



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:22 AM UTC

PDB ID : 3UXN / pdb_00003uxn
Title : Crystal Structure of Rat DNA Polymerase Beta, Wild Type Apoenzyme
Authors : Gridley, C.L.; Firbank, S.; Jaeger, J.
Deposited on : 2011-12-05
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

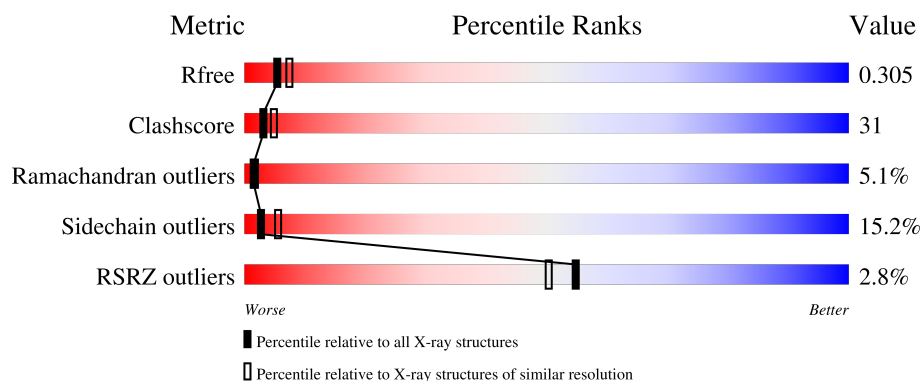
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	2% 54% 34% 8% ..
1	B	335	4% 41% 41% 13% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5379 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	325	Total	C	N	O	S	0	0	0
			2610	1647	461	493	9			
1	B	325	Total	C	N	O	S	0	0	0
			2610	1647	461	493	9			

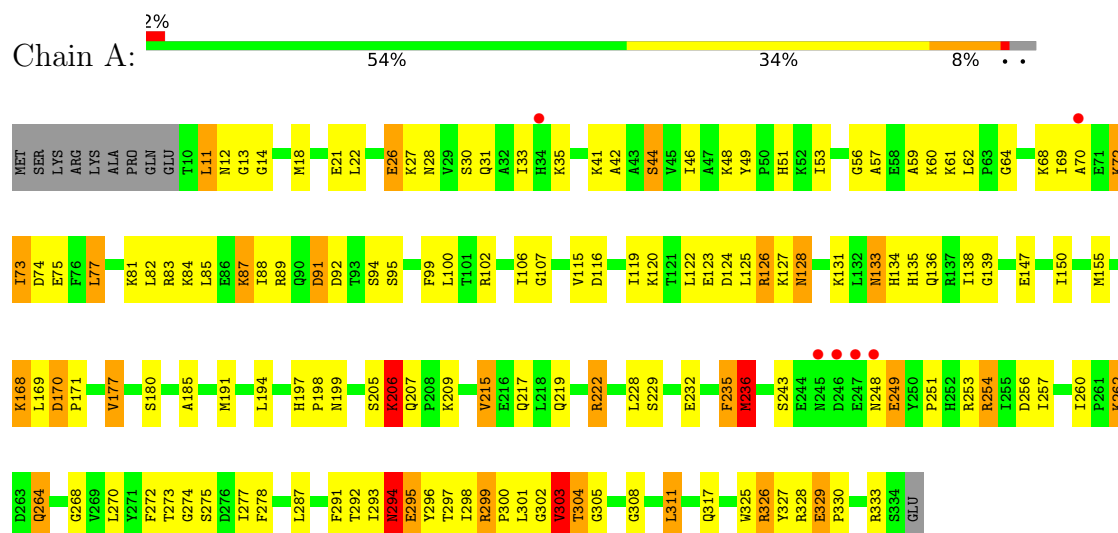
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	64	Total	O	0	0
			64	64		

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.95Å 67.45Å 83.36Å 90.00° 116.14° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	83.9 (15.00-2.50) 83.5 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.250 , 0.317 0.238 , 0.305	Depositor DCC
R_{free} test set	2018 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5379	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6824e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/2658	1.01	11/3577 (0.3%)
1	B	0.54	0/2658	0.95	6/3577 (0.2%)
All	All	0.60	0/5316	0.98	17/7154 (0.2%)

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	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	329	GLU	CA-C-N	8.01	127.57	119.24
1	A	329	GLU	C-N-CA	8.01	127.57	119.24
1	B	49	TYR	CA-C-N	6.71	126.39	119.82
1	B	49	TYR	C-N-CA	6.71	126.39	119.82
1	A	170	ASP	CA-C-N	6.14	125.76	119.56
1	A	170	ASP	C-N-CA	6.14	125.76	119.56
1	A	294	ASN	N-CA-CB	-6.00	100.90	111.39
1	A	243	SER	N-CA-C	5.86	116.16	108.07
1	A	273	THR	N-CA-C	-5.83	104.29	111.40
1	A	236	MET	CA-C-N	-5.82	117.68	122.16
1	A	236	MET	C-N-CA	-5.82	117.68	122.16
1	B	37	ASN	N-CA-C	5.62	118.12	111.33
1	B	207	GLN	CA-C-N	5.34	124.95	119.56
1	B	207	GLN	C-N-CA	5.34	124.95	119.56
1	A	107	GLY	CA-C-N	5.26	126.41	119.84
1	A	107	GLY	C-N-CA	5.26	126.41	119.84
1	B	15	ILE	N-CA-C	5.03	115.25	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	GLY	Peptide

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	2610	0	2629	138	0
1	B	2610	0	2629	190	0
2	A	95	0	0	6	0
2	B	64	0	0	14	0
All	All	5379	0	5258	328	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 31.

