



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:19 PM UTC

PDB ID : 4EVA / pdb_00004eva
Title : Crystal Structure of Mouse Catenin beta-59 in 5.6M urea
Authors : Wang, C.; Zhang, G.Y.
Deposited on : 2012-04-26
Resolution : 2.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

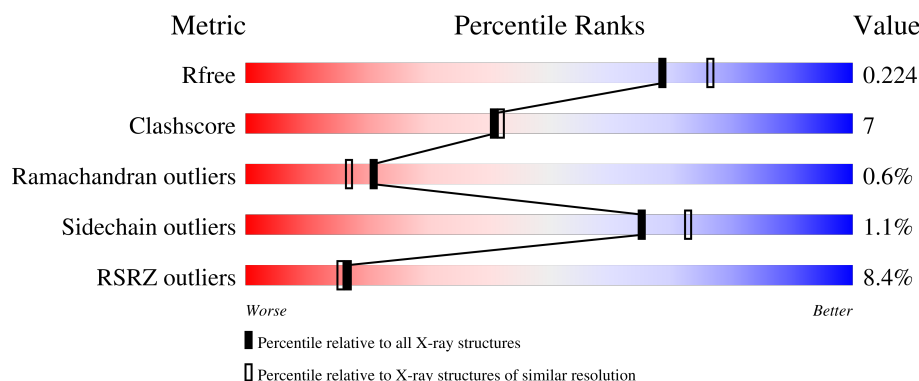
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	538	
1	C	538	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URE	A	726	-	-	X	-
2	URE	A	732	-	-	X	-
2	URE	A	737	-	-	X	-
2	URE	C	706	-	-	X	-
2	URE	C	710	-	-	X	-
2	URE	C	717	-	-	X	-
2	URE	C	730	-	-	X	-

2 Entry composition [i](#)

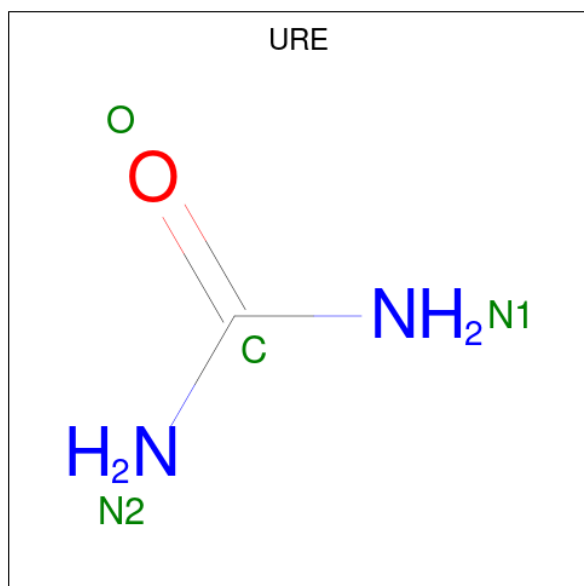
There are 3 unique types of molecules in this entry. The entry contains 8423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3738	2346	682	684	26			
1	C	488	Total	C	N	O	S	0	0	0
			3717	2335	678	678	26			

- Molecule 2 is UREA (CCD ID: URE) (formula: CH₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	A	1	Total	C	N	O	0	0
			4	1	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 4	C 1	N 2	O 1	1	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	1	0
2	A	1	Total 4	C 1	N 2	O 1	1	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	1	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0
2	C	1	Total 4	C 1	N 2	O 1	0	0

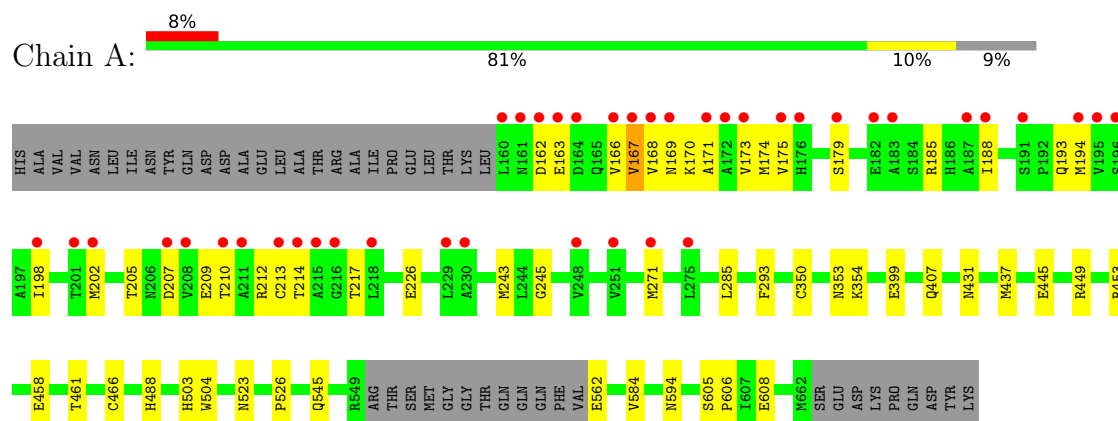
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	400	Total 400	O 400	0	0
3	C	280	Total 280	O 280	0	0

