



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:28 AM UTC

PDB ID : 1UFQ / pdb_00001ufq
Title : Crystal structure of ligand-free human uridine-cytidine kinase 2
Authors : Suzuki, N.N.; Koizumi, K.; Fukushima, M.; Matsuda, A.; Inagaki, F.
Deposited on : 2003-06-06
Resolution : 2.50 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
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

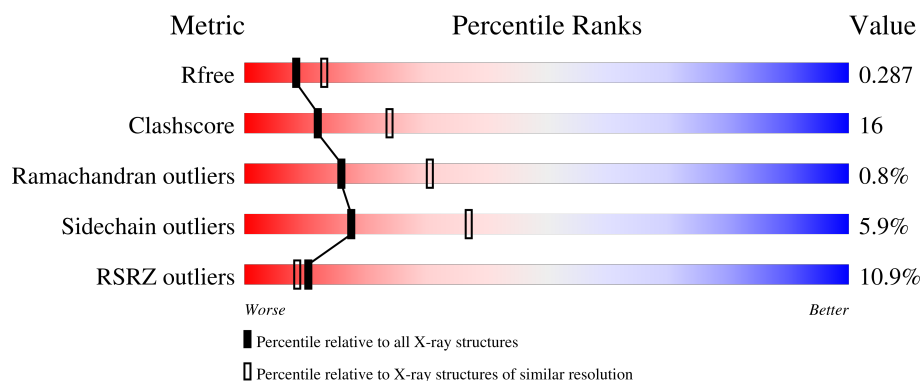
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	252	12% 54% 27% • 16%
1	B	252	6% 56% 24% • 17%
1	C	252	6% 56% 26% • 16%
1	D	252	12% 53% 29% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6633 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 Uridine-cytidine kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1641	1051	274	313	3			
1	B	208	Total	C	N	O	S	0	0	0
			1615	1040	267	305	3			
1	C	212	Total	C	N	O	S	0	0	0
			1651	1061	275	312	3			
1	D	210	Total	C	N	O	S	0	0	0
			1596	1028	270	295	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	cloning artifact	UNP Q9BZX2
A	0	GLY	-	cloning artifact	UNP Q9BZX2
B	-1	PRO	-	cloning artifact	UNP Q9BZX2
B	0	GLY	-	cloning artifact	UNP Q9BZX2
C	-1	PRO	-	cloning artifact	UNP Q9BZX2
C	0	GLY	-	cloning artifact	UNP Q9BZX2
D	-1	PRO	-	cloning artifact	UNP Q9BZX2
D	0	GLY	-	cloning artifact	UNP Q9BZX2

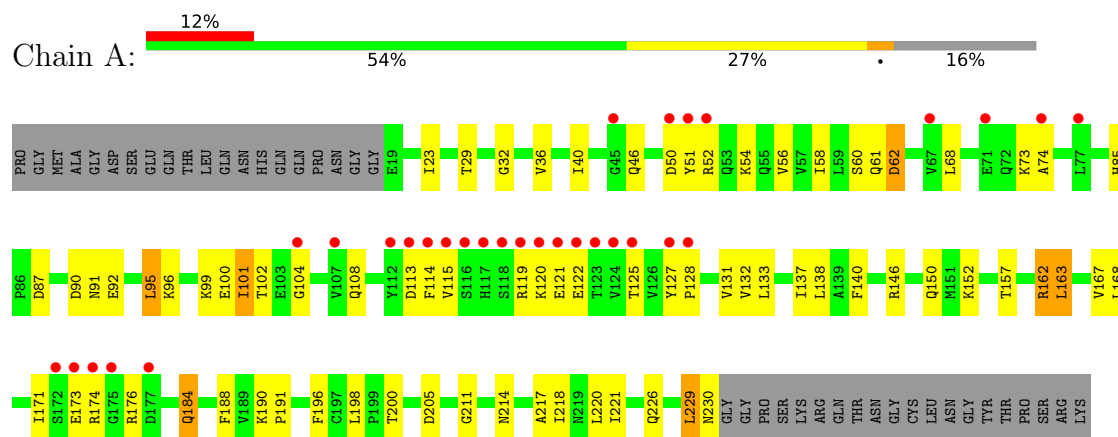
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	32	Total	O	0	0
			32	32		
2	C	38	Total	O	0	0
			38	38		
2	D	30	Total	O	0	0
			30	30		

