



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 PM UTC

PDB ID : 1ZQZ / pdb_00001zqz
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7), 31-KD DOMAIN;
SOAKED IN THE PRESENCE OF MNCL2 (50 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 2.70 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

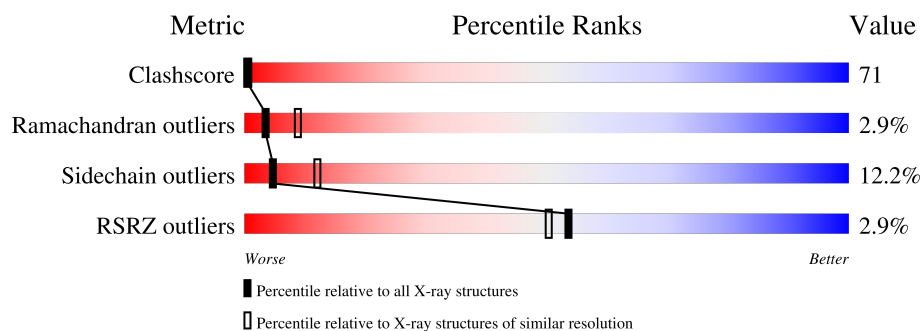
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	248	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2039 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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

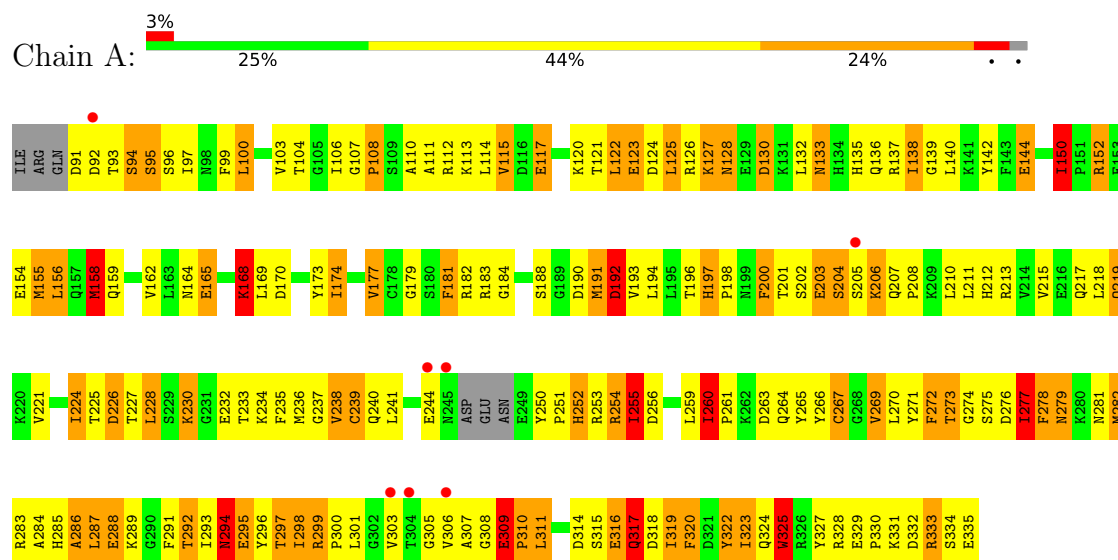
- Molecule 3 is water.

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

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: 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	118.56Å 62.73Å 37.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.70) 94.5 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.04 (at 2.22Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 133.1	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	2039	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: MN

