



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 PM UTC

PDB ID : 3K9E / pdb_00003k9e
Title : Crystal structure of a putative Ribokinase II (Apo Form) from E.coli
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-10-15
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

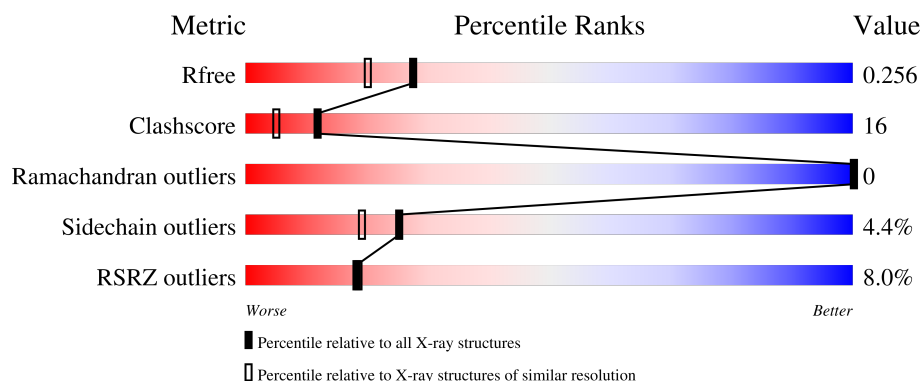
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	4% 68% 24% • 7%
1	B	330	10% 59% 33% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4900 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 PUTATIVE RIBOKINASE II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	Se	0	0	0
			2350	1491	405	439	7	8			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2376	1506	409	446	7	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MSE	-	expression tag	UNP Q8FD38
A	-3	SER	-	expression tag	UNP Q8FD38
A	-2	LEU	-	expression tag	UNP Q8FD38
A	321	GLU	-	expression tag	UNP Q8FD38
A	322	GLY	-	expression tag	UNP Q8FD38
A	323	HIS	-	expression tag	UNP Q8FD38
A	324	HIS	-	expression tag	UNP Q8FD38
A	325	HIS	-	expression tag	UNP Q8FD38
A	326	HIS	-	expression tag	UNP Q8FD38
A	327	HIS	-	expression tag	UNP Q8FD38
A	328	HIS	-	expression tag	UNP Q8FD38
B	-4	MSE	-	expression tag	UNP Q8FD38
B	-3	SER	-	expression tag	UNP Q8FD38
B	-2	LEU	-	expression tag	UNP Q8FD38
B	321	GLU	-	expression tag	UNP Q8FD38
B	322	GLY	-	expression tag	UNP Q8FD38
B	323	HIS	-	expression tag	UNP Q8FD38
B	324	HIS	-	expression tag	UNP Q8FD38
B	325	HIS	-	expression tag	UNP Q8FD38
B	326	HIS	-	expression tag	UNP Q8FD38
B	327	HIS	-	expression tag	UNP Q8FD38
B	328	HIS	-	expression tag	UNP Q8FD38