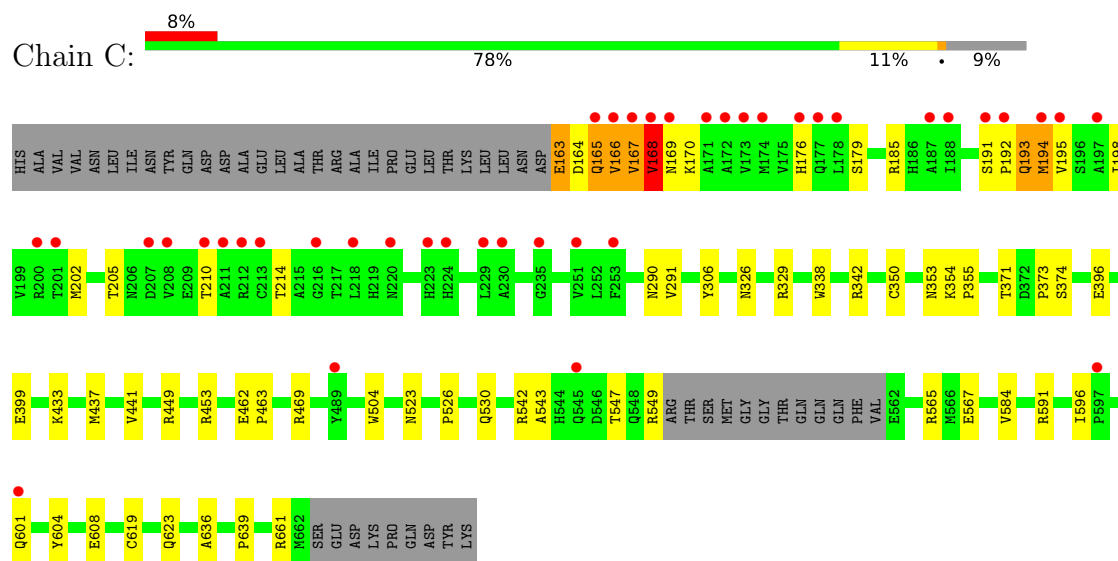
3 Residue-property plots

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: Catenin beta-1



• Molecule 1: Catenin beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.27Å 102.72Å 187.56Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	28.61 – 2.00 28.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	85.8 (28.61-2.00) 60.1 (28.61-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.200 , 0.228 (Not available) , 0.224	Depositor DCC
R_{free} test set	3543 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.397 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8423	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 5.58% 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](#)

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

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	0.31	0/3790	0.71	0/5142
1	C	0.33	0/3769	0.76	2/5113 (0.0%)
All	All	0.32	0/7559	0.73	2/10255 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	VAL	N-CA-C	10.81	121.65	110.62
1	C	166	VAL	CB-CA-C	-5.36	103.86	112.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3738	0	3872	44	0
1	C	3717	0	3860	56	0
2	A	152	0	152	11	0
2	C	136	0	136	15	0
3	A	400	0	0	9	0
3	C	280	0	0	5	0
All	All	8423	0	8020	103	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 7.