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	1.75	31/1973 (1.6%)	2.06	54/2662 (2.0%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	TRP	CA-C	-7.62	1.43	1.52
1	A	224	ILE	CA-CB	-6.35	1.47	1.54
1	A	251	PRO	CA-C	-6.33	1.45	1.52
1	A	314	ASP	CA-C	-6.23	1.44	1.52
1	A	237	GLY	C-O	-6.20	1.17	1.23
1	A	279	ASN	CA-C	-6.16	1.44	1.52
1	A	287	LEU	N-CA	-6.08	1.38	1.46
1	A	269	VAL	CA-CB	-6.07	1.46	1.54
1	A	128	ASN	C-O	6.06	1.29	1.24
1	A	239	CYS	CA-C	-5.99	1.45	1.52
1	A	165	GLU	C-N	-5.87	1.26	1.33
1	A	294	ASN	CA-C	-5.82	1.45	1.53
1	A	255	ILE	N-CA	-5.78	1.39	1.46
1	A	286	ALA	C-N	-5.70	1.26	1.33
1	A	252	HIS	CA-C	-5.55	1.45	1.52
1	A	238	VAL	N-CA	-5.51	1.39	1.46
1	A	239	CYS	C-O	-5.44	1.18	1.23
1	A	250	TYR	C-N	-5.39	1.26	1.33
1	A	276	ASP	CA-C	-5.37	1.45	1.52
1	A	255	ILE	CA-C	-5.33	1.46	1.52
1	A	267	CYS	N-CA	-5.30	1.40	1.46
1	A	320	PHE	N-CA	-5.30	1.40	1.46
1	A	260	ILE	CA-C	-5.23	1.47	1.52
1	A	254	ARG	CA-CB	-5.22	1.45	1.53
1	A	200	PHE	N-CA	-5.21	1.39	1.46
1	A	298	ILE	C-O	-5.19	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	TYR	CA-C	-5.16	1.46	1.52
1	A	278	PHE	N-CA	-5.07	1.40	1.46
1	A	228	LEU	CA-C	-5.03	1.46	1.52
1	A	259	LEU	CA-C	-5.02	1.46	1.52
1	A	322	TYR	CA-C	-5.00	1.45	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PHE	CA-CB-CG	-12.05	101.75	113.80
1	A	279	ASN	CA-CB-CG	-8.78	103.82	112.60
1	A	193	VAL	N-CA-C	8.40	120.25	107.99
1	A	150	ILE	N-CA-CB	8.23	121.45	111.08
1	A	177	VAL	CB-CA-C	-8.22	102.39	111.35
1	A	94	SER	N-CA-C	-8.21	102.29	111.82
1	A	191	MET	CA-C-N	-7.67	111.96	122.77
1	A	191	MET	C-N-CA	-7.67	111.96	122.77
1	A	226	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	333	ARG	N-CA-C	7.28	121.02	112.72
1	A	294	ASN	N-CA-CB	7.06	121.99	110.97
1	A	127	LYS	N-CA-C	-6.98	104.85	113.15
1	A	192	ASP	CB-CA-C	6.94	121.24	110.14
1	A	244	GLU	N-CA-C	-6.76	105.58	114.31
1	A	158	MET	N-CA-CB	6.57	119.54	110.01
1	A	319	ILE	N-CA-CB	6.50	118.15	110.55
1	A	168	LYS	CA-C-N	-6.49	109.59	121.52
1	A	168	LYS	C-N-CA	-6.49	109.59	121.52
1	A	193	VAL	CB-CA-C	-6.43	102.16	110.98
1	A	162	VAL	CB-CA-C	-6.32	103.61	112.14
1	A	309	GLU	CA-C-N	6.18	127.56	119.84
1	A	309	GLU	C-N-CA	6.18	127.56	119.84
1	A	117	GLU	N-CA-C	-5.88	105.42	113.30
1	A	124	ASP	N-CA-C	-5.84	104.60	110.97
1	A	130	ASP	CA-C-N	-5.81	112.22	122.26
1	A	130	ASP	C-N-CA	-5.81	112.22	122.26
1	A	123	GLU	N-CA-C	-5.77	105.08	111.71
1	A	316	GLU	N-CA-C	-5.75	104.92	111.07
1	A	297	THR	N-CA-C	5.72	117.76	109.07
1	A	152	ARG	N-CA-CB	5.70	119.00	110.22
1	A	138	ILE	N-CA-CB	5.57	117.69	110.57
1	A	277	ILE	O-C-N	5.57	127.56	121.83
1	A	266	TYR	N-CA-C	5.53	117.74	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	THR	N-CA-CB	5.51	118.59	110.33
1	A	325	TRP	N-CA-C	-5.48	99.75	109.06
1	A	181	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	155	MET	CB-CA-C	-5.36	101.89	110.79
1	A	138	ILE	O-C-N	5.36	127.47	121.90
1	A	168	LYS	O-C-N	-5.34	115.44	122.39
1	A	197	HIS	CA-C-O	5.29	124.42	119.13
1	A	200	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	309	GLU	C-N-CD	-5.28	103.34	125.00
1	A	254	ARG	CB-CA-C	-5.22	100.71	109.53
1	A	158	MET	CB-CA-C	5.19	119.03	110.88
1	A	95	SER	N-CA-C	-5.19	105.11	111.75
1	A	323	ILE	O-C-N	5.19	127.17	122.14
1	A	272	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	150	ILE	N-CA-C	5.13	112.94	107.76
1	A	317	GLN	N-CA-CB	5.13	118.14	109.78
1	A	125	LEU	CB-CA-C	-5.10	102.65	110.81
1	A	128	ASN	N-CA-C	5.09	116.42	110.41
1	A	230	LYS	CA-C-N	5.06	128.94	121.96
1	A	230	LYS	C-N-CA	5.06	128.94	121.96
1	A	174	ILE	N-CA-CB	5.02	117.02	110.99

