU:HD13	2.02	0.41
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.92	0.41
1:B:45:THR:HG23	1:B:110:VAL:HG22	2.02	0.41
1:A:80:ALA:N	1:A:81:PRO:HD2	2.36	0.41
1:B:191:LYS:HG2	1:B:192:PRO:HD2	2.02	0.41
1:B:103:VAL:HG11	1:B:118:ALA:CB	2.50	0.41
1:B:269:ILE:HG23	1:B:288:VAL:HG13	2.03	0.41
1:C:130:GLN:HA	1:C:151:ALA:HB2	2.03	0.41
1:C:288:VAL:HA	1:C:314:LYS:O	2.20	0.41
1:A:141:LEU:HA	1:A:141:LEU:HD12	1.82	0.41
1:C:187:GLU:O	1:C:188:GLN:OE1	2.39	0.41
1:C:241:ALA:O	1:C:244:PRO:HD3	2.20	0.41
1:A:212:PRO:HG3	1:A:240:TYR:CZ	2.56	0.41
1:B:234:GLU:H	1:B:234:GLU:HG2	1.44	0.41
1:B:322:THR:CG2	1:B:325:VAL:H	2.34	0.41
1:A:49:MET:HE2	1:A:52:ARG:HH22	1.82	0.41
1:B:215:LEU:HD21	1:B:224:ILE:CD1	2.50	0.41
1:B:247:LEU:O	1:B:247:LEU:HD12	2.21	0.41
1:C:95:MET:HE1	1:C:114:GLY:O	2.21	0.41
1:A:79:ALA:HB3	1:A:82:PHE:HD1	1.86	0.41
1:B:272:ALA:HB2	1:B:304:ALA:HB2	2.03	0.40
1:B:118:ALA:HB1	1:B:123:ILE:HG13	2.03	0.40
1:C:317:GLN:O	1:C:321:MET:HB2	2.22	0.40
1:B:162:VAL:HG22	1:B:162:VAL:O	2.21	0.40
1:C:13:MET:HE1	1:C:95:MET:HG2	2.03	0.40
1:C:215:LEU:HD23	1:C:215:LEU:HA	1.87	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	343/365 (94%)	330 (96%)	11 (3%)	2 (1%)	25 63
1	B	326/365 (89%)	314 (96%)	11 (3%)	1 (0%)	41 75
1	C	337/365 (92%)	326 (97%)	11 (3%)	0	100 100
All	All	1006/1095 (92%)	970 (96%)	33 (3%)	3 (0%)	41 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	ILE
1	A	273	GLY
1	A	178	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	275/292 (94%)	248 (90%)	27 (10%)	8 31
1	B	260/292 (89%)	237 (91%)	23 (9%)	10 36
1	C	270/292 (92%)	243 (90%)	27 (10%)	7 30
All	All	805/876 (92%)	728 (90%)	77 (10%)	8 32

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	54	LEU
1	A	74	VAL
1	A	75	ILE
1	A	90	SER
1	A	101	ASP
1	A	109	TYR

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Mol	Chain	Res	Type
1	A	141	LEU
1	A	160	GLU
1	A	164	THR
1	A	180	LYS
1	A	181	TRP
1	A	182	ARG
1	A	183	TYR
1	A	184	ASP
1	A	186	ARG
1	A	193	LEU
1	A	194	ASN
1	A	202	LEU
1	A	210	ARG
1	A	222	LEU
1	A	239	LEU
1	A	242	ASP
1	A	247	LEU
1	A	248	THR
1	A	278	THR
1	A	319	SER
1	B	12	VAL
1	B	31	LYS
1	B	63	GLN
1	B	64	ILE
1	B	65	ASP
1	B	76	ARG
1	B	121	LEU
1	B	123	ILE
1	B	141	LEU
1	B	147	VAL
1	B	159	SER
1	B	164	THR
1	B	165	THR
1	B	167	ASN
1	B	202	LEU
1	B	228	CYS
1	B	232	GLN
1	B	234	GLU
1	B	275	LEU
1	B	278	THR
1	B	300	GLN
1	B	309	ASP

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Mol	Chain	Res	Type
1	B	347	ARG
1	C	12	VAL
1	C	64	ILE
1	C	103	VAL
1	C	133	VAL
1	C	141	LEU
1	C	147	VAL
1	C	159	SER
1	C	163	VAL
1	C	164	THR
1	C	178	SER
1	C	180	LYS
1	C	183	TYR
1	C	185	GLU
1	C	187	GLU
1	C	191	LYS
1	C	202	LEU
1	C	210	ARG
1	C	227	GLN
1	C	248	THR
1	C	256	GLU
1	C	275	LEU
1	C	276	THR
1	C	299	HIS
1	C	319	SER
1	C	327	ASN
1	C	333	LEU
1	C	347	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	188	GLN
1	A	194	ASN
1	A	223	ASN
1	C	36	GLN

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 monosaccharides 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, 95^{th} 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	347/365 (95%)	0.13	5 (1%)	75	71	38, 66, 107, 163	0
1	B	332/365 (90%)	-0.04	5 (1%)	73	70	37, 61, 110, 148	0
1	C	343/365 (93%)	0.07	3 (0%)	84	80	33, 63, 103, 141	0
All	All	1022/1095 (93%)	0.05	13 (1%)	77	73	33, 64, 107, 163	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	THR	3.9
1	C	310	ILE	3.0
1	A	222	LEU	2.7
1	B	203	GLY	2.6
1	A	240	TYR	2.6
1	B	201	SER	2.5
1	A	247	LEU	2.4
1	C	312	ALA	2.4
1	B	240	TYR	2.4
1	A	218	LEU	2.3
1	B	75	ILE	2.1
1	C	230	GLN	2.1
1	A	251	VAL	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 monosaccharides 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.