



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 AM UTC

PDB ID : 1NOM / pdb_00001nom
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7), 31-KD DOMAIN;
SOAKED IN THE PRESENCE OF MNCL2 (5 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 3.00 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

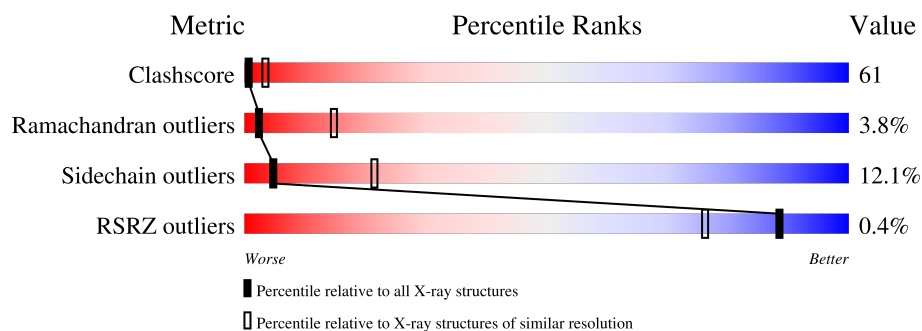
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

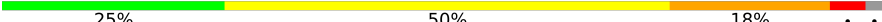
The reported resolution of this entry is 3.00 Å.

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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 2046 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	4	1	0
			1939	1221	343	367	8			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

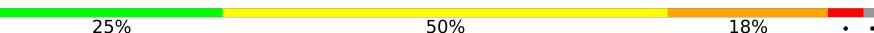
- Molecule 3 is water.

