



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 5K1C / pdb_00005k1c
Title : Crystal structure of the UAF1/WDR20/USP12 complex
Authors : Li, H.; D'Andrea, A.D.; Zheng, N.
Deposited on : 2016-05-18
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
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

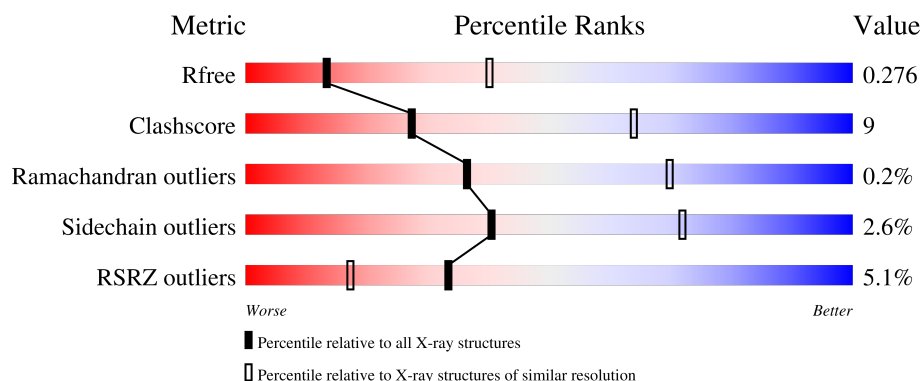
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	2672 (3.00-3.00)
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	355	7% 66% 17% • 15%
2	B	563	3% 76% 13% •• 9%
3	C	569	3% 56% 13% • 28%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9633 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 Ubiquitin carboxyl-terminal hydrolase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2374	1510	398	452	14			

- Molecule 2 is a protein called WD repeat-containing protein 48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	515	Total	C	N	O	S	0	0	0
			4001	2521	698	761	21			

- Molecule 3 is a protein called WD repeat-containing protein 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	407	Total	C	N	O	S	0	0	0
			3166	2019	540	589	18			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

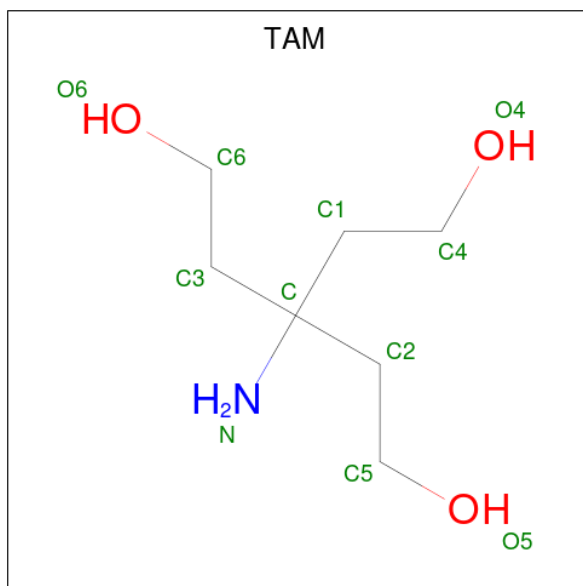
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			11	7	1	3		

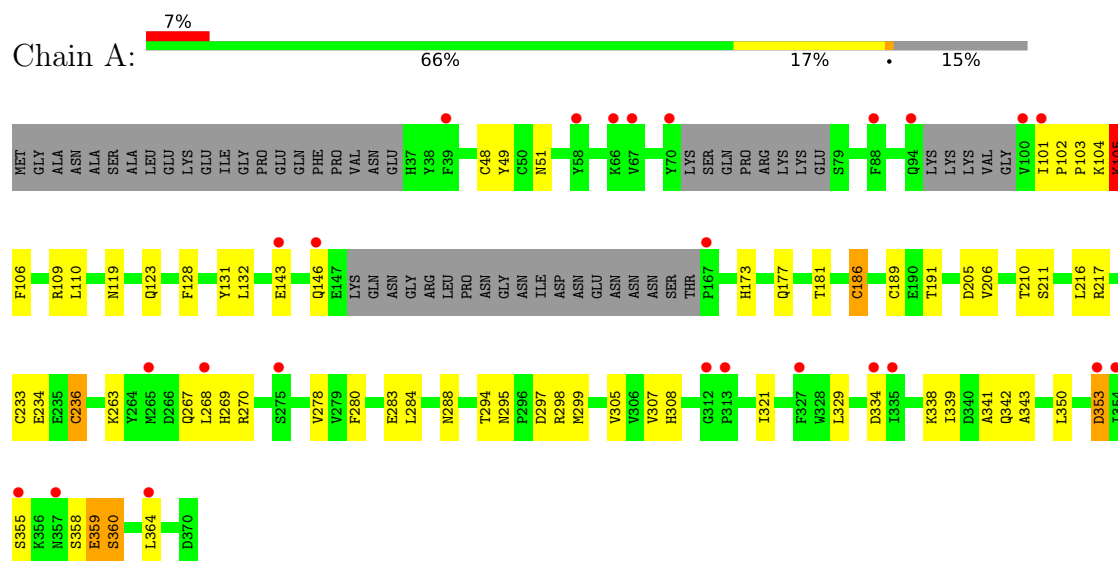
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total 6	O 6	0	0
7	B	42	Total 42	O 42	0	0
7	C	27	Total 27	O 27	0	0