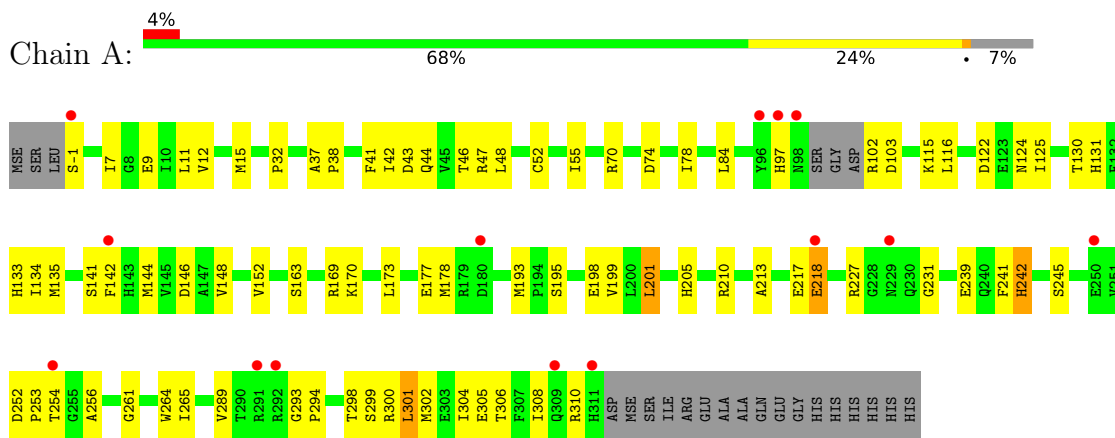
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total 103	O 103	0	0
2	B	71	Total 71	O 71	0	0

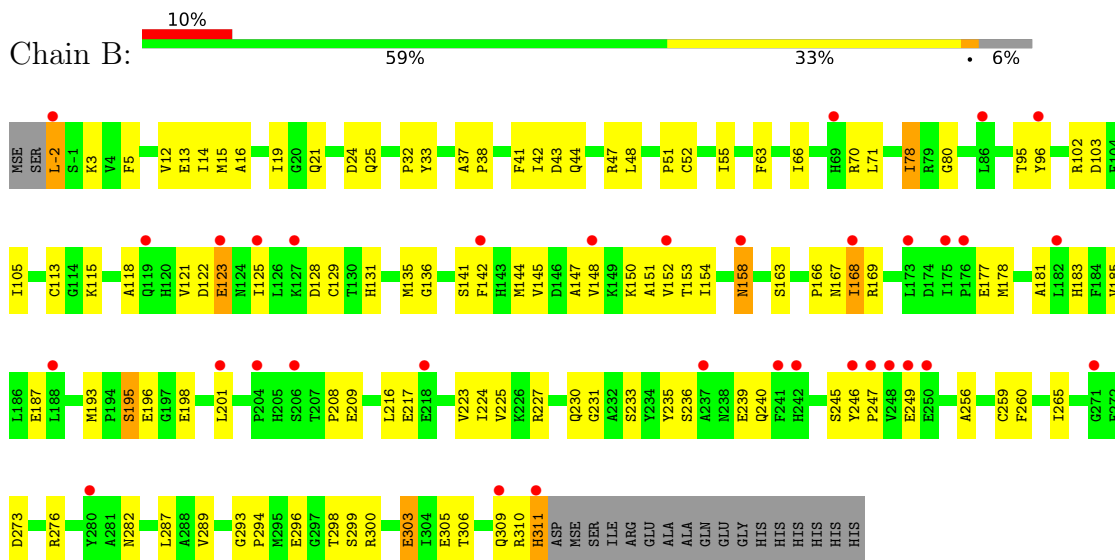
3 Residue-property plots [i](#)

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: PUTATIVE RIBOKINASE II



• Molecule 1: PUTATIVE RIBOKINASE II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.73Å 87.67Å 112.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 2.05 47.33 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.9 (47.33-2.05) 90.0 (47.33-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.257 0.228 , 0.256	Depositor DCC
R_{free} test set	1452 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4900	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/2394	0.92	8/3229 (0.2%)
1	B	0.40	0/2421	0.90	5/3267 (0.2%)
All	All	0.41	0/4815	0.91	13/6496 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	SER	N-CA-C	-7.31	100.68	110.55
1	B	303	GLU	N-CA-C	-6.52	104.26	111.36
1	A	239	GLU	N-CA-C	6.16	116.69	108.38
1	A	84	LEU	CA-C-N	5.96	126.11	119.32
1	A	84	LEU	C-N-CA	5.96	126.11	119.32
1	B	3	LYS	N-CA-C	5.72	118.79	109.24
1	A	169	ARG	N-CA-C	-5.50	99.77	108.73
1	B	195	SER	N-CA-C	-5.37	102.58	110.52
1	B	105	ILE	N-CA-C	-5.34	98.22	106.72
1	A	15	MSE	N-CA-C	5.26	117.55	109.07
1	A	199	VAL	N-CA-C	5.17	115.89	110.62
1	B	78	ILE	N-CA-C	5.15	117.13	112.29
1	A	78	ILE	N-CA-C	5.09	117.07	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2350	0	2306	56	0
1	B	2376	0	2330	92	0
2	A	103	0	0	3	0
2	B	71	0	0	22	0
All	All	4900	0	4636	148	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 16.