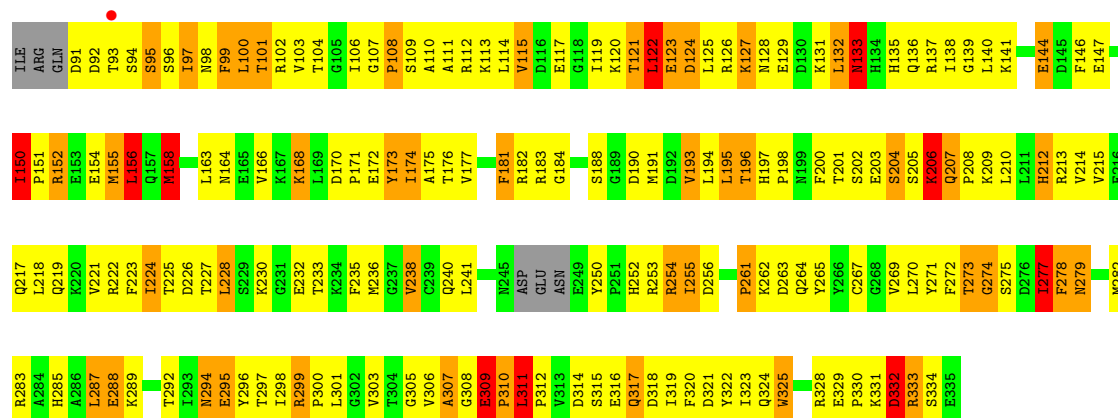
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.18Å 62.88Å 38.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-3.00) 96.6 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.61Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	(Not available) , (Not available) 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 187.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2046	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 6.68% 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	1.38	3/1977 (0.2%)	1.98	63/2666 (2.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	PHE	N-CA	-5.48	1.40	1.46
1	A	228	LEU	CA-C	-5.47	1.46	1.52
1	A	287	LEU	N-CA	-5.29	1.39	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PHE	CA-CB-CG	-12.82	100.98	113.80
1	A	124	ASP	N-CA-C	-8.71	101.75	111.07
1	A	132	LEU	CB-CA-C	-8.43	95.62	109.53
1	A	94	SER	N-CA-C	-8.29	102.17	111.71
1	A	193	VAL	N-CA-C	7.35	118.72	107.99
1	A	309	GLU	CA-C-N	7.22	128.86	119.84
1	A	309	GLU	C-N-CA	7.22	128.86	119.84
1	A	206	LYS	CA-C-N	-6.99	114.83	122.59
1	A	206	LYS	C-N-CA	-6.99	114.83	122.59
1	A	277	ILE	O-C-N	6.73	128.90	121.90
1	A	124	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	127	LYS	N-CA-C	-6.40	105.34	113.02
1	A	146	PHE	CA-CB-CG	-6.34	107.46	113.80
1	A	95	SER	N-CA-C	-6.28	104.49	111.71
1	A	212	HIS	CA-CB-CG	-6.25	107.55	113.80
1	A	272	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	228	LEU	N-CA-C	-6.18	104.45	112.68
1	A	279	ASN	CA-CB-CG	-6.06	106.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	N-CA-CB	6.04	120.59	110.32
1	A	177	VAL	CB-CA-C	-5.94	104.81	111.23
1	A	99	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	264	GLN	CA-C-N	5.85	128.12	120.28
1	A	264	GLN	C-N-CA	5.85	128.12	120.28
1	A	238	VAL	N-CA-CB	-5.81	101.73	112.43
1	A	321	ASP	CB-CA-C	-5.75	101.24	110.79
1	A	224	ILE	N-CA-C	-5.72	102.20	109.58
1	A	267	CYS	N-CA-C	-5.67	105.19	111.71
1	A	195	LEU	N-CA-C	5.63	118.39	109.50
1	A	261	PRO	N-CA-CB	5.61	108.31	103.31
1	A	176	THR	N-CA-C	5.59	117.52	108.41
1	A	320	PHE	N-CA-C	-5.56	105.12	111.07
1	A	273	THR	N-CA-CB	5.55	118.53	110.26
1	A	131	LYS	CA-C-N	5.50	130.22	122.09
1	A	131	LYS	C-N-CA	5.50	130.22	122.09
1	A	241	LEU	N-CA-CB	5.46	118.08	110.11
1	A	133	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	265	TYR	N-CA-C	5.44	117.21	111.28
1	A	311	LEU	CA-C-N	5.44	126.92	120.23
1	A	311	LEU	C-N-CA	5.44	126.92	120.23
1	A	307	ALA	N-CA-C	5.43	115.71	108.38
1	A	150	ILE	CA-C-N	5.42	125.18	119.76
1	A	150	ILE	C-N-CA	5.42	125.18	119.76
1	A	151	PRO	CB-CA-C	-5.41	104.02	111.21
1	A	174	ILE	N-CA-CB	5.41	118.60	111.25
1	A	147	GLU	CB-CA-C	5.38	121.22	109.99
1	A	123	GLU	N-CA-C	-5.37	105.83	112.38
1	A	147	GLU	N-CA-CB	5.33	119.10	110.40
1	A	175	ALA	N-CA-C	5.33	117.50	108.02
1	A	274	GLY	CA-C-N	5.33	131.28	121.70
1	A	274	GLY	C-N-CA	5.33	131.28	121.70
1	A	254	ARG	CB-CA-C	-5.29	99.81	109.54
1	A	131	LYS	CB-CA-C	5.27	118.81	109.65
1	A	163	LEU	N-CA-CB	5.26	117.70	110.07
1	A	314	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	333	ARG	N-CA-C	5.21	119.32	112.92
1	A	158	MET	CB-CA-C	5.18	119.39	110.79
1	A	109	SER	N-CA-C	-5.17	105.76	111.71
1	A	156	LEU	N-CA-CB	5.13	117.52	110.07
1	A	94	SER	CA-C-N	5.13	127.66	120.28
1	A	94	SER	C-N-CA	5.13	127.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	LEU	N-CA-CB	5.09	117.84	110.26
1	A	200	PHE	N-CA-C	5.03	116.71	108.52
1	A	207	GLN	O-C-N	5.00	125.40	121.20

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	1939	0	1875	231	0
2	A	1	0	0	0	0
3	A	106	0	0	11	2
All	All	2046	0	1875	231	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 61.