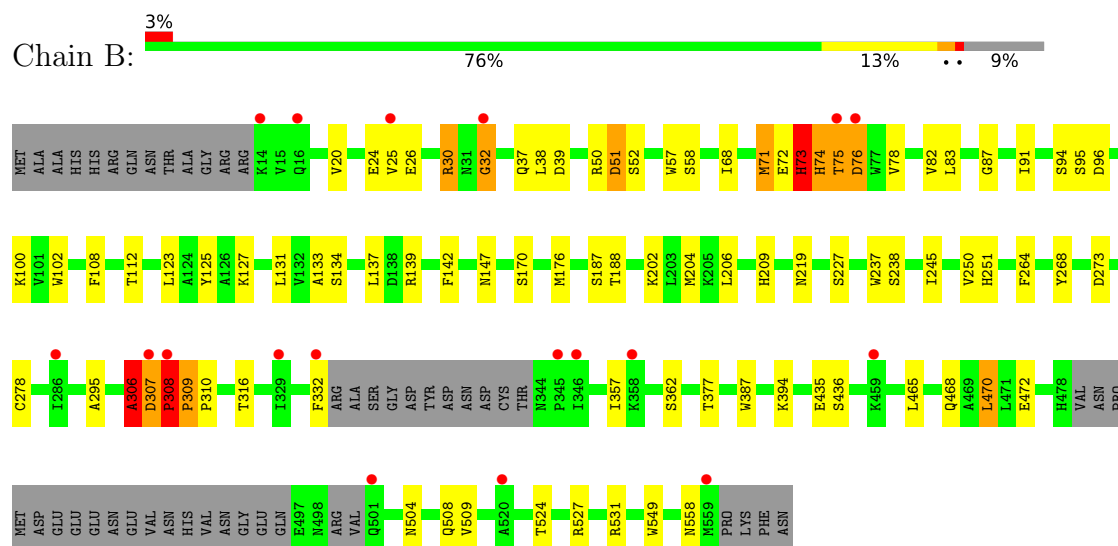
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 12