All (103) 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:C:371:THR:OG1	3:C:1019:HOH:O	1.82	0.98
1:C:168:VAL:HG13	1:C:170:LYS:H	1.31	0.95
1:C:168:VAL:HG13	1:C:169:ASN:N	1.91	0.85
1:C:165:GLN:OE1	1:C:167:VAL:HB	1.81	0.80
1:A:584:VAL:H	2:A:732:URE:HN12	1.31	0.76
1:C:608:GLU:HG3	2:C:730:URE:HN22	1.52	0.75
1:A:608:GLU:HG3	2:A:737:URE:HN22	1.50	0.74
1:A:594:ASN:OD1	3:A:924:HOH:O	2.06	0.73
1:A:169:ASN:O	1:A:173:VAL:HG23	1.89	0.73
1:A:466:CYS:SG	3:A:1160:HOH:O	2.46	0.72
1:C:542:ARG:HG2	2:C:720:URE:HN21	1.53	0.72
1:A:245:GLY:HA2	2:A:709:URE:HN12	1.57	0.70
1:A:167:VAL:O	1:A:167:VAL:HG12	1.92	0.69
1:C:163:GLU:O	2:C:710:URE:N1	2.28	0.66
2:A:733:URE:HN21	2:A:734:URE:HN22	1.44	0.65
1:A:205:THR:HG22	1:A:207:ASP:H	1.61	0.65
1:A:179:SER:O	1:A:185:ARG:NE	2.29	0.64
1:A:163:GLU:N	1:A:163:GLU:OE1	2.30	0.64
1:A:504:TRP:H	2:A:726:URE:HN22	1.48	0.60
1:C:202:MET:HB2	1:C:214:THR:HG21	1.83	0.60
1:A:166:VAL:O	1:A:167:VAL:HB	2.00	0.59
1:A:168:VAL:HG12	1:A:170:LYS:H	1.67	0.59
1:C:168:VAL:CG1	1:C:170:LYS:H	2.11	0.59
1:A:445:GLU:OE1	3:A:1043:HOH:O	2.17	0.59
1:A:545:GLN:NE2	3:A:938:HOH:O	2.36	0.59
1:C:163:GLU:O	2:C:710:URE:C	2.51	0.58
1:C:591:ARG:NH1	3:C:1050:HOH:O	2.21	0.58
1:A:354:LYS:NZ	3:A:926:HOH:O	2.36	0.58
2:A:717:URE:HN22	2:C:701:URE:HN22	1.51	0.58
1:C:168:VAL:HG13	1:C:170:LYS:N	2.13	0.57
1:A:210:THR:O	1:A:214:THR:OG1	2.19	0.57
1:C:166:VAL:HG13	1:C:167:VAL:N	2.20	0.57
1:A:175:VAL:HG11	1:A:198:ILE:HD11	1.86	0.56
1:C:399:GLU:HG3	1:C:437:MET:SD	2.45	0.56
1:A:488:HIS:HE1	3:A:1141:HOH:O	1.88	0.56
1:C:530:GLN:OE1	2:C:719:URE:N2	2.39	0.56
1:C:549:ARG:HB2	2:C:726:URE:HN11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:VAL:HG13	2:C:718:URE:HN21	1.71	0.55
1:C:291:VAL:H	2:C:706:URE:HN12	1.54	0.55
1:C:166:VAL:CG1	1:C:167:VAL:N	2.71	0.54
1:A:213:CYS:O	1:A:217:THR:OG1	2.25	0.54
1:C:176:HIS:O	1:C:179:SER:OG	2.24	0.54
1:C:601:GLN:NE2	3:C:868:HOH:O	2.32	0.53
1:A:503:HIS:HA	2:A:726:URE:HN12	1.74	0.52
2:A:729:URE:N1	3:A:1143:HOH:O	2.34	0.52
1:A:608:GLU:H	2:A:737:URE:HN12	1.59	0.51
1:C:396:GLU:OE1	1:C:433:LYS:NZ	2.44	0.51
1:C:604:TYR:CZ	1:C:639:PRO:HG3	2.46	0.50
1:A:202:MET:HG2	1:A:243:MET:SD	2.52	0.50
1:A:169:ASN:O	1:A:173:VAL:CG2	2.58	0.50
1:A:167:VAL:O	1:A:167:VAL:CG1	2.58	0.50
1:C:191:SER:C	1:C:193:GLN:H	2.20	0.49
1:C:164:ASP:O	1:C:164:ASP:OD1	2.30	0.49
1:C:591:ARG:HG3	1:C:596:ILE:HD13	1.95	0.49
1:A:399:GLU:HG3	1:A:437:MET:SD	2.52	0.49