All (231) 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	1.42	1.18
1:A:317:GLN:HE21	1:A:317:GLN:N	1.56	1.03
1:A:103:VAL:HB	1:A:106:ILE:HD13	1.38	1.02
1:A:294:ASN:HD22	1:A:296:TYR:H	1.02	0.93
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.33	0.92
1:A:294:ASN:ND2	1:A:296:TYR:H	1.73	0.86
1:A:122:LEU:HD12	1:A:123:GLU:N	1.91	0.85
1:A:279:ASN:O	1:A:283:ARG:HG2	1.77	0.85
1:A:103:VAL:CB	1:A:106:ILE:HD13	2.06	0.84
1:A:277:ILE:HD13	1:A:277:ILE:H	1.41	0.83
1:A:292:THR:HG22	1:A:301:LEU:HD11	1.59	0.83
1:A:138:ILE:HB	1:A:228:LEU:HD23	1.59	0.83
1:A:329:GLU:HB3	1:A:330:PRO:HD2	1.61	0.82
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:HH11	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HA	1:A:221:VAL:CG2	2.13	0.78
1:A:292:THR:HG22	1:A:301:LEU:CD1	2.13	0.78
1:A:274:GLY:HA2	1:A:279:ASN:OD1	1.83	0.77
1:A:110:ALA:O	1:A:114:LEU:HD13	1.88	0.74
1:A:150:ILE:HG12	1:A:253:ARG:HG2	1.71	0.73
1:A:218:LEU:HA	1:A:221:VAL:HG22	1.69	0.73
1:A:204:SER:C	1:A:206:LYS:HE2	2.14	0.72
1:A:317:GLN:H	1:A:317:GLN:HE21	0.78	0.72
1:A:92:ASP:C	1:A:95:SER:HB3	2.15	0.72
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.72	0.72
1:A:99:PHE:O	1:A:102:ARG:HB2	1.90	0.71
1:A:104:THR:HG22	3:A:435:HOH:O	1.88	0.71
1:A:270:LEU:HD12	1:A:333:ARG:NH1	2.05	0.71
1:A:138:ILE:HB	1:A:228:LEU:CD2	2.20	0.70
1:A:123:GLU:O	1:A:127:LYS:HG2	1.92	0.70
1:A:215:VAL:O	1:A:219:GLN:HG3	1.93	0.69
1:A:323:ILE:C	1:A:324:GLN:HG2	2.15	0.69
1:A:92:ASP:O	1:A:95:SER:HB3	1.92	0.69
1:A:170:ASP:O	1:A:173:TYR:HB2	1.94	0.68
1:A:104:THR:HG23	1:A:139:GLY:HA3	1.75	0.68
1:A:295:GLU:CD	1:A:295:GLU:H	2.02	0.68
1:A:271:TYR:CG	1:A:295:GLU:HB3	2.29	0.67
1:A:133:ASN:ND2	1:A:135:HIS:HB3	2.06	0.67
1:A:158:MET:HB2	1:A:191:MET:HE1	1.77	0.67
1:A:294:ASN:OD1	1:A:299[A]:ARG:NH2	2.28	0.67
1:A:100:LEU:O	1:A:103:VAL:HG23	1.94	0.66
1:A:144:GLU:OE1	1:A:144:GLU:N	2.29	0.66
1:A:158:MET:HB2	1:A:191:MET:CE	2.25	0.66
1:A:263:ASP:OD1	1:A:263:ASP:N	2.29	0.65
1:A:107:GLY:O	1:A:111:ALA:N	2.30	0.65
1:A:129:GLU:O	1:A:132:LEU:HB2	1.96	0.64
1:A:271:TYR:CD2	1:A:295:GLU:HB3	2.32	0.64
1:A:270:LEU:HD12	1:A:333:ARG:HH12	1.62	0.64
1:A:204:SER:CA	1:A:206:LYS:HE2	2.28	0.64
1:A:174:ILE:O	1:A:195:LEU:HD12	1.97	0.64
1:A:141:LYS:HB2	3:A:472:HOH:O	1.98	0.64
1:A:193:VAL:C	1:A:194:LEU:HD12	2.22	0.64
