



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 09:06 AM GMT

PDB ID : 1K5H
Title : 1-deoxy-D-xylulose-5-phosphatereductoisomerase
Authors : Reuter, K.; Sanderbrand, S.; Jomaa, H.; Wiesner, J.; Steinbrecher, I.; Beck, E.; Hintz, M.; Klebe, G.; Stubbs, M.T.
Deposited on : 2001-10-10
Resolution : 2.50 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>

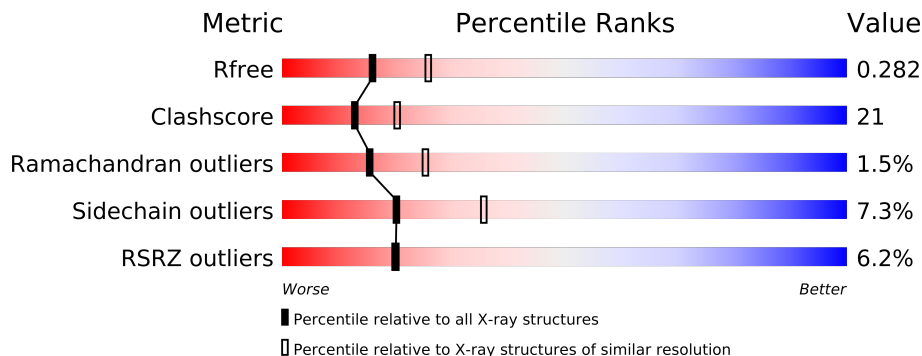
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	398	
1	B	398	
1	C	398	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9126 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 1-deoxy-D-xylulose-5-phosphatereductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3030	1892	534	577	27			
1	B	391	Total	C	N	O	S	0	0	0
			2978	1860	526	567	25			
1	C	398	Total	C	N	O	S	0	0	0
			3030	1892	534	577	27			

- Molecule 2 is water.

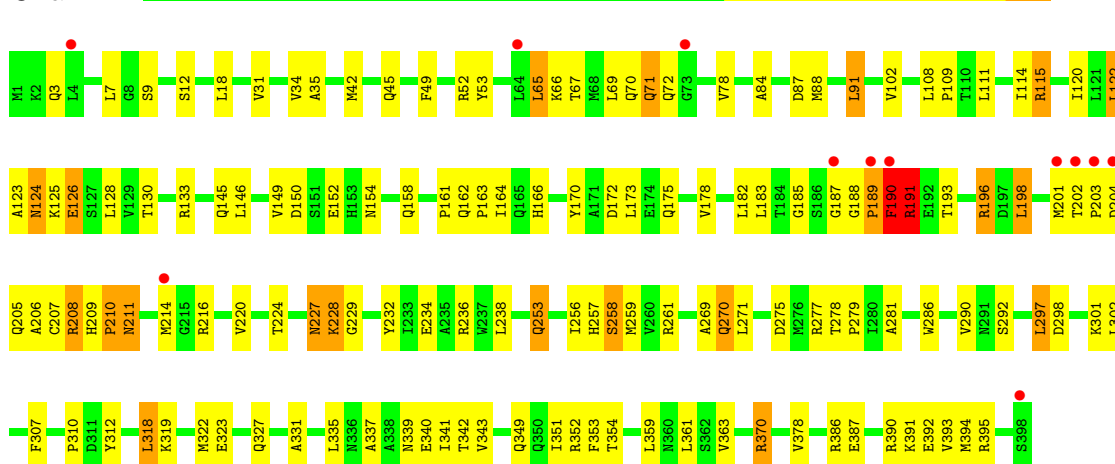
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	25	Total	O	0	0
			25	25		
2	C	40	Total	O	0	0
			40	40		

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.

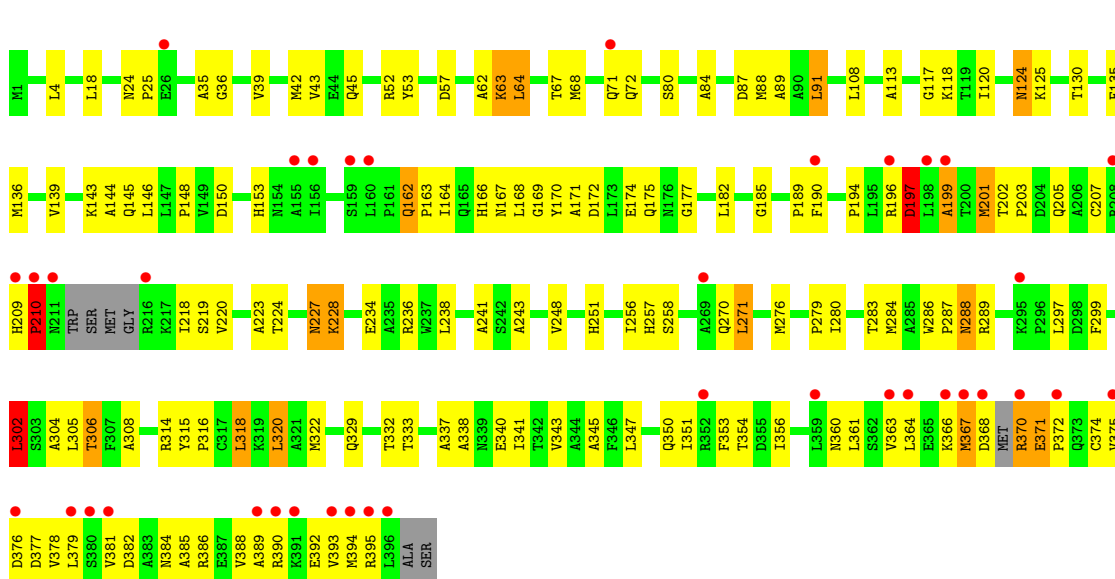
- Molecule 1: 1-deoxy-D-xylulose-5-phosphatereductoisomerase

Chain A:



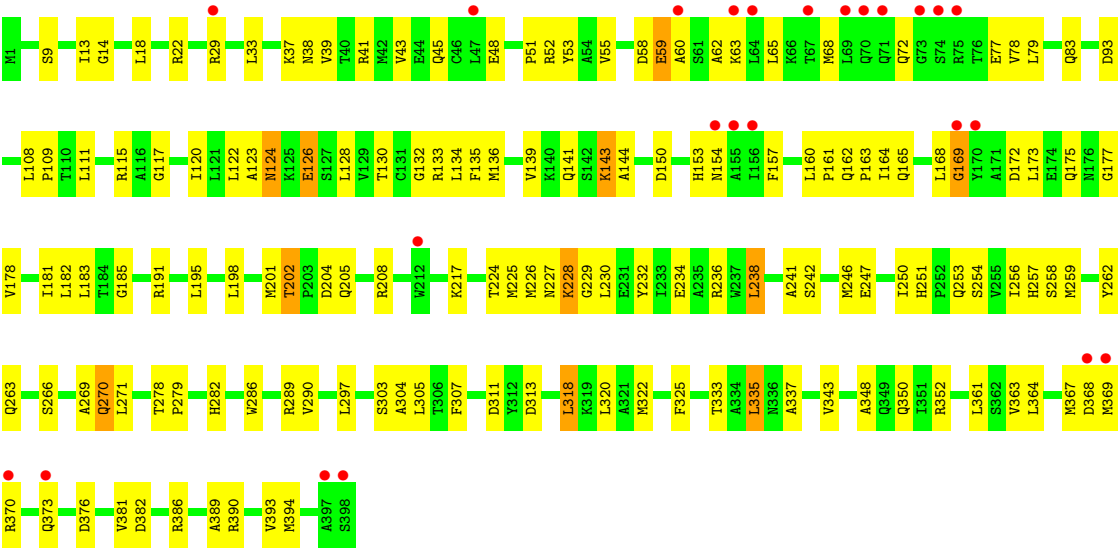
- Molecule 1: 1-deoxy-D-xylulose-5-phosphatereductoisomerase

Chain B:



- Molecule 1: 1-deoxy-D-xylulose-5-phosphatereductoisomerase

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.27Å 249.26Å 132.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.50 33.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.6 (33.45-2.50) 90.5 (33.45-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.284 0.233 , 0.282	Depositor DCC
R_{free} test set	5343 reflections (10.14%)	DCC
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57245 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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	0.35	0/3078	0.61	0/4171
1	B	0.36	0/3022	0.66	2/4094 (0.0%)
1	C	0.39	0/3078	0.64	0/4171
All	All	0.37	0/9178	0.64	2/12436 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	PRO	CA-N-CD	-14.82	90.75	111.50
1	B	302	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3030	0	3053	135	0
1	B	2978	0	3007	139	0
1	C	3030	0	3055	117	0
2	A	23	0	0	0	0
2	B	25	0	0	0	0
2	C	40	0	0	2	0
All	All	9126	0	9115	378	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 21.