1:C:290:ASN:HA	2:C:706:URE:HN12	1.78	0.49
1:A:175:VAL:HG12	1:A:217:THR:HG21	1.94	0.48
1:A:171:ALA:O	1:A:175:VAL:HG23	2.13	0.48
1:C:469:ARG:NH1	3:C:841:HOH:O	2.46	0.48
1:A:194:MET:HB2	1:A:194:MET:HE3	1.68	0.48
1:C:374:SER:HA	2:C:717:URE:HN21	1.79	0.48
1:A:163:GLU:H	1:A:163:GLU:CD	2.22	0.48
1:A:584:VAL:N	2:A:732:URE:HN12	2.07	0.48
1:A:170:LYS:O	1:A:174:MET:HG3	2.15	0.47
1:C:202:MET:HB2	1:C:214:THR:CG2	2.44	0.47
1:C:373:PRO:O	2:C:717:URE:N2	2.47	0.47
1:A:449:ARG:HH11	1:A:453:ARG:HD3	1.80	0.46
1:C:504:TRP:H	2:C:721:URE:HN22	1.61	0.46
1:A:350:CYS:HB3	1:A:353:ASN:HB2	1.98	0.46
1:A:243:MET:HA	1:A:243:MET:HE2	1.97	0.46
1:C:168:VAL:HG22	1:C:169:ASN:H	1.80	0.46
1:C:164:ASP:OD1	1:C:164:ASP:C	2.58	0.46
1:A:271:MET:HE1	3:A:1044:HOH:O	2.15	0.45
1:C:449:ARG:HH11	1:C:453:ARG:HD3	1.81	0.45
1:C:179:SER:O	1:C:185:ARG:NE	2.50	0.44
1:C:306:TYR:O	3:C:869:HOH:O	2.21	0.44
1:C:636:ALA:C	1:C:639:PRO:HD2	2.43	0.43
1:A:285:LEU:HD13	1:A:293:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:TRP:CE2	1:C:342:ARG:HD2	2.54	0.43
1:A:445:GLU:OE2	3:A:1054:HOH:O	2.22	0.43
1:C:165:GLN:H	1:C:165:GLN:HG3	1.39	0.42
1:C:194:MET:HE3	1:C:194:MET:HB2	1.72	0.42
1:C:350:CYS:HB3	1:C:353:ASN:HB2	2.01	0.42
1:A:209:GLU:OE1	1:A:212:ARG:NE	2.52	0.42
1:C:326:ASN:OD1	1:C:329:ARG:NH2	2.52	0.42
1:C:623:GLN:HB3	1:C:661:ARG:NH1	2.34	0.42
1:C:462:GLU:HB3	1:C:463:PRO:HD3	2.02	0.42
1:A:605:SER:HA	1:A:606:PRO:HD3	1.91	0.42
1:C:584:VAL:HG23	2:C:729:URE:HN21	1.84	0.42
1:C:619:CYS:O	1:C:661:ARG:NH1	2.52	0.42
1:C:523:ASN:C	1:C:526:PRO:HD2	2.45	0.41
1:C:604:TYR:OH	1:C:639:PRO:HG3	2.21	0.41
1:C:194:MET:O	1:C:198:ILE:HG13	2.20	0.41
1:C:205:THR:HG21	1:C:210:THR:HG23	2.01	0.41
1:A:431:ASN:HD21	2:A:716:URE:HN21	1.68	0.41
1:C:354:LYS:HB3	1:C:355:PRO:HD3	2.03	0.41
1:C:565:ARG:HB3	1:C:567:GLU:OE1	2.21	0.41
1:A:523:ASN:C	1:A:526:PRO:HD2	2.46	0.41
1:C:543:ALA:O	1:C:547:THR:HG23	2.21	0.41
1:A:458:GLU:HA	1:A:461:THR:OG1	2.21	0.40
1:A:163:GLU:N	1:A:163:GLU:CD	2.79	0.40
1:C:191:SER:O	1:C:193:GLN:N	2.55	0.40
1:C:608:GLU:H	2:C:730:URE:HN12	1.69	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	487/538 (90%)	481 (99%)	3 (1%)	3 (1%)	21 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	484/538 (90%)	475 (98%)	6 (1%)	3 (1%)	21	17
All	All	971/1076 (90%)	956 (98%)	9 (1%)	6 (1%)	21	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	VAL
1	A	162	ASP
1	A	193	GLN
1	C	193	GLN
1	C	192	PRO
1	C	168	VAL