1:A:224:ILE:HD13	1:A:235:PHE:CE2	2.33	0.63
1:A:150:ILE:HG12	1:A:253:ARG:CG	2.29	0.62
1:A:120:LYS:N	1:A:124:ASP:OD2	2.29	0.62
1:A:174:ILE:HB	1:A:196:THR:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:O	1:A:324:GLN:HG2	1.99	0.62
1:A:129:GLU:HA	1:A:132:LEU:HD12	1.80	0.62
1:A:135:HIS:ND1	1:A:228:LEU:HB3	2.14	0.62
1:A:277:ILE:HG12	1:A:278:PHE:H	1.65	0.61
1:A:301:LEU:HD12	1:A:301:LEU:N	2.15	0.61
1:A:113:LYS:HG3	1:A:114:LEU:HD12	1.81	0.61
1:A:152:ARG:NH2	1:A:181:PHE:O	2.33	0.61
1:A:278:PHE:HB2	1:A:333:ARG:O	1.99	0.61
1:A:287:LEU:HD12	1:A:287:LEU:O	2.00	0.61
1:A:254:ARG:NH1	1:A:255:ILE:H	1.97	0.61
1:A:317:GLN:NE2	1:A:317:GLN:N	2.27	0.61
1:A:292:THR:CG2	1:A:301:LEU:HD11	2.31	0.60
1:A:217:GLN:NE2	1:A:217:GLN:HA	2.15	0.60
1:A:97:ILE:HD11	1:A:112:ARG:HG2	1.82	0.60
1:A:182:ARG:HD3	1:A:273:THR:CG2	2.32	0.60
1:A:224:ILE:HD13	1:A:235:PHE:HE2	1.65	0.60
1:A:283:ARG:HD3	3:A:410:HOH:O	2.01	0.60
1:A:183:ARG:NE	3:A:499:HOH:O	2.34	0.59
1:A:254:ARG:CZ	1:A:254:ARG:HB3	2.31	0.59
1:A:155:MET:HA	1:A:158:MET:HG3	1.83	0.59
1:A:254:ARG:NH1	1:A:254:ARG:HB3	2.18	0.59
1:A:164:ASN:O	1:A:168:LYS:HG3	2.02	0.59
1:A:315:SER:HB2	1:A:317:GLN:HE22	1.67	0.58
1:A:102:ARG:HD3	3:A:458:HOH:O	2.03	0.58
1:A:122:LEU:O	1:A:125:LEU:HB2	2.04	0.58
1:A:150:ILE:N	1:A:188:SER:O	2.28	0.58
1:A:194:LEU:HD12	1:A:194:LEU:N	2.19	0.57
1:A:289:LYS:HD2	1:A:323:ILE:O	2.04	0.57
1:A:299[B]:ARG:HD2	1:A:308:GLY:HA3	1.85	0.57
1:A:277:ILE:HD13	1:A:277:ILE:N	2.14	0.57
1:A:103:VAL:CG1	1:A:106:ILE:HD13	2.33	0.57
1:A:209:LYS:O	1:A:213:ARG:HB2	2.05	0.57
1:A:103:VAL:HB	1:A:106:ILE:CD1	2.24	0.56
1:A:150:ILE:HD11	1:A:190:ASP:HA	1.87	0.56
1:A:207:GLN:O	1:A:210:LEU:HB2	2.05	0.56
1:A:303:VAL:C	1:A:305:GLY:H	2.13	0.56
1:A:294:ASN:ND2	1:A:297:THR:H	2.04	0.56
1:A:328:ARG:NH2	3:A:470:HOH:O	2.39	0.56
1:A:182:ARG:HD3	1:A:273:THR:HG21	1.88	0.55
1:A:106:ILE:CG2	1:A:111:ALA:HB2	2.37	0.55
1:A:285:HIS:O	1:A:288:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD12	1:A:114:LEU:N	2.23	0.54
1:A:104:THR:HG23	1:A:139:GLY:CA	2.37	0.54
1:A:250:TYR:HB3	3:A:404:HOH:O	2.06	0.54
1:A:98:ASN:O	1:A:101:THR:HG22	2.07	0.54
1:A:112:ARG:O	1:A:115:VAL:HG23	2.07	0.54
1:A:135:HIS:CE1	1:A:228:LEU:HB3	2.43	0.53
1:A:254:ARG:NH1	1:A:255:ILE:N	2.56	0.53
1:A:113:LYS:HG3	1:A:114:LEU:CD1	2.38	0.53