All (378) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:288:ASN:ND2	1:B:289:ARG:H	1.59	1.00
1:C:59:GLU:HA	1:C:62:ALA:HB3	1.46	0.97
1:B:210:PRO:HG3	1:B:219:SER:OG	1.64	0.97
1:A:208:ARG:H	1:A:208:ARG:HD2	1.30	0.96
1:A:256:ILE:HG12	1:A:271:LEU:HD22	1.52	0.91
1:C:202:THR:HG22	1:C:205:GLN:HG3	1.52	0.90
1:A:124:ASN:H	1:A:124:ASN:HD22	1.18	0.88
1:A:370:ARG:H	1:A:370:ARG:HD2	1.36	0.88
1:C:363:VAL:O	1:C:367:MET:HG2	1.72	0.87
1:B:288:ASN:HD22	1:B:289:ARG:N	1.72	0.86
1:B:288:ASN:HD22	1:B:289:ARG:H	0.87	0.85
1:C:181:ILE:HB	1:C:246:MET:HE2	1.60	0.82
1:A:297:LEU:HD21	1:A:302:LEU:HD21	1.60	0.82
1:A:256:ILE:HG12	1:A:271:LEU:CD2	2.08	0.82
1:C:256:ILE:HG12	1:C:271:LEU:HD22	1.61	0.82
1:B:130:THR:HG22	1:B:333:THR:HG23	1.62	0.81
1:B:220:VAL:HG11	1:B:343:VAL:HG13	1.61	0.80
1:A:211:ASN:ND2	1:A:214:MET:HB2	1.96	0.80
1:C:236:ARG:HD2	1:C:241:ALA:O	1.83	0.79
1:A:187:GLY:HA2	1:A:190:PHE:HA	1.65	0.78
1:B:227:ASN:ND2	1:B:228:LYS:H	1.82	0.78
1:A:257:HIS:HD2	1:A:270:GLN:HE22	1.31	0.78
1:B:118:LYS:O	1:B:120:ILE:HD12	1.85	0.76
1:A:278:THR:HB	1:A:279:PRO:HD3	1.68	0.76
1:C:177:GLY:HA2	1:C:263:GLN:NE2	2.01	0.76
1:A:319:LYS:HA	1:A:322:MET:HE2	1.68	0.75
1:B:218:ILE:HD12	1:B:218:ILE:H	1.51	0.75
1:B:146:LEU:HB2	1:B:168:LEU:HD12	1.69	0.73
1:B:39:VAL:O	1:B:43:VAL:HG23	1.89	0.73
1:B:52:ARG:HD2	1:B:53:TYR:CE1	2.23	0.73
1:C:52:ARG:HD2	1:C:53:TYR:HE1	1.52	0.73
1:C:52:ARG:HD2	1:C:53:TYR:CE1	2.24	0.73
1:A:204:ASP:OD1	1:A:205:GLN:HG3	1.88	0.72
1:A:257:HIS:CD2	1:A:270:GLN:HE22	2.07	0.72
1:C:41:ARG:HH11	1:C:41:ARG:HG2	1.53	0.72
1:A:120:ILE:HB	1:A:146:LEU:HD23	1.72	0.71
1:A:193:THR:HG23	1:A:196:ARG:H	1.53	0.71
1:C:181:ILE:HB	1:C:246:MET:CE	2.20	0.71
1:A:208:ARG:CD	1:A:208:ARG:H	2.01	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39:VAL:O	1:C:43:VAL:HG23	1.90	0.70
1:B:377:ASP:O	1:B:381:VAL:HG23	1.92	0.70
1:C:172:ASP:OD2	1:C:175:GLN:HG2	1.91	0.69
1:B:271:LEU:N	1:B:271:LEU:HD23	2.08	0.69
1:C:256:ILE:HG12	1:C:271:LEU:CD2	2.23	0.69
1:B:338:ALA:HB1	1:B:363:VAL:HG21	1.74	0.69
1:B:299:PHE:HA	1:B:302:LEU:HD22	1.74	0.69
1:C:133:ARG:HH11	1:C:133:ARG:HG3	1.58	0.68
1:B:148:PRO:HG3	1:B:238:LEU:HD21	1.74	0.68
1:A:203:PRO:HD3	1:C:373:GLN:O	1.94	0.68
1:A:12:SER:HB2	1:A:208:ARG:HG3	1.76	0.67
1:A:370:ARG:H	1:A:370:ARG:CD	2.07	0.67
1:A:359:LEU:O	1:A:363:VAL:HG23	1.94	0.67
1:A:319:LYS:O	1:A:323:GLU:HG3	1.95	0.67
1:B:360:ASN:O	1:B:364:LEU:HD23	1.95	0.67
1:A:253:GLN:H	1:A:253:GLN:CD	1.97	0.67
1:A:124:ASN:N	1:A:124:ASN:HD22	1.86	0.67
1:C:143:LYS:HA	1:C:143:LYS:NZ	2.10	0.67
1:B:305:LEU:HB2	1:C:305:LEU:HB2	1.75	0.66
1:A:188:GLY:H	1:A:189:PRO:C	1.98	0.66
1:A:84:ALA:O	1:A:88:MET:HG2	1.95	0.66
1:B:389:ALA:O	1:B:393:VAL:HG23	1.96	0.66
1:A:198:LEU:HD22	1:C:111:LEU:HD23	1.79	0.66
1:B:227:ASN:N	1:B:227:ASN:HD22	1.93	0.65
1:A:390:ARG:HA	1:A:393:VAL:HG12	1.78	0.65
1:A:162:GLN:HB3	1:A:163:PRO:HD3	1.78	0.65
1:C:143:LYS:HA	1:C:143:LYS:HZ3	1.62	0.65
1:A:3:GLN:HB3	1:A:31:VAL:CG2	2.26	0.65
1:A:318:LEU:HD22	1:A:322:MET:HE1	1.79	0.65
1:A:9:SER:HB2	1:A:45:GLN:HE22	1.62	0.65
1:A:196:ARG:HA	1:A:196:ARG:HE	1.61	0.65
1:B:185:GLY:HA3	1:B:228:LYS:HD3	1.79	0.64
1:B:288:ASN:ND2	1:B:289:ARG:N	2.40	0.64
1:B:36:GLY:HA2	1:B:57:ASP:HB2	1.80	0.64
1:A:208:ARG:HD2	1:A:208:ARG:N	2.11	0.63
1:B:62:ALA:HB2	1:B:80:SER:HB3	1.79	0.63
1:A:256:ILE:HA	1:A:271:LEU:HD22	1.81	0.63
1:A:185:GLY:HA3	1:A:228:LYS:HE2	1.81	0.62
1:C:185:GLY:HA3	1:C:228:LYS:HE2	1.80	0.62
1:C:22:ARG:HD3	1:C:48:GLU:OE1	1.99	0.62
1:B:18:LEU:HD12	1:B:45:GLN:NE2	2.13	0.62
1:C:202:THR:HG23	1:C:204:ASP:H	1.64	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:154:ASN:HD21	1:C:282:HIS:CD2	2.17	0.61
1:A:172:ASP:OD1	1:A:175:GLN:HG3	2.00	0.61
1:B:67:THR:O	1:B:71:GLN:HG2	1.99	0.61
1:A:210:PRO:HB3	1:C:115:ARG:HB3	1.82	0.61
1:C:55:VAL:HG22	1:C:79:LEU:HB2	1.82	0.61
1:A:124:ASN:H	1:A:124:ASN:ND2	1.92	0.61
1:C:29:ARG:HH11	1:C:29:ARG:HG2	1.66	0.60
1:C:253:GLN:O	1:C:254:SER:HB2	2.02	0.59
1:C:217:LYS:HG3	1:C:343:VAL:HG11	1.85	0.59
1:B:175:GLN:HA	1:B:175:GLN:HE21	1.68	0.59
1:C:165:GLN:NE2	1:C:286:TRP:HE1	2.00	0.59
1:C:227:ASN:OD1	1:C:228:LYS:N	2.35	0.58
1:B:251:HIS:HD2	1:B:306:THR:O	1.86	0.58
1:B:251:HIS:HE1	1:B:256:ILE:H	1.51	0.58
