



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:34 PM GMT

PDB ID : 2B9R
Title : Crystal Structure of Human Cyclin B1
Authors : Basavappa, R.; Petri, E.
Deposited on : 2005-10-12
Resolution : 2.90 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>

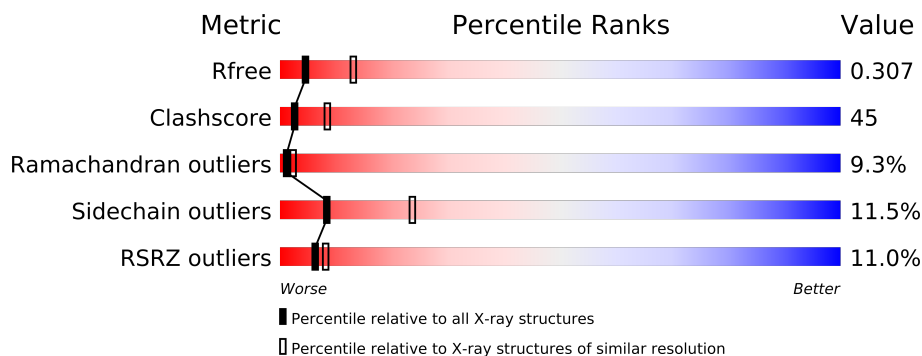
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	269	
1	B	269	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4030 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 Human cyclin B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1952	1259	329	348	16			
1	B	255	Total	C	N	O	S	0	0	0
			1984	1280	336	352	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	ENGINEERED	UNP P14635
A	19	ALA	GLU	ENGINEERED	UNP P14635
A	20	ALA	GLU	ENGINEERED	UNP P14635
A	74	SER	CYS	ENGINEERED	UNP P14635
A	186	SER	CYS	ENGINEERED	UNP P14635
B	3	SER	CYS	ENGINEERED	UNP P14635
B	19	ALA	GLU	ENGINEERED	UNP P14635
B	20	ALA	GLU	ENGINEERED	UNP P14635
B	74	SER	CYS	ENGINEERED	UNP P14635
B	186	SER	CYS	ENGINEERED	UNP P14635

- Molecule 2 is water.

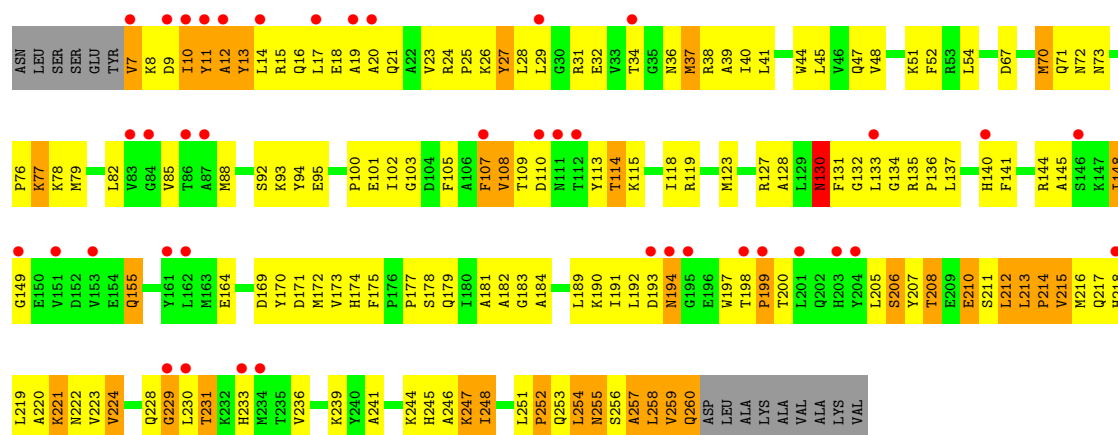
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	50	Total	O	0	0
			50	50		

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.

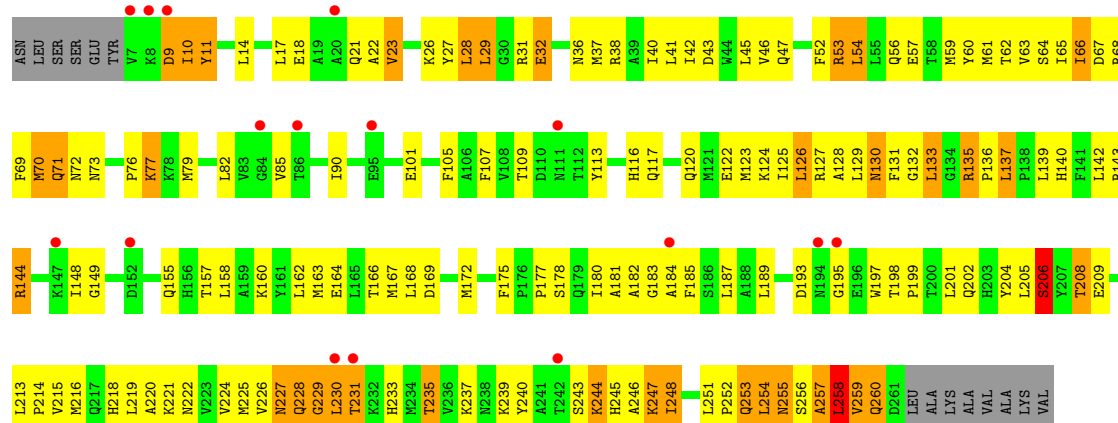
• Molecule 1: Human cyclin B1

Chain A: 



