



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:45 PM UTC

PDB ID : 1XIK / pdb_00001xik
Title : RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 BETA CHAIN
Authors : Logan, D.T.; Su, X.-D.; Aberg, A.; Regnstrom, K.; Hajdu, J.; Eklund, H.; Nordlund, P.
Deposited on : 1996-08-06
Resolution : 1.70 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

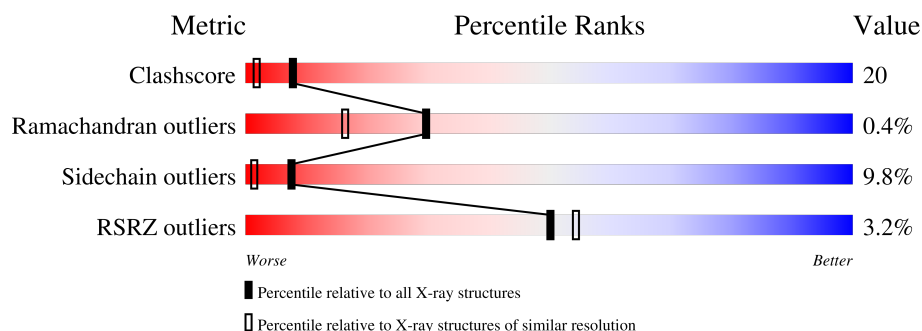
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	375	3% 55% 28% 7% 9%
1	B	375	2% 58% 24% 8% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5931 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 PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	1	0
			2789	1784	464	527	14			
1	B	341	Total	C	N	O	S	0	3	0
			2802	1790	468	529	15			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Hg	0	0
			6	6		
3	B	4	Total	Hg	0	0
			4	4		

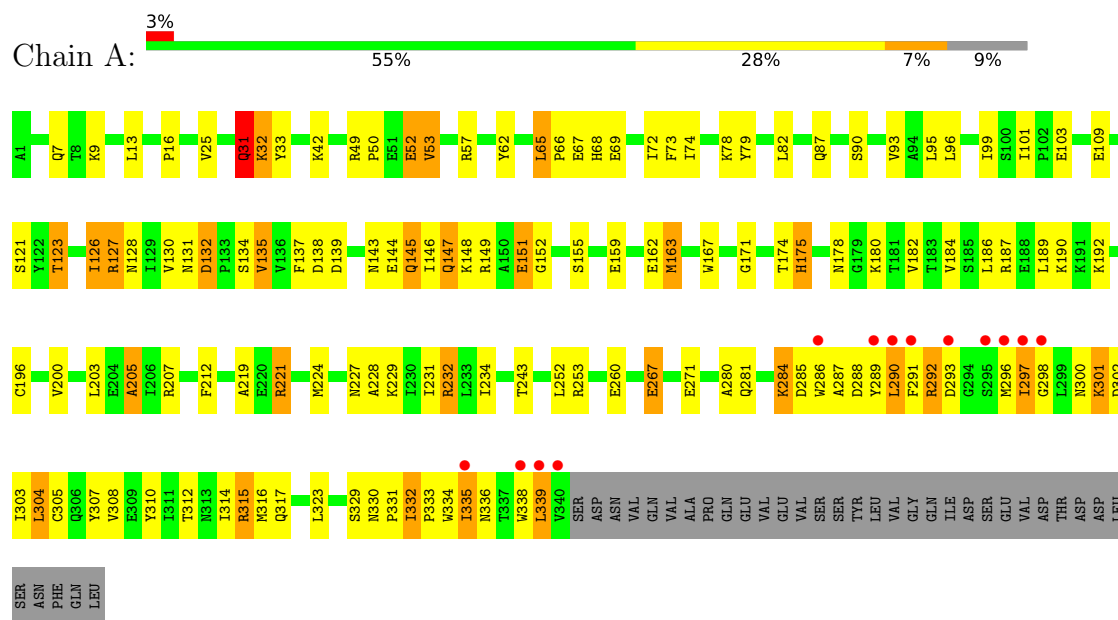
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		
4	B	178	Total	O	0	0
			178	178		