1:A:183:ARG:NH1	1:A:275:SER:N	2.56	0.53
1:A:331:LYS:C	1:A:333:ARG:H	2.17	0.52
1:A:183:ARG:HD3	1:A:274:GLY:O	2.10	0.52
1:A:195:LEU:HG	1:A:196:THR:N	2.25	0.52
1:A:93:THR:O	1:A:96:SER:N	2.40	0.51
1:A:158:MET:C	1:A:191:MET:HE1	2.35	0.51
1:A:113:LYS:O	1:A:117:GLU:HG2	2.10	0.51
1:A:208:PRO:HD2	3:A:473:HOH:O	2.11	0.51
1:A:217:GLN:O	1:A:221:VAL:HG22	2.11	0.51
1:A:262:LYS:O	1:A:262:LYS:HG3	2.10	0.51
1:A:270:LEU:HD22	1:A:319:ILE:HD13	1.92	0.51
1:A:292:THR:N	1:A:301:LEU:HD11	2.26	0.51
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:NH1	2.15	0.51
1:A:97:ILE:CD1	1:A:112:ARG:HG2	2.40	0.50
1:A:334:SER:HA	3:A:499:HOH:O	2.11	0.50
1:A:108:PRO:O	1:A:112:ARG:HG3	2.12	0.50
1:A:285:HIS:CD2	1:A:325:TRP:NE1	2.80	0.50
1:A:150:ILE:O	1:A:188:SER:N	2.29	0.50
1:A:240:GLN:NE2	1:A:252:HIS:CE1	2.79	0.50
1:A:183:ARG:HH11	1:A:274:GLY:C	2.20	0.50
1:A:275:SER:OG	1:A:277:ILE:HG12	2.12	0.50
1:A:155:MET:HB3	1:A:181:PHE:CE2	2.47	0.49
1:A:278:PHE:CE2	1:A:282:MET:HE2	2.47	0.49
1:A:133:ASN:ND2	1:A:136:GLN:H	2.09	0.49
1:A:100:LEU:HD11	1:A:120:LYS:O	2.13	0.49
1:A:154:GLU:O	1:A:158:MET:HG2	2.12	0.49
1:A:127:LYS:C	1:A:128:ASN:HD22	2.21	0.49
1:A:172:GLU:HG3	1:A:198:PRO:HG2	1.94	0.49
1:A:329:GLU:HB3	1:A:330:PRO:CD	2.38	0.49
1:A:122:LEU:HD12	1:A:123:GLU:H	1.73	0.49
1:A:127:LYS:O	1:A:128:ASN:ND2	2.46	0.49
1:A:93:THR:C	1:A:96:SER:H	2.20	0.49
1:A:101:THR:C	1:A:103:VAL:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD12	1:A:287:LEU:C	2.38	0.49
1:A:121:THR:O	1:A:124:ASP:HB2	2.14	0.48
1:A:172:GLU:CG	1:A:198:PRO:HG2	2.43	0.48
1:A:133:ASN:ND2	1:A:136:GLN:HG3	2.29	0.48
1:A:172:GLU:HG3	1:A:198:PRO:CG	2.44	0.48
1:A:194:LEU:N	1:A:194:LEU:CD1	2.77	0.47
1:A:315:SER:HB2	1:A:317:GLN:NE2	2.29	0.47
1:A:255:ILE:HG13	1:A:256:ASP:N	2.29	0.47
1:A:285:HIS:NE2	1:A:325:TRP:CD1	2.82	0.47
1:A:122:LEU:HD12	1:A:122:LEU:C	2.40	0.47
1:A:297:THR:OG1	1:A:299[A]:ARG:NH1	2.47	0.47
1:A:103:VAL:O	1:A:106:ILE:N	2.47	0.47
1:A:91:ASP:C	1:A:93:THR:H	2.21	0.47
1:A:114:LEU:N	1:A:114:LEU:CD1	2.78	0.47
1:A:277:ILE:H	1:A:277:ILE:CD1	2.09	0.47
1:A:299[B]:ARG:HD2	1:A:308:GLY:CA	2.45	0.47
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.59	0.47
1:A:104:THR:CG2	1:A:139:GLY:HA3	2.43	0.47
1:A:155:MET:CA	1:A:158:MET:HG3	2.44	0.46
1:A:311:LEU:HD13	1:A:311:LEU:N	2.30	0.46
