



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:52 PM UTC

PDB ID : 1ZQY / pdb_00001zqy
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7), 31-KD DOMAIN;
SOAKED IN THE PRESENCE OF MGCL2 (50 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 2.30 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

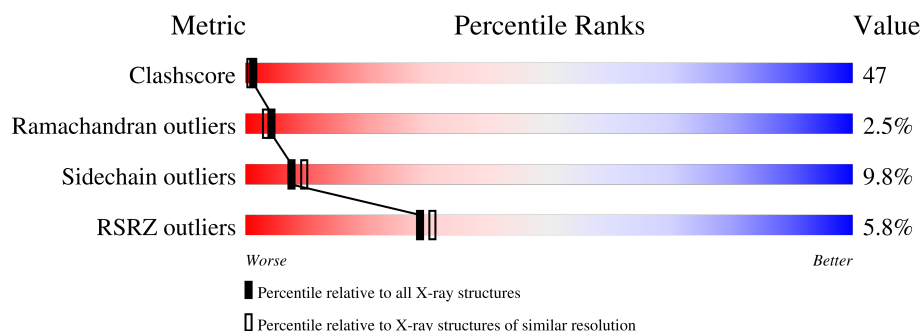
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	248	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2037 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 DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1935	1218	342	367	8			

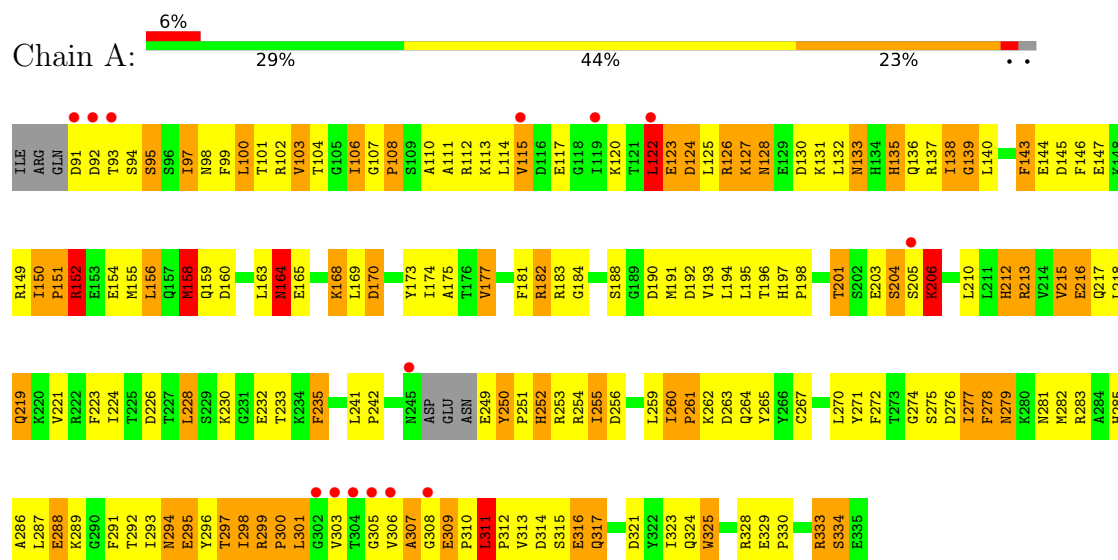
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total	O	0	0
			102	102		

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: DNA POLYMERASE BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.56Å 63.24Å 38.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.30) 91.6 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.11Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	(Not available) , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 111.7	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	0.94	EDS
Total number of atoms	2037	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 6.92% 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 i