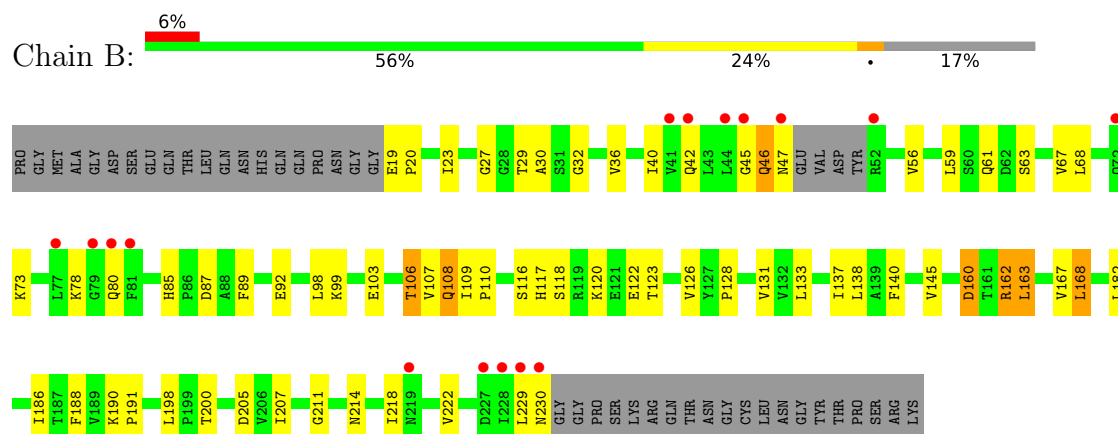
3 Residue-property plots [i](#)

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.