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	1935	0	1868	271	0
2	A	2	0	0	0	0
3	A	102	0	0	15	3
All	All	2039	0	1868	271	3

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 71.

All (271) 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:H	1:A:317:GLN:NE2	1.48	1.10
1:A:103:VAL:HB	1:A:106:ILE:HD13	1.41	0.99
1:A:317:GLN:H	1:A:317:GLN:HE21	1.01	0.98
1:A:317:GLN:HE21	1:A:317:GLN:N	1.61	0.97
1:A:174:ILE:HB	1:A:196:THR:HG22	1.47	0.95
1:A:294:ASN:HD22	1:A:296:TYR:H	1.14	0.94
1:A:277:ILE:HD13	1:A:277:ILE:H	1.33	0.92
1:A:155:MET:HA	1:A:158:MET:HG3	1.55	0.86
1:A:260:ILE:HG22	1:A:261:PRO:HD2	1.58	0.86
1:A:150:ILE:HG12	1:A:253:ARG:HG2	1.57	0.86
1:A:122:LEU:HD12	1:A:123:GLU:N	1.91	0.85
1:A:294:ASN:ND2	1:A:296:TYR:H	1.74	0.84
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:HH11	1.42	0.84
1:A:103:VAL:CB	1:A:106:ILE:HD13	2.10	0.80
1:A:279:ASN:O	1:A:283:ARG:HG2	1.81	0.79
1:A:315:SER:HB2	1:A:317:GLN:NE2	1.98	0.78
1:A:289:LYS:HZ2	1:A:324:GLN:HG3	1.47	0.78
1:A:315:SER:HB2	1:A:317:GLN:HE22	1.50	0.77
1:A:274:GLY:HA2	1:A:279:ASN:OD1	1.85	0.77
1:A:92:ASP:O	1:A:95:SER:HB3	1.85	0.76
1:A:110:ALA:O	1:A:114:LEU:HD13	1.87	0.75
1:A:123:GLU:O	1:A:127:LYS:HG2	1.84	0.75
1:A:329:GLU:HB3	1:A:330:PRO:HD2	1.69	0.75
1:A:104:THR:HG22	3:A:435:HOH:O	1.87	0.74
1:A:292:THR:HG22	1:A:301:LEU:CD1	2.17	0.74
1:A:133:ASN:ND2	1:A:136:GLN:H	1.85	0.73
1:A:159:GLN:HB2	1:A:177:VAL:HG21	1.70	0.73
1:A:289:LYS:NZ	1:A:324:GLN:HG3	2.04	0.72
1:A:155:MET:SD	1:A:158:MET:HE2	2.30	0.71
1:A:253:ARG:HG3	3:A:402:HOH:O	1.92	0.70
1:A:292:THR:N	1:A:301:LEU:HD11	2.06	0.70
1:A:202:SER:N	1:A:261:PRO:HB3	2.07	0.69
1:A:92:ASP:C	1:A:95:SER:HB3	2.17	0.69
1:A:113:LYS:O	1:A:117:GLU:HG2	1.93	0.68
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.58	0.68
1:A:292:THR:HG22	1:A:301:LEU:HD11	1.75	0.68
1:A:112:ARG:O	1:A:115:VAL:HG23	1.93	0.68
1:A:106:ILE:CG2	1:A:111:ALA:HB2	2.23	0.68
1:A:217:GLN:O	1:A:221:VAL:HG22	1.94	0.67
1:A:297:THR:O	1:A:299[A]:ARG:NH1	2.27	0.67
1:A:296:TYR:HA	3:A:449:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:THR:HB	3:A:414:HOH:O	1.93	0.67
1:A:281:ASN:O	1:A:284:ALA:HB3	1.94	0.66
1:A:154:GLU:O	1:A:158:MET:HG2	1.94	0.66
1:A:260:ILE:CG2	1:A:261:PRO:HD2	2.25	0.66
1:A:182:ARG:HH12	1:A:316:GLU:CD	2.03	0.66
1:A:207:GLN:O	1:A:210:LEU:HB2	1.96	0.66
1:A:323:ILE:C	1:A:324:GLN:HG2	2.19	0.66
1:A:150:ILE:CG1	1:A:253:ARG:HG2	2.23	0.66