All (328) 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:264:GLN:HB2	1:A:296:TYR:O	1.62	0.99
1:A:12:ASN:HD21	1:A:53:ILE:H	1.12	0.94
1:B:197:HIS:HD2	1:B:199:ASN:H	1.15	0.92
1:B:62:LEU:HD12	1:B:62:LEU:H	1.32	0.92
1:A:294:ASN:HD22	1:A:296:TYR:H	1.16	0.91
1:B:69:ILE:HD12	1:B:69:ILE:H	1.37	0.89
1:B:119:ILE:HG22	1:B:125:LEU:HD23	1.52	0.89
1:A:294:ASN:ND2	1:A:296:TYR:H	1.71	0.89
1:A:134:HIS:CD2	1:A:138:ILE:HD11	2.08	0.88
1:B:22:LEU:HD11	1:B:85:LEU:HD11	1.55	0.87
1:B:87:LYS:C	1:B:87:LYS:HD2	2.00	0.87
1:A:168:LYS:HE3	1:A:168:LYS:HA	1.59	0.85
1:B:266:TYR:HA	1:B:269:VAL:HG22	1.59	0.83
1:A:197:HIS:HD2	1:A:199:ASN:H	1.30	0.80
1:A:197:HIS:CD2	1:A:199:ASN:H	1.99	0.80
1:A:133:ASN:C	1:A:133:ASN:HD22	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:SER:O	1:B:206:LYS:HB2	1.82	0.79
1:A:304:THR:HG22	1:A:305:GLY:H	1.47	0.79
1:B:75:GLU:HG2	1:B:82:LEU:HD12	1.65	0.78
1:B:283:ARG:HD3	2:B:389:HOH:O	1.82	0.78
1:A:18:MET:O	1:A:22:LEU:HD13	1.85	0.77
1:B:162:VAL:HB	2:B:349:HOH:O	1.85	0.76
1:A:42:ALA:O	1:A:46:ILE:HD13	1.87	0.75
1:A:100:LEU:HD11	1:A:120:LYS:HA	1.67	0.75
1:B:197:HIS:CD2	1:B:199:ASN:H	2.03	0.75
1:B:115:VAL:HG13	1:B:120:LYS:HB3	1.69	0.74
1:B:105:GLY:HA3	1:B:136:GLN:HA	1.69	0.73
1:A:133:ASN:HD21	1:A:136:GLN:H	1.35	0.73
1:B:159:GLN:C	2:B:349:HOH:O	2.32	0.73
1:B:87:LYS:H	1:B:89:ARG:HH21	1.37	0.73
1:B:183:ARG:NH1	2:B:354:HOH:O	2.22	0.73
1:B:29:VAL:O	1:B:29:VAL:HG12	1.89	0.72
1:B:244:GLU:O	1:B:245:ASN:HB3	1.87	0.72
1:B:275:SER:HB3	1:B:278:PHE:HB3	1.70	0.72
1:A:133:ASN:ND2	1:A:136:GLN:H	1.87	0.71
1:B:26:GLU:HA	1:B:30:SER:HB3	1.73	0.70
1:B:16:THR:O	1:B:20:VAL:HG12	1.91	0.70
1:B:56:GLY:HA2	1:B:59:ALA:HB3	1.73	0.70
1:B:62:LEU:HD12	1:B:62:LEU:N	2.05	0.69
1:B:186:GLU:OE1	1:B:187:SER:HB2	1.92	0.69
1:B:87:LYS:HD2	1:B:87:LYS:O	1.93	0.69
1:B:162:VAL:O	1:B:166:VAL:HG23	1.92	0.69
1:B:216:GLU:OE1	2:B:386:HOH:O	2.11	0.69
1:A:125:LEU:C	1:A:127:LYS:H	2.02	0.68
1:B:75:GLU:HG3	1:B:75:GLU:O	1.89	0.68
1:B:167:LYS:NZ	2:B:365:HOH:O	2.27	0.68
1:B:87:LYS:HB2	1:B:90:GLN:CD	2.17	0.68
1:B:162:VAL:N	2:B:349:HOH:O	2.26	0.68
1:B:246:ASP:HB2	1:B:249:GLU:HB3	1.76	0.67
1:A:300:PRO:HD3	1:A:311:LEU:HD21	1.76	0.67
1:A:139:GLY:O	2:A:360:HOH:O	2.12	0.67
1:B:110:ALA:O	1:B:114:LEU:HD22	1.94	0.67
1:B:106:ILE:HG12	1:B:136:GLN:CD	2.20	0.67
1:A:106:ILE:HG12	1:A:136:GLN:HG2	1.78	0.66
1:B:276:ASP:OD1	2:B:372:HOH:O	2.14	0.66
1:B:103:VAL:HG12	1:B:105:GLY:H	1.59	0.66