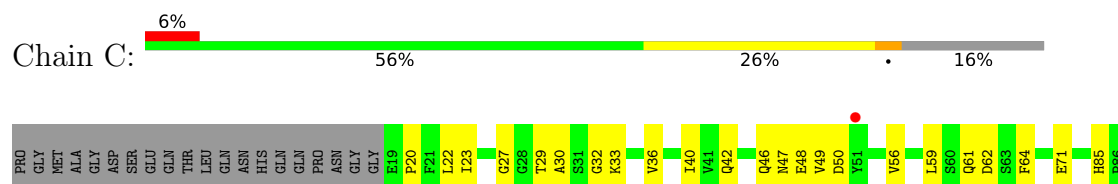
- Molecule 1: Uridine-cytidine kinase 2

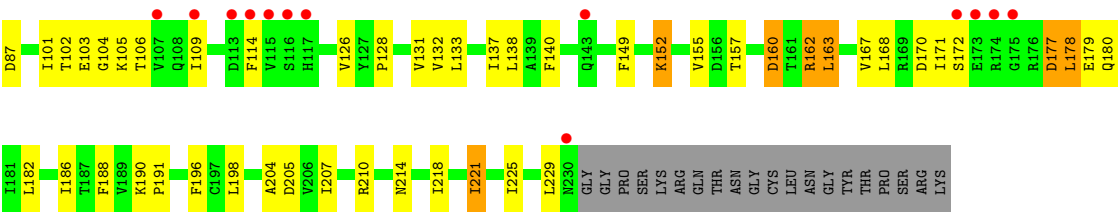


- Molecule 1: Uridine-cytidine kinase 2

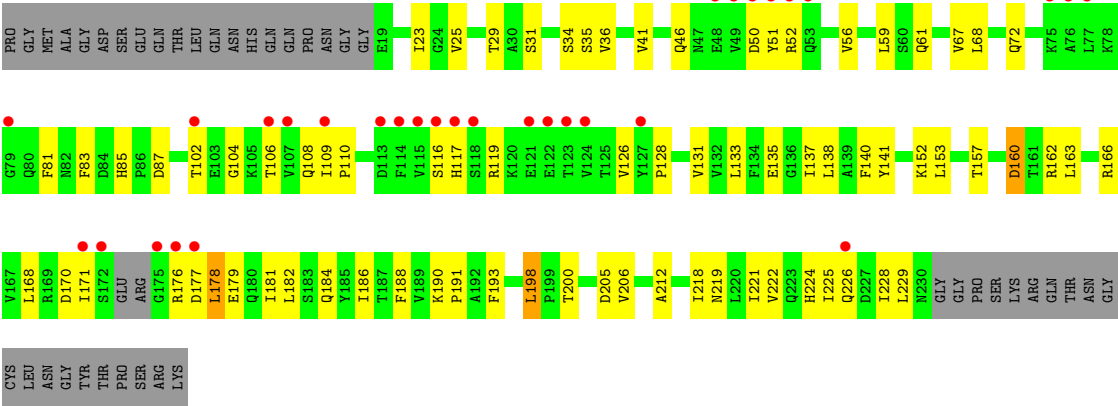


- Molecule 1: Uridine-cytidine kinase 2





● Molecule 1: Uridine-cytidine kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	84.06Å 94.26Å 156.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.41 – 2.50 40.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (40.41-2.50) 85.7 (40.41-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.287 0.236 , 0.287	Depositor DCC
R_{free} test set	3769 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6633	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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	0.46	0/1668	1.02	11/2261 (0.5%)
1	B	0.44	0/1642	0.94	5/2227 (0.2%)
1	C	0.47	0/1680	0.93	6/2281 (0.3%)
1	D	0.45	0/1622	0.93	5/2202 (0.2%)
All	All	0.46	0/6612	0.96	27/8971 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	N-CA-C	-9.49	101.83	113.97
1	A	211	GLY	N-CA-C	8.71	120.35	111.56
1	C	109	ILE	N-CA-C	7.25	115.08	107.76
1	D	67	VAL	N-CA-C	-6.17	99.86	108.12
1	A	73	LYS	N-CA-C	-6.08	105.36	112.89
1	D	188	PHE	N-CA-C	6.07	121.00	112.93
1	C	188	PHE	N-CA-C	6.02	120.94	112.93
1	D	205	ASP	N-CA-C	-5.73	105.39	112.90
1	B	211	GLY	N-CA-C	5.64	117.08	111.21
1	C	27	GLY	N-CA-C	-5.59	104.30	110.96
1	C	196	PHE	N-CA-C	5.55	120.54	113.55
1	A	188	PHE	N-CA-C	5.54	120.30	112.93
1	B	106	THR	N-CA-C	-5.45	102.82	110.50
1	C	114	PHE	N-CA-C	5.37	119.10	112.54
1	B	188	PHE	N-CA-C	5.27	119.47	112.72
1	A	205	ASP	N-CA-C	-5.27	106.99	113.41
1	B	205	ASP	N-CA-C	-5.24	106.03	112.90
1	A	74	ALA	N-CA-C	-5.23	105.50	111.14
1	A	58	ILE	N-CA-C	5.19	115.33	107.75
1	C	205	ASP	N-CA-C	-5.18	105.32	111.69
1	B	27	GLY	N-CA-C	-5.14	106.40	111.85
1	A	68	LEU	N-CA-C	5.08	117.67	110.50
1	D	31	SER	N-CA-C	-5.07	106.61	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	141	TYR	N-CA-C	5.03	116.46	111.07
1	A	173	GLU	N-CA-C	5.03	119.36	112.68
1	A	196	PHE	N-CA-C	5.01	119.74	113.43
1	A	101	ILE	N-CA-C	-5.00	105.52	110.62