• Molecule 1: Human cyclin B1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.17Å 117.17Å 197.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.90) 98.2 (19.95-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.243 , 0.308 0.241 , 0.307	Depositor DCC
R_{free} test set	1773 reflections (10.89%)	DCC
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 129.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 18051 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4030	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.55	2/1991 (0.1%)	0.65	0/2703
1	B	0.49	0/2025	0.71	1/2748 (0.0%)
All	All	0.52	2/4016 (0.0%)	0.68	1/5451 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	VAL	N-CA	8.52	1.63	1.46
1	A	7	VAL	C-N	5.43	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	CA-CB-CG	-5.20	103.33	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	VAL	Mainchain

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	1952	0	1942	176	0
1	B	1984	0	1989	184	0
2	A	44	0	0	13	0
2	B	50	0	0	17	0
All	All	4030	0	3931	352	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 45.

All (352) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:MET:O	1:A:72:ASN:N	1.58	1.34
1:B:70:MET:O	1:B:72:ASN:N	1.63	1.31
1:B:143:ARG:HH21	1:B:160:LYS:NZ	1.29	1.30
1:A:252:PRO:HG2	2:A:273:HOH:O	1.32	1.27
1:B:253:GLN:HA	1:B:255:ASN:ND2	1.64	1.11
1:B:53:ARG:HH11	1:B:53:ARG:CG	1.65	1.09
1:B:79:MET:HG3	2:B:293:HOH:O	1.53	1.06
1:B:53:ARG:NH1	1:B:53:ARG:HG3	1.51	1.03
1:B:253:GLN:HA	1:B:255:ASN:HD21	1.15	1.02
1:B:254:LEU:O	1:B:256:SER:N	1.94	1.01
1:B:177:PRO:HA	2:B:308:HOH:O	1.62	0.99
1:B:79:MET:HE1	2:B:317:HOH:O	1.63	0.99
1:A:131:PHE:HA	2:B:313:HOH:O	1.63	0.97
1:B:178:SER:N	2:B:308:HOH:O	1.96	0.97
1:B:143:ARG:HH21	1:B:160:LYS:HZ2	1.04	0.97
1:B:43:ASP:OD1	1:B:235:THR:HG23	1.67	0.94
1:B:79:MET:CE	2:B:317:HOH:O	2.16	0.94
1:B:143:ARG:HH21	1:B:160:LYS:HZ1	1.09	0.93
1:B:253:GLN:C	1:B:255:ASN:H	1.69	0.93
1:B:47:GLN:HE21	1:B:235:THR:HG21	1.33	0.93
1:B:143:ARG:NH2	1:B:160:LYS:NZ	2.15	0.93
1:B:64:SER:O	1:B:68:ARG:HG3	1.70	0.92
1:B:124:LYS:NZ	2:B:283:HOH:O	2.02	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:TYR:HB3	1:A:212:LEU:HD21	1.54	0.89
1:B:253:GLN:CA	1:B:255:ASN:ND2	2.35	0.89
1:B:77:LYS:HE2	1:B:77:LYS:H	1.36	0.88
1:B:18:GLU:OE2	1:B:177:PRO:HD2	1.72	0.88
1:B:177:PRO:O	1:B:178:SER:HB2	1.71	0.87
1:A:251:LEU:HB3	1:A:252:PRO:HD2	1.54	0.86
1:A:251:LEU:C	1:A:253:GLN:H	1.76	0.86
1:A:254:LEU:O	1:A:256:SER:N	2.08	0.86
1:B:132:GLY:N	2:B:273:HOH:O	2.09	0.85
1:A:216:MET:HA	1:A:219:LEU:HD12	1.57	0.85
1:B:57:GLU:N	1:B:57:GLU:OE2	2.08	0.85
1:A:253:GLN:C	1:A:255:ASN:H	1.78	0.84
1:B:32:GLU:H	1:B:32:GLU:CD	1.80	0.83
1:B:143:ARG:NH2	1:B:160:LYS:HZ2	1.74	0.83
1:A:257:ALA:O	1:A:259:VAL:N	2.13	0.82
1:B:26:LYS:O	1:B:29:LEU:HB2	1.80	0.82
1:A:77:LYS:HE2	1:A:78:LYS:H	1.44	0.82
1:A:133:LEU:H	1:B:131:PHE:CB	1.93	0.82
1:B:23:VAL:HA	1:B:71:GLN:OE1	1.78	0.82
1:B:228:GLN:HG3	1:B:229:GLY:H	1.45	0.80
1:B:70:MET:C	1:B:72:ASN:H	1.83	0.79
1:B:256:SER:O	1:B:259:VAL:HG23	1.83	0.79
1:B:199:PRO:HA	1:B:202:GLN:HG2	1.64	0.79
1:A:27:TYR:C	1:A:27:TYR:HD2	1.86	0.79
1:B:177:PRO:CA	2:B:308:HOH:O	2.22	0.77
1:A:13:TYR:HA	2:A:310:HOH:O	1.85	0.77