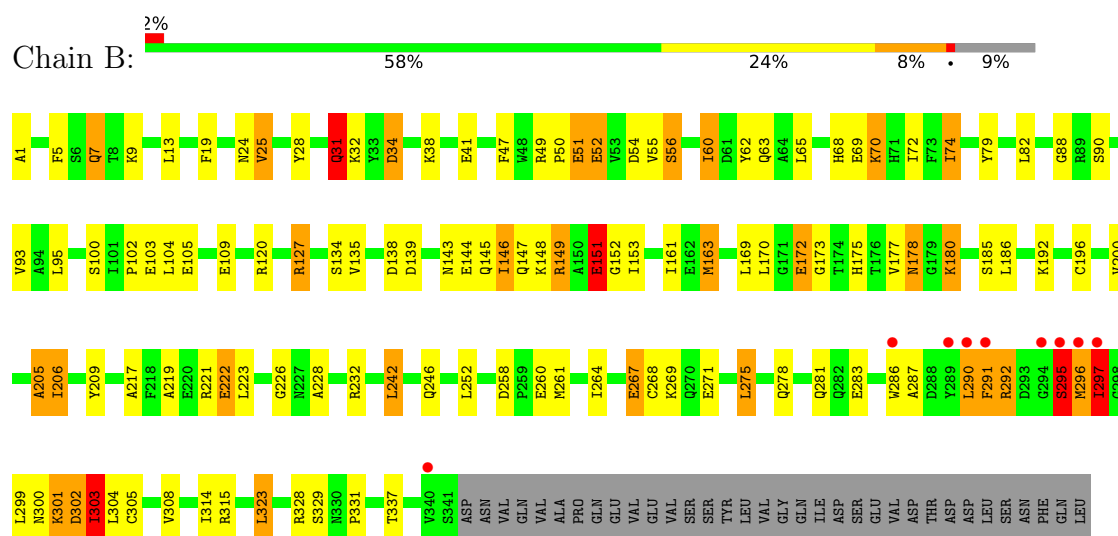
3 Residue-property plots

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: PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE



• Molecule 1: PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.44Å 83.53Å 113.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.70 15.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-1.70) 98.5 (15.00-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.206 , 0.280 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 95.7	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	0.97	EDS
Total number of atoms	5931	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, HG