1:A:137:ARG:HB2	3:A:434:HOH:O	1.95	0.65
1:A:311:LEU:HD23	1:A:322:TYR:CD1	2.32	0.65
1:A:285:HIS:O	1:A:288:GLU:N	2.28	0.65
1:A:133:ASN:HD21	1:A:136:GLN:H	1.44	0.64
1:A:152:ARG:NH2	1:A:181:PHE:O	2.29	0.64
1:A:294:ASN:OD1	1:A:299[A]:ARG:NH2	2.30	0.64
1:A:238:VAL:HA	1:A:253:ARG:O	1.98	0.64
1:A:205:SER:O	1:A:206:LYS:HD3	1.97	0.64
1:A:218:LEU:HA	1:A:221:VAL:CG2	2.28	0.64
1:A:204:SER:C	1:A:206:LYS:HE2	2.23	0.63
1:A:292:THR:O	1:A:299[A]:ARG:NH1	2.31	0.63
1:A:107:GLY:O	1:A:111:ALA:N	2.29	0.63
1:A:194:LEU:HD21	1:A:272:PHE:CD1	2.34	0.62
1:A:323:ILE:O	1:A:324:GLN:HG2	1.99	0.62
1:A:125:LEU:HD13	1:A:140:LEU:HD13	1.80	0.62
1:A:138:ILE:HB	1:A:228:LEU:CD2	2.29	0.62
1:A:133:ASN:C	1:A:133:ASN:HD22	2.07	0.62
1:A:270:LEU:HD12	1:A:333:ARG:NH1	2.15	0.62
1:A:152:ARG:NH2	1:A:184:GLY:HA2	2.15	0.61
1:A:277:ILE:HG12	1:A:278:PHE:N	2.15	0.61
1:A:277:ILE:HG12	1:A:278:PHE:H	1.66	0.61
1:A:174:ILE:HG21	1:A:265:TYR:CE2	2.36	0.61
1:A:169:LEU:HD21	1:A:217:GLN:HG2	1.81	0.60
1:A:236:MET:HE2	1:A:254:ARG:NH2	2.17	0.60
1:A:194:LEU:HD12	1:A:194:LEU:N	2.17	0.60
1:A:135:HIS:CE1	1:A:228:LEU:HD13	2.37	0.60
1:A:150:ILE:O	1:A:188:SER:N	2.28	0.60
1:A:277:ILE:CG1	1:A:335:GLU:HA	2.32	0.59
1:A:294:ASN:HD22	1:A:294:ASN:C	2.10	0.59
1:A:294:ASN:ND2	1:A:297:THR:H	2.00	0.59
1:A:303:VAL:C	1:A:305:GLY:H	2.11	0.59
1:A:311:LEU:HD23	1:A:322:TYR:CE1	2.38	0.59
1:A:301:LEU:HD12	1:A:301:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:CYS:O	1:A:270:LEU:HB3	2.02	0.58
1:A:103:VAL:HB	1:A:106:ILE:CD1	2.25	0.58
1:A:200:PHE:HB2	1:A:210:LEU:CD1	2.34	0.58
1:A:213:ARG:HD3	3:A:444:HOH:O	2.03	0.58
1:A:207:GLN:HB2	1:A:210:LEU:HD12	1.84	0.58
1:A:263:ASP:N	1:A:263:ASP:OD1	2.34	0.57
1:A:294:ASN:HD22	1:A:296:TYR:N	1.94	0.57
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.39	0.57
1:A:328:ARG:HG3	3:A:430:HOH:O	2.05	0.57
1:A:135:HIS:HE1	1:A:228:LEU:HD13	1.69	0.57
1:A:113:LYS:HG3	1:A:114:LEU:HD12	1.85	0.57
1:A:100:LEU:O	1:A:103:VAL:HG23	2.03	0.56
1:A:317:GLN:NE2	1:A:317:GLN:N	2.28	0.56
1:A:106:ILE:HG22	1:A:111:ALA:HB2	1.86	0.56
1:A:238:VAL:CG1	1:A:252:HIS:HB3	2.35	0.56
1:A:287:LEU:HD12	1:A:287:LEU:O	2.06	0.56
1:A:299[B]:ARG:HG2	1:A:310:PRO:N	2.21	0.56
1:A:182:ARG:HD3	1:A:273:THR:HG21	1.87	0.56
1:A:182:ARG:NH1	1:A:316:GLU:OE2	2.35	0.55
1:A:316:GLU:O	1:A:319:ILE:N	2.34	0.55
1:A:278:PHE:CZ	1:A:282:MET:HE2	2.41	0.55
1:A:114:LEU:HD12	1:A:114:LEU:N	2.20	0.55