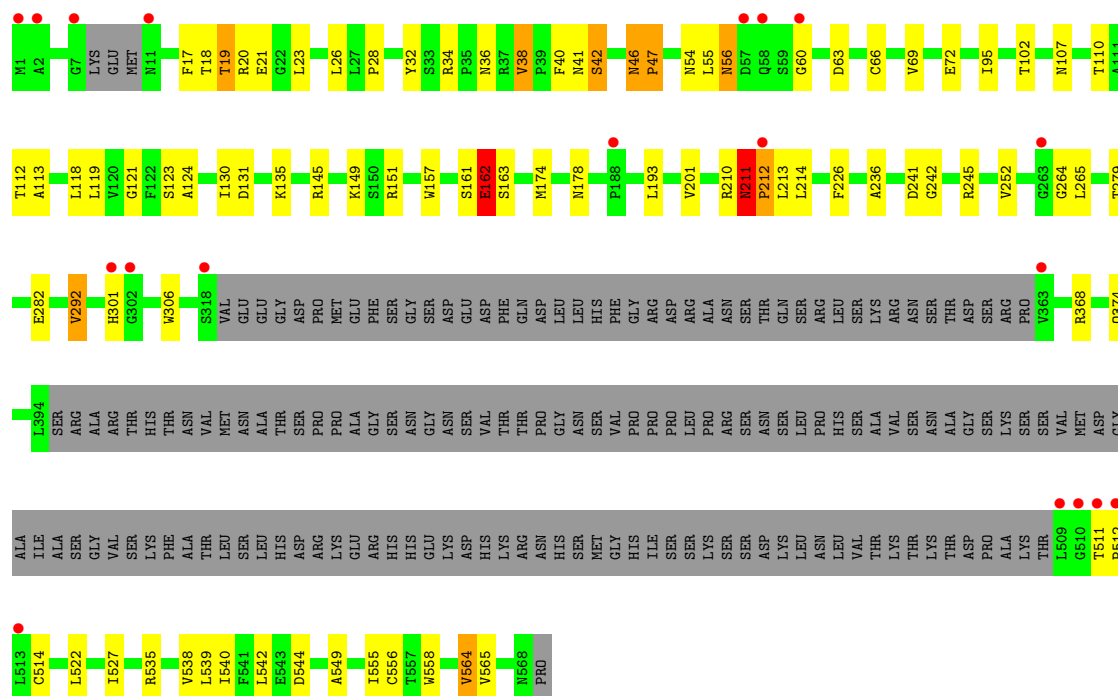


- Molecule 2: WD repeat-containing protein 48



- Molecule 3: WD repeat-containing protein 20





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	217.90Å 217.90Å 223.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.00 50.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.01-3.00) 97.7 (50.01-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.230 , 0.271 0.237 , 0.276	Depositor DCC
R_{free} test set	3014 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9633	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: PO4, ZN, TAM

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	0.89	7/2425 (0.3%)	1.22	23/3293 (0.7%)
2	B	0.95	8/4083 (0.2%)	1.15	27/5558 (0.5%)
3	C	0.82	1/3245 (0.0%)	1.06	13/4406 (0.3%)
All	All	0.90	16/9753 (0.2%)	1.14	63/13257 (0.5%)

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	5
2	B	0	1
All	All	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	PHE	C-N	12.57	1.50	1.33
2	B	307	ASP	C-O	12.43	1.37	1.24
2	B	75	THR	C-N	11.94	1.50	1.33
2	B	71	MET	C-N	11.57	1.49	1.33
2	B	76	ASP	C-O	-10.27	1.11	1.24
1	A	105	LYS	C-O	9.95	1.36	1.24
2	B	73	HIS	C-N	8.38	1.44	1.33
1	A	102	PRO	CA-C	7.75	1.59	1.52
1	A	186	CYS	N-CA	6.89	1.54	1.46
2	B	72	GLU	C-O	5.82	1.30	1.24
1	A	104	LYS	C-N	5.59	1.41	1.34
2	B	332	PHE	C-O	5.45	1.34	1.23
1	A	105	LYS	C-N	5.42	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	54	ASN	C-N	-5.33	1.27	1.33
2	B	76	ASP	CA-C	5.20	1.59	1.52
1	A	236	CYS	CA-C	5.18	1.59	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	306	ALA	CA-C-N	-14.27	102.09	119.78
2	B	306	ALA	C-N-CA	-14.27	102.09	119.78
1	A	359	GLU	N-CA-C	-14.26	89.59	110.42
1	A	104	LYS	O-C-N	13.56	136.20	122.09
1	A	359	GLU	CB-CA-C	11.05	125.07	109.71
1	A	353	ASP	N-CA-C	10.93	126.33	111.24
3	C	162	GLU	CB-CA-C	10.37	125.83	109.03
1	A	104	LYS	N-CA-C	9.74	122.79	111.11
2	B	72	GLU	O-C-N	-9.43	110.67	123.12
2	B	75	THR	CA-C-O	9.23	129.68	119.15
2	B	74	HIS	CB-CA-C	-8.98	93.54	109.62
3	C	162	GLU	N-CA-C	-8.80	103.05	113.88
2	B	436	SER	N-CA-C	8.44	120.17	110.97
2	B	307	ASP	N-CA-C	-8.18	101.40	112.35
1	A	105	LYS	CA-C-N	-8.15	109.36	120.44
1	A	105	LYS	C-N-CA	-8.15	109.36	120.44
1	A	101	ILE	CA-C-N	8.03	128.65	120.38
1	A	101	ILE	C-N-CA	8.03	128.65	120.38
3	C	42	SER	N-CA-C	-7.99	98.82	110.64
1	A	186	CYS	N-CA-C	-7.84	98.55	110.30
2	B	75	THR	CA-C-N	-7.52	107.19	121.54
2	B	75	THR	C-N-CA	-7.52	107.19	121.54
3	C	42	SER	CB-CA-C	7.45	118.97	109.80
2	B	74	HIS	N-CA-C	7.44	120.47	110.35
1	A	119	ASN	N-CA-C	7.22	121.33	112.23
3	C	211	ASN	N-CA-C	6.91	125.09	109.81
1	A	105	LYS	O-C-N	6.80	130.18	122.22
3	C	60	GLY	N-CA-C	-6.79	106.32	113.58
2	B	32	GLY	N-CA-C	6.75	129.19	113.18
1	A	269	HIS	N-CA-C	-6.69	102.00	111.56
1	A	342	GLN	CB-CA-C	6.50	124.75	110.18
3	C	46	ASN	CA-C-N	6.44	126.20	119.76
3	C	46	ASN	C-N-CA	6.44	126.20	119.76
2	B	558	ASN	N-CA-C	6.43	118.37	111.36
2	B	307	ASP	N-CA-CB	6.36	117.93	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	MET	CA-C-N	-6.35	113.84	122.86
2	B	71	MET	C-N-CA	-6.35	113.84	122.86
2	B	307	ASP	C-N-CD	-6.28	99.23	125.00
1	A	101	ILE	O-C-N	-6.28	116.11	121.57
1	A	294	THR	CA-C-N	-6.12	116.68	122.37
1	A	294	THR	C-N-CA	-6.12	116.68	122.37
1	A	186	CYS	CA-CB-SG	5.98	128.16	114.40
2	B	75	THR	O-C-N	-5.72	114.93	122.42
1	A	106	PHE	O-C-N	5.71	128.26	122.09
2	B	147	ASN	N-CA-C	5.67	117.47	111.28
1	A	267	GLN	N-CA-C	-5.66	103.89	112.04
3	C	46	ASN	N-CA-C	5.62	115.36	108.11
1	A	284	LEU	N-CA-C	5.60	117.50	108.32
2	B	394	LYS	N-CA-C	-5.58	103.02	110.55
2	B	20	VAL	N-CA-C	5.53	116.08	108.12
2	B	108	PHE	N-CA-C	5.42	118.29	109.24
3	C	38	VAL	CB-CA-C	5.42	115.98	110.94
2	B	38	LEU	N-CA-C	5.41	122.33	110.80
3	C	47	PRO	N-CA-C	5.40	119.67	111.19
2	B	306	ALA	N-CA-C	5.29	117.12	108.76
3	C	292	VAL	N-CA-CB	5.27	116.72	110.55
2	B	72	GLU	CA-C-N	5.24	131.55	121.54
2	B	72	GLU	C-N-CA	5.24	131.55	121.54
1	A	360	SER	N-CA-C	5.08	116.77	108.55
2	B	51	ASP	CB-CA-C	-5.07	104.93	111.22
1	A	359	GLU	N-CA-CB	-5.07	101.59	109.34
2	B	308	PRO	N-CA-C	-5.03	104.56	110.70
3	C	19	THR	N-CA-C	-5.02	101.43	109.07