5.1 Standard geometry i

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	1.86	34/1973 (1.7%)	2.17	76/2662 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	VAL	CA-CB	-7.12	1.46	1.54
1	A	321	ASP	CA-C	-7.05	1.43	1.52
1	A	228	LEU	N-CA	-6.96	1.37	1.46
1	A	212	HIS	CA-C	-6.71	1.43	1.52
1	A	230	LYS	CA-C	-6.66	1.46	1.53
1	A	311	LEU	CA-C	-6.60	1.44	1.53
1	A	250	TYR	CA-C	-6.36	1.44	1.52
1	A	334	SER	C-O	-6.16	1.17	1.24
1	A	286	ALA	CA-C	-6.12	1.44	1.52
1	A	254	ARG	N-CA	-6.00	1.38	1.45
1	A	276	ASP	CA-C	-5.97	1.45	1.52
1	A	313	VAL	C-O	-5.83	1.18	1.24
1	A	193	VAL	CA-C	-5.79	1.45	1.52
1	A	150	ILE	CA-C	5.70	1.57	1.53
1	A	316	GLU	CA-CB	5.70	1.62	1.53
1	A	228	LEU	CA-C	-5.66	1.45	1.53
1	A	259	LEU	CA-C	-5.61	1.46	1.52
1	A	164	ASN	N-CA	-5.55	1.39	1.46
1	A	279	ASN	CA-C	-5.50	1.45	1.52
1	A	146	PHE	CA-C	-5.48	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	THR	CA-C	-5.46	1.45	1.52
1	A	213	ARG	C-O	5.41	1.30	1.24
1	A	130	ASP	CG-OD1	5.39	1.35	1.25
1	A	250	TYR	C-N	-5.38	1.26	1.33
1	A	128	ASN	C-O	5.37	1.30	1.24
1	A	145	ASP	C-O	-5.25	1.17	1.24
1	A	194	LEU	CA-C	5.20	1.59	1.52
1	A	139	GLY	C-O	5.19	1.29	1.23
1	A	219	GLN	C-N	-5.17	1.27	1.34
1	A	235	PHE	CA-CB	-5.14	1.44	1.53
1	A	255	ILE	CA-C	-5.11	1.46	1.52
1	A	124	ASP	CG-OD1	5.07	1.34	1.25
1	A	135	HIS	C-O	5.05	1.29	1.24
1	A	160	ASP	CG-OD1	5.01	1.34	1.25