1:B:248:ILE:HD13	1:B:248:ILE:O	1.85	0.76
1:B:257:ALA:O	1:B:259:VAL:N	2.12	0.76
1:A:17:LEU:HD23	1:A:136:PRO:HD3	1.69	0.75
1:B:169:ASP:HB3	1:B:172:MET:HG2	1.69	0.75
1:B:253:GLN:C	1:B:255:ASN:N	2.38	0.75
1:A:155:GLN:HE22	1:A:189:LEU:HD12	1.51	0.74
1:B:40:ILE:HG13	1:B:41:LEU:N	2.02	0.74
1:A:131:PHE:O	1:B:132:GLY:HA2	1.87	0.74
1:A:27:TYR:C	1:A:27:TYR:CD2	2.58	0.74
1:B:227:ASN:HD22	1:B:254:LEU:HG	1.53	0.73
1:B:254:LEU:HD13	2:B:318:HOH:O	1.89	0.73
1:A:193:ASP:O	1:A:194:ASN:HB3	1.87	0.73
1:A:257:ALA:C	1:A:259:VAL:H	1.91	0.72
1:B:143:ARG:NH2	1:B:160:LYS:HZ1	1.84	0.71
1:B:228:GLN:O	1:B:229:GLY:O	2.09	0.71
1:A:212:LEU:C	1:A:214:PRO:HD2	2.12	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:132:GLY:N	2:B:273:HOH:O	2.24	0.70
1:A:253:GLN:HA	1:A:255:ASN:ND2	2.06	0.70
1:A:123:MET:CE	1:A:127:ARG:HH22	2.05	0.69
1:B:193:ASP:HB3	1:B:195:GLY:H	1.58	0.68
1:A:257:ALA:C	1:A:259:VAL:N	2.46	0.68
1:B:256:SER:OG	1:B:258:LEU:HA	1.94	0.67
1:B:260:GLN:HE21	1:B:260:GLN:N	1.90	0.67
1:B:253:GLN:O	1:B:255:ASN:N	2.28	0.67
1:B:43:ASP:CG	1:B:235:THR:HG23	2.15	0.67
1:B:53:ARG:HH11	1:B:53:ARG:HG3	0.71	0.67
1:A:70:MET:C	1:A:72:ASN:N	2.48	0.67
1:B:226:VAL:HG13	1:B:237:LYS:HD2	1.76	0.67
1:B:163:MET:O	1:B:166:THR:OG1	2.12	0.66
1:B:187:LEU:HB2	1:B:216:MET:HG2	1.78	0.66
1:B:253:GLN:CA	1:B:255:ASN:HD21	1.99	0.66
1:A:212:LEU:HD23	1:A:212:LEU:N	2.10	0.66
1:B:243:SER:O	1:B:245:HIS:N	2.30	0.65
1:A:251:LEU:C	1:A:253:GLN:N	2.48	0.65
1:A:198:THR:C	1:A:200:THR:H	1.99	0.65
1:B:123:MET:HE3	1:B:127:ARG:HH12	1.62	0.65
1:A:179:GLN:HB2	1:A:207:TYR:OH	1.96	0.64
1:A:219:LEU:O	1:A:223:VAL:HG23	1.96	0.64
1:A:193:ASP:O	1:A:194:ASN:CB	2.45	0.64
1:B:251:LEU:HB3	1:B:252:PRO:HD2	1.79	0.64
1:A:245:HIS:O	1:A:248:ILE:HB	1.97	0.64
1:A:37:MET:O	1:A:40:ILE:HG12	1.98	0.64
1:A:253:GLN:C	1:A:255:ASN:N	2.48	0.63
1:B:177:PRO:O	1:B:178:SER:CB	2.43	0.63
1:B:82:LEU:HB2	1:B:113:TYR:CE1	2.34	0.63
1:A:241:ALA:O	1:A:247:LYS:HG2	1.98	0.62
1:A:213:LEU:N	1:A:214:PRO:CD	2.62	0.62
1:A:82:LEU:HB2	1:A:113:TYR:CZ	2.35	0.62
1:B:137:LEU:HB2	1:B:140:HIS:CD2	2.35	0.62
1:B:213:LEU:HB3	1:B:214:PRO:HD3	1.80	0.61
1:A:256:SER:C	1:A:258:LEU:N	2.52	0.61
1:A:169:ASP:HB3	1:A:172:MET:HG2	1.82	0.61
1:A:255:ASN:O	1:A:256:SER:HB3	2.00	0.61
1:B:27:TYR:CE2	1:B:28:LEU:HD13	2.35	0.61
1:A:179:GLN:HB2	1:A:207:TYR:CZ	2.35	0.61
1:B:77:LYS:N	1:B:77:LYS:HE2	2.10	0.61
1:A:251:LEU:HB3	1:A:252:PRO:CD	2.26	0.61
1:A:191:ILE:HG22	1:A:192:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:LYS:O	1:B:123:MET:HG2	2.01	0.61
1:B:135:ARG:HG2	1:B:136:PRO:HD2	1.82	0.61
1:B:228:GLN:CG	1:B:229:GLY:H	2.12	0.60
1:A:38:ARG:HB3	2:A:289:HOH:O	2.02	0.60
1:B:53:ARG:NH1	1:B:53:ARG:CG	2.35	0.60
1:A:131:PHE:CB	1:B:133:LEU:H	2.15	0.60
1:B:47:GLN:NE2	1:B:235:THR:HG21	2.12	0.60
1:B:42:ILE:CG2	1:B:168:LEU:HD23	2.32	0.60
1:A:256:SER:O	1:A:259:VAL:N	2.35	0.59
1:A:101:GLU:CD	1:A:102:ILE:HG22	2.23	0.59
1:A:128:ALA:C	1:A:130:ASN:H	2.05	0.59
1:A:253:GLN:O	1:A:255:ASN:N	2.36	0.59
1:A:251:LEU:CB	1:A:252:PRO:HD2	2.32	0.58
1:A:253:GLN:HA	1:A:255:ASN:HD21	1.66	0.58
1:B:254:LEU:C	1:B:256:SER:N	2.56	0.58
1:B:62:THR:O	1:B:66:ILE:HG22	2.03	0.58
1:A:217:GLN:O	1:A:220:ALA:HB3	2.03	0.58
1:A:132:GLY:HA2	1:B:131:PHE:O	2.03	0.58