1:C:278:THR:HB	1:C:279:PRO:CD	2.34	0.58
1:A:327:GLN:HB2	1:A:331:ALA:CB	2.34	0.58
1:B:372:PRO:HB3	1:B:378:VAL:HG22	1.86	0.57
1:B:87:ASP:O	1:B:91:LEU:HD13	2.05	0.57
1:B:384:ASN:O	1:B:388:VAL:HG23	2.05	0.57
1:C:136:MET:CE	1:C:169:GLY:HA2	2.35	0.56
1:B:370:ARG:HG2	1:B:371:GLU:N	2.19	0.56
1:B:236:ARG:NH2	1:B:243:ALA:HB2	2.21	0.56
1:C:59:GLU:HA	1:C:62:ALA:CB	2.29	0.56
1:C:133:ARG:NH1	1:C:133:ARG:HG3	2.18	0.56
1:C:386:ARG:O	1:C:390:ARG:HG3	2.05	0.56
1:C:177:GLY:HA2	1:C:263:GLN:HE21	1.70	0.56
1:B:366:LYS:NZ	1:B:395:ARG:HH22	2.04	0.56
1:C:128:LEU:CD1	1:C:238:LEU:HD13	2.36	0.56
1:C:182:LEU:HD23	1:C:247:GLU:HB2	1.86	0.56
1:C:154:ASN:HD21	1:C:282:HIS:HD2	1.54	0.56
1:A:387:GLU:HG3	1:A:391:LYS:HE3	1.87	0.56
1:B:162:GLN:CD	1:C:162:GLN:HG3	2.26	0.56
1:B:388:VAL:O	1:B:392:GLU:HG2	2.06	0.55
1:B:125:LYS:HD2	1:B:234:GLU:OE1	2.05	0.55
1:B:314:ARG:C	1:B:316:PRO:HD3	2.27	0.55
1:C:128:LEU:HD11	1:C:238:LEU:HD13	1.89	0.55
1:C:257:HIS:HD2	1:C:270:GLN:HE22	1.55	0.55
1:C:173:LEU:HD22	1:C:178:VAL:HG11	1.89	0.55
1:B:271:LEU:HD11	1:C:259:MET:HE1	1.87	0.55
1:A:202:THR:HB	1:A:203:PRO:HD2	1.88	0.55
1:A:67:THR:O	1:A:71:GLN:HG2	2.07	0.55
1:B:190:PHE:CZ	1:B:201:MET:HG2	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:ALA:HB1	1:A:386:ARG:HG3	1.90	0.54
1:B:218:ILE:CD1	1:B:218:ILE:H	2.19	0.54
1:A:259:MET:HG2	1:A:269:ALA:HB2	1.89	0.54
1:B:218:ILE:HD12	1:B:218:ILE:N	2.21	0.54
1:A:227:ASN:ND2	1:A:228:LYS:N	2.56	0.54
1:C:236:ARG:NH2	1:C:325:PHE:CD2	2.76	0.54
1:B:341:ILE:HB	1:B:389:ALA:HB1	1.89	0.54
1:A:256:ILE:CG1	1:A:271:LEU:HD22	2.33	0.54
1:A:370:ARG:N	1:A:370:ARG:HD2	2.14	0.54
1:C:13:ILE:HD13	1:C:123:ALA:HB1	1.90	0.53
1:C:134:LEU:HD21	1:C:373:GLN:O	2.09	0.53
1:B:139:VAL:O	1:B:143:LYS:N	2.40	0.53
1:C:135:PHE:O	1:C:139:VAL:HG23	2.09	0.53
1:C:369:MET:SD	1:C:381:VAL:HA	2.49	0.53
1:B:124:ASN:H	1:B:124:ASN:HD22	1.55	0.53
1:A:298:ASP:OD2	1:A:301:LYS:HD3	2.09	0.53
1:B:227:ASN:HD22	1:B:228:LYS:H	1.52	0.53
1:B:270:GLN:HE21	1:C:266:SER:HB2	1.74	0.53
1:A:18:LEU:HD22	1:A:49:PHE:CE1	2.44	0.53
1:C:389:ALA:O	1:C:393:VAL:HG23	2.09	0.53
1:B:124:ASN:N	1:B:124:ASN:HD22	2.07	0.52
1:A:87:ASP:O	1:A:91:LEU:HD13	2.09	0.52
1:B:148:PRO:CG	1:B:238:LEU:HD21	2.39	0.52
1:C:253:GLN:H	1:C:253:GLN:CD	2.12	0.52
1:B:386:ARG:O	1:B:390:ARG:NH1	2.42	0.52
1:C:117:GLY:HA2	1:C:144:ALA:HB2	1.89	0.52
1:B:320:LEU:HD11	1:B:361:LEU:HA	1.90	0.52
1:A:256:ILE:HG12	1:A:271:LEU:HD21	1.92	0.52
1:C:37:LYS:O	1:C:39:VAL:HG23	2.09	0.52
1:B:189:PRO:HD2	1:B:223:ALA:HA	1.92	0.52
1:A:122:LEU:HD22	1:A:124:ASN:ND2	2.24	0.52
1:C:162:GLN:HB2	1:C:163:PRO:HD3	1.92	0.52
1:C:65:LEU:HD13	1:C:65:LEU:C	2.30	0.52
1:C:33:LEU:HD12	1:C:51:PRO:HG3	1.92	0.52
1:B:84:ALA:O	1:B:88:MET:HG2	2.09	0.52
1:C:311:ASP:HB3	1:C:313:ASP:OD1	2.10	0.52
1:B:175:GLN:HA	1:B:175:GLN:NE2	2.25	0.52
1:A:70:GLN:C	1:A:72:GLN:H	2.13	0.52
1:B:236:ARG:HD2	1:B:241:ALA:O	2.11	0.51
1:B:64:LEU:O	1:B:68:MET:HG3	2.10	0.51
1:A:130:THR:HB	1:A:378:VAL:CG1	2.40	0.51
1:B:338:ALA:CB	1:B:363:VAL:HG21	2.39	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:GLN:N	1:A:253:GLN:CD	2.63	0.51
1:C:150:ASP:OD2	1:C:153:HIS:ND1	2.44	0.51
1:C:282:HIS:HE1	2:C:423:HOH:O	1.93	0.51
1:B:172:ASP:OD2	1:B:175:GLN:HB2	2.11	0.51
1:A:125:LYS:HD3	1:A:150:ASP:HB2	1.92	0.51
1:A:130:THR:HB	1:A:378:VAL:HG11	1.92	0.51
1:C:172:ASP:HB3	1:C:175:GLN:CG	2.41	0.51
1:B:36:GLY:CA	1:B:57:ASP:HB2	2.40	0.51
1:A:3:GLN:HB3	1:A:31:VAL:HG23	1.93	0.51
1:B:227:ASN:ND2	1:B:228:LYS:N	2.54	0.50
1:C:172:ASP:HB3	1:C:175:GLN:HG3	1.93	0.50
1:B:370:ARG:HD2	1:B:370:ARG:N	2.25	0.50
1:B:35:ALA:HB2	1:B:42:MET:HE2	1.93	0.50
1:B:374:CYS:C	1:B:376:ASP:H	2.14	0.50
1:B:366:LYS:HZ1	1:B:395:ARG:HH22	1.57	0.50
1:B:361:LEU:HD22	1:B:361:LEU:O	2.12	0.50
1:A:154:ASN:O	1:A:158:GLN:HG3	2.12	0.50
1:B:210:PRO:HA	1:B:219:SER:HB3	1.93	0.50
1:B:196:ARG:NH2	1:B:199:ALA:HB3	2.26	0.50
1:B:374:CYS:HB3	1:B:377:ASP:OD2	2.11	0.50
1:A:387:GLU:CG	1:A:391:LYS:HE3	2.41	0.50
1:A:133:ARG:HH11	1:A:133:ARG:HG3	1.75	0.50
1:C:259:MET:HG2	1:C:269:ALA:HB2	1.94	0.50
1:B:297:LEU:HD12	1:B:299:PHE:CE1	2.47	0.50
1:B:304:ALA:HB1	1:C:304:ALA:HB1	1.94	0.50
1:C:124:ASN:N	1:C:124:ASN:HD22	2.10	0.49
1:A:188:GLY:H	1:A:190:PHE:N	2.10	0.49