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	1641	0	1622	44	0
1	B	1615	0	1601	56	0
1	C	1651	0	1627	47	0
1	D	1596	0	1564	55	0
2	A	30	0	0	1	0
2	B	32	0	0	2	0
2	C	38	0	0	2	0
2	D	30	0	0	2	0
All	All	6633	0	6414	201	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 (201) 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:D:85:HIS:HD2	1:D:87:ASP:H	1.14	0.89
1:C:85:HIS:HD2	1:C:87:ASP:H	1.15	0.89
1:C:46:GLN:HG3	1:C:56:VAL:HG12	1.60	0.82
1:D:219:ASN:HA	1:D:222:VAL:HG22	1.61	0.82
1:C:46:GLN:HG3	1:C:56:VAL:CG1	2.11	0.81
1:D:61:GLN:HE22	1:D:138:LEU:H	1.29	0.80
1:C:61:GLN:HE22	1:C:138:LEU:H	1.28	0.79
1:B:46:GLN:HG3	1:B:56:VAL:HG12	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:HIS:CD2	1:C:87:ASP:H	2.00	0.78
1:C:131:VAL:HG21	1:C:225:ILE:HG23	1.64	0.78
1:C:171:ILE:HG13	1:C:172:SER:N	1.99	0.77
1:B:61:GLN:HE22	1:B:138:LEU:H	1.31	0.76
1:D:59:LEU:HD11	1:D:109:ILE:HG12	1.67	0.76
1:A:85:HIS:HD2	1:A:87:ASP:H	1.36	0.74
1:D:85:HIS:CD2	1:D:87:ASP:H	2.03	0.74
1:C:210:ARG:HD2	2:C:285:HOH:O	1.89	0.72
1:B:36:VAL:O	1:B:40:ILE:HG13	1.90	0.72
1:B:23:ILE:HB	1:B:133:LEU:HD23	1.72	0.71
1:C:171:ILE:HG13	1:C:172:SER:H	1.56	0.70
1:B:120:LYS:HG2	1:B:122:GLU:HG2	1.74	0.69
1:D:171:ILE:HD11	1:D:178:LEU:HG	1.75	0.69
1:B:36:VAL:HG13	1:B:218:ILE:CD1	2.23	0.69
1:A:61:GLN:HE22	1:A:138:LEU:H	1.41	0.68
1:D:137:ILE:HG13	1:D:138:LEU:HG	1.73	0.68
1:D:176:ARG:HH12	1:D:184:GLN:NE2	1.91	0.68
1:B:182:LEU:O	1:B:186:ILE:HG12	1.95	0.67
1:B:46:GLN:HG3	1:B:56:VAL:CG1	2.23	0.66
1:A:120:LYS:HD3	1:A:122:GLU:OE2	1.96	0.65
1:D:140:PHE:CE1	1:D:152:LYS:HG2	2.32	0.65
1:D:190:LYS:HB3	1:D:191:PRO:HD3	1.79	0.65
1:A:23:ILE:HB	1:A:133:LEU:HD23	1.78	0.64
1:B:46:GLN:CG	1:B:56:VAL:HG12	2.28	0.63
1:D:29:THR:HB	1:D:166:ARG:HH12	1.61	0.63
1:A:108:GLN:HE22	1:A:125:THR:HG23	1.63	0.62
1:B:229:LEU:C	1:B:230:ASN:HD22	2.09	0.61
1:C:40:ILE:HD13	1:C:221:ILE:HG21	1.81	0.61
1:D:110:PRO:HB2	1:D:119:ARG:HD3	1.82	0.61
1:C:29:THR:O	1:C:30:ALA:HB3	2.00	0.61
1:A:46:GLN:HG3	1:A:56:VAL:CG1	2.30	0.61
1:B:29:THR:O	1:B:30:ALA:HB3	1.99	0.61
1:C:149:PHE:HB2	1:C:152:LYS:HD2	1.82	0.61
1:D:23:ILE:HB	1:D:133:LEU:HD23	1.82	0.61
1:A:46:GLN:HG3	1:A:56:VAL:HG13	1.82	0.60
1:A:113:ASP:C	1:A:115:VAL:H	2.07	0.60
1:B:78:LYS:CB	1:B:80:GLN:HE21	2.14	0.60
1:C:140:PHE:CE1	1:C:152:LYS:HG3	2.37	0.60