1:B:243:SER:C	1:B:245:HIS:N	2.56	0.58
1:A:37:MET:O	1:A:40:ILE:CG1	2.51	0.58
1:A:164:GLU:HG2	1:A:236:VAL:CG1	2.33	0.58
1:A:244:LYS:O	1:A:244:LYS:HG2	2.03	0.57
1:A:198:THR:HB	1:A:199:PRO:HD2	1.86	0.57
1:B:123:MET:HB3	1:B:127:ARG:NH1	2.19	0.57
1:B:255:ASN:O	1:B:256:SER:HB3	2.03	0.57
1:A:212:LEU:C	1:A:214:PRO:CD	2.72	0.57
1:A:246:ALA:O	1:A:248:ILE:N	2.38	0.57
1:B:254:LEU:CD1	2:B:318:HOH:O	2.48	0.56
1:B:260:GLN:NE2	1:B:260:GLN:N	2.53	0.56
1:A:14:LEU:HD22	1:A:136:PRO:HB3	1.86	0.56
1:B:257:ALA:C	1:B:259:VAL:H	2.07	0.56
1:A:208:THR:HB	1:A:211:SER:H	1.71	0.56
1:B:256:SER:C	1:B:258:LEU:N	2.57	0.56
1:B:46:VAL:HG22	1:B:59:MET:HE2	1.88	0.56
1:B:202:GLN:O	1:B:206:SER:HA	2.06	0.56
1:B:243:SER:C	1:B:245:HIS:H	2.09	0.56
1:B:21:GLN:CB	1:B:135:ARG:HD2	2.35	0.56
1:B:63:VAL:HA	1:B:66:ILE:CG2	2.36	0.56
1:B:253:GLN:O	1:B:255:ASN:ND2	2.40	0.55
1:B:65:ILE:HG23	1:B:129:LEU:HD11	1.88	0.55
1:B:131:PHE:C	2:B:273:HOH:O	2.40	0.55
1:A:172:MET:SD	1:A:218:HIS:HB3	2.47	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:GLY:H	1:B:131:PHE:CB	2.19	0.55
1:A:11:TYR:O	1:A:14:LEU:HB2	2.07	0.55
1:B:227:ASN:O	1:B:228:GLN:HB3	2.06	0.55
1:B:253:GLN:C	1:B:255:ASN:ND2	2.60	0.55
1:B:128:ALA:C	1:B:130:ASN:H	2.08	0.55
1:A:103:GLY:HA2	1:A:115:LYS:HE2	1.89	0.55
1:B:197:TRP:CE3	1:B:201:LEU:HD13	2.42	0.55
1:B:70:MET:O	1:B:73:ASN:N	2.35	0.54
1:A:123:MET:CE	1:A:127:ARG:NH2	2.70	0.54
1:A:251:LEU:O	1:A:253:GLN:N	2.39	0.54
1:A:27:TYR:HE2	1:A:28:LEU:HD13	1.72	0.54
1:B:63:VAL:HA	1:B:66:ILE:HG23	1.89	0.54
1:A:198:THR:O	1:A:200:THR:N	2.41	0.54
1:B:42:ILE:HG21	1:B:168:LEU:HD23	1.90	0.54
1:A:48:VAL:HA	1:A:51:LYS:HD3	1.89	0.54
1:A:31:ARG:HH11	1:A:31:ARG:HG3	1.73	0.54
1:A:40:ILE:HG13	1:A:41:LEU:N	2.23	0.54
1:A:70:MET:O	1:A:73:ASN:N	2.38	0.54
1:B:244:LYS:HG3	1:B:245:HIS:CE1	2.43	0.53
1:B:228:GLN:HG3	1:B:229:GLY:N	2.18	0.53
1:B:76:PRO:HD2	1:B:79:MET:HE2	1.91	0.53
1:A:132:GLY:HA2	1:B:131:PHE:C	2.29	0.53
1:B:155:GLN:HE22	1:B:189:LEU:N	2.07	0.53
1:A:44:TRP:HA	1:A:47:GLN:HE21	1.72	0.53
1:A:36:ASN:HA	1:A:39:ALA:HB3	1.90	0.53
1:B:148:ILE:O	1:B:148:ILE:HG13	2.09	0.53
1:A:27:TYR:HD2	1:A:28:LEU:N	2.07	0.53
1:A:177:PRO:O	1:A:178:SER:CB	2.56	0.52
1:B:158:LEU:O	1:B:162:LEU:HG	2.09	0.52
1:B:14:LEU:HD23	1:B:136:PRO:HG3	1.91	0.52
1:A:102:ILE:HD11	1:A:118:ILE:HB	1.91	0.52
1:A:18:GLU:O	1:A:21:GLN:N	2.21	0.52
1:A:79:MET:HG3	2:A:304:HOH:O	2.09	0.52
1:A:215:VAL:HB	2:A:284:HOH:O	2.08	0.52
1:A:205:LEU:O	1:A:206:SER:C	2.48	0.52
1:A:164:GLU:HG2	1:A:236:VAL:HG13	1.91	0.52
1:A:24:ARG:O	1:A:27:TYR:HB3	2.09	0.52
1:B:185:PHE:HD2	1:B:197:TRP:HZ3	1.57	0.52
1:A:198:THR:C	1:A:200:THR:N	2.64	0.51
1:B:259:VAL:O	1:B:260:GLN:HG3	2.10	0.51
1:A:101:GLU:CD	1:A:102:ILE:H	2.13	0.51
1:A:172:MET:HB2	1:A:175:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:ASN:O	1:B:228:GLN:CB	2.59	0.51
1:B:9:ASP:O	1:B:10:ILE:C	2.49	0.51
1:B:157:THR:HG22	1:B:248:ILE:HG21	1.94	0.50
1:A:12:ALA:C	1:A:14:LEU:H	2.14	0.50
1:B:177:PRO:C	2:B:308:HOH:O	2.28	0.50
1:B:130:ASN:O	1:B:131:PHE:CB	2.60	0.50
1:A:244:LYS:CG	1:A:244:LYS:O	2.59	0.50
1:A:76:PRO:O	1:A:77:LYS:C	2.49	0.50
1:A:27:TYR:CD2	1:A:28:LEU:N	2.80	0.50
1:A:12:ALA:O	1:A:14:LEU:N	2.44	0.50
1:B:17:LEU:HD23	1:B:136:PRO:HD3	1.93	0.50
1:A:130:ASN:O	1:A:131:PHE:CB	2.60	0.49