1:A:311:LEU:N	1:A:311:LEU:CD1	2.79	0.46
1:A:126:ARG:HG2	1:A:140:LEU:HD21	1.97	0.46
1:A:202:SER:N	1:A:261:PRO:HB3	2.31	0.46
1:A:182:ARG:HH12	1:A:316:GLU:CD	2.23	0.46
1:A:294:ASN:HD22	1:A:294:ASN:C	2.24	0.46
1:A:270:LEU:O	1:A:273:THR:N	2.36	0.45
1:A:278:PHE:CE2	1:A:282:MET:CE	2.98	0.45
1:A:288:GLU:N	1:A:288:GLU:OE1	2.49	0.45
1:A:212:HIS:CD2	1:A:230:LYS:HE3	2.52	0.45
1:A:319:ILE:O	1:A:323:ILE:HG12	2.17	0.45
1:A:137:ARG:NH1	3:A:468:HOH:O	2.49	0.45
1:A:218:LEU:CB	1:A:224:ILE:HG13	2.47	0.45
1:A:168:LYS:CB	1:A:168:LYS:NZ	2.80	0.45
1:A:218:LEU:CA	1:A:221:VAL:HG22	2.43	0.45
1:A:298:ILE:C	1:A:299[A]:ARG:HG3	2.42	0.45
1:A:309:GLU:HA	1:A:310:PRO:HD3	1.65	0.45
1:A:99:PHE:CD1	1:A:99:PHE:C	2.95	0.45
1:A:100:LEU:HB3	1:A:106:ILE:HG21	1.99	0.44
1:A:269:VAL:O	1:A:273:THR:OG1	2.31	0.44
1:A:301:LEU:CD1	1:A:301:LEU:N	2.79	0.44
1:A:207:GLN:HB2	1:A:210:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PRO:C	1:A:301:LEU:HD12	2.42	0.44
1:A:114:LEU:CD1	1:A:114:LEU:H	2.31	0.44
1:A:170:ASP:HA	1:A:171:PRO:HD3	1.77	0.44
1:A:182:ARG:HB3	1:A:273:THR:HG23	1.99	0.44
1:A:217:GLN:HA	1:A:217:GLN:HE21	1.81	0.44
1:A:218:LEU:O	1:A:221:VAL:HG23	2.18	0.44
1:A:137:ARG:HD3	3:A:434:HOH:O	2.18	0.43
1:A:204:SER:HB2	1:A:205:SER:H	1.44	0.43
1:A:133:ASN:HD22	1:A:135:HIS:H	1.66	0.43
1:A:227:THR:HG23	1:A:235:PHE:CE1	2.54	0.43
1:A:119:ILE:HA	1:A:124:ASP:OD2	2.18	0.43
1:A:292:THR:HG22	1:A:299[A]:ARG:O	2.19	0.43
1:A:301:LEU:C	1:A:307:ALA:HB3	2.44	0.43
1:A:133:ASN:ND2	1:A:135:HIS:H	2.17	0.43
1:A:271:TYR:CD1	1:A:271:TYR:C	2.97	0.43
1:A:299[B]:ARG:HB3	1:A:308:GLY:HA2	2.01	0.43
1:A:127:LYS:C	1:A:128:ASN:ND2	2.77	0.43
1:A:285:HIS:CD2	1:A:325:TRP:CD1	3.06	0.43
1:A:166:VAL:CG1	1:A:173:TYR:HB3	2.49	0.42
1:A:152:ARG:HA	1:A:155:MET:HB2	2.01	0.42
1:A:182:ARG:NH1	1:A:316:GLU:OE2	2.45	0.42
1:A:201:THR:C	1:A:203:GLU:H	2.28	0.42
1:A:205:SER:O	1:A:206:LYS:HB3	2.19	0.42
1:A:277:ILE:HG12	1:A:278:PHE:N	2.32	0.42
1:A:225:THR:OG1	1:A:238:VAL:HG12	2.19	0.42
1:A:275:SER:O	1:A:279:ASN:OD1	2.38	0.42
1:A:225:THR:O	1:A:226:ASP:OD1	2.37	0.42
1:A:330:PRO:O	1:A:333:ARG:HB2	2.20	0.42
1:A:104:THR:CG2	1:A:139:GLY:CA	2.98	0.42
1:A:133:ASN:HD22	1:A:135:HIS:N	2.17	0.41
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.55	0.41
1:A:181:PHE:HB2	1:A:188:SER:OG	2.20	0.41