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	PRO	Mainchain
1	A	105	LYS	Mainchain
1	A	205	ASP	Peptide
1	A	295	ASN	Peptide
1	A	334	ASP	Peptide
2	B	306	ALA	Mainchain

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	2374	0	2188	40	0
2	B	4001	0	3913	65	0
3	C	3166	0	3067	64	0
4	A	1	0	0	0	0
5	B	5	0	0	0	0
6	C	11	0	17	5	0
7	A	6	0	0	1	0
7	B	42	0	0	4	0
7	C	27	0	0	3	0
All	All	9633	0	9185	168	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 9.

All (168) 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)
2:B:307:ASP:CB	2:B:308:PRO:HD3	1.52	1.21
2:B:307:ASP:HB3	2:B:308:PRO:CD	1.70	1.21
7:A:502:HOH:O	2:B:188:THR:HG21	1.60	1.01
2:B:307:ASP:CB	2:B:308:PRO:CD	2.35	0.96
3:C:110:THR:CG2	3:C:162:GLU:HG2	1.94	0.96
2:B:308:PRO:O	2:B:309:PRO:O	1.90	0.89
3:C:110:THR:HG21	3:C:162:GLU:HG2	1.53	0.86
1:A:358:SER:O	1:A:359:GLU:C	2.21	0.84
3:C:110:THR:CG2	3:C:162:GLU:CG	2.57	0.82
1:A:105:LYS:O	1:A:109:ARG:CB	2.28	0.81
2:B:273:ASP:HB3	7:B:705:HOH:O	1.80	0.80
2:B:306:ALA:O	2:B:307:ASP:C	2.23	0.77
2:B:308:PRO:O	2:B:309:PRO:C	2.29	0.75
3:C:211:ASN:O	3:C:213:LEU:N	2.20	0.73
3:C:55:LEU:O	3:C:56:ASN:HB2	1.87	0.73
2:B:468:GLN:HB3	2:B:504:ASN:ND2	2.03	0.72
2:B:74:HIS:HD2	2:B:78:VAL:HG22	1.55	0.71
1:A:233:CYS:HB3	1:A:236:CYS:HB2	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:HD22	1:A:270:ARG:HD3	1.72	0.70
1:A:173:HIS:O	1:A:177:GLN:HB3	1.91	0.70
2:B:26:GLU:OE1	2:B:30:ARG:NH1	2.24	0.70
3:C:542:LEU:HD23	6:C:601:TAM:H31	1.72	0.70
2:B:307:ASP:HB3	2:B:308:PRO:HD3	0.74	0.69
2:B:307:ASP:N	2:B:308:PRO:CD	2.55	0.67
2:B:307:ASP:N	2:B:308:PRO:HD2	2.07	0.67
2:B:307:ASP:O	2:B:309:PRO:HD3	1.95	0.67
3:C:511:THR:N	3:C:512:PRO:CD	2.60	0.65
3:C:69:VAL:HG23	3:C:69:VAL:O	1.96	0.65
2:B:307:ASP:O	2:B:309:PRO:CD	2.44	0.65
3:C:540:ILE:HG22	3:C:542:LEU:CD1	2.28	0.63
1:A:268:LEU:CD2	1:A:270:ARG:HD3	2.27	0.63
3:C:110:THR:HG23	3:C:162:GLU:CG	2.28	0.63
3:C:212:PRO:O	3:C:213:LEU:C	2.36	0.62
1:A:358:SER:O	1:A:360:SER:HB3	2.00	0.62
3:C:542:LEU:HD23	6:C:601:TAM:C3	2.30	0.61
3:C:265:LEU:HD22	3:C:279:THR:HG22	1.83	0.60
2:B:75:THR:HG21	2:B:524:THR:CB	2.31	0.60
2:B:32:GLY:O	2:B:50:ARG:HG3	2.02	0.59
2:B:209:HIS:HE2	2:B:227:SER:HG	1.48	0.59
1:A:189:CYS:N	1:A:236:CYS:SG	2.74	0.59
3:C:511:THR:H	3:C:512:PRO:HD3	1.68	0.58
2:B:73:HIS:CD2	2:B:100:LYS:HZ2	2.22	0.57
3:C:242:GLY:HA2	3:C:264:GLY:HA2	1.87	0.57
3:C:28:PRO:HD2	7:C:702:HOH:O	2.03	0.57
1:A:353:ASP:OD1	1:A:353:ASP:C	2.47	0.56
3:C:110:THR:HG23	3:C:162:GLU:HG3	1.88	0.56
1:A:268:LEU:HB2	1:A:270:ARG:HG2	1.86	0.55
2:B:307:ASP:O	2:B:309:PRO:N	2.41	0.54