1:B:172:MET:HB2	1:B:175:PHE:CD1	2.47	0.49
1:B:105:PHE:O	1:B:109:THR:HG23	2.12	0.49
1:A:85:VAL:HG21	1:A:109:THR:HG22	1.92	0.49
1:B:18:GLU:OE2	1:B:177:PRO:CD	2.55	0.49
1:B:43:ASP:OD2	1:B:235:THR:CG2	2.60	0.49
1:A:101:GLU:OE2	1:A:102:ILE:HG22	2.12	0.49
1:A:9:ASP:O	1:A:10:ILE:CB	2.60	0.49
1:A:220:ALA:O	1:A:224:VAL:HG23	2.13	0.48
1:A:220:ALA:HB1	1:A:260:GLN:NE2	2.28	0.48
1:B:254:LEU:HD22	2:B:318:HOH:O	2.12	0.48
1:A:215:VAL:CG2	1:A:216:MET:N	2.76	0.48
1:A:31:ARG:NH1	1:A:31:ARG:HG3	2.28	0.48
1:A:115:LYS:HB3	1:A:119:ARG:HH21	1.77	0.48
1:B:41:LEU:HG	1:B:45:LEU:HD12	1.96	0.48
1:B:21:GLN:CB	1:B:135:ARG:CD	2.92	0.48
1:B:205:LEU:O	1:B:206:SER:C	2.52	0.48
1:A:25:PRO:HD3	1:A:174:HIS:HB3	1.96	0.47
1:A:181:ALA:O	1:A:182:ALA:C	2.51	0.47
1:A:107:PHE:O	1:A:110:ASP:N	2.45	0.47
1:A:255:ASN:C	1:A:257:ALA:N	2.67	0.47
1:B:158:LEU:HB2	1:B:248:ILE:HD11	1.96	0.47
1:A:82:LEU:HB2	1:A:113:TYR:CE1	2.50	0.47
1:B:231:THR:C	1:B:233:HIS:N	2.67	0.47
1:B:256:SER:O	1:B:257:ALA:C	2.52	0.47
1:A:220:ALA:O	1:A:221:LYS:C	2.52	0.47
1:B:77:LYS:CE	1:B:77:LYS:H	2.20	0.47
1:B:52:PHE:HB3	1:B:54:LEU:HD13	1.96	0.47
1:B:219:LEU:O	1:B:220:ALA:C	2.53	0.47
1:B:260:GLN:HE21	1:B:260:GLN:H	1.62	0.47
1:A:255:ASN:C	1:A:257:ALA:H	2.18	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:ARG:NH2	1:B:204:TYR:HD2	2.14	0.46
1:B:189:LEU:O	1:B:193:ASP:HB2	2.15	0.46
1:A:220:ALA:CB	1:A:260:GLN:NE2	2.78	0.46
1:A:82:LEU:HD13	1:A:113:TYR:CG	2.50	0.46
1:B:90:ILE:HD13	1:B:126:LEU:HD13	1.97	0.46
1:A:172:MET:HB2	1:A:175:PHE:CD1	2.49	0.46
1:B:189:LEU:O	1:B:193:ASP:CB	2.64	0.46
1:A:257:ALA:O	1:A:258:LEU:C	2.53	0.46
1:B:38:ARG:NH1	1:B:67:ASP:OD1	2.48	0.46
1:B:204:TYR:O	1:B:205:LEU:HD23	2.16	0.46
1:B:246:ALA:O	1:B:247:LYS:C	2.53	0.46
1:B:31:ARG:HG3	1:B:31:ARG:HH11	1.80	0.46
1:B:199:PRO:HA	1:B:202:GLN:CG	2.40	0.46
1:A:27:TYR:HE1	1:A:67:ASP:OD2	1.99	0.46
1:A:77:LYS:NZ	2:A:306:HOH:O	2.02	0.46
1:B:14:LEU:CD2	1:B:136:PRO:HB3	2.46	0.46
1:A:241:ALA:O	1:A:247:LYS:HA	2.16	0.45
1:B:213:LEU:N	1:B:214:PRO:HD2	2.31	0.45
1:A:123:MET:HE1	1:A:127:ARG:HH22	1.82	0.45
1:B:27:TYR:OH	1:B:67:ASP:OD2	2.31	0.45
1:A:24:ARG:HA	1:A:25:PRO:HD2	1.76	0.45
1:A:254:LEU:C	1:A:256:SER:N	2.70	0.45
1:A:258:LEU:HD12	2:A:286:HOH:O	2.15	0.45
1:B:175:PHE:HB2	1:B:180:ILE:HD11	1.99	0.45
1:B:181:ALA:O	1:B:182:ALA:C	2.55	0.45
1:A:135:ARG:CB	2:A:293:HOH:O	2.63	0.45
1:A:135:ARG:HG3	2:A:293:HOH:O	2.17	0.45
1:B:239:LYS:HD3	1:B:240:TYR:CE1	2.52	0.45
1:B:224:VAL:HG12	1:B:225:MET:N	2.32	0.45
1:B:28:LEU:O	1:B:29:LEU:C	2.55	0.45
1:A:246:ALA:O	1:A:247:LYS:C	2.55	0.45
1:A:175:PHE:HB3	1:A:179:GLN:OE1	2.16	0.45
1:B:22:ALA:O	1:B:23:VAL:HB	2.17	0.45
1:A:170:TYR:HA	1:A:173:VAL:CG2	2.47	0.45
1:A:94:TYR:CE2	1:B:126:LEU:HB3	2.52	0.45
1:A:144:ARG:O	1:A:148:ILE:HG13	2.17	0.45
1:B:122:GLU:HG2	1:B:126:LEU:HD22	1.98	0.44
1:B:69:PHE:CD1	1:B:125:ILE:HG12	2.52	0.44
1:B:228:GLN:CG	1:B:229:GLY:N	2.79	0.44
1:A:135:ARG:HB2	2:A:293:HOH:O	2.17	0.44
1:B:140:HIS:N	1:B:140:HIS:CD2	2.86	0.44
1:A:141:PHE:HB3	2:A:288:HOH:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:PRO:HG2	1:A:105:PHE:CE2	2.53	0.44
1:A:256:SER:HB3	1:A:258:LEU:HD23	1.99	0.44
1:B:116:HIS:CE1	1:B:120:GLN:OE1	2.70	0.44
1:B:218:HIS:O	1:B:221:LYS:HB3	2.18	0.44