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	405/447 (91%)	401 (99%)	4 (1%)	68	75
1	C	403/447 (90%)	398 (99%)	5 (1%)	63	70
All	All	808/894 (90%)	799 (99%)	9 (1%)	65	73

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ILE
1	A	226	GLU
1	A	407	GLN
1	A	562	GLU
1	C	163	GLU
1	C	165	GLN
1	C	168	VAL
1	C	194	MET
1	C	195	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	HIS
1	A	379	GLN
1	A	585	HIS
1	C	186	HIS
1	C	220	ASN
1	C	224	HIS
1	C	516	ASN

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](#)

72 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	URE	C	708	-	3,3,3	1.28	1 (33%)	3,3,3	0.81	0
2	URE	A	717	-	3,3,3	1.29	1 (33%)	3,3,3	0.90	0
2	URE	C	711	-	3,3,3	1.31	1 (33%)	3,3,3	0.83	0
2	URE	A	711	-	3,3,3	1.28	1 (33%)	3,3,3	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	URE	C	709	-	3,3,3	1.28	1 (33%)	3,3,3	0.82	0
2	URE	A	737	-	3,3,3	1.29	1 (33%)	3,3,3	0.86	0
2	URE	C	720	-	3,3,3	1.29	1 (33%)	3,3,3	0.73	0
2	URE	A	707	-	3,3,3	1.29	1 (33%)	3,3,3	0.81	0
2	URE	C	733	-	3,3,3	1.29	1 (33%)	3,3,3	0.76	0
2	URE	A	723	-	3,3,3	1.28	1 (33%)	3,3,3	0.76	0
2	URE	C	714	-	3,3,3	1.30	1 (33%)	3,3,3	0.79	0
2	URE	A	710	-	3,3,3	1.29	1 (33%)	3,3,3	0.83	0
2	URE	C	710	-	3,3,3	1.24	1 (33%)	3,3,3	0.80	0
2	URE	A	704	-	3,3,3	1.29	1 (33%)	3,3,3	0.81	0
2	URE	A	720	-	3,3,3	1.30	1 (33%)	3,3,3	0.82	0
2	URE	C	726	-	3,3,3	1.29	1 (33%)	3,3,3	0.74	0
2	URE	A	736	-	3,3,3	1.28	1 (33%)	3,3,3	0.78	0
2	URE	A	705	-	3,3,3	1.30	1 (33%)	3,3,3	0.80	0
2	URE	A	702	-	3,3,3	1.28	1 (33%)	3,3,3	0.82	0
2	URE	C	707	-	3,3,3	1.27	0	3,3,3	0.83	0
2	URE	A	714	-	3,3,3	1.29	1 (33%)	3,3,3	0.80	0
2	URE	C	727	-	3,3,3	1.28	1 (33%)	3,3,3	0.77	0
2	URE	C	724	-	3,3,3	1.29	1 (33%)	3,3,3	0.82	0
2	URE	C	731	-	3,3,3	1.28	1 (33%)	3,3,3	0.80	0
2	URE	C	716	-	3,3,3	1.28	1 (33%)	3,3,3	0.83	0
2	URE	A	706	-	3,3,3	1.28	1 (33%)	3,3,3	0.81	0
2	URE	C	718	-	3,3,3	1.29	1 (33%)	3,3,3	0.76	0
2	URE	C	729	-	3,3,3	1.30	1 (33%)	3,3,3	0.78	0
2	URE	C	706	-	3,3,3	1.29	1 (33%)	3,3,3	0.80	0
2	URE	A	701	-	3,3,3	1.30	1 (33%)	3,3,3	0.87	0
2	URE	A	734	-	3,3,3	1.30	1 (33%)	3,3,3	0.86	0
2	URE	A	730	-	3,3,3	1.26	1 (33%)	3,3,3	0.78	0
2	URE	C	705	-	3,3,3	1.30	1 (33%)	3,3,3	0.84	0
2	URE	C	721	-	3,3,3	1.29	1 (33%)	3,3,3	0.84	0
2	URE	C	725	-	3,3,3	1.29	1 (33%)	3,3,3	0.82	0
2	URE	A	728	-	3,3,3	1.30	1 (33%)	3,3,3	0.81	0
2	URE	C	704	-	3,3,3	1.29	1 (33%)	3,3,3	0.79	0
2	URE	A	715	-	3,3,3	1.28	1 (33%)	3,3,3	0.83	0
2	URE	C	712	-	3,3,3	1.30	1 (33%)	3,3,3	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	URE	A	721	-	3,3,3	1.31	1 (33%)	3,3,3	0.84	0
2	URE	C	715	-	3,3,3	1.29	1 (33%)	3,3,3	0.82	0
2	URE	C	719	-	3,3,3	1.30	1 (33%)	3,3,3	0.84	0
2	URE	C	728	-	3,3,3	1.29	1 (33%)	3,3,3	0.87	0
2	URE	C	734	-	3,3,3	1.29	1 (33%)	3,3,3	0.84	0
2	URE	C	723	-	3,3,3	1.28	1 (33%)	3,3,3	0.80	0
2	URE	C	730	-	3,3,3	1.29	1 (33%)	3,3,3	0.82	0
2	URE	A	732	-	3,3,3	1.30	1 (33%)	3,3,3	0.86	0
2	URE	C	732	-	3,3,3	1.27	0	3,3,3	0.80	0
2	URE	A	716	-	3,3,3	1.29	1 (33%)	3,3,3	0.84	0
2	URE	C	717	-	3,3,3	1.29	1 (33%)	3,3,3	0.78	0
2	URE	A	719	-	3,3,3	1.29	1 (33%)	3,3,3	0.80	0
2	URE	A	722	-	3,3,3	1.30	1 (33%)	3,3,3	0.86	0
2	URE	A	733	-	3,3,3	1.28	1 (33%)	3,3,3	0.79	0
2	URE	A	729	-	3,3,3	1.27	1 (33%)	3,3,3	0.79	0