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	0.91	3/2858 (0.1%)	1.51	29/3877 (0.7%)
1	B	0.92	1/2881 (0.0%)	1.47	41/3907 (1.0%)
All	All	0.92	4/5739 (0.1%)	1.49	70/7784 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ILE	CA-CB	-6.43	1.46	1.54
1	A	163	MET	SD-CE	5.62	1.93	1.79
1	B	163	MET	SD-CE	5.34	1.92	1.79
1	A	126	ILE	CA-CB	-5.22	1.48	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	LYS	N-CA-C	-10.73	98.30	111.40
1	A	334	TRP	N-CA-C	-8.54	102.05	111.36
1	B	90	SER	N-CA-C	8.30	124.94	113.16
1	A	293	ASP	N-CA-C	-8.00	103.08	112.92
1	B	297	ILE	CB-CA-C	7.84	122.00	111.88
1	B	302	ASP	N-CA-C	7.69	119.29	111.07
1	B	25	VAL	CB-CA-C	-7.68	101.16	111.15
1	B	206	ILE	N-CA-C	7.67	118.56	112.12
1	A	25	VAL	CB-CA-C	-7.46	101.45	111.15
1	B	295	SER	N-CA-C	7.43	121.79	109.46
1	B	70	LYS	N-CA-C	-7.08	103.50	111.07
1	A	53	VAL	N-CA-C	6.98	118.02	109.30
1	A	90	SER	N-CA-C	6.86	122.17	113.25
1	B	205	ALA	CA-C-N	-6.84	115.59	122.77
1	B	205	ALA	C-N-CA	-6.84	115.59	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	GLU	N-CA-C	6.70	120.09	110.24
1	B	120	ARG	N-CA-CB	-6.57	100.46	110.12
1	B	55	VAL	N-CA-C	-6.38	106.56	112.43
1	A	128	ASN	CA-C-N	-6.35	112.64	121.53
1	A	128	ASN	C-N-CA	-6.35	112.64	121.53
1	A	243	THR	N-CA-C	-6.32	104.48	111.36
1	A	7	GLN	N-CA-C	6.22	120.87	113.16
1	B	217	ALA	N-CA-C	-6.20	104.43	111.07
1	B	291	PHE	N-CA-C	6.11	120.73	113.16
1	B	178	ASN	N-CA-C	6.00	119.69	111.54
1	B	314	ILE	CB-CA-C	-5.99	104.30	111.97
1	A	95	LEU	N-CA-C	5.95	120.72	112.45
1	B	25	VAL	N-CA-C	5.95	116.74	108.89
1	A	65	LEU	N-CA-C	5.92	117.16	109.64
1	A	292	ARG	N-CA-C	5.92	117.82	111.36
1	B	292	ARG	N-CA-C	5.86	118.62	111.82
1	B	32	LYS	N-CA-C	-5.84	104.83	111.14
1	A	16	PRO	N-CA-C	-5.82	102.72	111.57
1	A	205	ALA	CA-C-N	-5.82	117.00	123.16
1	A	205	ALA	C-N-CA	-5.82	117.00	123.16
1	A	174	THR	N-CA-C	-5.73	100.07	109.40
1	B	34	ASP	N-CA-C	5.69	119.83	113.01
1	A	284	LYS	N-CA-C	-5.67	105.02	111.14
1	B	226	GLY	N-CA-C	-5.65	105.65	112.49
1	B	120	ARG	CA-CB-CG	5.49	125.08	114.10
1	B	161	ILE	N-CA-C	-5.47	105.17	110.42
1	A	99	ILE	N-CA-C	5.43	116.59	109.21
1	B	329	SER	N-CA-C	-5.42	102.73	110.59
1	B	297	ILE	N-CA-C	5.41	115.43	107.15
1	A	151	GLU	N-CA-C	5.36	118.01	110.23
1	B	1	ALA	CA-C-N	-5.35	114.18	122.09
1	B	1	ALA	C-N-CA	-5.35	114.18	122.09
1	B	303	ILE	N-CA-C	-5.24	105.43	110.72
1	B	135	VAL	N-CA-CB	5.23	116.67	110.55
1	B	102	PRO	N-CA-C	5.22	120.78	113.53
1	B	28	TYR	CA-CB-CG	-5.21	104.53	113.90
1	A	308	VAL	CB-CA-C	-5.20	105.23	112.04
1	A	132	ASP	C-N-CD	-5.16	103.84	125.00
1	B	31	GLN	N-CA-C	5.15	117.08	108.99
1	B	308	VAL	CB-CA-C	-5.14	105.39	111.97
1	B	13	LEU	CA-C-N	-5.14	114.58	122.60
1	B	13	LEU	C-N-CA	-5.14	114.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ILE	N-CA-C	-5.13	105.60	110.42
1	A	189	LEU	N-CA-C	-5.12	105.78	111.36
1	B	93	VAL	N-CA-C	5.11	115.83	110.62
1	B	209	TYR	CA-CB-CG	-5.11	104.71	113.90
1	A	31	GLN	CG-CD-NE2	-5.06	108.81	116.40
1	A	31	GLN	CB-CG-CD	-5.05	104.01	112.60
1	B	19	PHE	CA-C-N	-5.05	116.29	122.75
1	B	19	PHE	C-N-CA	-5.05	116.29	122.75
1	A	175	HIS	N-CA-CB	-5.01	103.50	111.62
1	A	267	GLU	CA-C-N	-5.01	114.63	122.65
1	A	267	GLU	C-N-CA	-5.01	114.63	122.65
1	B	7	GLN	N-CA-C	5.00	119.23	113.18
1	A	291	PHE	N-CA-C	5.00	119.52	112.72

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	2789	0	2731	111	0
1	B	2802	0	2749	115	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
4	A	148	0	0	2	0
4	B	178	0	0	11	0
All	All	5931	0	5480	218	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 20.

