



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:02 PM GMT

PDB ID : 1HPU  
Title : 5'-NUCLEOTIDASE (CLOSED FORM), COMPLEX WITH AMPCP  
Authors : Knoefel, T.; Straeter, N.  
Deposited on : 2000-12-13  
Resolution : 1.85 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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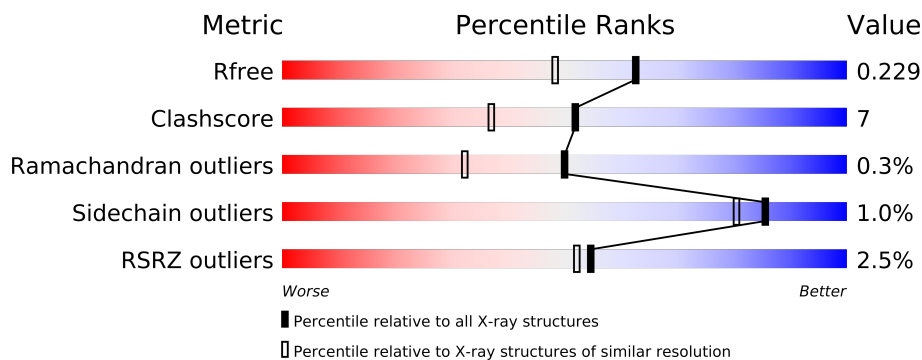
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.85 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	525	
1	B	525	
1	C	525	
1	D	525	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17735 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

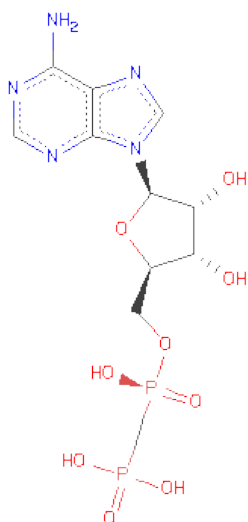
- Molecule 1 is a protein called 5'-NUCLEOTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4100	2590	703	790	17			
1	B	525	Total	C	N	O	S	0	0	0
			4100	2590	703	790	17			
1	C	525	Total	C	N	O	S	0	0	0
			4100	2590	703	790	17			
1	D	525	Total	C	N	O	S	0	0	0
			4100	2590	703	790	17			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: A12) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>5</sub>O<sub>9</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
3	B	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
3	C	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
3	D	1	Total	C	N	O	P	0	0
			27	11	5	9	2		

- Molecule 4 is water.

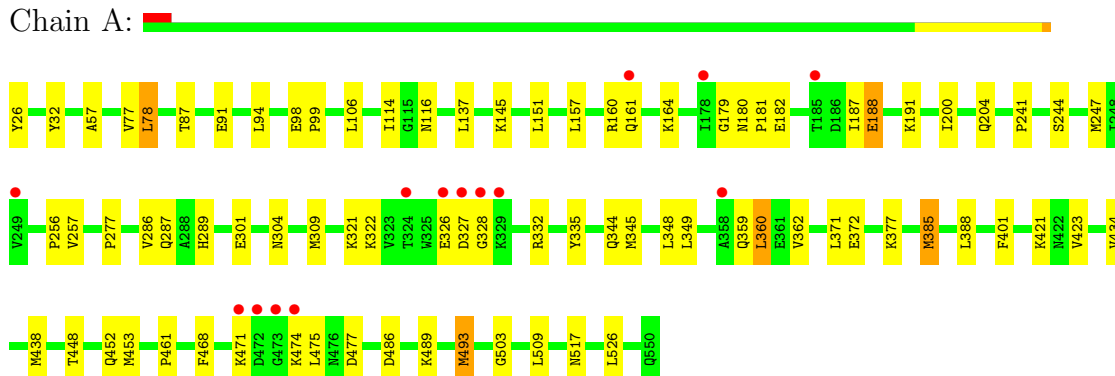
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	267	Total	O	0	0
			267	267		
4	B	305	Total	O	0	0
			305	305		
4	C	304	Total	O	0	0
			304	304		
4	D	343	Total	O	0	0
			343	343		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