3:C:511:THR:O	3:C:514:CYS:O	2.24	0.54
2:B:435:GLU:HG3	2:B:549:TRP:CG	2.43	0.54
2:B:24:GLU:OE1	2:B:531:ARG:NH2	2.42	0.53
2:B:472:GLU:OE2	2:B:508:GLN:NE2	2.41	0.53
1:A:353:ASP:C	1:A:355:SER:H	2.16	0.53
2:B:123:LEU:HD23	2:B:134:SER:HA	1.91	0.53
2:B:206:LEU:HB3	2:B:237:TRP:CZ3	2.44	0.53
3:C:151:ARG:HD2	7:C:724:HOH:O	2.09	0.53
2:B:306:ALA:HB3	2:B:310:PRO:HD3	1.92	0.52
3:C:174:MET:HE3	3:C:226:PHE:CD2	2.45	0.52
1:A:305:VAL:HG12	1:A:321:ILE:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASP:OD1	1:A:353:ASP:O	2.29	0.51
1:A:49:TYR:CG	1:A:123:GLN:HB3	2.45	0.51
1:A:216:LEU:HB3	1:A:288:ASN:HD21	1.75	0.51
2:B:75:THR:HG21	2:B:524:THR:HB	1.91	0.51
2:B:75:THR:OG1	2:B:96:ASP:HB2	2.10	0.51
3:C:242:GLY:CA	3:C:264:GLY:HA2	2.40	0.51
2:B:39:ASP:HB2	2:B:83:LEU:HD21	1.92	0.51
3:C:301:HIS:HB3	3:C:522:LEU:HD21	1.93	0.50
1:A:358:SER:O	1:A:360:SER:N	2.44	0.50
1:A:48:CYS:HA	1:A:51:ASN:HB2	1.93	0.50
1:A:49:TYR:CZ	1:A:123:GLN:HG2	2.47	0.50
3:C:41:ASN:O	3:C:42:SER:C	2.53	0.50
1:A:329:LEU:HD23	1:A:338:LYS:HA	1.94	0.50
1:A:353:ASP:O	1:A:353:ASP:CG	2.53	0.50
3:C:241:ASP:OD2	3:C:245:ARG:NH2	2.44	0.49
3:C:21:GLU:CD	3:C:368:ARG:HH12	2.21	0.49
3:C:17:PHE:CD1	3:C:527:ILE:HD13	2.47	0.49
3:C:511:THR:N	3:C:512:PRO:HD3	2.25	0.49
1:A:307:VAL:HG12	1:A:308:HIS:N	2.28	0.49
3:C:374:GLN:HA	3:C:535:ARG:HB2	1.94	0.48
2:B:307:ASP:H	2:B:308:PRO:HD2	1.75	0.48
1:A:339:ILE:CG1	1:A:343:ALA:CB	2.91	0.48
2:B:74:HIS:CD2	2:B:94:SER:HB2	2.48	0.48
3:C:564:VAL:HG12	3:C:565:VAL:HG23	1.94	0.48
1:A:233:CYS:CB	1:A:236:CYS:HB2	2.43	0.48
1:A:280:PHE:CG	1:A:364:LEU:HD21	2.49	0.48
1:A:283:GLU:HG2	1:A:299:MET:SD	2.54	0.48
3:C:32:TYR:HB2	3:C:555:ILE:HB	1.94	0.48
1:A:143:GLU:HG3	1:A:146:GLN:NE2	2.29	0.47
2:B:25:VAL:HG23	2:B:26:GLU:N	2.29	0.47
2:B:142:PHE:HB3	7:B:722:HOH:O	2.13	0.47
2:B:131:LEU:HD23	2:B:176:MET:SD	2.55	0.47
2:B:100:LYS:NZ	2:B:112:THR:OG1	2.48	0.47
3:C:211:ASN:C	3:C:213:LEU:N	2.73	0.47
3:C:539:LEU:O	3:C:540:ILE:HD13	2.14	0.47
3:C:130:ILE:HG22	3:C:131:ASP:N	2.30	0.47
3:C:282:GLU:HA	3:C:306:TRP:CD1	2.49	0.47
1:A:217:ARG:NH2	3:C:301:HIS:CE1	2.83	0.46
1:A:339:ILE:HG13	1:A:343:ALA:HB3	1.96	0.46
2:B:295:ALA:HB3	2:B:316:THR:HB	1.97	0.46
3:C:538:VAL:HB	3:C:549:ALA:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:HIS:HD2	2:B:100:LYS:NZ	2.14	0.46
1:A:210:THR:HG22	1:A:211:SER:N	2.31	0.46
1:A:341:ALA:C	1:A:343:ALA:H	2.23	0.46
2:B:273:ASP:HB2	7:B:714:HOH:O	2.16	0.46
3:C:211:ASN:O	3:C:213:LEU:HD12	2.15	0.46
2:B:32:GLY:O	2:B:50:ARG:CG	2.63	0.46
2:B:71:MET:HB3	2:B:102:TRP:CZ3	2.51	0.46
3:C:212:PRO:O	3:C:214:LEU:N	2.49	0.46