All (218) 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:A:205:ALA:HB1	1:A:315:ARG:HD3	1.26	1.12
1:A:287:ALA:HB2	1:A:304:LEU:HD12	1.27	1.10
1:B:72:ILE:HG12	1:B:290:LEU:HD13	1.33	1.08
1:B:205:ALA:HB1	1:B:315[B]:ARG:HG3	1.41	1.02
1:B:301:LYS:H	1:B:301:LYS:HD3	1.28	0.99
1:B:246:GLN:HE22	1:B:315[B]:ARG:HH21	1.17	0.88
1:A:221:ARG:NH1	1:A:296:MET:HE3	1.90	0.86
1:A:205:ALA:HB1	1:A:315:ARG:CD	2.06	0.85
1:B:286:TRP:CZ2	1:B:290:LEU:HG	2.12	0.84
1:A:287:ALA:HB2	1:A:304:LEU:CD1	2.08	0.83
1:A:286:TRP:CD1	1:A:290:LEU:HD22	2.13	0.83
1:A:145:GLN:HG2	1:A:289:TYR:CG	2.13	0.83
1:B:72:ILE:HG23	1:B:290:LEU:HD11	1.61	0.83
1:B:72:ILE:HG12	1:B:290:LEU:CD1	2.08	0.81
1:B:68:HIS:CE1	1:B:69:GLU:HG3	2.16	0.80
1:B:163:MET:HG3	1:B:192:LYS:HE3	1.63	0.79
1:B:144:GLU:HG2	1:B:148:LYS:HE3	1.64	0.78
1:B:221:ARG:NH1	1:B:297:ILE:HG13	1.99	0.77
1:B:290:LEU:HB3	1:B:291:PHE:CD1	2.19	0.77
1:A:205:ALA:CB	1:A:315:ARG:HD3	2.12	0.77
1:B:258:ASP:OD2	1:B:261:MET:HB2	1.85	0.75
1:A:219:ALA:HB1	1:A:338:TRP:CH2	2.21	0.75
1:A:143:ASN:O	1:A:147:GLN:HG3	1.87	0.75
1:A:286:TRP:NE1	1:A:290:LEU:HD22	2.00	0.74
1:B:221:ARG:CZ	1:B:297:ILE:HG13	2.17	0.74
1:B:79:TYR:CE1	1:B:149:ARG:HG2	2.22	0.73
1:B:301:LYS:H	1:B:301:LYS:CD	2.02	0.72
1:A:228:ALA:O	1:A:232:ARG:HG3	1.91	0.71
1:A:163:MET:SD	1:A:192:LYS:HG3	2.32	0.70
1:B:51:GLU:CD	1:B:51:GLU:H	1.99	0.70
1:A:307:TYR:O	1:A:310:TYR:HB3	1.92	0.69
1:A:335:ILE:HD13	1:A:339:LEU:HD22	1.76	0.68
1:A:227:ASN:O	1:A:231:ILE:HG12	1.94	0.68
1:A:300:ASN:OD1	1:A:303:ILE:HD12	1.95	0.67
1:A:335:ILE:HD13	1:A:339:LEU:CD2	2.25	0.67
1:B:296:MET:HE3	1:B:299:LEU:HB3	1.77	0.66
1:B:62:TYR:O	1:B:70:LYS:HE3	1.96	0.66
1:B:246:GLN:NE2	1:B:315[B]:ARG:HH21	1.93	0.66
1:B:205:ALA:O	1:B:315[A]:ARG:NH1	2.29	0.66
1:A:126:ILE:HD12	1:A:137:PHE:CZ	2.31	0.65
1:B:286:TRP:CH2	1:B:290:LEU:HG	2.31	0.65
1:A:287:ALA:CB	1:A:304:LEU:HD12	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG12	1:A:131:ASN:N	2.12	0.65
1:A:132:ASP:O	1:A:135:VAL:HG23	1.97	0.65
1:B:290:LEU:HD12	1:B:291:PHE:CE1	2.33	0.63
1:B:301:LYS:HD3	1:B:301:LYS:N	2.09	0.63
1:A:149:ARG:HD2	1:A:286:TRP:CD2	2.34	0.63
1:B:291:PHE:HB2	1:B:301:LYS:HD2	1.80	0.63
1:A:32:LYS:HD3	1:A:33:TYR:CE2	2.34	0.63
1:A:145:GLN:HG2	1:A:289:TYR:CB	2.29	0.62
1:A:145:GLN:HG2	1:A:289:TYR:HB2	1.81	0.62
1:B:72:ILE:HG23	1:B:290:LEU:CD1	2.30	0.62
1:A:287:ALA:CB	1:A:301:LYS:HG3	2.31	0.61
1:B:139:ASP:O	1:B:143:ASN:HB2	2.00	0.61
1:A:82:LEU:HD12	1:B:5:PHE:CE2	2.36	0.60
1:A:307:TYR:CG	1:A:332:ILE:HD11	2.36	0.60
1:B:147:GLN:HG2	4:B:494:HOH:O	2.01	0.60
1:B:300:ASN:OD1	1:B:302:ASP:N	2.34	0.60
1:B:163:MET:SD	1:B:192:LYS:HD2	2.42	0.60
1:B:299:LEU:HD21	1:B:304:LEU:HD13	1.83	0.60
1:A:280:ALA:O	1:A:284:LYS:HG3	2.01	0.60
1:A:187:ARG:HD2	1:A:260:GLU:OE2	2.01	0.60
1:B:149:ARG:HD3	1:B:286:TRP:HB2	1.82	0.59
1:A:130:VAL:HG12	1:A:131:ASN:H	1.66	0.59
1:A:159:GLU:O	1:A:163:MET:HG3	2.03	0.59
1:B:145:GLN:HA	1:B:145:GLN:NE2	2.16	0.59
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.18	0.59
1:B:296:MET:HG2	1:B:297:ILE:N	2.18	0.58
1:B:54:ASP:OD1	1:B:56:SER:HB3	2.02	0.58
1:B:82:LEU:C	1:B:82:LEU:HD23	2.28	0.58
1:B:24:ASN:OD1	1:B:25:VAL:N	2.29	0.58
1:A:232:ARG:HD2	1:A:338:TRP:HE3	1.70	0.57
1:B:177:VAL:O	1:B:180:LYS:HG2	2.05	0.57
1:B:127:ARG:NH1	1:B:127:ARG:HG3	2.20	0.57