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PHE	CA-CB-CG	-10.10	103.70	113.80
1	A	206	LYS	CA-C-N	-10.01	111.67	122.89
1	A	206	LYS	C-N-CA	-10.01	111.67	122.89
1	A	226	ASP	CA-CB-CG	9.14	121.75	112.60
1	A	150	ILE	CA-C-O	9.09	125.83	119.20
1	A	124	ASP	N-CA-C	-8.94	101.22	110.97
1	A	94	SER	N-CA-C	-8.43	102.26	112.54
1	A	272	PHE	CA-CB-CG	-8.04	105.77	113.80
1	A	152	ARG	N-CA-CB	7.97	122.78	109.78
1	A	130	ASP	CA-C-N	-7.95	108.51	122.26
1	A	130	ASP	C-N-CA	-7.95	108.51	122.26
1	A	235	PHE	CB-CA-C	-7.33	96.44	109.70
1	A	265	TYR	N-CA-C	7.23	119.16	111.28
1	A	147	GLU	N-CA-CB	7.15	121.04	110.53
1	A	279	ASN	CA-CB-CG	-7.08	105.52	112.60
1	A	160	ASP	CA-C-N	-6.96	109.41	120.55
1	A	160	ASP	C-N-CA	-6.96	109.41	120.55
1	A	279	ASN	N-CA-C	6.96	119.46	111.11
1	A	170	ASP	CA-C-N	6.95	126.64	119.82
1	A	170	ASP	C-N-CA	6.95	126.64	119.82
1	A	228	LEU	N-CA-C	-6.95	102.03	112.04
1	A	182	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	A	260	ILE	CB-CA-C	-6.85	98.89	111.36
1	A	213	ARG	CA-C-O	6.79	127.75	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	CD-NE-CZ	-6.75	114.94	124.40
1	A	261	PRO	N-CA-CB	6.71	109.28	103.31
1	A	106	ILE	N-CA-C	6.67	118.04	107.98
1	A	216	GLU	CA-C-N	-6.54	110.37	120.31
1	A	216	GLU	C-N-CA	-6.54	110.37	120.31
1	A	150	ILE	CA-C-N	6.53	127.04	119.99
1	A	150	ILE	C-N-CA	6.53	127.04	119.99
1	A	132	LEU	CB-CA-C	-6.50	98.81	109.53
1	A	122	LEU	N-CA-CB	6.43	119.84	110.26
1	A	195	LEU	CA-C-N	-6.35	111.45	121.87
1	A	195	LEU	C-N-CA	-6.35	111.45	121.87
1	A	297	THR	N-CA-C	6.34	117.80	108.86
1	A	333	ARG	N-CA-C	6.25	119.85	112.72
1	A	223	PHE	N-CA-C	-6.13	104.52	112.68
1	A	123	GLU	N-CA-C	-6.06	104.99	112.38
1	A	151	PRO	CB-CA-C	-6.05	102.32	110.85
1	A	307	ALA	N-CA-C	5.92	117.96	109.14
1	A	311	LEU	CA-C-O	-5.89	115.30	120.60
1	A	252	HIS	N-CA-C	-5.82	101.06	110.32
1	A	321	ASP	N-CA-CB	5.81	118.43	110.01
1	A	138	ILE	O-C-N	5.75	127.45	121.87
1	A	192	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	267	CYS	N-CA-CB	-5.72	101.41	110.22
1	A	291	PHE	N-CA-C	5.72	118.78	109.06
1	A	314	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	215	VAL	N-CA-CB	-5.64	104.25	110.51
1	A	127	LYS	N-CA-C	-5.60	106.49	113.15
1	A	103	VAL	CB-CA-C	-5.58	102.81	110.96
1	A	131	LYS	CB-CA-C	5.57	119.35	109.65
1	A	300	PRO	CB-CA-C	-5.56	102.68	110.63
1	A	152	ARG	N-CA-C	5.54	120.51	111.37
1	A	173	TYR	CB-CA-C	-5.49	101.11	109.89
1	A	259	LEU	CA-C-O	-5.46	114.52	120.36
1	A	219	GLN	N-CA-CB	5.39	118.14	110.16
1	A	126	ARG	CA-CB-CG	-5.38	103.34	114.10
1	A	265	TYR	N-CA-CB	-5.35	102.25	110.12
1	A	163	LEU	N-CA-CB	5.34	117.75	110.01
1	A	251	PRO	CA-C-O	-5.27	115.20	122.15
1	A	194	LEU	O-C-N	-5.25	117.33	123.27
1	A	147	GLU	CB-CA-C	5.22	118.79	109.29
1	A	177	VAL	CB-CA-C	-5.21	105.60	111.23
1	A	143	PHE	CA-CB-CG	-5.21	108.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	PRO	N-CA-C	-5.18	103.41	111.13
1	A	175	ALA	CA-C-N	-5.17	115.48	122.77
1	A	175	ALA	C-N-CA	-5.17	115.48	122.77
1	A	94	SER	CA-C-O	5.14	125.71	119.38
1	A	98	ASN	N-CA-CB	5.12	117.74	110.16
1	A	158	MET	N-CA-CB	5.12	117.64	110.12
1	A	311	LEU	N-CA-C	-5.05	103.32	110.29
1	A	158	MET	CB-CA-C	5.05	119.17	110.79
1	A	95	SER	N-CA-C	-5.05	105.91	111.71
1	A	264	GLN	CA-C-O	5.03	125.12	119.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	152	ARG	CA

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	1935	0	1868	178	0
2	A	102	0	0	13	2
All	All	2037	0	1868	178	2

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 47.