1:A:85:HIS:CD2	1:A:87:ASP:H	2.19	0.59
1:A:150:GLN:HA	1:A:150:GLN:OE1	2.01	0.59
1:C:137:ILE:O	1:C:138:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLY:O	1:C:36:VAL:HG23	2.02	0.58
1:D:153:LEU:HD23	1:D:206:VAL:HB	1.85	0.58
1:A:56:VAL:HA	1:A:131:VAL:O	2.04	0.58
1:C:214:ASN:O	1:C:218:ILE:HG12	2.02	0.58
1:C:177:ASP:H	1:C:180:GLN:HE21	1.52	0.57
1:B:45:GLY:C	1:B:47:ASN:H	2.11	0.57
1:A:40:ILE:HD13	1:A:221:ILE:HG21	1.86	0.57
1:C:182:LEU:O	1:C:186:ILE:HG12	2.04	0.57
1:B:19:GLU:N	1:B:20:PRO:HD3	2.20	0.57
1:B:73:LYS:HE2	1:B:117:HIS:HB2	1.86	0.57
1:A:91:ASN:O	1:A:95:LEU:HB2	2.06	0.56
1:A:157:THR:HB	1:A:162:ARG:HD3	1.88	0.56
1:C:177:ASP:H	1:C:180:GLN:NE2	2.03	0.56
1:A:190:LYS:HB3	1:A:191:PRO:HD3	1.87	0.56
1:B:42:GLN:HA	1:B:47:ASN:HD22	1.69	0.55
1:A:96:LYS:HE2	1:A:100:GLU:OE2	2.06	0.55
1:D:46:GLN:HG3	1:D:56:VAL:HB	1.88	0.55
1:C:42:GLN:HG2	1:C:47:ASN:HD22	1.72	0.55
1:C:56:VAL:HA	1:C:131:VAL:O	2.07	0.55
1:D:219:ASN:HA	1:D:222:VAL:CG2	2.36	0.55
1:A:46:GLN:O	1:A:54:LYS:NZ	2.40	0.54
1:B:137:ILE:HG13	1:B:138:LEU:HG	1.89	0.54
1:C:23:ILE:HB	1:C:133:LEU:HD23	1.89	0.53
1:C:62:ASP:C	1:C:64:PHE:H	2.16	0.53
1:D:36:VAL:HG22	1:D:218:ILE:HD11	1.90	0.53
1:D:153:LEU:CD2	1:D:206:VAL:HB	2.39	0.53
1:A:146:ARG:O	1:A:152:LYS:HE3	2.09	0.52
1:C:46:GLN:HA	1:C:49:VAL:HG23	1.90	0.52
1:D:157:THR:O	1:D:162:ARG:HD3	2.09	0.52
1:C:157:THR:HB	1:C:162:ARG:HD3	1.91	0.52
1:B:190:LYS:HB3	1:B:191:PRO:HD3	1.91	0.52
1:C:61:GLN:NE2	1:C:138:LEU:H	2.04	0.52
1:D:171:ILE:CD1	1:D:178:LEU:HG	2.39	0.52
1:B:67:VAL:HG13	1:B:118:SER:HA	1.92	0.52
1:B:99:LYS:O	1:B:103:GLU:HG3	2.10	0.52
1:D:109:ILE:HD12	1:D:109:ILE:N	2.26	0.51
1:D:35:SER:OG	1:D:212:ALA:HB2	2.10	0.51
1:A:120:LYS:HD3	1:A:122:GLU:CD	2.35	0.51
1:A:113:ASP:O	1:A:115:VAL:N	2.44	0.51
1:D:177:ASP:OD1	1:D:179:GLU:HG3	2.11	0.51
1:D:221:ILE:N	1:D:221:ILE:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:NE2	1:A:125:THR:HG23	2.27	0.50
1:B:117:HIS:HD2	2:B:260:HOH:O	1.94	0.50
1:D:190:LYS:HD3	2:D:271:HOH:O	2.12	0.50
1:A:113:ASP:C	1:A:115:VAL:N	2.70	0.49
1:A:137:ILE:HG12	2:A:276:HOH:O	2.13	0.49
1:C:61:GLN:HE22	1:C:138:LEU:N	2.04	0.49
1:A:174:ARG:CB	1:A:176:ARG:HG3	2.42	0.49
1:B:85:HIS:CD2	1:B:87:ASP:H	2.30	0.49
1:C:190:LYS:HB3	1:C:191:PRO:HD3	1.94	0.49
1:B:85:HIS:HD2	1:B:87:ASP:H	1.61	0.49
1:C:126:VAL:HG23	1:C:126:VAL:O	2.13	0.48