1:B:252:LEU:HD22	1:B:261:MET:HG2	1.86	0.57
1:A:149:ARG:NH1	1:A:286:TRP:NE1	2.53	0.57
1:A:139:ASP:O	1:A:143:ASN:HB2	2.05	0.56
1:B:242:LEU:HD11	1:B:315[B]:ARG:NH2	2.22	0.55
1:B:60:ILE:HD12	4:B:552:HOH:O	2.07	0.55
1:A:221:ARG:CZ	1:A:296:MET:HE3	2.36	0.55
1:A:155:SER:O	1:A:159:GLU:HG3	2.07	0.55
1:B:172:GLU:OE2	1:B:185:SER:HA	2.07	0.55
1:B:323:LEU:N	1:B:323:LEU:HD23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLU:HG2	1:A:152:GLY:N	2.21	0.54
1:A:149:ARG:HD2	1:A:286:TRP:CE3	2.42	0.54
1:B:275:LEU:HD12	1:B:275:LEU:C	2.32	0.54
1:A:62:TYR:O	1:A:65:LEU:HB2	2.08	0.54
1:B:105:GLU:O	1:B:109:GLU:HG3	2.08	0.54
1:B:5:PHE:HD1	1:B:7:GLN:HE21	1.55	0.53
1:A:300:ASN:CG	1:A:303:ILE:HD12	2.32	0.53
1:A:335:ILE:HG23	1:A:339:LEU:HD22	1.90	0.53
1:B:281:GLN:NE2	4:B:445:HOH:O	2.41	0.53
1:A:138:ASP:O	1:B:9:LYS:HE3	2.09	0.53
1:B:268:CYS:HA	4:B:549:HOH:O	2.07	0.53
1:B:291:PHE:HD2	1:B:295:SER:HB3	1.73	0.53
1:A:9:LYS:HG3	4:B:384:HOH:O	2.09	0.53
1:A:203:LEU:HD23	1:A:203:LEU:C	2.33	0.53
1:A:330:ASN:ND2	1:A:336:ASN:HD21	2.07	0.52
1:B:79:TYR:CZ	1:B:149:ARG:HG2	2.44	0.52
1:B:267:GLU:HG2	4:B:523:HOH:O	2.09	0.52
1:B:290:LEU:HB3	1:B:291:PHE:HD1	1.71	0.52
1:B:5:PHE:HD1	1:B:7:GLN:NE2	2.08	0.52
1:A:134:SER:O	1:A:138:ASP:HB2	2.10	0.52
1:A:187:ARG:HG2	1:A:187:ARG:HH11	1.73	0.52
1:B:178:ASN:HB2	1:B:180:LYS:HE2	1.91	0.52
1:B:291:PHE:HB2	1:B:301:LYS:CD	2.40	0.52
1:A:333:PRO:HA	1:A:336:ASN:ND2	2.25	0.51
1:A:317:GLN:HB2	1:A:323:LEU:HD21	1.92	0.51
1:A:297:ILE:O	1:A:297:ILE:HG22	2.11	0.51
1:B:286:TRP:NE1	4:B:499:HOH:O	2.43	0.51
1:B:151:GLU:OE2	1:B:152:GLY:N	2.44	0.51
1:B:232:ARG:NH2	1:B:337:THR:O	2.44	0.51
1:B:286:TRP:CE2	1:B:290:LEU:HG	2.45	0.50
1:A:93:VAL:HG13	4:A:454:HOH:O	2.11	0.50
1:B:221:ARG:NH2	1:B:296:MET:HG3	2.27	0.50
1:A:50:PRO:O	1:A:53:VAL:N	2.43	0.50
1:A:149:ARG:NH1	1:A:286:TRP:CE2	2.79	0.50
1:A:187:ARG:NH2	1:A:267:GLU:OE2	2.34	0.50
1:B:143:ASN:ND2	4:B:518:HOH:O	2.42	0.49
1:B:143:ASN:O	1:B:147:GLN:HG3	2.12	0.49
1:B:178:ASN:HB2	1:B:180:LYS:NZ	2.27	0.49
1:B:31:GLN:HG3	1:B:34:ASP:HA	1.95	0.49
1:B:271:GLU:HB2	4:B:549:HOH:O	2.13	0.49
1:B:221:ARG:HH21	1:B:296:MET:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD12	1:A:103:GLU:CD	2.38	0.48
1:B:72:ILE:CG1	1:B:290:LEU:HD13	2.24	0.48
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.78	0.48
1:A:68:HIS:O	1:A:72:ILE:HG13	2.13	0.48
1:A:287:ALA:HB1	1:A:301:LYS:HG3	1.95	0.48
1:B:127:ARG:HH11	1:B:127:ARG:CG	2.25	0.48
1:B:149:ARG:O	1:B:149:ARG:HG3	2.12	0.48
1:A:286:TRP:HE1	1:A:290:LEU:HD22	1.77	0.48
1:A:171:GLY:O	1:A:175:HIS:HE1	1.97	0.48
1:B:221:ARG:O	1:B:222:GLU:HB3	2.13	0.48
1:A:123:THR:O	1:A:127:ARG:HG2	2.13	0.47
1:A:288:ASP:OD1	1:A:301:LYS:HD3	2.13	0.47
1:B:52:GLU:O	1:B:52:GLU:HG2	2.14	0.47
1:A:178:ASN:HD21	1:B:175:HIS:CD2	2.33	0.47
1:A:287:ALA:HB3	1:A:301:LYS:CD	2.44	0.47
1:B:328:ARG:CZ	1:B:331:PRO:HB3	2.45	0.47
1:B:172:GLU:HG3	1:B:173:GLY:N	2.30	0.47
1:B:219:ALA:HB2	1:B:228:ALA:HB2	1.96	0.47
1:A:50:PRO:HG3	1:A:121:SER:HB3	1.97	0.47
1:A:62:TYR:HA	1:A:65:LEU:HG	1.96	0.47
1:A:149:ARG:NH1	1:A:286:TRP:CD1	2.83	0.47
1:A:31:GLN:HE21	1:A:31:GLN:HB3	1.11	0.46
1:A:109:GLU:OE2	1:B:88:GLY:O	2.33	0.46
1:B:260:GLU:HG2	1:B:264:ILE:HD11	1.97	0.46
1:B:74:ILE:HD13	1:B:74:ILE:HA	1.75	0.46