1:A:319:LYS:HA	1:A:322:MET:CE	2.40	0.49
1:B:166:HIS:CD2	1:B:286:TRP:HZ2	2.29	0.49
1:B:341:ILE:HG13	1:B:389:ALA:HB3	1.93	0.49
1:B:135:PHE:O	1:B:139:VAL:HG23	2.13	0.49
1:C:124:ASN:H	1:C:124:ASN:HD22	1.60	0.49
1:B:276:MET:HE2	1:B:276:MET:HA	1.93	0.49
1:C:58:ASP:OD2	1:C:60:ALA:HB3	2.13	0.49
1:B:318:LEU:O	1:B:322:MET:HG3	2.12	0.49
1:A:211:ASN:HD22	1:A:214:MET:HB2	1.71	0.49
1:A:150:ASP:OD2	1:A:152:GLU:HG2	2.12	0.49
1:A:102:VAL:HA	1:A:126:GLU:OE1	2.12	0.49
1:A:18:LEU:HD11	1:A:45:GLN:NE2	2.27	0.49
1:C:160:LEU:HD13	1:C:164:ILE:HG21	1.95	0.49
1:A:392:GLU:O	1:A:395:ARG:HG2	2.13	0.49
1:B:89:ALA:HB1	1:B:113:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:251:HIS:CD2	1:B:306:THR:O	2.66	0.48
1:C:259:MET:HG2	1:C:269:ALA:CB	2.43	0.48
1:A:18:LEU:HD22	1:A:49:PHE:CD1	2.48	0.48
1:A:161:PRO:CG	1:A:164:ILE:HD12	2.43	0.48
1:A:229:GLY:O	1:A:232:TYR:HB3	2.14	0.48
1:A:281:ALA:HB2	1:A:292:SER:HB3	1.95	0.48
1:B:337:ALA:O	1:B:340:GLU:HB2	2.13	0.48
1:A:188:GLY:N	1:A:190:PHE:N	2.62	0.48
1:A:209:HIS:ND1	1:A:210:PRO:HD2	2.28	0.48
1:C:130:THR:HG22	1:C:333:THR:HA	1.95	0.48
1:B:341:ILE:HG22	1:B:393:VAL:HG21	1.96	0.48
1:A:125:LYS:HB2	1:A:234:GLU:OE1	2.13	0.48
1:B:167:ASN:HA	1:B:170:TYR:CZ	2.49	0.48
1:B:150:ASP:OD1	1:B:153:HIS:ND1	2.46	0.48
1:C:124:ASN:ND2	1:C:124:ASN:H	2.11	0.48
1:B:62:ALA:CB	1:B:80:SER:HB3	2.43	0.48
1:C:136:MET:HE3	1:C:169:GLY:HA2	1.96	0.47
1:C:153:HIS:HE1	1:C:234:GLU:OE1	1.96	0.47
1:B:374:CYS:C	1:B:376:ASP:N	2.67	0.47
1:A:191:ARG:HD3	1:A:191:ARG:C	2.35	0.47
1:B:337:ALA:HB2	1:B:382:ASP:OD1	2.13	0.47
1:A:52:ARG:HD2	1:A:53:TYR:CE1	2.49	0.47
1:C:318:LEU:HD22	1:C:322:MET:HE3	1.96	0.47
1:B:361:LEU:HD13	1:B:361:LEU:C	2.35	0.47
1:A:220:VAL:HG11	1:A:343:VAL:HG13	1.97	0.47
1:A:216:ARG:O	1:A:220:VAL:HG23	2.15	0.47
1:C:202:THR:HG23	1:C:204:ASP:N	2.30	0.47
1:A:189:PRO:O	1:A:191:ARG:N	2.47	0.47
1:A:318:LEU:HD22	1:A:322:MET:CE	2.45	0.47
1:B:194:PRO:HG2	1:B:197:ASP:HB2	1.97	0.47
1:C:157:PHE:CD1	1:C:168:LEU:HD11	2.50	0.46
1:A:122:LEU:HD22	1:A:124:ASN:HD21	1.81	0.46
1:A:340:GLU:HG3	1:A:386:ARG:NH2	2.30	0.46
1:C:122:LEU:HD12	1:C:124:ASN:HD21	1.81	0.46
1:C:18:LEU:HD12	1:C:45:GLN:NE2	2.31	0.46
1:C:41:ARG:NH1	1:C:41:ARG:HG2	2.24	0.46
1:A:216:ARG:NH1	1:C:83:GLN:HE21	2.14	0.46
1:A:162:GLN:HG3	1:A:166:HIS:HD2	1.80	0.46
1:A:173:LEU:HB3	1:A:178:VAL:HB	1.98	0.46
1:A:145:GLN:NE2	1:A:286:TRP:CH2	2.84	0.46
1:C:191:ARG:HD3	2:C:430:HOH:O	2.16	0.46
1:B:271:LEU:HD11	1:C:259:MET:CE	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:LEU:HB2	1:A:109:PRO:HD3	1.98	0.46
1:A:352:ARG:HB2	1:A:352:ARG:HH11	1.80	0.46
1:A:35:ALA:HB3	1:A:42:MET:HE2	1.97	0.46
1:B:227:ASN:N	1:B:227:ASN:ND2	2.61	0.46
1:A:206:ALA:HA	1:A:208:ARG:CD	2.46	0.46
1:C:318:LEU:HD13	1:C:322:MET:HE3	1.97	0.46
1:C:335:LEU:HG	1:C:364:LEU:HD11	1.97	0.46
1:B:256:ILE:HA	1:B:271:LEU:HB3	1.99	0.45
1:C:318:LEU:HD22	1:C:322:MET:CE	2.46	0.45
1:A:190:PHE:N	1:A:190:PHE:CD1	2.84	0.45
1:C:29:ARG:HH11	1:C:29:ARG:CG	2.29	0.45
1:A:259:MET:HG2	1:A:269:ALA:CB	2.46	0.45
1:C:224:THR:O	1:C:225:MET:HB2	2.16	0.45
1:A:227:ASN:ND2	1:A:228:LYS:H	2.13	0.45
1:B:145:GLN:HE22	1:B:166:HIS:HA	1.81	0.45
1:B:117:GLY:HA2	1:B:144:ALA:HB2	1.98	0.45
1:A:390:ARG:O	1:A:393:VAL:HG12	2.17	0.45
1:A:170:TYR:CD1	1:A:170:TYR:N	2.84	0.45
1:A:270:GLN:C	1:A:271:LEU:HD23	2.36	0.45
1:B:251:HIS:CE1	1:B:256:ILE:H	2.32	0.45
1:A:327:GLN:HB2	1:A:331:ALA:HB2	1.98	0.45
1:A:164:ILE:HD13	1:A:173:LEU:HD23	1.99	0.45
1:A:128:LEU:CD1	1:A:238:LEU:HG	2.46	0.45
1:B:177:GLY:HA3	1:C:289:ARG:HB2	1.99	0.45
1:B:136:MET:CE	1:B:169:GLY:HA3	2.46	0.45
1:C:168:LEU:O	1:C:169:GLY:C	2.55	0.45
1:B:257:HIS:HD2	1:B:270:GLN:OE1	1.99	0.45
1:C:120:ILE:N	1:C:120:ILE:HD12	2.32	0.45
1:A:275:ASP:OD1	1:A:277:ARG:HD3	2.16	0.45
1:B:207:CYS:C	1:B:209:HIS:H	2.21	0.45
1:C:29:ARG:CZ	1:C:29:ARG:HB2	2.47	0.45
1:C:77:GLU:HG3	1:C:78:VAL:H	1.82	0.45
1:C:226:MET:O	1:C:230:LEU:HG	2.17	0.45
1:C:198:LEU:HA	1:C:201:MET:HG2	1.99	0.44
1:B:248:VAL:HG11	1:B:318:LEU:HD11	1.99	0.44
1:B:271:LEU:N	1:B:271:LEU:CD2	2.79	0.44
1:B:210:PRO:HD3	1:B:219:SER:CB	2.47	0.44
1:A:352:ARG:NH1	1:A:352:ARG:CB	2.81	0.44
1:A:310:PRO:HG2	1:A:312:TYR:CZ	2.53	0.44