1:B:73:LYS:HE2	1:B:116:SER:O	2.13	0.48
1:D:182:LEU:O	1:D:186:ILE:HG12	2.13	0.48
1:B:230:ASN:HD22	1:B:230:ASN:N	2.10	0.48
1:C:85:HIS:HD2	1:C:87:ASP:N	1.98	0.48
1:B:56:VAL:O	1:B:56:VAL:HG13	2.14	0.48
1:C:46:GLN:HA	1:C:49:VAL:CG2	2.42	0.48
1:D:85:HIS:HD2	1:D:87:ASP:N	1.95	0.48
1:D:193:PHE:CE1	1:D:198:LEU:HG	2.49	0.48
1:A:61:GLN:NE2	1:A:138:LEU:H	2.09	0.47
1:B:140:PHE:HB2	1:B:200:THR:HB	1.96	0.47
1:C:62:ASP:C	1:C:64:PHE:N	2.72	0.47
1:C:221:ILE:O	1:C:225:ILE:HG13	2.13	0.47
1:D:224:HIS:O	1:D:228:ILE:HG13	2.14	0.47
1:C:33:LYS:HA	1:C:155:VAL:HG21	1.97	0.47
1:A:32:GLY:O	1:A:36:VAL:HG23	2.14	0.46
1:B:68:LEU:HB2	1:B:117:HIS:HB3	1.97	0.46
1:B:120:LYS:CG	1:B:122:GLU:HG2	2.45	0.46
1:B:230:ASN:N	1:B:230:ASN:ND2	2.63	0.46
1:D:25:VAL:O	1:D:135:GLU:HA	2.15	0.46
1:A:184:GLN:HE21	1:A:184:GLN:HB3	1.51	0.46
1:A:217:ALA:O	1:A:220:LEU:HB3	2.15	0.46
1:A:60:SER:C	1:A:62:ASP:N	2.71	0.46
1:B:214:ASN:O	1:B:218:ILE:HG12	2.15	0.46
1:D:29:THR:HB	1:D:166:ARG:NH1	2.28	0.46
1:A:214:ASN:O	1:A:218:ILE:HG12	2.16	0.46
1:D:68:LEU:HD22	1:D:72:GLN:HB3	1.97	0.46
1:B:56:VAL:HA	1:B:131:VAL:O	2.15	0.46
1:D:110:PRO:CB	1:D:119:ARG:HD3	2.45	0.46
1:B:29:THR:O	1:B:30:ALA:CB	2.65	0.45
1:B:108:GLN:HG3	1:B:123:THR:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HD11	1:D:178:LEU:CG	2.45	0.45
1:A:29:THR:O	1:A:162:ARG:HG2	2.16	0.45
1:B:63:SER:O	1:B:110:PRO:HG2	2.16	0.45
1:A:99:LYS:O	1:A:102:THR:HB	2.15	0.45
1:D:170:ASP:HB2	1:D:181:ILE:HD13	1.98	0.45
1:B:163:LEU:HD22	1:B:167:VAL:HG23	1.98	0.45
1:A:102:THR:C	1:A:104:GLY:H	2.25	0.45
1:D:176:ARG:HH12	1:D:184:GLN:HE22	1.63	0.45
1:A:90:ASP:OD2	1:A:119:ARG:NH2	2.37	0.45
1:D:177:ASP:O	1:D:181:ILE:HG13	2.17	0.45
1:A:163:LEU:O	1:A:167:VAL:HG23	2.16	0.45
1:C:152:LYS:HB3	1:C:204:ALA:HA	1.99	0.45
1:B:108:GLN:HG3	1:B:123:THR:HB	1.99	0.44
1:D:219:ASN:CA	1:D:222:VAL:HG22	2.41	0.44
1:A:146:ARG:HG2	1:A:152:LYS:CE	2.48	0.44
1:B:23:ILE:HB	1:B:133:LEU:CD2	2.46	0.44
1:C:29:THR:O	1:C:30:ALA:CB	2.65	0.44
1:A:229:LEU:O	1:A:230:ASN:OD1	2.36	0.44
1:C:20:PRO:HG2	1:C:101:ILE:O	2.17	0.44
1:A:127:TYR:O	1:A:128:PRO:C	2.59	0.44
1:C:152:LYS:HD3	2:C:281:HOH:O	2.18	0.44
1:D:36:VAL:HG13	1:D:218:ILE:HD13	2.00	0.44
1:B:109:ILE:HD12	1:B:109:ILE:N	2.33	0.43
1:D:59:LEU:HD11	1:D:109:ILE:CG1	2.45	0.43
1:A:140:PHE:HB2	1:A:200:THR:HB	1.99	0.43