1:A:210:GLU:OE1	1:A:210:GLU:N	2.51	0.44
1:A:256:SER:O	1:A:257:ALA:C	2.56	0.44
1:B:158:LEU:HB2	1:B:248:ILE:CD1	2.48	0.44
1:A:133:LEU:HD22	1:A:133:LEU:N	2.32	0.44
1:A:95:GLU:HA	1:A:95:GLU:OE2	2.17	0.44
1:B:113:TYR:HA	1:B:117:GLN:OE1	2.18	0.43
1:A:39:ALA:O	1:A:40:ILE:C	2.56	0.43
1:A:220:ALA:HB1	1:A:260:GLN:HE21	1.82	0.43
1:A:108:VAL:C	1:A:110:ASP:H	2.21	0.43
1:B:139:LEU:O	1:B:143:ARG:HG2	2.18	0.43
1:A:211:SER:C	1:A:212:LEU:HD23	2.38	0.43
1:B:172:MET:HB2	1:B:175:PHE:HD1	1.83	0.43
1:B:243:SER:O	1:B:244:LYS:C	2.56	0.43
1:A:228:GLN:HG3	1:A:229:GLY:N	2.33	0.43
1:A:14:LEU:O	1:A:16:GLN:N	2.51	0.43
1:A:101:GLU:CG	1:A:102:ILE:H	2.31	0.43
1:A:101:GLU:CG	1:A:102:ILE:N	2.81	0.43
1:A:190:LYS:HD2	2:A:290:HOH:O	2.17	0.43
1:B:56:GLN:HB3	1:B:139:LEU:HD11	2.00	0.43
1:A:40:ILE:HG13	1:A:41:LEU:H	1.84	0.43
1:A:231:THR:C	1:A:233:HIS:H	2.22	0.43
1:B:252:PRO:HG2	1:B:255:ASN:OD1	2.18	0.43
1:A:230:LEU:O	1:A:231:THR:O	2.36	0.43
1:B:208:THR:O	1:B:209:GLU:C	2.56	0.43
1:A:88:MET:O	1:A:92:SER:OG	2.33	0.43
1:A:25:PRO:HD3	1:A:174:HIS:CB	2.49	0.42
1:B:248:ILE:HD11	1:B:251:LEU:HD11	2.01	0.42
1:B:164:GLU:HG3	1:B:167:MET:HE2	2.00	0.42
1:A:215:VAL:HG22	1:A:216:MET:N	2.34	0.42
1:A:12:ALA:C	1:A:14:LEU:N	2.72	0.42
1:A:14:LEU:C	1:A:16:GLN:N	2.70	0.42
1:A:114:THR:OG1	1:A:115:LYS:N	2.52	0.42
1:A:183:GLY:O	1:A:184:ALA:C	2.57	0.42
1:B:216:MET:O	1:B:219:LEU:HB2	2.19	0.42
1:B:251:LEU:C	1:B:253:GLN:H	2.22	0.42
1:A:26:LYS:HA	1:A:170:TYR:CZ	2.55	0.42
1:B:60:TYR:O	1:B:61:MET:C	2.57	0.42
1:B:28:LEU:HD12	1:B:28:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:MET:HB3	1:A:123:MET:HE2	1.67	0.42
1:B:254:LEU:CD2	2:B:318:HOH:O	2.67	0.42
1:A:216:MET:HE3	1:A:216:MET:HB3	1.95	0.42
1:B:226:VAL:HG12	1:B:227:ASN:N	2.35	0.42
1:A:36:ASN:HA	1:A:39:ALA:CB	2.50	0.42
1:B:82:LEU:HB2	1:B:113:TYR:CD1	2.54	0.41
1:A:258:LEU:HD23	1:A:258:LEU:H	1.84	0.41
1:A:18:GLU:O	1:A:20:ALA:N	2.52	0.41
1:B:11:TYR:C	1:B:11:TYR:CD1	2.94	0.41
1:A:164:GLU:HG2	1:A:236:VAL:HG11	2.02	0.41
1:B:142:LEU:HA	1:B:142:LEU:HD12	1.81	0.41
1:B:257:ALA:C	1:B:259:VAL:N	2.70	0.41
1:B:79:MET:HE2	2:B:317:HOH:O	2.03	0.41
1:A:135:ARG:HG2	1:A:136:PRO:HD2	2.02	0.41
1:B:101:GLU:OE1	1:B:101:GLU:HA	2.20	0.41
1:B:158:LEU:HG	1:B:162:LEU:HD11	2.03	0.41
1:A:218:HIS:O	1:A:219:LEU:C	2.57	0.41
1:A:28:LEU:HA	1:A:31:ARG:HG2	2.03	0.41
1:B:183:GLY:O	1:B:184:ALA:C	2.59	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.89	0.41
1:A:212:LEU:N	1:A:212:LEU:CD2	2.81	0.41
1:A:248:ILE:O	1:A:248:ILE:HD13	2.21	0.40
1:B:198:THR:O	1:B:201:LEU:N	2.53	0.40
1:A:52:PHE:CE2	1:A:108:VAL:HG11	2.56	0.40
1:A:137:LEU:H	1:A:140:HIS:HD2	1.68	0.40
1:B:107:PHE:C	1:B:107:PHE:CD1	2.94	0.40
1:B:128:ALA:C	1:B:130:ASN:N	2.74	0.40
1:A:217:GLN:CB	1:A:260:GLN:HG2	2.51	0.40
1:B:259:VAL:C	1:B:260:GLN:HG3	2.42	0.40
1:A:82:LEU:HB2	1:A:113:TYR:CE2	2.56	0.40
1:B:231:THR:C	1:B:233:HIS:H	2.23	0.40
1:A:128:ALA:C	1:A:130:ASN:N	2.73	0.40
1:A:169:ASP:OD1	1:A:171:ASP:N	2.41	0.40
1:B:219:LEU:O	1:B:222:ASN:N	2.55	0.40
1:A:145:ALA:CB	2:A:307:HOH:O	2.70	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	252/269 (94%)	188 (75%)	38 (15%)	26 (10%)	1	2
1	B	253/269 (94%)	204 (81%)	28 (11%)	21 (8%)	1	3
All	All	505/538 (94%)	392 (78%)	66 (13%)	47 (9%)	1	2