1:A:204:SER:CA	1:A:206:LYS:HE2	2.37	0.55
1:A:174:ILE:HB	1:A:196:THR:CG2	2.29	0.55
1:A:291:PHE:HA	1:A:301:LEU:HD13	1.89	0.54
1:A:298:ILE:C	1:A:299[A]:ARG:HG3	2.32	0.54
1:A:218:LEU:O	1:A:221:VAL:HG23	2.06	0.54
1:A:127:LYS:O	1:A:128:ASN:ND2	2.40	0.54
1:A:292:THR:HG22	1:A:301:LEU:HD12	1.88	0.54
1:A:144:GLU:OE1	1:A:144:GLU:N	2.41	0.54
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.90	0.54
1:A:174:ILE:HD12	1:A:196:THR:CG2	2.38	0.54
1:A:182:ARG:HD3	1:A:273:THR:CG2	2.38	0.54
1:A:207:GLN:N	1:A:208:PRO:HD3	2.23	0.53
1:A:260:ILE:HG22	1:A:261:PRO:CD	2.34	0.53
1:A:278:PHE:HB2	1:A:333:ARG:O	2.07	0.53
1:A:291:PHE:CA	1:A:301:LEU:HD13	2.39	0.53
1:A:289:LYS:HD2	1:A:323:ILE:O	2.08	0.53
1:A:230:LYS:HG2	1:A:230:LYS:O	2.09	0.53
1:A:240:GLN:HG2	1:A:241:LEU:O	2.09	0.52
1:A:155:MET:HE2	1:A:188:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG12	1:A:335:GLU:HA	1.90	0.52
1:A:164:ASN:OD1	1:A:165:GLU:HG2	2.10	0.52
1:A:212:HIS:CD2	1:A:230:LYS:HE3	2.44	0.52
1:A:320:PHE:CD2	1:A:327:TYR:CD1	2.98	0.52
1:A:277:ILE:HD13	1:A:277:ILE:N	2.14	0.52
1:A:295:GLU:CD	1:A:295:GLU:H	2.18	0.52
1:A:308:GLY:O	1:A:309:GLU:HB2	2.10	0.52
1:A:150:ILE:N	1:A:188:SER:O	2.27	0.51
1:A:224:ILE:HD13	1:A:235:PHE:CE2	2.46	0.51
1:A:261:PRO:HG2	1:A:264:GLN:OE1	2.10	0.51
1:A:285:HIS:CD2	1:A:325:TRP:NE1	2.78	0.51
1:A:158:MET:HB2	1:A:191:MET:CE	2.40	0.51
1:A:320:PHE:CD2	1:A:327:TYR:HD1	2.28	0.51
1:A:234:LYS:CG	1:A:235:PHE:N	2.74	0.51
1:A:183:ARG:NH1	1:A:275:SER:N	2.59	0.51
1:A:318:ASP:O	1:A:322:TYR:HD2	1.94	0.51
1:A:330:PRO:HA	1:A:333:ARG:HG3	1.92	0.50
1:A:155:MET:HE1	1:A:191:MET:HA	1.93	0.50
1:A:218:LEU:HB3	1:A:224:ILE:HG13	1.94	0.50
1:A:159:GLN:N	1:A:191:MET:HE1	2.26	0.50
1:A:204:SER:HB3	1:A:207:GLN:HE21	1.75	0.50
1:A:331:LYS:HG3	1:A:332:ASP:OD1	2.12	0.50
1:A:218:LEU:HA	1:A:221:VAL:HG22	1.93	0.50
1:A:285:HIS:CD2	1:A:325:TRP:CE2	2.99	0.50
1:A:240:GLN:NE2	1:A:252:HIS:CE1	2.80	0.50
1:A:127:LYS:C	1:A:128:ASN:HD22	2.19	0.49
1:A:164:ASN:O	1:A:168:LYS:HG3	2.11	0.49
1:A:270:LEU:O	1:A:273:THR:N	2.37	0.49
1:A:301:LEU:C	1:A:307:ALA:HB3	2.36	0.49
1:A:278:PHE:CE2	1:A:282:MET:CE	2.95	0.49
1:A:301:LEU:CD1	1:A:301:LEU:N	2.76	0.49
1:A:103:VAL:CG1	1:A:106:ILE:HD13	2.41	0.49
1:A:133:ASN:ND2	1:A:135:HIS:HB3	2.26	0.49
1:A:224:ILE:CG2	1:A:225:THR:N	2.76	0.49
1:A:296:TYR:HD1	3:A:449:HOH:O	1.95	0.49
1:A:334:SER:HA	3:A:499:HOH:O	2.12	0.49
1:A:158:MET:HB2	1:A:191:MET:HE1	1.95	0.49