All (178) 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:317:GLN:NE2	1:A:317:GLN:H	1.43	1.16
1:A:277:ILE:H	1:A:277:ILE:HD13	1.26	0.97
1:A:317:GLN:HE21	1:A:317:GLN:N	1.63	0.95
1:A:317:GLN:H	1:A:317:GLN:HE21	0.97	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:ND2	1:A:296:TYR:H	1.75	0.84
1:A:294:ASN:HD22	1:A:296:TYR:H	1.25	0.84
1:A:103:VAL:HB	1:A:106:ILE:HD13	1.61	0.80
1:A:279:ASN:O	1:A:283:ARG:HG2	1.79	0.80
1:A:133:ASN:ND2	1:A:136:GLN:H	1.79	0.80
1:A:270:LEU:HD21	1:A:282:MET:CE	2.13	0.79
1:A:154:GLU:O	1:A:158:MET:HG2	1.84	0.78
1:A:97:ILE:HD11	1:A:112:ARG:HG2	1.70	0.72
1:A:110:ALA:O	1:A:114:LEU:HD13	1.90	0.71
1:A:103:VAL:HB	1:A:106:ILE:CD1	2.21	0.71
1:A:278:PHE:CE2	1:A:282:MET:HE2	2.27	0.70
1:A:277:ILE:HD13	1:A:277:ILE:N	2.05	0.70
1:A:100:LEU:O	1:A:103:VAL:HG23	1.91	0.70
1:A:92:ASP:O	1:A:95:SER:HB3	1.93	0.68
1:A:144:GLU:N	1:A:144:GLU:OE1	2.25	0.68
1:A:270:LEU:HD21	1:A:282:MET:HE3	1.74	0.68
1:A:295:GLU:H	1:A:295:GLU:CD	2.02	0.68
1:A:133:ASN:C	1:A:133:ASN:HD22	2.03	0.67
1:A:330:PRO:HD2	2:A:429:HOH:O	1.95	0.67
1:A:97:ILE:CD1	1:A:112:ARG:HG2	2.25	0.66
1:A:270:LEU:HD12	1:A:333:ARG:NH1	2.11	0.65
1:A:107:GLY:O	1:A:111:ALA:N	2.29	0.65
1:A:317:GLN:NE2	1:A:317:GLN:N	2.26	0.65
1:A:120:LYS:N	1:A:124:ASP:OD2	2.27	0.64
1:A:155:MET:HE2	1:A:188:SER:HB2	1.79	0.64
1:A:263:ASP:OD1	1:A:263:ASP:N	2.26	0.64
1:A:122:LEU:HD12	1:A:123:GLU:N	2.12	0.63
1:A:123:GLU:O	1:A:127:LYS:HG2	1.99	0.63
1:A:183:ARG:NE	2:A:499:HOH:O	2.31	0.62
1:A:133:ASN:HD21	1:A:136:GLN:H	1.45	0.62
1:A:315:SER:HB2	1:A:317:GLN:HE22	1.65	0.62
1:A:305:GLY:O	1:A:307:ALA:N	2.34	0.61
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.82	0.61
1:A:204:SER:C	1:A:206:LYS:HE2	2.26	0.60
1:A:323:ILE:C	1:A:324:GLN:HG2	2.27	0.60
1:A:133:ASN:H	1:A:136:GLN:NE2	2.00	0.59
1:A:103:VAL:CB	1:A:106:ILE:HD13	2.32	0.59
1:A:294:ASN:HD22	1:A:294:ASN:C	2.10	0.59
1:A:294:ASN:HD22	1:A:295:GLU:N	2.01	0.58
1:A:150:ILE:HG22	1:A:151:PRO:HD2	1.84	0.58
1:A:164:ASN:OD1	1:A:165:GLU:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:N	1:A:301:LEU:HD12	2.19	0.58
1:A:277:ILE:HG12	1:A:278:PHE:H	1.69	0.57
1:A:204:SER:CA	1:A:206:LYS:HE2	2.34	0.57
1:A:138:ILE:HB	1:A:228:LEU:CD2	2.34	0.57
1:A:274:GLY:HA2	1:A:279:ASN:OD1	2.05	0.57
1:A:150:ILE:CG2	1:A:151:PRO:HD2	2.35	0.57
1:A:152:ARG:NH2	1:A:181:PHE:O	2.39	0.56
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:HH11	1.70	0.55
1:A:285:HIS:HD2	1:A:323:ILE:HD12	1.71	0.55
1:A:156:LEU:HD13	1:A:181:PHE:HE1	1.71	0.54
1:A:249:GLU:HG3	2:A:455:HOH:O	2.07	0.54
1:A:143:PHE:HB3	1:A:144:GLU:OE1	2.07	0.54
1:A:262:LYS:O	1:A:262:LYS:HG3	2.07	0.54
1:A:122:LEU:HD12	1:A:122:LEU:C	2.32	0.54
1:A:277:ILE:H	1:A:277:ILE:CD1	2.07	0.53