All (148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:O	1:B:95:THR:HG21	1.60	0.99
1:A:305:GLU:HB2	2:A:397:HOH:O	1.69	0.92
1:A:44:GLN:HE22	1:A:299:SER:H	1.14	0.90
1:B:15:MSE:HE3	1:B:33:TYR:CD2	2.09	0.87
1:B:233:SER:HB2	2:B:380:HOH:O	1.75	0.86
1:B:298:THR:HG22	2:B:352:HOH:O	1.78	0.83
1:B:15:MSE:HE1	1:B:293:GLY:HA2	1.59	0.83
1:B:168:ILE:HG22	1:B:169:ARG:H	1.44	0.81
1:B:225:VAL:HB	2:B:380:HOH:O	1.79	0.81
1:B:141:SER:OG	1:B:144:MSE:HG2	1.83	0.77
1:A:134:ILE:HD11	1:A:152:VAL:CG2	2.14	0.77
1:A:218:GLU:O	1:A:218:GLU:HG2	1.87	0.75
1:B:44:GLN:HB2	2:B:352:HOH:O	1.87	0.72
1:B:183:HIS:O	1:B:187:GLU:HG2	1.88	0.72
1:B:168:ILE:H	1:B:168:ILE:HD12	1.54	0.71
1:B:177:GLU:HG2	1:B:178:MSE:HE2	1.73	0.71
1:B:259:CYS:SG	2:B:352:HOH:O	2.49	0.70
1:A:205:HIS:HB3	1:A:210:ARG:HD3	1.74	0.69
1:B:168:ILE:HG22	1:B:169:ARG:N	2.07	0.69
1:A:134:ILE:HD11	1:A:152:VAL:HG22	1.75	0.69
1:B:123:GLU:H	1:B:123:GLU:CD	1.98	0.69
1:A:44:GLN:HE22	1:A:299:SER:N	1.91	0.68
1:A:115:LYS:HD3	2:A:401:HOH:O	1.92	0.68
1:B:163:SER:HB2	1:B:193:MSE:HE2	1.76	0.68
1:B:55:ILE:HG12	2:B:370:HOH:O	1.93	0.68
1:A:173:LEU:HD11	1:A:201:LEU:HG	1.76	0.68
1:B:235:TYR:HE2	2:B:380:HOH:O	1.76	0.67
1:B:15:MSE:HE2	1:B:294:PRO:HD3	1.77	0.66
1:B:150:LYS:HG2	2:B:351:HOH:O	1.94	0.66
1:B:55:ILE:HG23	2:B:370:HOH:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:HA	1:A:201:LEU:HD22	1.78	0.65
1:A:252:ASP:OD1	1:A:254:THR:HG23	1.98	0.64
1:B:249:GLU:O	1:B:249:GLU:HG2	1.97	0.63
1:A:141:SER:OG	1:A:144:MSE:HG2	1.99	0.63
1:A:142:PHE:CZ	1:A:146:ASP:OD2	2.51	0.63
1:A:177:GLU:HG2	1:A:178:MSE:HE2	1.80	0.62
1:B:305:GLU:HG2	2:B:367:HOH:O	2.00	0.61
1:B:247:PRO:HA	2:B:358:HOH:O	2.02	0.59
1:B:41:PHE:HB2	1:B:135:MSE:HE2	1.83	0.59
1:B:44:GLN:HE22	1:B:299:SER:H	1.49	0.59
1:B:235:TYR:CD1	1:B:240:GLN:HG3	2.39	0.58
1:B:153:THR:HB	2:B:386:HOH:O	2.05	0.57
1:A:227:ARG:HB2	1:A:231:GLY:O	2.05	0.57
1:B:236:SER:OG	1:B:239:GLU:HG2	2.04	0.57
1:A:116:LEU:HD23	1:A:144:MSE:HE1	1.88	0.56
1:B:166:PRO:C	1:B:168:ILE:HD12	2.31	0.56
1:B:208:PRO:HG2	1:B:209:GLU:OE2	2.06	0.56
1:A:170:LYS:HE2	1:A:201:LEU:HD21	1.86	0.56