2	URE	A	726	-	3,3,3	1.28	1 (33%)	3,3,3	0.85	0
2	URE	C	701	-	3,3,3	1.31	1 (33%)	3,3,3	0.79	0
2	URE	A	727	-	3,3,3	1.27	1 (33%)	3,3,3	0.83	0
2	URE	A	724	-	3,3,3	1.30	1 (33%)	3,3,3	0.73	0
2	URE	A	731	-	3,3,3	1.30	1 (33%)	3,3,3	0.89	0
2	URE	A	738	-	3,3,3	1.29	1 (33%)	3,3,3	0.83	0
2	URE	C	722	-	3,3,3	1.30	1 (33%)	3,3,3	0.80	0
2	URE	A	713	-	3,3,3	1.28	1 (33%)	3,3,3	0.82	0
2	URE	C	713	-	3,3,3	1.28	1 (33%)	3,3,3	0.82	0
2	URE	C	703	-	3,3,3	1.29	1 (33%)	3,3,3	0.79	0
2	URE	A	703	-	3,3,3	1.29	1 (33%)	3,3,3	0.81	0
2	URE	A	718	-	3,3,3	1.29	1 (33%)	3,3,3	0.80	0
2	URE	A	708	-	3,3,3	1.29	1 (33%)	3,3,3	0.79	0
2	URE	A	709	-	3,3,3	1.29	1 (33%)	3,3,3	0.81	0
2	URE	A	725	-	3,3,3	1.27	0	3,3,3	0.84	0
2	URE	A	735	-	3,3,3	1.28	1 (33%)	3,3,3	0.79	0
2	URE	C	702	-	3,3,3	1.28	1 (33%)	3,3,3	0.85	0
2	URE	A	712	-	3,3,3	1.29	1 (33%)	3,3,3	0.82	0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	731	URE	O-C	-2.06	1.18	1.26
2	A	720	URE	O-C	-2.06	1.18	1.26
2	A	721	URE	O-C	-2.06	1.18	1.26
2	A	705	URE	O-C	-2.06	1.18	1.26
2	C	701	URE	O-C	-2.05	1.18	1.26
2	A	717	URE	O-C	-2.05	1.18	1.26
2	A	722	URE	O-C	-2.05	1.18	1.26
2	C	711	URE	O-C	-2.05	1.18	1.26
2	C	719	URE	O-C	-2.05	1.18	1.26
2	C	722	URE	O-C	-2.05	1.18	1.26
2	A	703	URE	O-C	-2.05	1.18	1.26
2	A	716	URE	O-C	-2.05	1.18	1.26
2	A	708	URE	O-C	-2.05	1.18	1.26
2	C	729	URE	O-C	-2.04	1.18	1.26
2	A	710	URE	O-C	-2.04	1.18	1.26
2	A	732	URE	O-C	-2.04	1.18	1.26
2	A	734	URE	O-C	-2.04	1.18	1.26
2	C	717	URE	O-C	-2.04	1.18	1.26
2	C	705	URE	O-C	-2.04	1.18	1.26
2	C	714	URE	O-C	-2.04	1.18	1.26
2	C	712	URE	O-C	-2.04	1.18	1.26
2	C	734	URE	O-C	-2.04	1.18	1.26
2	C	728	URE	O-C	-2.04	1.18	1.26
2	C	725	URE	O-C	-2.04	1.18	1.26
2	C	724	URE	O-C	-2.03	1.18	1.26
2	A	719	URE	O-C	-2.03	1.18	1.26
2	C	718	URE	O-C	-2.03	1.18	1.26
2	C	730	URE	O-C	-2.03	1.18	1.26
2	A	701	URE	O-C	-2.03	1.18	1.26
2	A	737	URE	O-C	-2.03	1.18	1.26
2	C	720	URE	O-C	-2.03	1.18	1.26
2	A	724	URE	O-C	-2.03	1.18	1.26
2	C	726	URE	O-C	-2.03	1.18	1.26
2	C	703	URE	O-C	-2.03	1.18	1.26
2	C	721	URE	O-C	-2.03	1.18	1.26
2	A	707	URE	O-C	-2.03	1.18	1.26
2	A	728	URE	O-C	-2.03	1.18	1.26
2	A	735	URE	O-C	-2.03	1.18	1.26
2	A	718	URE	O-C	-2.03	1.18	1.26
2	C	708	URE	O-C	-2.03	1.18	1.26
2	A	712	URE	O-C	-2.03	1.18	1.26
2	A	704	URE	O-C	-2.03	1.19	1.26
2	C	702	URE	O-C	-2.02	1.19	1.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	713	URE	O-C	-2.02	1.19	1.26
2	A	709	URE	O-C	-2.02	1.19	1.26
2	C	704	URE	O-C	-2.02	1.19	1.26
2	A	706	URE	O-C	-2.02	1.19	1.26
2	C	715	URE	O-C	-2.02	1.19	1.26
2	A	738	URE	O-C	-2.02	1.19	1.26
2	C	733	URE	O-C	-2.02	1.19	1.26
2	C	706	URE	O-C	-2.02	1.19	1.26
2	C	731	URE	O-C	-2.02	1.19	1.26
2	C	727	URE	O-C	-2.02	1.19	1.26
2	C	723	URE	O-C	-2.02	1.19	1.26
2	C	709	URE	O-C	-2.02	1.19	1.26
2	A	714	URE	O-C	-2.02	1.19	1.26
2	A	723	URE	O-C	-2.02	1.19	1.26
2	A	726	URE	O-C	-2.01	1.19	1.26
2	A	729	URE	O-C	-2.01	1.19	1.26
2	A	736	URE	O-C	-2.01	1.19	1.26
2	A	727	URE	O-C	-2.01	1.19	1.26
2	C	716	URE	O-C	-2.01	1.19	1.26
2	A	733	URE	O-C	-2.01	1.19	1.26
2	A	711	URE	O-C	-2.01	1.19	1.26
2	A	715	URE	O-C	-2.01	1.19	1.26
2	A	702	URE	O-C	-2.01	1.19	1.26
2	A	713	URE	O-C	-2.00	1.19	1.26
2	C	710	URE	O-C	-2.00	1.19	1.26
2	A	730	URE	O-C	-2.00	1.19	1.26