2:B:206:LEU:HB3	2:B:237:TRP:CE3	2.50	0.46
3:C:556:CYS:HA	7:C:708:HOH:O	2.16	0.46
3:C:34:ARG:NH2	3:C:40:PHE:HA	2.31	0.46
3:C:145:ARG:NH1	3:C:149:LYS:O	2.48	0.46
2:B:73:HIS:CD2	2:B:100:LYS:NZ	2.84	0.45
2:B:76:ASP:HB3	2:B:95:SER:HB2	1.99	0.45
2:B:125:TYR:CZ	2:B:127:LYS:HA	2.52	0.45
3:C:19:THR:HG22	3:C:20:ARG:N	2.32	0.45
1:A:339:ILE:HG13	1:A:343:ALA:CB	2.47	0.45
3:C:46:ASN:HB2	3:C:47:PRO:HD2	1.99	0.45
3:C:201:VAL:HG21	3:C:252:VAL:CG1	2.47	0.45
1:A:49:TYR:CD1	1:A:123:GLN:HB3	2.52	0.45
2:B:133:ALA:HA	2:B:142:PHE:O	2.17	0.45
1:A:128:PHE:CZ	1:A:132:LEU:HD22	2.53	0.44
1:A:206:VAL:HG13	1:A:278:VAL:HG21	1.99	0.44
1:A:350:LEU:HD13	1:A:358:SER:HA	1.99	0.44
2:B:37:GLN:NE2	2:B:37:GLN:HA	2.32	0.44
3:C:34:ARG:HH22	3:C:40:PHE:HA	1.83	0.44
2:B:83:LEU:HD11	2:B:87:GLY:HA2	1.99	0.44
1:A:297:ASP:O	1:A:298:ARG:C	2.58	0.44
2:B:30:ARG:O	2:B:362:SER:OG	2.22	0.44
3:C:36:ASN:CG	3:C:38:VAL:HG12	2.43	0.44
3:C:544:ASP:CG	6:C:601:TAM:H42	2.42	0.44
2:B:307:ASP:C	2:B:309:PRO:N	2.74	0.44
3:C:36:ASN:OD1	3:C:38:VAL:HG12	2.16	0.44
2:B:202:LYS:HE3	7:B:724:HOH:O	2.18	0.44
3:C:112:THR:OG1	3:C:113:ALA:N	2.51	0.44
3:C:26:LEU:HB2	3:C:558:TRP:CZ3	2.52	0.43
1:A:341:ALA:C	1:A:343:ALA:N	2.76	0.43
3:C:102:THR:HG22	3:C:121:GLY:C	2.43	0.43
2:B:468:GLN:HB3	2:B:504:ASN:CG	2.42	0.43
3:C:161:SER:OG	3:C:162:GLU:N	2.52	0.43
2:B:268:TYR:CE1	2:B:278:CYS:SG	3.11	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:ASN:O	3:C:211:ASN:OD1	2.36	0.43
2:B:238:SER:HB2	2:B:245:ILE:HD11	1.99	0.43
2:B:187:SER:OG	2:B:188:THR:N	2.51	0.43
2:B:57:TRP:CZ3	2:B:357:ILE:HG23	2.54	0.43
3:C:63:ASP:CG	6:C:601:TAM:O6	2.62	0.42
1:A:131:TYR:O	1:A:132:LEU:C	2.62	0.42
3:C:212:PRO:C	3:C:214:LEU:N	2.77	0.42
2:B:73:HIS:O	2:B:527:ARG:NE	2.53	0.42
3:C:34:ARG:HH21	3:C:38:VAL:HG13	1.85	0.42
3:C:107:ASN:HB2	3:C:157:TRP:CE2	2.55	0.42
2:B:204:MET:SD	2:B:206:LEU:HD21	2.60	0.42
3:C:124:ALA:HB1	3:C:145:ARG:HD3	2.02	0.42
1:A:173:HIS:HA	1:A:177:GLN:HB2	2.00	0.41
2:B:137:LEU:HA	2:B:170:SER:HB3	2.03	0.41
2:B:51:ASP:OD1	2:B:51:ASP:O	2.37	0.41
3:C:123:SER:HA	3:C:151:ARG:HB2	2.02	0.41
2:B:58:SER:HB2	2:B:68:ILE:HD11	2.02	0.41
2:B:470:LEU:HD12	2:B:509:VAL:HG21	2.03	0.40
3:C:69:VAL:CG2	3:C:72:GLU:HB2	2.51	0.40
3:C:542:LEU:HG	6:C:601:TAM:H32	2.04	0.40
2:B:377:THR:HG23	2:B:387:TRP:CD1	2.56	0.40
2:B:250:VAL:HG23	2:B:251:HIS:CD2	2.56	0.40
3:C:18:THR:HG22	3:C:23:LEU:HD13	2.02	0.40
3:C:265:LEU:HD22	3:C:279:THR:CG2	2.49	0.40
1:A:339:ILE:CG1	1:A:343:ALA:HB3	2.50	0.40
2:B:219:ASN:HB3	2:B:264:PHE:CD2	2.57	0.40
3:C:226:PHE:HA	3:C:236:ALA:O	2.21	0.40