1:B:122:LEU:HD12	1:B:125:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ASN:O	2:B:374:HOH:O	2.14	0.65
1:B:117:GLU:HG2	1:B:131:LYS:HE2	1.78	0.65
1:B:62:LEU:HD13	1:B:65:VAL:HG21	1.78	0.65
1:B:93:THR:HG22	1:B:112:ARG:NH2	2.12	0.65
1:A:69:ILE:O	1:A:73:ILE:HG13	1.98	0.64
1:A:12:ASN:O	1:A:14:GLY:N	2.29	0.64
1:A:294:ASN:HD21	1:A:296:TYR:HB2	1.62	0.64
1:B:106:ILE:HG12	1:B:136:GLN:NE2	2.12	0.64
1:B:299:ARG:HA	1:B:311:LEU:CD2	2.28	0.64
1:B:125:LEU:C	1:B:127:LYS:H	2.07	0.63
1:B:325:TRP:HA	1:B:325:TRP:CE3	2.33	0.63
1:A:294:ASN:HD22	1:A:296:TYR:N	1.92	0.62
1:A:205:SER:O	1:A:206:LYS:HB3	1.99	0.62
1:B:133:ASN:CG	1:B:137:ARG:HH12	2.06	0.62
1:A:294:ASN:HD22	1:A:297:THR:H	1.47	0.62
1:B:299:ARG:HH11	1:B:310:PRO:HG3	1.64	0.62
1:B:201:THR:H	1:B:204:SER:HB2	1.63	0.62
1:B:113:LYS:HG3	1:B:114:LEU:HD13	1.81	0.61
1:A:235:PHE:C	1:A:235:PHE:CD2	2.77	0.61
1:B:36:TYR:HD2	1:B:37:ASN:ND2	1.98	0.61
1:A:72:LYS:O	1:A:75:GLU:HB3	1.99	0.61
1:A:56:GLY:HA2	1:A:59:ALA:HB3	1.82	0.61
1:B:93:THR:HG22	1:B:112:ARG:HH21	1.65	0.61
1:B:193:VAL:HG13	1:B:257:ILE:HG23	1.83	0.60
1:A:248:ASN:O	1:A:249:GLU:C	2.44	0.60
1:B:243:SER:C	1:B:245:ASN:H	2.06	0.60
1:B:243:SER:HB3	1:B:249:GLU:HG3	1.83	0.60
1:B:247:GLU:O	1:B:248:ASN:HB2	2.02	0.60
1:A:30:SER:O	1:A:31:GLN:HB2	2.01	0.60
1:A:134:HIS:O	1:A:138:ILE:HD12	2.01	0.60
1:A:300:PRO:HD3	1:A:311:LEU:CD2	2.32	0.60
1:A:119:ILE:HG23	1:A:124:ASP:HB3	1.83	0.60
1:B:189:GLY:O	1:B:190:ASP:HB3	2.01	0.60
1:B:114:LEU:HD21	1:B:132:LEU:HD12	1.83	0.60
1:A:294:ASN:ND2	1:A:296:TYR:N	2.47	0.59
1:A:299:ARG:NH1	2:A:390:HOH:O	2.36	0.59
1:B:69:ILE:H	1:B:69:ILE:CD1	2.10	0.59
1:B:325:TRP:HA	1:B:325:TRP:HE3	1.68	0.58
1:A:83:ARG:O	1:A:87:LYS:HE3	2.03	0.58
1:A:198:PRO:HA	1:A:262:LYS:HG3	1.85	0.58
1:A:264:GLN:HA	2:A:397:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:HA	1:B:86:GLU:HB2	1.85	0.58
1:A:133:ASN:H	1:A:136:GLN:NE2	2.02	0.58
1:A:205:SER:O	1:A:206:LYS:CB	2.51	0.58
1:B:330:PRO:O	1:B:333:ARG:HB2	2.04	0.58
1:A:304:THR:CG2	1:A:305:GLY:H	2.12	0.58
1:B:208:PRO:HB3	1:B:232:GLU:OE1	2.03	0.58
1:B:216:GLU:O	1:B:216:GLU:HG3	2.04	0.58
1:A:304:THR:HG22	1:A:305:GLY:N	2.18	0.57
1:A:150:ILE:CB	1:A:155:MET:HE3	2.35	0.57
1:B:122:LEU:CD1	1:B:125:LEU:HD12	2.34	0.57
1:A:150:ILE:HG21	1:A:155:MET:CE	2.34	0.57
1:A:150:ILE:HB	1:A:155:MET:HE3	1.86	0.57
1:A:292:THR:OG1	1:A:301:LEU:HD12	2.04	0.57
1:B:174:ILE:HB	1:B:196:THR:HG22	1.87	0.56
1:A:177:VAL:CG1	1:A:191:MET:HG3	2.35	0.56
1:B:168:LYS:HZ3	1:B:168:LYS:HB2	1.70	0.56