1:A:287:LEU:HD12	1:A:287:LEU:O	2.08	0.53
1:A:114:LEU:HD12	1:A:114:LEU:N	2.21	0.53
1:A:137:ARG:NH1	2:A:468:HOH:O	2.41	0.53
1:A:288:GLU:N	1:A:288:GLU:OE1	2.41	0.53
1:A:270:LEU:HD21	1:A:282:MET:HE1	1.90	0.52
1:A:315:SER:HB2	1:A:317:GLN:NE2	2.24	0.52
1:A:252:HIS:NE2	2:A:483:HOH:O	2.34	0.52
1:A:285:HIS:O	1:A:288:GLU:N	2.42	0.52
1:A:150:ILE:O	1:A:188:SER:N	2.33	0.52
1:A:205:SER:O	1:A:206:LYS:HD3	2.10	0.52
1:A:289:LYS:NZ	1:A:324:GLN:HG3	2.26	0.51
1:A:299[B]:ARG:HD2	1:A:308:GLY:HA3	1.92	0.51
1:A:150:ILE:HD13	1:A:253:ARG:HG2	1.92	0.51
1:A:215:VAL:O	1:A:219:GLN:HG3	2.10	0.51
1:A:271:TYR:CG	1:A:295:GLU:HB3	2.46	0.51
1:A:329:GLU:HB3	1:A:330:PRO:HD2	1.92	0.51
1:A:106:ILE:CG2	1:A:111:ALA:HB2	2.41	0.51
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.46	0.51
1:A:169:LEU:O	1:A:170:ASP:HB2	2.10	0.51
1:A:285:HIS:NE2	1:A:325:TRP:CD1	2.79	0.51
1:A:334:SER:HA	2:A:499:HOH:O	2.10	0.50
1:A:152:ARG:NH1	2:A:463:HOH:O	2.28	0.50
1:A:108:PRO:O	1:A:111:ALA:N	2.44	0.50
1:A:241:LEU:CD2	1:A:242:PRO:HD2	2.42	0.49
1:A:297:THR:O	1:A:299[A]:ARG:NH1	2.45	0.49
1:A:92:ASP:C	1:A:95:SER:HB3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:O	1:A:115:VAL:HG23	2.13	0.49
1:A:156:LEU:CD1	1:A:181:PHE:CE1	2.96	0.49
1:A:224:ILE:HD13	1:A:235:PHE:CE2	2.48	0.49
1:A:275:SER:OG	1:A:277:ILE:HG12	2.12	0.48
1:A:317:GLN:H	1:A:317:GLN:CD	2.09	0.48
1:A:138:ILE:HB	1:A:228:LEU:HD23	1.95	0.48
1:A:289:LYS:HZ2	1:A:324:GLN:HG3	1.77	0.48
1:A:323:ILE:O	1:A:324:GLN:HG2	2.12	0.48
1:A:150:ILE:HA	1:A:151:PRO:HD3	1.66	0.48
1:A:255:ILE:HG12	1:A:256:ASP:N	2.29	0.48
1:A:270:LEU:HD12	1:A:333:ARG:HH11	1.78	0.48
1:A:299[B]:ARG:HD2	1:A:308:GLY:CA	2.44	0.48
1:A:110:ALA:HA	1:A:113:LYS:HE3	1.96	0.48
1:A:204:SER:HB3	1:A:206:LYS:HE2	1.95	0.47
1:A:212:HIS:O	1:A:216:GLU:HG3	2.13	0.47
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.73	0.47
1:A:156:LEU:CD1	1:A:181:PHE:HE1	2.26	0.47
1:A:217:GLN:O	1:A:221:VAL:HG22	2.14	0.47
1:A:126:ARG:H	1:A:126:ARG:HG3	1.47	0.47
1:A:260:ILE:HG22	1:A:261:PRO:N	2.28	0.47
1:A:299[B]:ARG:CD	1:A:309:GLU:H	2.28	0.47
1:A:155:MET:HA	1:A:158:MET:HG3	1.96	0.47
1:A:114:LEU:N	1:A:114:LEU:CD1	2.78	0.47
1:A:122:LEU:O	1:A:125:LEU:HB2	2.14	0.47
1:A:126:ARG:C	1:A:128:ASN:H	2.23	0.47
1:A:126:ARG:HG2	1:A:140:LEU:HD21	1.97	0.47
1:A:104:THR:HG23	1:A:139:GLY:HA3	1.96	0.46
1:A:104:THR:HG22	2:A:435:HOH:O	2.15	0.46
1:A:150:ILE:N	1:A:188:SER:O	2.30	0.46
1:A:270:LEU:CD1	1:A:333:ARG:NH1	2.77	0.46
1:A:103:VAL:HA	2:A:435:HOH:O	2.14	0.46
1:A:174:ILE:HB	1:A:196:THR:HG22	1.98	0.46
1:A:303:VAL:C	1:A:305:GLY:H	2.23	0.46
1:A:308:GLY:O	1:A:309:GLU:HB2	2.16	0.46
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.82	0.46