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	71	GLN
1	A	206	SER
1	A	247	LYS
1	A	255	ASN
1	A	258	LEU
1	A	259	VAL
1	B	9	ASP
1	B	10	ILE
1	B	29	LEU
1	B	71	GLN
1	B	206	SER
1	B	228	GLN
1	B	229	GLY
1	B	244	LYS
1	B	253	GLN
1	B	254	LEU
1	B	255	ASN
1	B	258	LEU
1	A	8	LYS
1	A	12	ALA
1	A	13	TYR
1	A	231	THR
1	A	254	LEU
1	A	257	ALA
1	B	230	LEU
1	B	247	LYS

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Mol	Chain	Res	Type
1	B	257	ALA
1	B	259	VAL
1	A	19	ALA
1	A	130	ASN
1	A	197	TRP
1	A	214	PRO
1	B	130	ASN
1	B	227	ASN
1	A	15	ARG
1	A	149	GLY
1	A	194	ASN
1	A	199	PRO
1	A	229	GLY
1	A	252	PRO
1	B	23	VAL
1	B	70	MET
1	B	149	GLY
1	A	23	VAL
1	A	70	MET
1	A	221	LYS

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	202/237 (85%)	178 (88%)	24 (12%)	8	21
1	B	208/237 (88%)	185 (89%)	23 (11%)	9	26
All	All	410/474 (86%)	363 (88%)	47 (12%)	8	23