1:B:29:VAL:O	1:B:29:VAL:CG1	2.53	0.56
1:B:276:ASP:HB2	2:B:372:HOH:O	2.06	0.56
1:B:267:CYS:HB3	2:B:374:HOH:O	2.06	0.56
1:B:130:ASP:OD1	1:B:131:LYS:HG3	2.06	0.55
1:B:36:TYR:HD2	1:B:37:ASN:HD22	1.54	0.55
1:B:72:LYS:HB3	1:B:82:LEU:HD11	1.88	0.55
1:B:155:MET:HE3	1:B:191:MET:HE3	1.89	0.55
1:A:150:ILE:HD13	1:A:155:MET:CE	2.37	0.55
1:B:159:GLN:O	1:B:163:LEU:HB2	2.07	0.55
1:B:170:ASP:OD2	1:B:197:HIS:HE1	1.90	0.55
1:B:27:LYS:HZ2	1:B:28:ASN:ND2	2.04	0.55
1:A:68:LYS:HG3	1:A:69:ILE:H	1.70	0.54
1:B:329:GLU:HG3	1:B:330:PRO:HD2	1.89	0.54
1:B:107:GLY:O	1:B:111:ALA:HB2	2.07	0.54
1:A:177:VAL:HG11	1:A:191:MET:HG3	1.89	0.54
1:A:100:LEU:HD22	1:A:115:VAL:HG23	1.89	0.54
1:B:82:LEU:HD23	1:B:84:LYS:HB3	1.87	0.54
1:B:294:ASN:HB3	1:B:296:TYR:H	1.72	0.54
1:B:133:ASN:HB2	1:B:137:ARG:NH1	2.23	0.54
1:B:202:SER:HB3	1:B:264:GLN:NE2	2.22	0.54
1:A:68:LYS:HG3	1:A:69:ILE:N	2.23	0.54
1:B:37:ASN:HD22	1:B:37:ASN:N	2.04	0.54
1:A:302:GLY:O	1:A:303:VAL:C	2.51	0.53
1:B:186:GLU:CD	1:B:187:SER:HB2	2.32	0.53
1:B:287:LEU:HD12	1:B:291:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:PHE:C	1:B:181:PHE:CD2	2.87	0.53
1:B:294:ASN:HB3	1:B:297:THR:H	1.73	0.53
1:A:81:LYS:HE2	1:A:89:ARG:NH2	2.24	0.53
1:B:134:HIS:H	1:B:137:ARG:NH2	2.07	0.53
1:A:91:ASP:N	1:A:91:ASP:OD2	2.41	0.53
1:A:236:MET:HB3	1:A:256:ASP:OD1	2.09	0.53
1:A:75:GLU:OE2	1:A:83:ARG:NE	2.42	0.52
1:A:150:ILE:CD1	1:A:155:MET:HE3	2.40	0.52
1:A:197:HIS:HD2	1:A:199:ASN:N	2.03	0.52
1:B:104:THR:HG22	1:B:139:GLY:CA	2.39	0.52
1:B:110:ALA:C	1:B:114:LEU:HD22	2.35	0.52
1:B:251:PRO:HG2	1:B:253:ARG:CZ	2.38	0.52
1:B:104:THR:HG22	1:B:139:GLY:HA3	1.91	0.52
1:A:42:ALA:O	1:A:46:ILE:CD1	2.57	0.52
1:B:84:LYS:O	1:B:87:LYS:HG2	2.09	0.52
1:A:131:LYS:HD2	1:A:131:LYS:O	2.10	0.52
1:A:317:GLN:HE22	1:A:327:TYR:HB2	1.74	0.52
1:B:160:ASP:O	1:B:164:ASN:HB2	2.09	0.52
1:A:299:ARG:HG2	1:A:308:GLY:O	2.09	0.52
1:B:201:THR:HB	1:B:263:ASP:OD2	2.10	0.52
1:A:73:ILE:O	1:A:77:LEU:HD13	2.10	0.51
1:B:22:LEU:CD1	1:B:85:LEU:HD11	2.33	0.51
1:B:106:ILE:N	1:B:136:GLN:HG2	2.26	0.51
1:A:215:VAL:O	1:A:219:GLN:HG3	2.10	0.51
1:B:111:ALA:O	1:B:115:VAL:HG23	2.10	0.51
1:A:229:SER:HB3	1:A:236:MET:HG3	1.92	0.51
1:B:177:VAL:HG23	1:B:177:VAL:O	2.10	0.51
1:A:56:GLY:HA3	1:A:74:ASP:HB3	1.92	0.51
1:A:317:GLN:NE2	1:A:327:TYR:HB2	2.26	0.51
1:B:54:LYS:O	1:B:77:LEU:HD12	2.11	0.51
1:B:87:LYS:C	1:B:89:ARG:N	2.67	0.50
1:B:106:ILE:HD12	1:B:110:ALA:HB3	1.92	0.50
1:B:279:ASN:O	1:B:283:ARG:HG2	2.11	0.50