1:A:315:SER:CB	1:A:317:GLN:NE2	2.79	0.46
1:A:298:ILE:C	1:A:299[A]:ARG:HG3	2.41	0.46
1:A:328:ARG:NH2	2:A:470:HOH:O	2.49	0.46
1:A:99:PHE:CD1	1:A:99:PHE:C	2.95	0.45
1:A:91:ASP:C	1:A:93:THR:H	2.24	0.45
1:A:113:LYS:HG3	1:A:114:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:O	1:A:117:GLU:HG2	2.17	0.45
1:A:278:PHE:CE2	1:A:282:MET:CE	2.98	0.45
1:A:255:ILE:CG1	1:A:256:ASP:N	2.80	0.45
1:A:277:ILE:HG12	1:A:278:PHE:N	2.30	0.45
1:A:283:ARG:NH2	1:A:294:ASN:HA	2.31	0.45
1:A:250:TYR:HB3	2:A:404:HOH:O	2.16	0.45
1:A:316:GLU:N	1:A:317:GLN:NE2	2.65	0.45
1:A:213:ARG:HD3	2:A:444:HOH:O	2.16	0.45
1:A:301:LEU:N	1:A:301:LEU:CD1	2.80	0.45
1:A:301:LEU:C	1:A:307:ALA:HB3	2.42	0.45
1:A:294:ASN:ND2	1:A:294:ASN:C	2.74	0.44
1:A:155:MET:HA	1:A:158:MET:CG	2.47	0.44
1:A:201:THR:C	1:A:203:GLU:H	2.26	0.44
1:A:159:GLN:HB2	1:A:177:VAL:HG21	2.00	0.44
1:A:182:ARG:HH12	1:A:316:GLU:CD	2.26	0.44
1:A:281:ASN:HD22	1:A:281:ASN:HA	1.65	0.44
1:A:299[B]:ARG:HG2	1:A:310:PRO:N	2.33	0.44
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.83	0.43
1:A:152:ARG:NH2	1:A:184:GLY:CA	2.82	0.43
1:A:316:GLU:CD	1:A:333:ARG:HH12	2.26	0.43
1:A:149:ARG:HG3	2:A:447:HOH:O	2.18	0.43
1:A:311:LEU:HA	1:A:311:LEU:HD12	1.70	0.43
1:A:133:ASN:ND2	1:A:133:ASN:C	2.75	0.43
1:A:205:SER:O	1:A:206:LYS:HB3	2.19	0.43
1:A:197:HIS:ND1	1:A:198:PRO:HD2	2.34	0.43
1:A:158:MET:HG2	1:A:158:MET:H	1.71	0.43
1:A:138:ILE:HG23	1:A:138:ILE:HD12	1.61	0.43
1:A:285:HIS:CD2	1:A:323:ILE:HD12	2.52	0.43
1:A:285:HIS:CD2	1:A:325:TRP:CE2	3.07	0.43
1:A:293:ILE:HG21	1:A:293:ILE:HD13	1.62	0.43
1:A:168:LYS:CB	1:A:168:LYS:NZ	2.81	0.43
1:A:299[B]:ARG:HB3	1:A:300:PRO:HD2	2.01	0.43
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.83	0.42
1:A:155:MET:HE1	1:A:190:ASP:O	2.20	0.42
1:A:127:LYS:HA	1:A:127:LYS:HD3	1.84	0.42
1:A:127:LYS:C	1:A:128:ASN:ND2	2.78	0.42
1:A:174:ILE:HD12	1:A:196:THR:CG2	2.50	0.42
1:A:150:ILE:CD1	1:A:253:ARG:HG2	2.50	0.42
1:A:152:ARG:NH2	1:A:184:GLY:HA2	2.35	0.42
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.88	0.41
1:A:91:ASP:C	1:A:93:THR:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:CD1	1:A:114:LEU:H	2.33	0.41
1:A:241:LEU:HD23	1:A:242:PRO:HD2	2.02	0.41
1:A:201:THR:C	1:A:203:GLU:N	2.77	0.41
1:A:158:MET:HB2	1:A:191:MET:HE1	2.02	0.41
1:A:168:LYS:NZ	1:A:168:LYS:HB2	2.35	0.41
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.77	0.41
1:A:126:ARG:C	1:A:128:ASN:N	2.79	0.40
1:A:292:THR:N	1:A:301:LEU:HD11	2.37	0.40
1:A:296:TYR:C	1:A:297:THR:HG23	2.46	0.40
1:A:299[B]:ARG:HD2	1:A:309:GLU:H	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:477:HOH:O	2:A:477:HOH:O[2_555]	0.72	1.48
2:A:502:HOH:O	2:A:502:HOH:O[2_555]	1.85	0.35