1:A:254:ARG:NH1	1:A:255:ILE:H	2.11	0.49
1:A:281:ASN:OD1	1:A:335:GLU:O	2.30	0.49
1:A:106:ILE:HG21	1:A:111:ALA:HB2	1.94	0.48
1:A:293:ILE:HG22	1:A:294:ASN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:C	1:A:96:SER:H	2.21	0.48
1:A:138:ILE:HB	1:A:228:LEU:HD23	1.95	0.48
1:A:91:ASP:C	1:A:93:THR:H	2.21	0.48
1:A:217:GLN:NE2	1:A:217:GLN:HA	2.29	0.48
1:A:238:VAL:HG13	1:A:252:HIS:HB3	1.96	0.48
1:A:215:VAL:O	1:A:219:GLN:HG3	2.14	0.48
1:A:122:LEU:HD12	1:A:122:LEU:C	2.38	0.48
1:A:132:LEU:HA	1:A:136:GLN:NE2	2.29	0.48
1:A:142:TYR:CE1	1:A:252:HIS:CD2	3.01	0.48
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.73	0.48
1:A:174:ILE:CG2	1:A:265:TYR:CE2	2.97	0.47
1:A:277:ILE:HG13	1:A:335:GLU:HA	1.96	0.47
1:A:201:THR:C	1:A:203:GLU:H	2.23	0.47
1:A:91:ASP:C	1:A:93:THR:N	2.73	0.47
1:A:108:PRO:O	1:A:111:ALA:N	2.48	0.47
1:A:133:ASN:HD21	1:A:136:GLN:HG3	1.80	0.47
1:A:285:HIS:NE2	1:A:325:TRP:CD1	2.83	0.47
1:A:97:ILE:HG12	1:A:115:VAL:HG21	1.96	0.47
1:A:122:LEU:HD12	1:A:123:GLU:H	1.71	0.47
1:A:300:PRO:O	1:A:308:GLY:HA2	2.15	0.47
1:A:114:LEU:N	1:A:114:LEU:CD1	2.78	0.47
1:A:194:LEU:N	1:A:194:LEU:CD1	2.78	0.47
1:A:289:LYS:HD3	1:A:324:GLN:OE1	2.15	0.47
1:A:230:LYS:HB2	1:A:235:PHE:HD1	1.80	0.46
1:A:182:ARG:HB3	1:A:273:THR:HG23	1.97	0.46
1:A:155:MET:CA	1:A:158:MET:HG3	2.36	0.46
1:A:201:THR:C	1:A:261:PRO:HB3	2.40	0.46
1:A:201:THR:C	1:A:203:GLU:N	2.73	0.46
1:A:135:HIS:ND1	1:A:228:LEU:HB3	2.31	0.46
1:A:269:VAL:O	1:A:273:THR:OG1	2.28	0.46
1:A:152:ARG:NH2	1:A:184:GLY:CA	2.79	0.46
1:A:174:ILE:HG21	1:A:265:TYR:HE2	1.79	0.46
1:A:133:ASN:ND2	1:A:136:GLN:HG3	2.30	0.46
1:A:299[A]:ARG:HH11	1:A:299[A]:ARG:CG	2.23	0.46
1:A:299[B]:ARG:HG2	1:A:309:GLU:H	1.80	0.46
1:A:227:THR:HG23	1:A:235:PHE:CE1	2.51	0.46
1:A:113:LYS:HG3	1:A:114:LEU:CD1	2.47	0.45
1:A:183:ARG:NH1	1:A:275:SER:CA	2.80	0.45
1:A:236:MET:HE3	1:A:256:ASP:OD2	2.17	0.45
1:A:255:ILE:O	1:A:256:ASP:OD1	2.34	0.45
1:A:93:THR:O	1:A:96:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HG22	1:A:225:THR:N	2.30	0.45
1:A:299[B]:ARG:HD2	1:A:308:GLY:HA3	1.97	0.45
1:A:225:THR:O	1:A:226:ASP:OD1	2.34	0.45
1:A:271:TYR:CG	1:A:295:GLU:HB3	2.52	0.45
1:A:137:ARG:NH1	3:A:468:HOH:O	2.50	0.45
1:A:331:LYS:NZ	1:A:332:ASP:OD2	2.49	0.45
1:A:292:THR:CG2	1:A:301:LEU:HD11	2.46	0.44
1:A:150:ILE:HD11	1:A:190:ASP:HA	1.99	0.44
1:A:200:PHE:HE1	1:A:205:SER:HA	1.82	0.44
1:A:204:SER:HB2	1:A:205:SER:H	1.19	0.44