1:A:150:ILE:HG21	1:A:155:MET:HE3	1.92	0.50
1:A:27:LYS:HG2	1:A:28:ASN:OD1	2.11	0.50
1:A:125:LEU:C	1:A:127:LYS:N	2.69	0.50
1:A:122:LEU:O	1:A:126:ARG:HG3	2.12	0.50
1:A:134:HIS:HD2	1:A:138:ILE:HD11	1.73	0.50
1:A:44:SER:O	1:A:48:LYS:HG2	2.11	0.50
1:A:60:LYS:HB2	1:A:70:ALA:HB1	1.94	0.49
1:B:87:LYS:C	1:B:89:ARG:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:HG2	1:B:82:LEU:CD1	2.39	0.49
1:B:159:GLN:O	1:B:159:GLN:HG2	2.10	0.49
1:B:244:GLU:O	1:B:245:ASN:CB	2.59	0.49
1:A:177:VAL:HG11	1:A:191:MET:HE2	1.93	0.49
1:A:100:LEU:HD11	1:A:120:LYS:CA	2.39	0.49
1:A:133:ASN:C	1:A:133:ASN:ND2	2.62	0.49
1:B:159:GLN:HE21	1:B:177:VAL:HG22	1.78	0.49
1:A:82:LEU:HD12	1:A:83:ARG:N	2.28	0.49
1:B:106:ILE:HG23	1:B:110:ALA:HB3	1.94	0.49
1:B:311:LEU:N	1:B:311:LEU:HD22	2.27	0.49
1:A:287:LEU:HD23	1:A:291:PHE:O	2.13	0.49
1:B:103:VAL:C	1:B:105:GLY:H	2.19	0.49
1:B:113:LYS:HG3	1:B:114:LEU:CD1	2.43	0.49
1:B:170:ASP:OD1	1:B:171:PRO:HD2	2.12	0.49
1:B:274:GLY:O	1:B:275:SER:CB	2.60	0.49
1:B:329:GLU:HG2	1:B:331:LYS:NZ	2.28	0.49
1:B:132:LEU:HB3	1:B:136:GLN:HE22	1.76	0.48
1:B:93:THR:CG2	1:B:112:ARG:HH21	2.26	0.48
1:B:260:ILE:HG23	1:B:261:PRO:HD2	1.95	0.48
1:B:66:GLY:H	1:B:69:ILE:HD13	1.78	0.48
1:A:115:VAL:HG12	1:A:116:ASP:N	2.27	0.48
1:B:182:ARG:HD3	1:B:273:THR:OG1	2.13	0.48
1:A:298:ILE:O	1:A:311:LEU:HD23	2.14	0.47
1:B:133:ASN:HB2	1:B:134:HIS:H	1.46	0.47
1:B:269:VAL:HG23	1:B:270:LEU:N	2.28	0.47
1:A:197:HIS:CD2	1:A:199:ASN:HB2	2.49	0.47
1:B:297:THR:HB	1:B:310:PRO:HB3	1.95	0.47
1:B:26:GLU:CA	1:B:30:SER:HB3	2.43	0.47
1:B:122:LEU:HA	1:B:125:LEU:HD12	1.96	0.47
1:A:125:LEU:O	1:A:127:LYS:N	2.47	0.47
1:A:150:ILE:CG2	1:A:155:MET:HE3	2.43	0.47
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.49	0.47
1:B:243:SER:C	1:B:245:ASN:N	2.73	0.47
1:B:159:GLN:NE2	2:B:377:HOH:O	2.47	0.47
1:B:193:VAL:CG1	1:B:257:ILE:HG12	2.44	0.47
1:A:91:ASP:O	1:A:92:ASP:C	2.57	0.47
1:B:249:GLU:O	1:B:250:TYR:C	2.57	0.47
1:A:294:ASN:ND2	1:A:296:TYR:HB2	2.27	0.47
1:A:328:ARG:O	1:A:329:GLU:C	2.55	0.47
1:B:27:LYS:NZ	1:B:28:ASN:ND2	2.62	0.47
1:B:42:ALA:O	1:B:46:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:O	1:A:127:LYS:HE2	2.15	0.47
1:A:293:ILE:HG22	1:A:294:ASN:N	2.30	0.47
1:B:62:LEU:HD13	1:B:65:VAL:CG2	2.44	0.47
1:B:173:TYR:CD2	1:B:195:LEU:HD11	2.49	0.46
1:A:150:ILE:HG21	1:A:155:MET:HE2	1.97	0.46
1:B:105:GLY:O	1:B:106:ILE:O	2.33	0.46
1:A:177:VAL:HG12	2:A:386:HOH:O	2.16	0.46
1:A:180:SER:O	1:A:185:ALA:HB3	2.15	0.46