1:A:285:HIS:HD2	1:A:323:ILE:HD12	1.84	0.41
1:A:181:PHE:CD1	1:A:181:PHE:C	2.97	0.41
1:A:214:VAL:O	1:A:217:GLN:HB3	2.21	0.41
1:A:230:LYS:HB2	1:A:235:PHE:HD1	1.83	0.41
1:A:292:THR:CB	1:A:301:LEU:HD11	2.50	0.41
1:A:156:LEU:CD1	1:A:181:PHE:CE2	3.04	0.41
1:A:292:THR:HG23	1:A:299[B]:ARG:HB2	2.03	0.41
1:A:100:LEU:C	1:A:102:ARG:N	2.78	0.41
1:A:183:ARG:NH1	1:A:274:GLY:C	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.88	0.41
1:A:255:ILE:CG1	1:A:256:ASP:N	2.81	0.41
1:A:294:ASN:ND2	1:A:296:TYR:N	2.54	0.41
1:A:152:ARG:NH2	1:A:184:GLY:HA2	2.36	0.41
1:A:236:MET:HE2	1:A:236:MET:HB3	1.82	0.41
1:A:285:HIS:O	1:A:288:GLU:HB2	2.21	0.40
1:A:331:LYS:HG3	1:A:332:ASP:OD1	2.22	0.40
1:A:108:PRO:O	1:A:111:ALA:N	2.53	0.40
1:A:309:GLU:HG3	1:A:310:PRO:HD2	2.04	0.40
1:A:168:LYS:NZ	1:A:168:LYS:HB2	2.35	0.40
1:A:93:THR:C	1:A:95:SER:N	2.75	0.40
1:A:318:ASP:O	1:A:322:TYR:CD2	2.74	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)
3:A:468:HOH:O	3:A:468:HOH:O[2_565]	0.71	1.49
3:A:502:HOH:O	3:A:502:HOH:O[2_555]	1.73	0.47

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	33 (14%)	9 (4%)	2 15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	SER
1	A	206	LYS
1	A	309	GLU

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Mol	Chain	Res	Type
1	A	306	VAL
1	A	108	PRO
1	A	144	GLU
1	A	222	ARG
1	A	332	ASP
1	A	310	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	207/226 (92%)	181 (87%)	26 (13%)	4 20

All (26) 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	121	THR
1	A	122	LEU
1	A	133	ASN
1	A	150	ILE
1	A	155	MET
1	A	156	LEU
1	A	158	MET
1	A	168	LYS
1	A	173	TYR
1	A	181	PHE
1	A	196	THR
1	A	255	ILE
1	A	277	ILE
1	A	288	GLU
1	A	294	ASN
1	A	295	GLU

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Mol	Chain	Res	Type
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	311	LEU
1	A	317	GLN
1	A	325	TRP
1	A	332	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	207	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 ⓘ

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.59	1 (0%)	88 76	3, 35, 89, 100	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	THR	2.5

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	340	1/1	0.97	0.03	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.