1:A:309:GLU:HA	1:A:310:PRO:HD3	1.73	0.44
1:A:284:ALA:HB2	3:A:509:HOH:O	2.18	0.44
1:A:291:PHE:HA	1:A:301:LEU:CD1	2.48	0.44
1:A:292:THR:HG23	1:A:299[B]:ARG:HB2	1.99	0.44
1:A:254:ARG:NH1	1:A:255:ILE:N	2.65	0.44
1:A:278:PHE:CZ	1:A:282:MET:CE	3.00	0.44
1:A:318:ASP:O	1:A:322:TYR:CD2	2.71	0.44
1:A:130:ASP:OD1	1:A:130:ASP:N	2.50	0.44
1:A:299[B]:ARG:CG	1:A:309:GLU:H	2.31	0.44
1:A:127:LYS:C	1:A:128:ASN:ND2	2.76	0.43
1:A:330:PRO:HD2	3:A:429:HOH:O	2.17	0.43
1:A:328:ARG:NH2	3:A:470:HOH:O	2.52	0.43
1:A:137:ARG:NE	3:A:445:HOH:O	2.51	0.43
1:A:174:ILE:HD12	1:A:196:THR:HG23	1.99	0.43
1:A:331:LYS:HZ3	1:A:332:ASP:CG	2.26	0.43
1:A:270:LEU:CD1	1:A:333:ARG:NH1	2.82	0.43
1:A:296:TYR:C	1:A:297:THR:CG2	2.91	0.42
1:A:192:ASP:HB2	1:A:256:ASP:HB2	1.99	0.42
1:A:133:ASN:H	1:A:136:GLN:NE2	2.17	0.42
1:A:182:ARG:HG3	3:A:443:HOH:O	2.19	0.42
1:A:289:LYS:NZ	1:A:324:GLN:CG	2.79	0.42
1:A:298:ILE:O	1:A:298:ILE:HG23	2.17	0.42
1:A:311:LEU:HB3	1:A:322:TYR:CZ	2.53	0.42
1:A:170:ASP:O	1:A:173:TYR:HB2	2.19	0.42
1:A:230:LYS:HB2	1:A:235:PHE:CD1	2.54	0.42
1:A:174:ILE:HG22	1:A:265:TYR:OH	2.19	0.42
1:A:179:GLY:C	1:A:181:PHE:N	2.77	0.42
1:A:254:ARG:HH11	1:A:255:ILE:H	1.66	0.42
1:A:330:PRO:O	1:A:333:ARG:HG3	2.20	0.42
1:A:219:GLN:HE21	1:A:219:GLN:HB3	1.55	0.42
1:A:126:ARG:C	1:A:128:ASN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HG13	1:A:256:ASP:N	2.35	0.42
1:A:183:ARG:NH1	1:A:275:SER:HA	2.36	0.41
1:A:294:ASN:ND2	1:A:296:TYR:N	2.56	0.41
1:A:142:TYR:CE1	1:A:252:HIS:CG	3.08	0.41
1:A:296:TYR:C	1:A:297:THR:HG23	2.45	0.41
1:A:100:LEU:HD11	1:A:120:LYS:O	2.21	0.41
1:A:165:GLU:O	1:A:169:LEU:HG	2.20	0.41
1:A:206:LYS:O	1:A:207:GLN:HG2	2.20	0.41
1:A:329:GLU:HB3	1:A:330:PRO:CD	2.46	0.41
1:A:91:ASP:O	1:A:94:SER:N	2.51	0.41
1:A:99:PHE:CD1	1:A:99:PHE:C	2.98	0.41
1:A:104:THR:CG2	1:A:139:GLY:HA3	2.50	0.41
1:A:291:PHE:HD1	1:A:299[B]:ARG:O	2.04	0.41
1:A:294:ASN:HD22	1:A:295:GLU:N	2.18	0.41
1:A:286:ALA:O	1:A:291:PHE:N	2.51	0.41
1:A:183:ARG:HD2	1:A:333:ARG:HB2	2.03	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.89	0.41
1:A:292:THR:N	1:A:301:LEU:CD1	2.79	0.41
1:A:183:ARG:HH11	1:A:274:GLY:C	2.28	0.40
1:A:133:ASN:ND2	1:A:133:ASN:C	2.78	0.40
1:A:218:LEU:HA	1:A:218:LEU:HD23	1.82	0.40
1:A:239:CYS:SG	1:A:255:ILE:HG21	2.61	0.40
1:A:282:MET:HE2	1:A:282:MET:HB2	1.83	0.40
1:A:291:PHE:C	1:A:301:LEU:HD11	2.45	0.40
1:A:183:ARG:HH11	1:A:275:SER:N	2.20	0.40