1:B:175:GLN:CA	1:B:175:GLN:HE21	2.29	0.44
1:A:161:PRO:HG2	1:A:164:ILE:HD12	1.99	0.44
1:A:65:LEU:HD13	1:A:78:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:LYS:O	1:A:70:GLN:HB2	2.18	0.44
1:B:367:MET:HE1	1:B:385:ALA:N	2.33	0.43
1:B:224:THR:HG22	1:B:353:PHE:CZ	2.53	0.43
1:A:228:LYS:HZ2	1:A:228:LYS:HA	1.83	0.43
1:C:68:MET:O	1:C:72:GLN:HG2	2.17	0.43
1:B:279:PRO:O	1:B:283:THR:HG23	2.19	0.43
1:A:257:HIS:HD2	1:A:270:GLN:NE2	2.06	0.43
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.87	0.43
1:A:352:ARG:NH1	1:A:352:ARG:HB2	2.34	0.43
1:C:9:SER:HA	1:C:14:GLY:HA3	2.00	0.43
1:C:108:LEU:HB2	1:C:109:PRO:HD3	2.01	0.43
1:C:182:LEU:HD12	1:C:259:MET:HB2	2.00	0.43
1:C:132:GLY:O	1:C:136:MET:HG2	2.19	0.43
1:C:352:ARG:HH11	1:C:352:ARG:HG2	1.83	0.43
1:B:356:ILE:HG22	1:B:360:ASN:ND2	2.34	0.43
1:A:352:ARG:NE	1:A:354:THR:HG22	2.34	0.43
1:A:65:LEU:HD22	1:A:69:LEU:HG	2.01	0.43
1:C:229:GLY:O	1:C:232:TYR:HB3	2.17	0.43
1:A:162:GLN:CB	1:A:163:PRO:HD3	2.46	0.43
1:A:391:LYS:HA	1:A:394:MET:HE3	2.01	0.43
1:B:270:GLN:HE21	1:C:266:SER:CB	2.32	0.43
1:A:352:ARG:CZ	1:A:352:ARG:HB3	2.49	0.43
1:A:65:LEU:HD13	1:A:78:VAL:CG2	2.49	0.43
1:A:257:HIS:O	1:A:258:SER:CB	2.67	0.42
1:B:363:VAL:O	1:B:367:MET:HG2	2.19	0.42
1:C:257:HIS:CD2	1:C:270:GLN:HE22	2.33	0.42
1:A:256:ILE:HD12	1:A:307:PHE:HZ	1.84	0.42
1:A:297:LEU:HD23	1:A:298:ASP:N	2.33	0.42
1:A:342:THR:O	1:A:351:ILE:HD11	2.19	0.42
1:A:228:LYS:NZ	1:A:228:LYS:HA	2.34	0.42
1:B:315:TYR:N	1:B:316:PRO:HD3	2.33	0.42
1:B:345:ALA:O	1:B:350:GLN:HB2	2.19	0.42
1:C:59:GLU:O	1:C:63:LYS:N	2.34	0.42
1:A:310:PRO:HG2	1:A:312:TYR:CE1	2.54	0.42
1:B:284:MET:HB2	1:B:284:MET:HE3	1.96	0.42
1:B:375:VAL:O	1:B:379:LEU:HG	2.19	0.42
1:C:236:ARG:HH11	1:C:242:SER:HA	1.84	0.42
1:B:35:ALA:HB2	1:B:42:MET:CE	2.49	0.42
1:B:167:ASN:HB2	1:B:171:ALA:HB2	2.01	0.42
1:B:196:ARG:HH22	1:B:199:ALA:HB3	1.84	0.42
1:A:114:ILE:O	1:A:115:ARG:C	2.58	0.42
1:B:356:ILE:O	1:B:360:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:394:MET:HA	1:B:394:MET:CE	2.50	0.42
1:B:182:LEU:N	1:B:182:LEU:HD12	2.35	0.42
1:B:280:ILE:CG2	1:B:284:MET:HE3	2.50	0.42
1:B:24:ASN:N	1:B:25:PRO:CD	2.83	0.42
1:A:188:GLY:N	1:A:189:PRO:C	2.70	0.42
1:B:63:LYS:HE3	1:B:67:THR:OG1	2.19	0.42
1:B:108:LEU:HA	1:B:108:LEU:HD23	1.82	0.42
1:B:162:GLN:N	1:B:163:PRO:HD2	2.35	0.41
1:B:201:MET:HG3	1:B:205:GLN:OE1	2.20	0.41
1:A:339:ASN:O	1:A:343:VAL:HG23	2.20	0.41
1:C:161:PRO:HD3	1:C:262:TYR:OH	2.19	0.41
1:C:337:ALA:HB2	1:C:382:ASP:OD1	2.20	0.41
1:A:182:LEU:HD11	1:A:261:ARG:HB2	2.03	0.41
1:B:36:GLY:C	1:B:57:ASP:HB2	2.41	0.41
1:A:391:LYS:HA	1:A:394:MET:CE	2.50	0.41
1:C:250:ILE:O	1:C:307:PHE:HA	2.20	0.41
1:B:203:PRO:HB3	1:B:347:LEU:HD23	2.02	0.41
1:B:209:HIS:N	1:B:210:PRO:HD2	2.35	0.41
1:C:202:THR:HG22	1:C:205:GLN:H	1.84	0.41
1:C:251:HIS:HE1	1:C:305:LEU:HD22	1.85	0.41
1:B:286:TRP:CD1	1:B:287:PRO:HA	2.55	0.41
1:B:164:ILE:HD13	1:B:171:ALA:HB3	2.02	0.41
1:C:236:ARG:NH2	1:C:325:PHE:HD2	2.18	0.41
1:C:236:ARG:NH1	1:C:242:SER:HA	2.36	0.41
1:A:202:THR:HG22	1:C:373:GLN:HB3	2.02	0.41
1:A:341:ILE:HD13	1:A:386:ARG:HG2	2.03	0.41
1:A:224:THR:HG22	1:A:353:PHE:CZ	2.55	0.41
1:A:7:LEU:HA	1:A:34:VAL:HB	2.03	0.41
1:B:207:CYS:C	1:B:210:PRO:HD2	2.41	0.41
1:A:123:ALA:HA	1:A:149:VAL:HB	2.03	0.41
1:A:190:PHE:H	1:A:190:PHE:HD1	1.61	0.41
1:B:124:ASN:N	1:B:124:ASN:ND2	2.69	0.41
1:B:136:MET:HE1	1:B:169:GLY:HA3	2.02	0.41
1:A:18:LEU:CD1	1:A:45:GLN:NE2	2.84	0.41
1:B:199:ALA:HA	1:B:354:THR:HB	2.02	0.41
1:B:345:ALA:HB3	1:B:351:ILE:HD11	2.01	0.41
1:B:210:PRO:HD3	1:B:219:SER:HB3	2.02	0.40
1:C:201:MET:HE3	1:C:205:GLN:HB3	2.02	0.40
1:B:202:THR:OG1	1:B:205:GLN:HG3	2.21	0.40
1:A:281:ALA:CB	1:A:292:SER:HB3	2.52	0.40
1:B:314:ARG:HD3	1:B:315:TYR:CZ	2.56	0.40
1:C:122:LEU:CD1	1:C:124:ASN:HD21	2.34	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:348:ALA:HB3	1:C:350:GLN:HG2	2.01	0.40
1:B:385:ALA:O	1:B:386:ARG:C	2.59	0.40
1:B:329:GLN:HA	1:B:332:THR:OG1	2.22	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	396/398 (100%)	367 (93%)	21 (5%)	8 (2%)	11	17
1	B	385/398 (97%)	351 (91%)	29 (8%)	5 (1%)	18	29
1	C	396/398 (100%)	378 (96%)	13 (3%)	5 (1%)	18	29
All	All	1177/1194 (99%)	1096 (93%)	63 (5%)	18 (2%)	15	25