1:B:37:ALA:HB3	1:B:38:PRO:HD3	1.87	0.56
1:A:70:ARG:NH1	1:A:74:ASP:OD2	2.39	0.56
1:B:14:ILE:HD12	1:B:14:ILE:N	2.21	0.55
1:A:134:ILE:HD11	1:A:152:VAL:HG21	1.88	0.55
1:A:48:LEU:HD22	1:A:301:LEU:HD13	1.88	0.55
1:A:300:ARG:HH22	1:A:302:MSE:CE	2.20	0.54
1:B:51:PRO:HG2	2:B:343:HOH:O	2.08	0.54
1:B:167:ASN:HA	1:B:198:GLU:OE2	2.08	0.54
1:B:80:GLY:HA3	2:B:370:HOH:O	2.07	0.54
1:A:231:GLY:H	1:A:245:SER:HB3	1.72	0.53
1:B:80:GLY:CA	2:B:370:HOH:O	2.56	0.53
1:A:12:VAL:HB	1:A:32:PRO:HB2	1.90	0.53
1:B:78:ILE:C	1:B:78:ILE:HD12	2.34	0.53
1:B:15:MSE:CE	1:B:293:GLY:HA2	2.34	0.53
1:B:-2:LEU:O	1:B:128:ASP:HB3	2.09	0.52
1:A:102:ARG:HH11	1:A:102:ARG:HG2	1.75	0.52
1:B:209:GLU:H	1:B:209:GLU:CD	2.17	0.52
1:B:43:ASP:O	1:B:47:ARG:HG3	2.09	0.52
1:A:43:ASP:O	1:A:47:ARG:HG3	2.10	0.52
1:B:168:ILE:HD12	1:B:168:ILE:N	2.23	0.51
1:A:131:HIS:CE1	1:A:265:ILE:HD12	2.45	0.51
1:A:242:HIS:N	1:A:242:HIS:CD2	2.78	0.51
1:B:95:THR:HG22	1:B:96:TYR:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:HD11	1:B:52:CYS:HB2	1.92	0.51
1:B:216:LEU:HD21	1:B:223:VAL:HG23	1.93	0.50
1:B:196:GLU:HB2	1:B:227:ARG:HA	1.91	0.50
1:B:305:GLU:O	1:B:309:GLN:HG3	2.11	0.50
1:A:300:ARG:HH22	1:A:302:MSE:HE1	1.77	0.50
1:A:193:MSE:HE1	1:A:261:GLY:HA2	1.93	0.50
1:A:37:ALA:HB3	1:A:38:PRO:HD3	1.94	0.49
1:B:260:PHE:C	1:B:260:PHE:CD2	2.90	0.49
1:B:142:PHE:HA	1:B:145:VAL:HG22	1.94	0.49
1:B:142:PHE:O	1:B:145:VAL:HG22	2.12	0.49
1:B:195:SER:OG	1:B:198:GLU:HG3	2.13	0.49
1:B:306:THR:O	1:B:310:ARG:HG3	2.13	0.49
1:A:42:ILE:HD11	1:A:52:CYS:HB2	1.95	0.48
1:B:224:ILE:N	1:B:224:ILE:HD12	2.28	0.48
1:B:5:PHE:HB2	1:B:129:CYS:SG	2.54	0.48
1:B:13:GLU:C	1:B:14:ILE:HD12	2.39	0.48
1:B:231:GLY:N	1:B:245:SER:HB3	2.29	0.48
1:A:231:GLY:N	1:A:245:SER:HB3	2.28	0.48
1:B:136:GLY:C	1:B:168:ILE:HG13	2.39	0.47
1:B:15:MSE:CE	1:B:294:PRO:HD3	2.43	0.47
1:A:9:GLU:O	1:A:9:GLU:HG2	2.13	0.47
1:B:305:GLU:OE1	1:B:309:GLN:CD	2.57	0.47
1:A:301:LEU:O	1:A:305:GLU:HG3	2.15	0.47
1:B:44:GLN:NE2	2:B:352:HOH:O	2.47	0.47
1:A:205:HIS:CD2	1:A:210:ARG:HE	2.32	0.47
1:B:131:HIS:CE1	1:B:265:ILE:HD12	2.49	0.47
1:A:306:THR:O	1:A:310:ARG:HG3	2.15	0.47