1:B:29:THR:HG23	1:B:137:ILE:CG2	2.48	0.43
1:B:126:VAL:O	1:B:126:VAL:HG23	2.18	0.43
1:B:207:ILE:HB	1:C:207:ILE:HB	2.00	0.43
1:D:36:VAL:HG13	1:D:218:ILE:CD1	2.48	0.43
1:D:50:ASP:C	1:D:52:ARG:H	2.26	0.43
1:C:40:ILE:CD1	1:C:221:ILE:HG21	2.49	0.43
1:A:50:ASP:O	1:A:52:ARG:N	2.52	0.43
1:C:103:GLU:HB2	1:C:105:LYS:HD3	1.99	0.43
1:D:41:VAL:HG12	1:D:56:VAL:HG12	2.01	0.43
1:D:116:SER:O	1:D:117:HIS:HB2	2.17	0.42
1:A:40:ILE:CD1	1:A:221:ILE:HG21	2.49	0.42
1:B:107:VAL:HG23	1:B:126:VAL:HG22	2.01	0.42
1:D:106:THR:OG1	1:D:128:PRO:HD3	2.19	0.42
1:C:163:LEU:HD22	1:C:167:VAL:HG23	2.01	0.42
1:D:56:VAL:HG22	1:D:131:VAL:HB	2.00	0.42
1:C:22:LEU:HD12	1:C:132:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:PHE:HB2	1:D:200:THR:HB	2.00	0.42
1:B:162:ARG:NH1	2:B:259:HOH:O	2.50	0.42
1:D:102:THR:C	1:D:104:GLY:H	2.27	0.42
1:B:56:VAL:CG1	1:B:56:VAL:O	2.68	0.42
1:D:109:ILE:HD13	1:D:126:VAL:HG23	2.01	0.42
1:D:131:VAL:HG21	1:D:225:ILE:HG23	2.01	0.42
1:B:45:GLY:C	1:B:47:ASN:N	2.77	0.41
1:B:106:THR:OG1	1:B:128:PRO:HD3	2.21	0.41
1:C:49:VAL:HG12	1:C:50:ASP:N	2.35	0.41
1:B:92:GLU:N	1:B:92:GLU:OE1	2.54	0.41
1:B:42:GLN:HA	1:B:47:ASN:ND2	2.36	0.41
1:C:102:THR:C	1:C:104:GLY:H	2.28	0.41
1:B:98:LEU:HD12	1:B:145:VAL:HG13	2.03	0.41
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.82	0.41
1:D:50:ASP:C	1:D:52:ARG:N	2.79	0.41
1:B:218:ILE:O	1:B:222:VAL:HG23	2.20	0.41
1:C:178:LEU:HD12	1:C:178:LEU:HA	1.91	0.41
1:D:109:ILE:N	1:D:109:ILE:CD1	2.84	0.41
1:D:171:ILE:HG13	1:D:181:ILE:HD12	2.02	0.41
1:A:101:ILE:HG21	1:A:132:VAL:HG21	2.03	0.41
1:C:106:THR:OG1	1:C:128:PRO:HD3	2.21	0.41
1:A:95:LEU:HD22	1:A:95:LEU:HA	1.93	0.40
1:A:36:VAL:O	1:A:40:ILE:HG13	2.22	0.40
1:B:61:GLN:HG2	1:B:89:PHE:CD2	2.56	0.40
1:D:34:SER:HB2	2:D:280:HOH:O	2.21	0.40
1:D:81:PHE:HD2	1:D:83:PHE:CZ	2.39	0.40
1:B:29:THR:HG23	1:B:137:ILE:HG21	2.02	0.40
1:B:32:GLY:O	1:B:36:VAL:HG23	2.21	0.40
1:B:108:GLN:HG3	1:B:123:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/252 (83%)	198 (94%)	10 (5%)	2 (1%)	12	24
1	B	204/252 (81%)	194 (95%)	8 (4%)	2 (1%)	12	24
1	C	210/252 (83%)	200 (95%)	9 (4%)	1 (0%)	24	43
1	D	206/252 (82%)	199 (97%)	5 (2%)	2 (1%)	12	24
All	All	830/1008 (82%)	791 (95%)	32 (4%)	7 (1%)	16	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	114	PHE
1	B	46	GLN
1	D	51	TYR
1	C	160	ASP
1	D	160	ASP
1	B	160	ASP