1:A:251:PRO:HG2	1:A:253:ARG:CZ	2.45	0.46
1:A:26:GLU:O	1:A:30:SER:HB2	2.16	0.46
1:B:103:VAL:C	1:B:105:GLY:N	2.74	0.46
1:B:116:ASP:C	1:B:118:GLY:H	2.23	0.46
1:A:135:HIS:CD2	1:A:228:LEU:HB3	2.51	0.46
1:B:133:ASN:CB	1:B:137:ARG:NH1	2.79	0.46
1:B:116:ASP:C	1:B:118:GLY:N	2.70	0.46
1:B:245:ASN:O	1:B:246:ASP:CG	2.59	0.46
1:A:294:ASN:ND2	1:A:297:THR:H	2.13	0.45
1:B:264:GLN:OE1	1:B:296:TYR:HB3	2.16	0.45
1:A:295:GLU:HG2	1:A:296:TYR:CD1	2.51	0.45
1:A:303:VAL:HG23	1:A:304:THR:H	1.81	0.45
1:A:49:TYR:CE2	1:A:51:HIS:HB2	2.52	0.45
1:B:267:CYS:CB	2:B:374:HOH:O	2.64	0.45
1:B:276:ASP:O	1:B:280:LYS:HG2	2.16	0.45
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.71	0.45
1:B:247:GLU:O	1:B:248:ASN:CB	2.65	0.45
1:A:206:LYS:HB2	1:A:206:LYS:NZ	2.31	0.45
1:A:268:GLY:O	1:A:272:PHE:HD1	2.00	0.45
1:B:133:ASN:HB2	1:B:137:ARG:CZ	2.47	0.45
1:B:15:ILE:HD11	1:B:77:LEU:HD21	1.98	0.45
1:B:209:LYS:O	1:B:213:ARG:HB2	2.16	0.45
1:B:313:VAL:O	1:B:313:VAL:CG2	2.65	0.45
1:A:135:HIS:HE1	1:A:236:MET:HE2	1.82	0.45
1:B:299:ARG:HA	1:B:311:LEU:HD23	1.99	0.45
1:B:150:ILE:HG21	1:B:155:MET:SD	2.57	0.45
1:B:49:TYR:HA	1:B:50:PRO:HD2	1.85	0.44
1:B:168:LYS:HB2	1:B:168:LYS:NZ	2.32	0.44
1:A:53:ILE:HG22	1:A:77:LEU:HD21	1.99	0.44
1:B:99:PHE:CZ	1:B:122:LEU:HD22	2.52	0.44
1:A:294:ASN:HB3	1:A:297:THR:O	2.17	0.44
1:A:11:LEU:HD13	1:A:51:HIS:C	2.43	0.44
1:B:26:GLU:C	1:B:30:SER:HB3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLN:O	1:A:222:ARG:NH1	2.51	0.44
1:B:299:ARG:HB2	1:B:300:PRO:CD	2.47	0.44
1:A:277:ILE:HD13	1:A:277:ILE:HA	1.81	0.43
1:B:107:GLY:O	1:B:111:ALA:CB	2.66	0.43
1:A:84:LYS:NZ	2:A:376:HOH:O	2.50	0.43
1:A:135:HIS:CG	1:A:228:LEU:HB3	2.53	0.43
1:B:87:LYS:HB2	1:B:90:GLN:NE2	2.31	0.43
1:B:311:LEU:HB3	1:B:312:PRO:HD2	2.00	0.43
1:B:147:GLU:H	1:B:147:GLU:HG2	1.70	0.43
1:A:170:ASP:HA	1:A:171:PRO:HD3	1.77	0.43
1:B:134:HIS:C	1:B:136:GLN:N	2.76	0.43
1:B:275:SER:HB3	1:B:278:PHE:CB	2.46	0.43
1:B:246:ASP:CB	1:B:249:GLU:HB3	2.47	0.43
1:B:18:MET:O	1:B:22:LEU:HD12	2.19	0.43
1:B:276:ASP:CB	2:B:372:HOH:O	2.63	0.43
1:B:125:LEU:C	1:B:127:LYS:N	2.72	0.43
1:B:269:VAL:O	1:B:270:LEU:C	2.62	0.43
1:A:169:LEU:HD21	1:A:217:GLN:HG2	2.01	0.42
1:A:264:GLN:HE21	1:A:264:GLN:HB3	1.68	0.42
1:B:133:ASN:O	1:B:135:HIS:CD2	2.72	0.42
1:A:12:ASN:ND2	1:A:53:ILE:H	1.96	0.42
1:A:68:LYS:HG3	1:A:69:ILE:HG13	2.02	0.42
1:A:254:ARG:NH2	1:A:256:ASP:OD1	2.53	0.42
1:A:68:LYS:HE3	1:A:69:ILE:HG13	2.02	0.42