1:A:145:GLN:HG2	1:A:289:TYR:CD2	2.49	0.46
1:A:307:TYR:HA	1:A:331:PRO:CG	2.45	0.46
1:A:339:LEU:HD12	1:A:339:LEU:HA	1.65	0.46
1:A:145:GLN:CG	1:A:289:TYR:HB2	2.45	0.46
1:B:323:LEU:N	1:B:323:LEU:CD2	2.79	0.46
1:B:296:MET:CG	1:B:297:ILE:N	2.79	0.45
1:A:335:ILE:HD13	1:A:339:LEU:HD21	1.97	0.45
1:A:49:ARG:O	1:A:52:GLU:HB2	2.16	0.45
1:B:152:GLY:N	4:B:430:HOH:O	2.44	0.45
1:A:57:ARG:O	1:A:57:ARG:HG2	2.17	0.45
1:A:82:LEU:CD1	1:B:5:PHE:CE2	2.99	0.45
1:B:5:PHE:CD1	1:B:7:GLN:NE2	2.85	0.45
1:A:82:LEU:CD1	1:B:5:PHE:CZ	3.00	0.45
1:A:312:THR:O	1:A:316:MET:HG3	2.16	0.45
1:B:178:ASN:HB2	1:B:180:LYS:CE	2.46	0.44
1:A:66:PRO:O	1:A:69:GLU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:HG2	1:B:104:LEU:N	2.33	0.44
1:B:286:TRP:CH2	1:B:290:LEU:CD1	3.00	0.44
1:A:144:GLU:O	1:A:148:LYS:HB2	2.18	0.44
1:A:186:LEU:O	1:A:190:LYS:HG3	2.18	0.44
1:B:299:LEU:HD11	1:B:304:LEU:HD13	1.98	0.44
1:B:287:ALA:HB2	1:B:304:LEU:HD23	1.99	0.44
1:A:96:LEU:HD21	1:A:109:GLU:HG3	1.99	0.44
1:B:82:LEU:HD13	1:B:146:ILE:HG22	2.00	0.44
1:A:196:CYS:O	1:A:200:VAL:HG23	2.18	0.43
1:B:242:LEU:O	1:B:242:LEU:HD22	2.18	0.43
1:B:134:SER:O	1:B:138:ASP:HB2	2.18	0.43
1:A:163:MET:HE2	1:A:163:MET:HB3	1.82	0.43
1:A:338:TRP:H	1:A:338:TRP:CD1	2.34	0.43
1:B:221:ARG:HH21	1:B:296:MET:CG	2.31	0.43
1:A:182:VAL:HA	4:A:461:HOH:O	2.18	0.43
1:A:175:HIS:CD2	1:B:178:ASN:HD21	2.36	0.43
1:B:196:CYS:O	1:B:200:VAL:HG23	2.19	0.43
1:B:261:MET:HA	1:B:264:ILE:HD12	2.00	0.43
1:A:145:GLN:NE2	1:A:145:GLN:CA	2.81	0.43
1:A:147:GLN:HE21	1:A:147:GLN:HB2	1.47	0.43
1:A:49:ARG:HH22	1:B:41:GLU:HB3	1.83	0.43
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.85	0.42
1:A:212:PHE:N	1:A:212:PHE:CD1	2.86	0.42
1:B:47:PHE:HE2	1:B:49:ARG:CZ	2.33	0.42
1:A:87:GLN:NE2	1:A:87:GLN:HA	2.33	0.42
1:A:145:GLN:CG	1:A:289:TYR:CD2	3.03	0.42
1:A:74:ILE:CG2	1:A:78:LYS:HE3	2.49	0.42
1:B:49:ARG:O	1:B:52:GLU:HB3	2.20	0.42
1:A:74:ILE:HG22	1:A:78:LYS:HE3	2.02	0.42
1:A:292:ARG:HD2	1:A:292:ARG:O	2.19	0.42
1:B:65:LEU:HD21	1:B:223:LEU:HD13	2.02	0.42
1:B:205:ALA:HB1	1:B:315[A]:ARG:HD2	2.00	0.42
1:A:74:ILE:HD13	1:A:74:ILE:HA	1.80	0.41
1:A:130:VAL:CG1	1:A:131:ASN:N	2.79	0.41
1:B:149:ARG:HD2	1:B:283:GLU:OE1	2.19	0.41
1:B:95:LEU:HA	1:B:95:LEU:HD23	1.82	0.41
1:B:291:PHE:CB	1:B:301:LYS:CD	2.99	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.94	0.41
1:A:281:GLN:NE2	1:A:285:ASP:OD1	2.53	0.41
1:A:147:GLN:HG3	1:A:147:GLN:H	1.55	0.41
1:A:286:TRP:NE1	1:A:290:LEU:CD2	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PHE:CD1	1:B:291:PHE:N	2.89	0.41
1:B:163:MET:SD	1:B:192:LYS:CD	3.09	0.41
1:A:79:TYR:OH	1:A:207:ARG:HD3	2.22	0.40
1:B:297:ILE:HD11	4:B:452:HOH:O	2.20	0.40
1:B:303:ILE:HG23	1:B:303:ILE:HD13	1.77	0.40
1:B:163:MET:SD	1:B:192:LYS:CE	3.09	0.40
1:B:300:ASN:ND2	1:B:303:ILE:HG13	2.37	0.40
1:A:73:PHE:CZ	1:A:224:MET:HE2	2.57	0.40
1:A:167:TRP:HA	1:A:184:VAL:HG11	2.04	0.40
1:A:301:LYS:O	1:A:305:CYS:SG	2.80	0.40
1:A:330:ASN:HD22	1:A:336:ASN:HD21	1.68	0.40
1:B:49:ARG:HA	1:B:50:PRO:HD2	1.95	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	339/375 (90%)	325 (96%)	12 (4%)	2 (1%)	21	9
1	B	342/375 (91%)	337 (98%)	4 (1%)	1 (0%)	36	22
All	All	681/750 (91%)	662 (97%)	16 (2%)	3 (0%)	30	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	MET
1	A	297	ILE
1	A	298	GLY