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	27	TYR
1	A	29	LEU
1	A	32	GLU
1	A	34	THR

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Mol	Chain	Res	Type
1	A	37	MET
1	A	54	LEU
1	A	77	LYS
1	A	107	PHE
1	A	108	VAL
1	A	114	THR
1	A	130	ASN
1	A	148	ILE
1	A	155	GLN
1	A	208	THR
1	A	210	GLU
1	A	212	LEU
1	A	213	LEU
1	A	215	VAL
1	A	222	ASN
1	A	224	VAL
1	A	239	LYS
1	A	248	ILE
1	A	260	GLN
1	B	11	TYR
1	B	28	LEU
1	B	32	GLU
1	B	36	ASN
1	B	37	MET
1	B	53	ARG
1	B	54	LEU
1	B	66	ILE
1	B	77	LYS
1	B	85	VAL
1	B	126	LEU
1	B	133	LEU
1	B	135	ARG
1	B	137	LEU
1	B	144	ARG
1	B	206	SER
1	B	208	THR
1	B	215	VAL
1	B	230	LEU
1	B	231	THR
1	B	235	THR
1	B	248	ILE
1	B	260	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	81	GLN
1	A	130	ASN
1	A	140	HIS
1	A	155	GLN
1	A	218	HIS
1	A	233	HIS
1	A	255	ASN
1	A	260	GLN
1	B	47	GLN
1	B	72	ASN
1	B	116	HIS
1	B	130	ASN
1	B	140	HIS
1	B	155	GLN
1	B	227	ASN
1	B	233	HIS
1	B	260	GLN

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	254/269 (94%)	0.70	40 (15%) 3 4	69, 87, 119, 150	0
1	B	255/269 (94%)	0.33	16 (6%) 19 23	68, 86, 117, 150	0
All	All	509/538 (94%)	0.52	56 (11%) 6 8	68, 86, 118, 150	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ASN	14.2
1	A	195	GLY	12.1
1	B	194	ASN	6.8
1	A	199	PRO	5.9
1	A	19	ALA	5.4
1	B	231	THR	5.1
1	A	11	TYR	4.3
1	A	14	LEU	4.3
1	B	20	ALA	4.2
1	A	34	THR	4.1
1	A	153	VAL	4.1
1	A	7	VAL	3.9
1	A	204	TYR	3.9
1	A	146	SER	3.6
1	A	29	LEU	3.6
1	A	203	HIS	3.4
1	A	20	ALA	3.4
1	A	84	GLY	3.3
1	A	110	ASP	3.2
1	B	86	THR	3.2
1	A	230	LEU	3.1
1	A	229	GLY	2.9
1	A	133	LEU	2.9
1	A	201	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	193	ASP	2.9
1	B	8	LYS	2.8
1	B	9	ASP	2.8
1	B	195	GLY	2.8
1	B	184	ALA	2.7
1	A	218	HIS	2.7
1	A	87	ALA	2.6
1	B	230	LEU	2.6
1	A	198	THR	2.5
1	A	162	LEU	2.5
1	A	149	GLY	2.5
1	A	111	ASN	2.5
1	B	152	ASP	2.5
1	A	9	ASP	2.4
1	A	17	LEU	2.4
1	A	151	VAL	2.4
1	A	107	PHE	2.4
1	B	147	LYS	2.3
1	A	233	HIS	2.3
1	A	161	TYR	2.3
1	A	83	VAL	2.2
1	A	86	THR	2.2
1	B	242	THR	2.2
1	B	84	GLY	2.1
1	A	10	ILE	2.1
1	A	112	THR	2.1
1	A	140	HIS	2.1
1	B	7	VAL	2.1
1	B	111	ASN	2.1
1	B	95	GLU	2.1
1	A	12	ALA	2.1
1	A	234	MET	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.