1:B:208:PRO:CB	1:B:232:GLU:OE1	2.67	0.42
1:A:150:ILE:HG12	1:A:253:ARG:NE	2.35	0.42
1:B:119:ILE:CG2	1:B:125:LEU:HD23	2.35	0.42
1:B:269:VAL:HG23	1:B:270:LEU:H	1.84	0.42
1:A:106:ILE:CG1	1:A:136:GLN:HG2	2.49	0.42
1:B:221:VAL:O	1:B:221:VAL:CG1	2.68	0.42
1:A:311:LEU:N	1:A:311:LEU:HD22	2.35	0.42
1:A:84:LYS:HE2	1:A:88:ILE:HD11	2.01	0.41
1:B:69:ILE:O	1:B:73:ILE:HG13	2.19	0.41
1:B:88:ILE:HG22	1:B:88:ILE:O	2.20	0.41
1:B:111:ALA:O	1:B:115:VAL:N	2.51	0.41
1:A:21:GLU:HG3	2:A:399:HOH:O	2.20	0.41
1:B:31:GLN:HA	1:B:31:GLN:NE2	2.36	0.41
1:B:138:ILE:HG21	1:B:228:LEU:HD21	2.02	0.41
1:A:135:HIS:NE2	1:A:228:LEU:HD13	2.35	0.41
1:B:150:ILE:CG2	1:B:154:GLU:HB3	2.50	0.41
1:B:216:GLU:O	1:B:216:GLU:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:O	1:A:61:LYS:HG3	2.20	0.41
1:A:81:LYS:HE2	1:A:89:ARG:HH21	1.85	0.41
1:A:30:SER:O	1:A:31:GLN:CB	2.66	0.41
1:A:325:TRP:CD1	1:A:326:ARG:NH2	2.89	0.41
1:A:33:ILE:HD12	1:A:33:ILE:N	2.35	0.41
1:B:105:GLY:HA3	1:B:136:GLN:CA	2.43	0.41
1:B:182:ARG:C	1:B:184:GLY:H	2.29	0.41
1:B:26:GLU:HG3	1:B:39:TYR:HE1	1.85	0.41
1:B:197:HIS:CD2	1:B:199:ASN:HB2	2.56	0.41
1:A:278:PHE:CE2	1:A:333:ARG:HD3	2.55	0.41
1:B:25:PHE:CD2	1:B:25:PHE:C	2.99	0.41
1:B:209:LYS:O	1:B:209:LYS:HD3	2.21	0.41
1:B:133:ASN:CG	1:B:137:ARG:NH1	2.78	0.41
1:B:321:ASP:O	1:B:322:TYR:C	2.64	0.41
1:A:150:ILE:HD13	1:A:155:MET:HE3	2.00	0.40
1:B:19:LEU:HB3	1:B:43:ALA:HB2	2.03	0.40
1:A:53:ILE:HD12	1:A:59:ALA:HB2	2.03	0.40
1:A:150:ILE:CD1	1:A:155:MET:CE	2.99	0.40
1:A:99:PHE:O	1:A:102:ARG:HG2	2.20	0.40
1:A:329:GLU:HA	1:A:330:PRO:HD3	1.94	0.40
1:B:99:PHE:HE2	1:B:122:LEU:HB2	1.87	0.40
1:B:313:VAL:O	1:B:313:VAL:HG22	2.21	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.63	0.40
1:A:150:ILE:HG12	1:A:253:ARG:CZ	2.52	0.40
1:B:121:THR:OG1	1:B:122:LEU:N	2.54	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	323/335 (96%)	275 (85%)	36 (11%)	12 (4%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	323/335 (96%)	271 (84%)	31 (10%)	21 (6%)	1	1
All	All	646/670 (96%)	546 (84%)	67 (10%)	33 (5%)	1	2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	206	LYS
1	A	249	GLU
1	A	303	VAL
1	B	87	LYS
1	B	106	ILE
1	B	204	SER
1	B	205	SER
1	B	245	ASN
1	B	248	ASN
1	B	250	TYR
1	B	275	SER
1	A	13	GLY
1	A	95	SER
1	A	126	ARG
1	B	108	PRO
1	B	121	THR
1	B	130	ASP
1	B	133	ASN
1	B	134	HIS
1	B	206	LYS
1	B	274	GLY
1	A	94	SER
1	A	275	SER
1	A	304	THR
1	B	61	LYS
1	B	86	GLU
1	B	126	ARG
1	B	129	GLU
1	B	132	LEU
1	B	190	ASP