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	PHE
1	A	210	PRO
1	A	258	SER
1	A	349	GLN
1	B	371	GLU
1	A	191	ARG
1	C	38	ASN
1	C	169	GLY
1	C	258	SER
1	A	211	ASN
1	B	197	ASP
1	A	71	GLN
1	B	199	ALA
1	C	126	GLU
1	B	308	ALA
1	B	367	MET

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Mol	Chain	Res	Type
1	C	368	ASP
1	A	189	PRO

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	328/328 (100%)	302 (92%)	26 (8%)	18	31
1	B	323/328 (98%)	301 (93%)	22 (7%)	22	39
1	C	328/328 (100%)	305 (93%)	23 (7%)	21	38
All	All	979/984 (100%)	908 (93%)	71 (7%)	20	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	91	LEU
1	A	111	LEU
1	A	115	ARG
1	A	122	LEU
1	A	124	ASN
1	A	126	GLU
1	A	183	LEU
1	A	190	PHE
1	A	191	ARG
1	A	196	ARG
1	A	198	LEU
1	A	201	MET
1	A	207	CYS
1	A	208	ARG
1	A	227	ASN
1	A	228	LYS
1	A	236	ARG
1	A	253	GLN
1	A	270	GLN
1	A	290	VAL

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Mol	Chain	Res	Type
1	A	297	LEU
1	A	318	LEU
1	A	335	LEU
1	A	361	LEU
1	A	370	ARG
1	B	4	LEU
1	B	63	LYS
1	B	64	LEU
1	B	72	GLN
1	B	91	LEU
1	B	124	ASN
1	B	162	GLN
1	B	174	GLU
1	B	197	ASP
1	B	201	MET
1	B	210	PRO
1	B	227	ASN
1	B	228	LYS
1	B	258	SER
1	B	271	LEU
1	B	288	ASN
1	B	302	LEU
1	B	306	THR
1	B	318	LEU
1	B	320	LEU
1	B	368	ASP
1	B	370	ARG
1	C	59	GLU
1	C	93	ASP
1	C	124	ASN
1	C	126	GLU
1	C	141	GLN
1	C	143	LYS
1	C	183	LEU
1	C	195	LEU
1	C	202	THR
1	C	208	ARG
1	C	228	LYS
1	C	238	LEU
1	C	270	GLN
1	C	290	VAL
1	C	297	LEU