1:B:41:PHE:HB2	1:B:135:MSE:CE	2.45	0.46
1:B:256:ALA:HB2	1:B:289:VAL:CG1	2.44	0.46
1:B:154:ILE:HD12	2:B:351:HOH:O	2.15	0.46
1:B:246:TYR:CE2	1:B:282:ASN:ND2	2.84	0.46
1:B:227:ARG:NH2	2:B:380:HOH:O	2.48	0.45
1:B:300:ARG:HB2	1:B:303:GLU:HG3	1.97	0.45
1:B:19:ILE:HD12	1:B:19:ILE:N	2.30	0.45
1:B:63:PHE:O	1:B:66:ILE:HG22	2.17	0.45
1:B:227:ARG:HH11	1:B:227:ARG:HG2	1.82	0.45
1:B:148:VAL:O	1:B:152:VAL:HG23	2.16	0.45
1:B:287:LEU:HB3	2:B:382:HOH:O	2.16	0.45
1:B:95:THR:HG22	1:B:96:TYR:N	2.32	0.45
1:B:122:ASP:HB3	1:B:125:ILE:HG13	1.99	0.45
1:B:311:HIS:ND1	1:B:311:HIS:C	2.73	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ASP:O	1:B:25:GLN:HG3	2.17	0.44
1:B:136:GLY:HA3	1:B:168:ILE:HG13	1.99	0.44
1:B:154:ILE:O	1:B:158:ASN:OD1	2.35	0.44
1:A:133:HIS:HD2	1:A:163:SER:OG	2.02	0.43
1:B:12:VAL:HB	1:B:32:PRO:HB2	2.02	0.42
1:A:177:GLU:HG3	2:A:411:HOH:O	2.18	0.42
1:B:181:ALA:O	1:B:185:VAL:HG23	2.20	0.42
1:A:213:ALA:O	1:A:217:GLU:HG3	2.19	0.42
1:A:241:PHE:C	1:A:242:HIS:CD2	2.97	0.42
1:B:118:ALA:HA	1:B:147:ALA:HA	2.01	0.42
1:B:151:ALA:HA	2:B:351:HOH:O	2.19	0.42
1:A:43:ASP:O	1:A:46:THR:HG22	2.20	0.42
1:A:116:LEU:HB3	1:A:144:MSE:SE	2.69	0.42
1:A:122:ASP:HB3	1:A:125:ILE:HG12	2.02	0.42
1:A:193:MSE:HE1	1:A:264:TRP:HB3	2.01	0.42
1:A:198:GLU:CA	1:A:201:LEU:HD22	2.49	0.42
1:A:293:GLY:HA2	1:A:294:PRO:HD3	1.90	0.42
1:B:70:ARG:HH22	1:B:296:GLU:CD	2.28	0.42
1:B:273:ASP:HB2	2:B:390:HOH:O	2.19	0.42
1:A:41:PHE:HB2	1:A:135:MSE:HE2	2.01	0.42
1:A:44:GLN:NE2	1:A:298:THR:HA	2.35	0.42
1:A:41:PHE:HB2	1:A:135:MSE:CE	2.50	0.41
1:A:205:HIS:ND1	1:A:210:ARG:HG2	2.35	0.41
1:A:7:ILE:HG13	1:A:55:ILE:O	2.20	0.41
1:A:-1:SER:HA	1:A:130:THR:HG21	2.03	0.41
1:A:304:ILE:O	1:A:308:ILE:HG13	2.20	0.41
1:B:16:ALA:CB	1:B:95:THR:HG23	2.51	0.41
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.90	0.41
1:A:148:VAL:O	1:A:152:VAL:HG23	2.21	0.41
1:B:121:VAL:HG11	2:B:351:HOH:O	2.19	0.41
1:B:198:GLU:HB3	1:B:201:LEU:HD12	2.02	0.41
1:B:208:PRO:HG2	1:B:209:GLU:CD	2.45	0.41
1:A:-1:SER:HA	1:A:130:THR:CG2	2.52	0.40
1:A:256:ALA:HB2	1:A:289:VAL:CG1	2.51	0.40