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	308/340 (91%)	281 (91%)	27 (9%)	9	2
1	B	311/340 (92%)	277 (89%)	34 (11%)	6	1
All	All	619/680 (91%)	558 (90%)	61 (10%)	7	1

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	42	LYS
1	A	52	GLU
1	A	67	GLU
1	A	123	THR
1	A	127	ARG
1	A	135	VAL
1	A	145	GLN
1	A	146	ILE
1	A	147	GLN
1	A	162	GLU
1	A	180	LYS
1	A	221	ARG
1	A	229	LYS
1	A	232	ARG
1	A	253	ARG
1	A	271	GLU
1	A	290	LEU
1	A	301	LYS
1	A	302	ASP
1	A	304	LEU
1	A	314	ILE
1	A	315	ARG
1	A	329	SER
1	A	332	ILE
1	A	335	ILE
1	A	339	LEU

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Mol	Chain	Res	Type
1	B	31	GLN
1	B	38	LYS
1	B	51	GLU
1	B	52	GLU
1	B	56	SER
1	B	60	ILE
1	B	63	GLN
1	B	74	ILE
1	B	100	SER
1	B	127	ARG
1	B	146	ILE
1	B	149	ARG
1	B	151	GLU
1	B	169	LEU
1	B	170	LEU
1	B	172	GLU
1	B	180	LYS
1	B	186	LEU
1	B	206	ILE
1	B	222	GLU
1	B	242	LEU
1	B	267	GLU
1	B	269	LYS
1	B	275	LEU
1	B	278	GLN
1	B	290	LEU
1	B	292	ARG
1	B	295	SER
1	B	297	ILE
1	B	301	LYS
1	B	303	ILE
1	B	305[A]	CYS
1	B	305[B]	CYS
1	B	323	LEU