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	239/248 (96%)	213 (89%)	20 (8%)	6 (2%)	4 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	306	VAL
1	A	309	GLU
1	A	204	SER
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	108	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	206/226 (91%)	185 (90%)	21 (10%)	7 8

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ILE
1	A	100	LEU
1	A	101	THR
1	A	115	VAL
1	A	122	LEU
1	A	133	ASN
1	A	152	ARG
1	A	156	LEU
1	A	158	MET
1	A	164	ASN
1	A	168	LYS
1	A	277	ILE
1	A	288	GLU
1	A	294	ASN
1	A	295	GLU
1	A	298	ILE
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	311	LEU
1	A	317	GLN
1	A	325	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	133	ASN
1	A	136	GLN
1	A	157	GLN
1	A	217	GLN
1	A	240	GLN
1	A	252	HIS
1	A	281	ASN
1	A	285	HIS
1	A	294	ASN
1	A	317	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	242/248 (97%)	-0.04	14 (5%) 29 31	14, 36, 89, 100	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	VAL	3.4
1	A	303	VAL	2.8
1	A	304	THR	2.6
1	A	122	LEU	2.5
1	A	115	VAL	2.5
1	A	92	ASP	2.5
1	A	305	GLY	2.4
1	A	308	GLY	2.3
1	A	91	ASP	2.3
1	A	93	THR	2.3
1	A	245	ASN	2.2
1	A	302	GLY	2.2
1	A	205	SER	2.2
1	A	119	ILE	2.1

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.