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	176/221 (80%)	165 (94%)	11 (6%)	16	34
1	B	174/221 (79%)	167 (96%)	7 (4%)	28	54
1	C	177/221 (80%)	162 (92%)	15 (8%)	10	22
1	D	165/221 (75%)	157 (95%)	8 (5%)	23	46
All	All	692/884 (78%)	651 (94%)	41 (6%)	18	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	92	GLU
1	A	95	LEU
1	A	162	ARG

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Mol	Chain	Res	Type
1	A	163	LEU
1	A	168	LEU
1	A	171	ILE
1	A	184	GLN
1	A	198	LEU
1	A	226	GLN
1	A	229	LEU
1	B	59	LEU
1	B	108	GLN
1	B	160	ASP
1	B	162	ARG
1	B	163	LEU
1	B	168	LEU
1	B	198	LEU
1	C	48	GLU
1	C	59	LEU
1	C	71	GLU
1	C	152	LYS
1	C	160	ASP
1	C	162	ARG
1	C	163	LEU
1	C	168	LEU
1	C	170	ASP
1	C	177	ASP
1	C	178	LEU
1	C	179	GLU
1	C	198	LEU
1	C	221	ILE
1	C	229	LEU
1	D	108	GLN
1	D	160	ASP
1	D	163	LEU
1	D	168	LEU
1	D	178	LEU
1	D	198	LEU
1	D	226	GLN
1	D	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	85	HIS
1	A	91	ASN
1	A	108	GLN
1	A	117	HIS
1	A	143	GLN
1	A	184	GLN
1	B	42	GLN
1	B	47	ASN
1	B	61	GLN
1	B	80	GLN
1	B	85	HIS
1	B	91	ASN
1	B	117	HIS
1	B	143	GLN
1	B	226	GLN
1	B	230	ASN
1	C	42	GLN
1	C	47	ASN
1	C	61	GLN
1	C	85	HIS
1	C	91	ASN
1	C	108	GLN
1	C	180	GLN
1	C	184	GLN
1	D	61	GLN
1	D	85	HIS
1	D	117	HIS
1	D	143	GLN
1	D	184	GLN
1	D	223	GLN
1	D	226	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	212/252 (84%)	0.72	31 (14%) 6 4	18, 38, 74, 80	0
1	B	208/252 (82%)	0.38	16 (7%) 19 17	20, 34, 58, 72	0
1	C	212/252 (84%)	0.44	14 (6%) 24 21	17, 38, 58, 68	0
1	D	210/252 (83%)	0.68	31 (14%) 5 4	16, 41, 70, 80	0
All	All	842/1008 (83%)	0.55	92 (10%) 10 9	16, 38, 67, 80	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ARG	5.7
1	A	115	VAL	4.5
1	A	175	GLY	4.5
1	D	52	ARG	4.3
1	D	116	SER	4.3
1	D	53	GLN	4.1
1	D	113	ASP	4.0
1	A	116	SER	4.0
1	C	173	GLU	3.9
1	D	172	SER	3.9
1	C	174	ARG	3.9
1	D	175	GLY	3.9
1	A	122	GLU	3.8
1	D	48	GLU	3.8
1	D	50	ASP	3.7
1	A	117	HIS	3.7
1	A	45	GLY	3.7
1	D	75	LYS	3.6
1	B	79	GLY	3.6
1	A	118	SER	3.5
1	D	51	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	72	GLN	3.4
1	B	45	GLY	3.4
1	B	227	ASP	3.4
1	A	121	GLU	3.3
1	C	114	PHE	3.3
1	A	113	ASP	3.3
1	D	121	GLU	3.2
1	D	76	ALA	3.1
1	C	116	SER	3.1
1	A	177	ASP	3.1
1	A	50	ASP	3.1
1	B	230	ASN	3.0
1	A	114	PHE	3.0
1	D	79	GLY	3.0
1	C	172	SER	3.0
1	A	123	THR	2.9
1	D	106	THR	2.9
1	A	71	GLU	2.9
1	D	118	SER	2.9
1	A	172	SER	2.9
1	D	107	VAL	2.9
1	A	125	THR	2.9
1	C	175	GLY	2.9
1	A	120	LYS	2.8
1	A	51	TYR	2.8
1	A	173	GLU	2.8
1	A	124	VAL	2.7
1	D	77	LEU	2.7
1	A	128	PRO	2.7
1	C	107	VAL	2.7
1	B	77	LEU	2.6
1	C	115	VAL	2.6
1	B	44	LEU	2.6
1	B	47	ASN	2.6
1	C	109	ILE	2.6
1	B	219	ASN	2.6
1	D	124	VAL	2.5
1	B	229	LEU	2.5
1	D	123	THR	2.5
1	A	112	TYR	2.4
1	B	42	GLN	2.4
1	C	230	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	127	TYR	2.4
1	D	114	PHE	2.4
1	A	107	VAL	2.4
1	D	117	HIS	2.3
1	A	104	GLY	2.2
1	C	117	HIS	2.2
1	D	177	ASP	2.2
1	B	41	VAL	2.2
1	D	171	ILE	2.2
1	A	67	VAL	2.2
1	B	228	ILE	2.2
1	A	52	ARG	2.2
1	D	176	ARG	2.2
1	D	49	VAL	2.1
1	A	74	ALA	2.1
1	D	226	GLN	2.1
1	D	102	THR	2.1
1	D	115	VAL	2.1
1	A	119	ARG	2.1
1	A	77	LEU	2.1
1	D	109	ILE	2.1
1	B	80	GLN	2.1
1	B	81	PHE	2.1
1	B	52	ARG	2.1
1	C	143	GLN	2.0
1	D	122	GLU	2.0
1	C	51	TYR	2.0
1	D	127	TYR	2.0
1	C	113	ASP	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.