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

Mol	Chain	Res	Type
1	A	7	GLN
1	A	30	GLN
1	A	31	GLN
1	A	68	HIS

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Mol	Chain	Res	Type
1	A	71	HIS
1	A	87	GLN
1	A	145	GLN
1	A	147	GLN
1	A	168	HIS
1	A	175	HIS
1	A	246	GLN
1	A	250	ASN
1	A	278	GLN
1	A	281	GLN
1	A	336	ASN
1	B	7	GLN
1	B	12	GLN
1	B	30	GLN
1	B	31	GLN
1	B	76	ASN
1	B	80	GLN
1	B	87	GLN
1	B	128	ASN
1	B	131	ASN
1	B	145	GLN
1	B	147	GLN
1	B	168	HIS
1	B	175	HIS
1	B	227	ASN
1	B	246	GLN
1	B	247	HIS
1	B	278	GLN
1	B	281	GLN
1	B	326	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](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	340/375 (90%)	0.08	13 (3%)	44 48	18, 31, 70, 93	1 (0%)
1	B	341/375 (90%)	-0.09	9 (2%)	57 61	16, 28, 61, 98	3 (0%)
All	All	681/750 (90%)	-0.00	22 (3%)	50 54	16, 30, 65, 98	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	GLY	4.4
1	B	290	LEU	4.2
1	A	338	TRP	3.4
1	B	291	PHE	3.3
1	B	340	VAL	3.0
1	A	339	LEU	3.0
1	A	297	ILE	2.7
1	A	295	SER	2.7
1	A	290	LEU	2.7
1	B	289	TYR	2.6
1	B	297	ILE	2.6
1	B	295	SER	2.5
1	A	340	VAL	2.4
1	A	286	TRP	2.4
1	A	335	ILE	2.4
1	A	293	ASP	2.3
1	B	296	MET	2.2
1	A	289	TYR	2.2
1	A	291	PHE	2.2
1	A	296	MET	2.1
1	B	286	TRP	2.1
1	A	298	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG	A	383	1/1	0.94	0.09	26,26,26,26	1
3	HG	A	382	1/1	0.97	0.06	32,32,32,32	1
3	HG	A	379	1/1	0.97	0.05	36,36,36,36	1
3	HG	B	381	1/1	0.97	0.07	37,37,37,37	1
3	HG	A	380	1/1	0.98	0.06	38,38,38,38	1
2	FE2	A	377	1/1	0.99	0.02	19,19,19,19	0
2	FE2	B	376	1/1	0.99	0.02	20,20,20,20	0
3	HG	B	378	1/1	0.99	0.03	35,35,35,35	1
3	HG	B	380	1/1	0.99	0.04	34,34,34,34	1
3	HG	A	381	1/1	0.99	0.03	27,27,27,27	1
3	HG	A	378	1/1	1.00	0.03	33,33,33,33	1
3	HG	B	379	1/1	1.00	0.03	36,36,36,36	1
2	FE2	A	376	1/1	1.00	0.01	17,17,17,17	0
2	FE2	B	377	1/1	1.00	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.