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	717	URE	1	0
2	A	737	URE	2	0
2	C	720	URE	1	0
2	C	710	URE	2	0
2	C	726	URE	1	0
2	C	718	URE	1	0
2	C	729	URE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	706	URE	2	0
2	A	734	URE	1	0
2	C	721	URE	1	0
2	C	719	URE	1	0
2	C	730	URE	2	0
2	A	732	URE	2	0
2	A	716	URE	1	0
2	C	717	URE	2	0
2	A	733	URE	1	0
2	A	729	URE	1	0
2	A	726	URE	2	0
2	C	701	URE	1	0
2	A	709	URE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	491/538 (91%)	0.22	41 (8%)	17 15	16, 29, 98, 115	1 (0%)
1	C	488/538 (90%)	0.30	41 (8%)	17 15	23, 36, 103, 116	2 (0%)
All	All	979/1076 (90%)	0.26	82 (8%)	17 15	16, 33, 101, 116	3 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ASP	5.9
1	C	216	GLY	5.5
1	A	183	ALA	5.0
1	A	171	ALA	5.0
1	A	166	VAL	5.0
1	A	191	SER	4.3
1	C	195	VAL	4.3
1	A	216	GLY	4.3
1	C	188	ILE	4.1
1	A	213	CYS	4.0
1	A	208	VAL	3.8
1	C	166	VAL	3.7
1	A	172	ALA	3.7
1	C	201	THR	3.6
1	A	160	LEU	3.5
1	A	207	ASP	3.5
1	C	178	LEU	3.4
1	C	235	GLY	3.4
1	C	172	ALA	3.4
1	A	173	VAL	3.3
1	C	171	ALA	3.3
1	A	182	GLU	3.3
1	A	167	VAL	3.2
1	A	161	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	197	ALA	3.2
1	C	165	GLN	3.2
1	C	211	ALA	3.1
1	C	173	VAL	3.1
1	A	248	VAL	3.0
1	C	169	ASN	3.0
1	A	187	ALA	3.0
1	C	168	VAL	3.0
1	C	191	SER	3.0
1	A	194	MET	3.0
1	A	229	LEU	2.9
1	C	213	CYS	2.8
1	C	210	THR	2.8
1	C	194	MET	2.7
1	A	215	ALA	2.7
1	A	251	VAL	2.7
1	A	218	LEU	2.7
1	A	211	ALA	2.7
1	A	202	MET	2.6
1	A	188	ILE	2.6
1	A	169	ASN	2.6
1	A	214	THR	2.5
1	A	163	GLU	2.5
1	C	174	MET	2.5
1	A	210	THR	2.5
1	A	176	HIS	2.5
1	C	177	GLN	2.5
1	C	545	GLN	2.5
1	C	253	PHE	2.5
1	C	207	ASP	2.4
1	C	208	VAL	2.4
1	C	223	HIS	2.4
1	C	220	ASN	2.4
1	C	167	VAL	2.4
1	C	200	ARG	2.4
1	A	168	VAL	2.3
1	A	175	VAL	2.3
1	A	201	THR	2.3
1	A	230	ALA	2.3
1	C	251	VAL	2.3
1	C	229	LEU	2.2
1	A	196	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	597	PRO	2.2
1	C	230	ALA	2.2
1	C	218	LEU	2.2
1	C	212	ARG	2.2
1	A	162	ASP	2.2
1	C	192	PRO	2.1
1	C	601	GLN	2.1
1	A	271	MET	2.1
1	C	489	TYR	2.1
1	A	198	ILE	2.1
1	A	195	VAL	2.1
1	C	187	ALA	2.1
1	C	224	HIS	2.1
1	A	179	SER	2.0
1	A	275	LEU	2.0
1	C	176	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](#)