1:B:227:ARG:HB2	1:B:231:GLY:O	2.21	0.40
1:B:235:TYR:CE1	1:B:240:GLN:HG3	2.55	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	303/330 (92%)	297 (98%)	6 (2%)	0	100	100
1	B	309/330 (94%)	294 (95%)	15 (5%)	0	100	100
All	All	612/660 (93%)	591 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	250/259 (96%)	241 (96%)	9 (4%)	31	26
1	B	253/259 (98%)	240 (95%)	13 (5%)	21	14
All	All	503/518 (97%)	481 (96%)	22 (4%)	25	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	97	HIS
1	A	103	ASP
1	A	124	ASN
1	A	201	LEU
1	A	218	GLU
1	A	242	HIS
1	A	253	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	301	LEU
1	B	-2	LEU
1	B	71	LEU
1	B	102	ARG
1	B	103	ASP
1	B	113	CYS
1	B	115	LYS
1	B	123	GLU
1	B	158	ASN
1	B	168	ILE
1	B	217	GLU
1	B	230	GLN
1	B	276	ARG
1	B	311	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	30	ASN
1	A	44	GLN
1	A	133	HIS
1	A	238	ASN
1	A	275	HIS
1	B	44	GLN
1	B	143	HIS
1	B	229	ASN
1	B	230	GLN
1	B	238	ASN
1	B	240	GLN
1	B	279	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/330 (90%)	0.29	14 (4%) 36 36	24, 35, 57, 72	0
1	B	303/330 (91%)	0.79	34 (11%) 10 9	26, 44, 69, 81	0
All	All	602/660 (91%)	0.54	48 (7%) 18 18	24, 39, 65, 81	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	HIS	4.8
1	B	241	PHE	4.3
1	B	311	HIS	4.0
1	B	242	HIS	3.9
1	B	237	ALA	3.8
1	B	123	GLU	3.4
1	B	119	GLN	3.3
1	B	168	ILE	3.3
1	B	-2	LEU	3.2
1	A	97	HIS	3.1
1	B	249	GLU	3.1
1	B	175	ILE	3.0
1	A	96	TYR	3.0
1	B	142	PHE	3.0
1	B	246	TYR	2.9
1	B	173	LEU	2.8
1	A	-1	SER	2.8
1	B	176	PRO	2.8
1	A	218	GLU	2.7
1	B	69	HIS	2.7
1	A	98	ASN	2.6
1	B	86	LEU	2.6
1	B	96	TYR	2.6
1	B	201	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	309	GLN	2.5
1	A	229	ASN	2.4
1	B	248	VAL	2.4
1	B	206	SER	2.4
1	B	182	LEU	2.3
1	B	247	PRO	2.3
1	B	218	GLU	2.3
1	A	142	PHE	2.2
1	B	204	PRO	2.2
1	A	250	GLU	2.2
1	A	254	THR	2.2
1	B	152	VAL	2.1
1	B	188	LEU	2.1
1	B	280	TYR	2.1
1	B	127	LYS	2.1
1	A	180	ASP	2.1
1	B	309	GLN	2.1
1	B	271	GLY	2.1
1	B	125	ILE	2.1
1	B	158	ASN	2.0
1	A	291	ARG	2.0
1	B	148	VAL	2.0
1	B	250	GLU	2.0
1	A	292	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.