All (3) 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)
3:A:468:HOH:O	3:A:468:HOH:O[2_565]	0.58	1.62
3:A:477:HOH:O	3:A:477:HOH:O[2_555]	0.58	1.62
3:A:502:HOH:O	3:A:502:HOH:O[2_555]	2.00	0.20

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%)	197 (82%)	35 (15%)	7 (3%)	3 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	309	GLU
1	A	204	SER
1	A	144	GLU
1	A	310	PRO
1	A	306	VAL
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%)	180 (87%)	26 (13%)	4 11

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	115	VAL
1	A	121	THR
1	A	122	LEU
1	A	133	ASN
1	A	150	ILE
1	A	156	LEU
1	A	158	MET
1	A	168	LYS
1	A	192	ASP

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Mol	Chain	Res	Type
1	A	203	GLU
1	A	211	LEU
1	A	219	GLN
1	A	255	ILE
1	A	260	ILE
1	A	277	ILE
1	A	282	MET
1	A	288	GLU
1	A	292	THR
1	A	294	ASN
1	A	295	GLU
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	133	ASN
1	A	135	HIS
1	A	136	GLN
1	A	157	GLN
1	A	217	GLN
1	A	219	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 ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 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 [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%)	-0.11	7 (2%) 53 50	14, 39, 85, 100	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	SER	3.8
1	A	245	ASN	3.3
1	A	303	VAL	2.6
1	A	92	ASP	2.5
1	A	304	THR	2.4
1	A	306	VAL	2.2
1	A	244	GLU	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](#)

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(Å ²)	Q<0.9
2	MN	A	343	1/1	0.89	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	340	1/1	0.93	0.11	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.