There are no symmetry-related clashes.

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	294/355 (83%)	259 (88%)	35 (12%)	0	100	100
2	B	507/563 (90%)	457 (90%)	49 (10%)	1 (0%)	43	76
3	C	399/569 (70%)	363 (91%)	34 (8%)	2 (0%)	24	60
All	All	1200/1487 (81%)	1079 (90%)	118 (10%)	3 (0%)	36	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	309	PRO
3	C	211	ASN
3	C	212	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	248/324 (76%)	242 (98%)	6 (2%)	43	73
2	B	438/492 (89%)	429 (98%)	9 (2%)	47	75
3	C	348/499 (70%)	336 (97%)	12 (3%)	32	66
All	All	1034/1315 (79%)	1007 (97%)	27 (3%)	40	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	181	THR
1	A	186	CYS
1	A	191	THR
1	A	234	GLU
1	A	263	LYS
2	B	30	ARG
2	B	52	SER
2	B	73	HIS
2	B	82	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	91	ILE
2	B	139	ARG
2	B	308	PRO
2	B	465	LEU
2	B	470	LEU
3	C	56	ASN
3	C	66	CYS
3	C	95	ILE
3	C	118	LEU
3	C	119	LEU
3	C	135	LYS
3	C	162	GLU
3	C	163	SER
3	C	193	LEU
3	C	210	ARG
3	C	292	VAL
3	C	564	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	51	ASN
1	A	119	ASN
1	A	146	GLN
1	A	209	ASN
1	A	288	ASN
2	B	60	ASN
2	B	73	HIS
2	B	74	HIS
2	B	167	ASN
2	B	178	GLN
2	B	283	ASN
2	B	367	HIS
2	B	381	ASN
2	B	548	GLN
3	C	16	GLN
3	C	41	ASN
3	C	61	ASN
3	C	128	GLN
3	C	301	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	PO4	B	601	-	4,4,4	0.74	0	6,6,6	1.69	2 (33%)
6	TAM	C	601	-	10,10,10	1.41	3 (30%)	12,12,12	2.81	4 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TAM	C	601	-	-	4/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	601	TAM	C2-C	2.84	1.57	1.53
6	C	601	TAM	C1-C	-2.11	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	601	TAM	C2-C5	2.02	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	TAM	C4-C1-C	-7.53	107.09	115.97
6	C	601	TAM	C5-C2-C	3.45	120.04	115.97
6	C	601	TAM	C2-C-N	3.14	116.11	108.22
6	C	601	TAM	C1-C-N	-2.93	100.88	108.22
5	B	601	PO4	O3-P-O1	-2.65	101.60	110.95
5	B	601	PO4	O4-P-O3	2.55	115.83	107.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	601	TAM	C1-C-C2-C5
6	C	601	TAM	C3-C-C1-C4
6	C	601	TAM	N-C-C2-C5
6	C	601	TAM	C3-C-C2-C5