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Mol	Chain	Res	Type
1	C	303	SER
1	C	318	LEU
1	C	320	LEU
1	C	335	LEU
1	C	361	LEU
1	C	370	ARG
1	C	376	ASP
1	C	394	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	72	GLN
1	A	124	ASN
1	A	145	GLN
1	A	205	GLN
1	A	211	ASN
1	A	227	ASN
1	A	257	HIS
1	A	270	GLN
1	A	329	GLN
1	A	373	GLN
1	B	70	GLN
1	B	71	GLN
1	B	72	GLN
1	B	124	ASN
1	B	145	GLN
1	B	162	GLN
1	B	165	GLN
1	B	175	GLN
1	B	227	ASN
1	B	251	HIS
1	B	257	HIS
1	B	270	GLN
1	B	288	ASN
1	B	291	ASN
1	B	384	ASN
1	C	3	GLN
1	C	71	GLN
1	C	83	GLN
1	C	124	ASN

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Mol	Chain	Res	Type
1	C	145	GLN
1	C	165	GLN
1	C	257	HIS
1	C	282	HIS

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	398/398 (100%)	0.28	12 (3%) 48 50	40, 60, 99, 116	0
1	B	391/398 (98%)	0.47	38 (9%) 8 7	35, 64, 121, 144	0
1	C	398/398 (100%)	0.22	24 (6%) 21 21	25, 52, 91, 109	0
All	All	1187/1194 (99%)	0.33	74 (6%) 20 20	25, 58, 107, 144	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	VAL	7.1
1	B	396	LEU	6.9
1	B	367	MET	6.2
1	B	370	ARG	5.8
1	C	170	TYR	5.3
1	B	209	HIS	5.1
1	A	190	PHE	5.0
1	A	203	PRO	4.8
1	C	63	LYS	4.8
1	B	364	LEU	4.4
1	B	381	VAL	4.4
1	C	64	LEU	4.3
1	B	393	VAL	4.3
1	B	210	PRO	3.8
1	C	398	SER	3.8
1	B	372	PRO	3.6
1	B	394	MET	3.6
1	B	211	ASN	3.5
1	C	369	MET	3.4
1	B	196	ARG	3.3
1	A	214	MET	3.3
1	B	368	ASP	3.2
1	A	189	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	169	GLY	2.9
1	C	75	ARG	2.9
1	B	359	LEU	2.8
1	B	380	SER	2.8
1	B	208	ARG	2.8
1	B	391	LYS	2.7
1	B	376	ASP	2.7
1	C	370	ARG	2.7
1	C	71	GLN	2.7
1	A	202	THR	2.6
1	C	67	THR	2.6
1	A	204	ASP	2.6
1	C	368	ASP	2.6
1	B	160	LEU	2.6
1	B	198	LEU	2.6
1	A	73	GLY	2.5
1	B	269	ALA	2.5
1	C	397	ALA	2.5
1	C	74	SER	2.5
1	A	398	SER	2.5
1	C	69	LEU	2.5
1	C	156	ILE	2.5
1	B	389	ALA	2.4
1	B	190	PHE	2.4
1	A	201	MET	2.4
1	B	352	ARG	2.4
1	C	60	ALA	2.4
1	B	156	ILE	2.4
1	C	373	GLN	2.4
1	C	154	ASN	2.4
1	B	375	VAL	2.3
1	B	379	LEU	2.3
1	B	155	ALA	2.3
1	C	155	ALA	2.3
1	B	390	ARG	2.3
1	C	212	TRP	2.2
1	B	26	GLU	2.2
1	B	366	LYS	2.2
1	B	71	GLN	2.2
1	C	47	LEU	2.2
1	A	4	LEU	2.1
1	B	395	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	199	ALA	2.1
1	A	187	GLY	2.1
1	B	295	LYS	2.1
1	C	29	ARG	2.1
1	B	159	SER	2.1
1	A	64	LEU	2.1
1	B	216	ARG	2.0
1	C	70	GLN	2.0
1	C	73	GLY	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.