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	URE	A	718	4/4	0.51	0.11	61,66,66,68	3
2	URE	C	710	4/4	0.55	0.14	102,103,107,112	0
2	URE	C	726	4/4	0.62	0.12	71,72,75,77	3
2	URE	C	732	4/4	0.64	0.15	60,65,66,68	1
2	URE	A	734	4/4	0.71	0.23	51,55,58,58	2
2	URE	C	701	4/4	0.75	0.15	53,57,57,60	4
2	URE	C	722	4/4	0.76	0.17	67,70,71,71	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	URE	A	712	4/4	0.78	0.21	68,71,72,78	2
2	URE	A	725	4/4	0.78	0.15	46,48,48,48	2
2	URE	C	733	4/4	0.78	0.15	59,64,65,68	3
2	URE	C	712	4/4	0.80	0.15	86,91,92,97	2
2	URE	C	714	4/4	0.80	0.16	58,60,62,62	4
2	URE	A	717	4/4	0.82	0.10	49,52,52,55	2
2	URE	A	713	4/4	0.82	0.13	60,63,63,64	3
2	URE	C	734	4/4	0.82	0.12	66,69,70,71	2
2	URE	A	719	4/4	0.83	0.14	48,50,50,53	3
2	URE	C	711	4/4	0.83	0.15	78,81,86,89	2
2	URE	A	730	4/4	0.83	0.14	45,50,53,54	1
2	URE	C	729	4/4	0.84	0.16	61,62,65,66	3
2	URE	C	725	4/4	0.84	0.08	86,93,94,96	0
2	URE	C	731	4/4	0.85	0.19	48,50,53,56	4
2	URE	C	708	4/4	0.85	0.12	56,56,57,59	3
2	URE	C	702	4/4	0.85	0.13	49,50,50,50	1
2	URE	C	723	4/4	0.85	0.14	59,62,65,72	2
2	URE	A	733	4/4	0.86	0.11	50,56,57,60	1
2	URE	A	732	4/4	0.86	0.15	45,46,49,58	3
2	URE	A	715	4/4	0.87	0.10	55,57,59,61	3
2	URE	A	716	4/4	0.87	0.11	47,49,50,52	3
2	URE	C	717	4/4	0.88	0.15	54,61,62,68	3
2	URE	C	720	4/4	0.88	0.09	53,59,62,64	2
2	URE	C	721	4/4	0.88	0.13	55,57,60,63	4
2	URE	A	726	4/4	0.88	0.10	48,52,54,54	1
2	URE	C	713	4/4	0.88	0.16	59,61,65,74	2
2	URE	A	711	4/4	0.88	0.10	48,48,49,53	2
2	URE	C	718	4/4	0.89	0.16	57,61,63,64	4
2	URE	A	721	4/4	0.89	0.13	63,68,69,76	3
2	URE	A	723	4/4	0.89	0.11	44,46,46,46	3
2	URE	A	736	4/4	0.89	0.11	63,64,64,65	3
2	URE	C	724	4/4	0.90	0.14	52,56,57,58	3
2	URE	A	705	4/4	0.90	0.11	34,36,37,37	1
2	URE	A	722	4/4	0.90	0.11	55,59,60,62	3
2	URE	C	715	4/4	0.90	0.12	52,53,54,58	3
2	URE	C	706	4/4	0.91	0.12	36,39,39,40	1
2	URE	C	727	4/4	0.91	0.12	51,53,55,57	2
2	URE	A	727	4/4	0.91	0.09	45,49,49,50	4
2	URE	A	724	4/4	0.91	0.14	45,50,55,59	2
2	URE	C	716	4/4	0.91	0.09	51,55,57,61	2
2	URE	A	720	4/4	0.91	0.16	54,56,57,61	4
2	URE	A	707	4/4	0.91	0.11	47,48,52,54	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	URE	A	729	4/4	0.92	0.09	47,49,51,52	1
2	URE	A	703	4/4	0.92	0.14	40,46,47,49	1
2	URE	C	705	4/4	0.92	0.07	33,33,34,37	2
2	URE	A	728	4/4	0.93	0.15	41,43,46,46	2
2	URE	C	730	4/4	0.93	0.13	58,61,63,67	4
2	URE	A	737	4/4	0.93	0.10	45,49,50,58	3
2	URE	A	714	4/4	0.94	0.11	46,47,47,47	4
2	URE	A	731	4/4	0.94	0.12	51,52,53,54	4
2	URE	A	702	4/4	0.94	0.08	32,33,33,34	1
2	URE	A	709	4/4	0.94	0.07	59,59,61,64	3
2	URE	A	710	4/4	0.94	0.11	53,55,57,65	3
2	URE	C	709	4/4	0.95	0.10	40,42,44,45	1
2	URE	C	703	4/4	0.95	0.10	33,34,35,36	1
2	URE	C	704	4/4	0.95	0.08	48,54,55,62	3
2	URE	A	738	4/4	0.95	0.10	49,53,53,61	3
2	URE	A	701	4/4	0.95	0.07	26,29,31,31	1
2	URE	A	735	4/4	0.95	0.09	50,51,52,52	2
2	URE	A	706	4/4	0.96	0.10	36,38,39,41	1
2	URE	A	704	4/4	0.96	0.08	32,32,35,35	1
2	URE	C	719	4/4	0.96	0.08	38,38,38,38	2
2	URE	C	728	4/4	0.96	0.11	46,50,52,53	3
2	URE	C	707	4/4	0.96	0.09	41,43,43,44	1
2	URE	A	708	4/4	0.97	0.09	35,35,37,39	2

6.5 Other polymers [i](#)

There are no such residues in this entry.