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	601	TAM	5	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	302/355 (85%)	0.64	25 (8%)	17 9	59, 129, 186, 207	0
2	B	515/563 (91%)	0.25	18 (3%)	47 27	49, 87, 140, 217	0
3	C	407/569 (71%)	0.21	19 (4%)	36 19	47, 85, 138, 177	0
All	All	1224/1487 (82%)	0.33	62 (5%)	33 17	47, 93, 168, 217	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	ASP	6.6
2	B	307	ASP	4.5
3	C	58	GLN	4.4
2	B	559	MET	4.3
1	A	355	SER	4.2
1	A	70	TYR	3.9
3	C	212	PRO	3.9
1	A	94	GLN	3.9
3	C	511	THR	3.8
3	C	60	GLY	3.7
1	A	146	GLN	3.7
3	C	188	PRO	3.6
2	B	76	ASP	3.6
1	A	67	VAL	3.5
1	A	364	LEU	3.5
1	A	268	LEU	3.4
2	B	332	PHE	3.3
1	A	357	ASN	3.3
1	A	39	PHE	3.2
2	B	501	GLN	3.2
2	B	75	THR	3.2
3	C	509	LEU	3.1
2	B	32	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	14	LYS	3.0
1	A	354	ILE	2.9
1	A	335	ILE	2.8
3	C	263	GLY	2.6
2	B	346	ILE	2.6
1	A	167	PRO	2.6
1	A	313	PRO	2.6
3	C	11	ASN	2.6
2	B	25	VAL	2.6
1	A	66	LYS	2.6
3	C	513	LEU	2.6
2	B	345	PRO	2.5
3	C	302	GLY	2.5
2	B	286	ILE	2.5
3	C	363	VAL	2.5
3	C	1	MET	2.4
3	C	301	HIS	2.4
3	C	318	SER	2.4
1	A	327	PHE	2.4
2	B	358	LYS	2.4
2	B	520	ALA	2.4
1	A	275	SER	2.4
2	B	459	LYS	2.3
1	A	312	GLY	2.3
3	C	7	GLY	2.3
1	A	100	VAL	2.3
3	C	510	GLY	2.3
1	A	334	ASP	2.3
2	B	329	ILE	2.2
2	B	308	PRO	2.2
2	B	16	GLN	2.2
1	A	265	MET	2.2
3	C	2	ALA	2.2
1	A	143	GLU	2.1
1	A	101	ILE	2.1
1	A	58	TYR	2.1
1	A	88	PHE	2.1
3	C	512	PRO	2.1
3	C	57	ASP	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($\text{\AA}^2$)	Q<0.9
6	TAM	C	601	11/11	0.87	0.24	90,108,133,148	0
5	PO4	B	601	5/5	0.96	0.07	68,69,84,85	0
4	ZN	A	401	1/1	0.96	0.26	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.