1	A	11	LEU
1	A	64	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	286/296 (97%)	251 (88%)	35 (12%)	5	10
1	B	286/296 (97%)	234 (82%)	52 (18%)	2	3
All	All	572/592 (97%)	485 (85%)	87 (15%)	3	5

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	35	LYS
1	A	44	SER
1	A	62	LEU
1	A	72	LYS
1	A	73	ILE
1	A	77	LEU
1	A	87	LYS
1	A	91	ASP
1	A	128	ASN
1	A	133	ASN
1	A	147	GLU
1	A	168	LYS
1	A	177	VAL
1	A	194	LEU
1	A	206	LYS
1	A	207	GLN
1	A	209	LYS
1	A	215	VAL
1	A	222	ARG
1	A	232	GLU
1	A	235	PHE
1	A	236	MET
1	A	254	ARG
1	A	257	ILE
1	A	260	ILE
1	A	262	LYS

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Mol	Chain	Res	Type
1	A	264	GLN
1	A	270	LEU
1	A	294	ASN
1	A	295	GLU
1	A	299	ARG
1	A	303	VAL
1	A	311	LEU
1	A	326	ARG
1	B	19	LEU
1	B	21	GLU
1	B	33	ILE
1	B	34	HIS
1	B	45	VAL
1	B	62	LEU
1	B	65	VAL
1	B	69	ILE
1	B	71	GLU
1	B	75	GLU
1	B	77	LEU
1	B	82	LEU
1	B	83	ARG
1	B	87	LYS
1	B	89	ARG
1	B	92	ASP
1	B	94	SER
1	B	97	ILE
1	B	106	ILE
1	B	113	LYS
1	B	114	LEU
1	B	119	ILE
1	B	133	ASN
1	B	135	HIS
1	B	136	GLN
1	B	140	LEU
1	B	147	GLU
1	B	148	LYS
1	B	154	GLU
1	B	168	LYS
1	B	169	LEU
1	B	174	ILE
1	B	186	GLU
1	B	187	SER

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Mol	Chain	Res	Type
1	B	205	SER
1	B	206	LYS
1	B	209	LYS
1	B	233	THR
1	B	260	ILE
1	B	287	LEU
1	B	288	GLU
1	B	292	THR
1	B	303	VAL
1	B	304	THR
1	B	306	VAL
1	B	313	VAL
1	B	317	GLN
1	B	324	GLN
1	B	325	TRP
1	B	329	GLU
1	B	331	LYS
1	B	334	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	98	ASN
1	A	128	ASN
1	A	133	ASN
1	A	136	GLN
1	A	197	HIS
1	A	219	GLN
1	A	248	ASN
1	A	264	GLN
1	A	294	ASN
1	A	317	GLN
1	A	324	GLN
1	B	28	ASN
1	B	31	GLN
1	B	37	ASN
1	B	134	HIS
1	B	135	HIS
1	B	136	GLN
1	B	159	GLN
1	B	197	HIS

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Mol	Chain	Res	Type
1	B	199	ASN
1	B	240	GLN
1	B	252	HIS
1	B	264	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	325/335 (97%)	-0.01	6 (1%) 67 64	13, 30, 70, 92	0
1	B	325/335 (97%)	0.26	12 (3%) 45 40	24, 42, 93, 105	0
All	All	650/670 (97%)	0.12	18 (2%) 55 50	13, 38, 86, 105	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ASP	4.5
1	A	247	GLU	3.9
1	B	248	ASN	3.7
1	A	248	ASN	3.6
1	B	119	ILE	3.3
1	B	132	LEU	2.9
1	B	107	GLY	2.7
1	B	114	LEU	2.6
1	B	32	ALA	2.6
1	A	245	ASN	2.5
1	B	69	ILE	2.2
1	B	94	SER	2.2
1	A	70	ALA	2.2
1	B	125	LEU	2.1
1	B	106	ILE	2.1
1	B	138	ILE	2.1
1	B	109	SER	2.1
1	A	34	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.