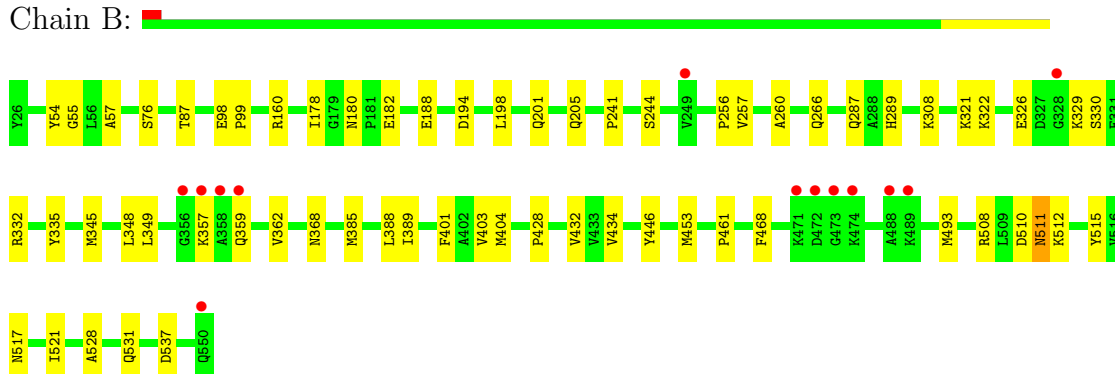
#### • Molecule 1: 5'-NUCLEOTIDASE

Chain A:



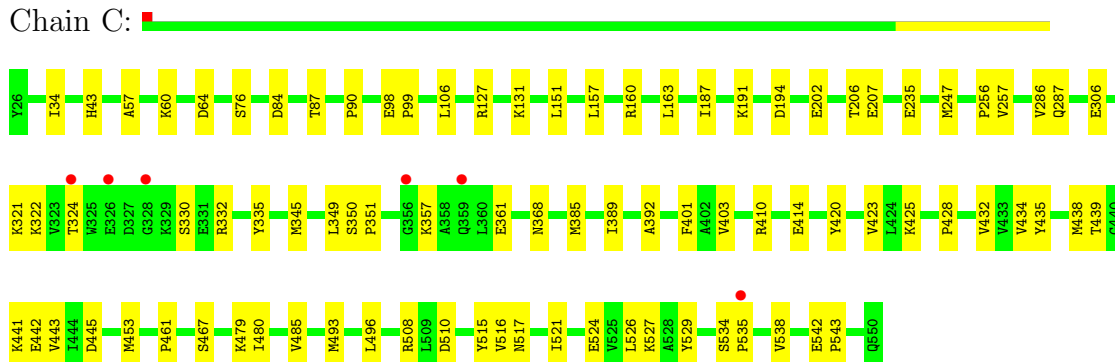
#### • Molecule 1: 5'-NUCLEOTIDASE

Chain B:



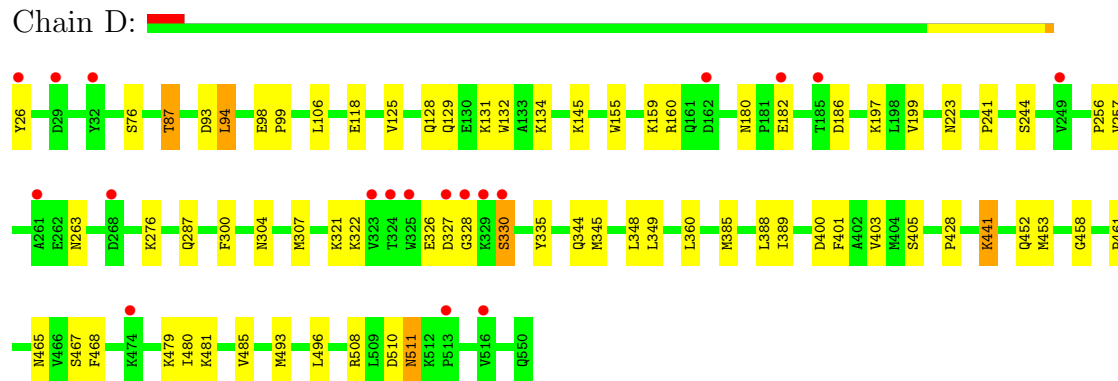
#### • Molecule 1: 5'-NUCLEOTIDASE

Chain C:



- Molecule 1: 5'-NUCLEOTIDASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.40Å 89.96Å 96.26Å 110.79° 106.43° 107.76°	Depositor
Resolution (Å)	28.59 – 1.85 28.59 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.59-1.85) 95.0 (28.59-1.78)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.78Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.234 0.204 , 0.229	Depositor DCC
$R_{free}$ test set	1981 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.9	EDS
Estimated twinning fraction	0.003 for k,h,-h-k-l 0.001 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 217522 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, A12

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	0.46	0/4188	0.72	2/5666 (0.0%)
1	B	0.50	0/4188	0.74	1/5666 (0.0%)
1	C	0.51	0/4188	0.73	1/5666 (0.0%)
1	D	0.49	0/4188	0.73	2/5666 (0.0%)
All	All	0.49	0/16752	0.73	6/22664 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	PRO	N-CA-C	-7.18	93.44	112.10
1	C	256	PRO	N-CA-C	-7.17	93.46	112.10
1	B	256	PRO	N-CA-C	-6.95	94.04	112.10
1	A	256	PRO	N-CA-C	-6.66	94.77	112.10
1	D	94	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	78	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4100	0	4019	72	0
1	B	4100	0	4019	46	0
1	C	4100	0	4019	65	0
1	D	4100	0	4019	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	27	0	14	0	0
3	B	27	0	14	1	0
3	C	27	0	14	0	0
3	D	27	0	14	0	0
4	A	267	0	0	5	0
4	B	305	0	0	1	0
4	C	304	0	0	3	0
4	D	343	0	0	4	0
All	All	17735	0	16132	236	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (236) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:345:MET:HE3	1:A:348:LEU:HD23	1.42	0.98
1:C:345:MET:HE2	1:C:349:LEU:HD11	1.49	0.95
1:B:345:MET:HE2	1:B:349:LEU:HG	1.50	0.92
1:C:322:LYS:HE3	1:C:330:SER:HB3	1.51	0.92
1:C:345:MET:HE2	1:C:349:LEU:CD1	2.04	0.88
1:D:345:MET:CE	1:D:348:LEU:HD23	2.04	0.88
1:B:359:GLN:O	1:B:362:VAL:HG12	1.75	0.87
1:A:322:LYS:HE3	1:A:332:ARG:NH2	1.92	0.83
1:A:345:MET:CE	1:A:348:LEU:HD23	2.09	0.83
1:B:345:MET:CE	1:B:348:LEU:HD23	2.09	0.82
1:A:345:MET:HE2	1:A:349:LEU:HG	1.60	0.82
1:A:385:MET:CE	1:A:385:MET:HA	2.09	0.82
1:A:471:LYS:O	1:A:474:LYS:HG2	1.79	0.81
1:C:368:ASN:HD22	1:C:538:VAL:HG22	1.49	0.78
1:D:345:MET:HE2	1:D:349:LEU:HG	1.66	0.77
1:A:385:MET:HA	1:A:385:MET:HE3	1.66	0.77
1:D:345:MET:HE1	1:D:348:LEU:HD23	1.64	0.77
1:B:345:MET:HE3	1:B:348:LEU:HD23	1.69	0.75
1:B:508:ARG:HD2	1:B:510:ASP:OD1	1.86	0.75
1:B:385:MET:HE2	1:B:389:ILE:HG13	1.68	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:MET:HE1	1:A:388:LEU:HD23	1.68	0.74
1:A:247:MET:HE3	1:A:309:MET:HE2	1.69	0.74
1:B:345:MET:CE	1:B:349:LEU:HG	2.18	0.74
1:B:308:LYS:NZ	1:C:324:THR:O	2.20	0.72
1:D:345:MET:HE3	1:D:348:LEU:HD23	1.71	0.72
1:A:322:LYS:HE3	1:A:332:ARG:HH22	1.56	0.71
1:A:486:ASP:OD2	1:A:489:LYS:HG3	1.90	0.71
1:C:247:MET:HE2	1:C:286:VAL:HG11	1.72	0.70
1:A:180:ASN:ND2	1:A:182:GLU:HG2	2.07	0.69
1:A:423:VAL:HG13	1:A:526:LEU:HD23	1.74	0.69
1:C:345:MET:HE2	1:C:349:LEU:CG	2.24	0.68
1:C:202:GLU:OE2	1:C:206:THR:HG21	1.94	0.68
1:D:441:LYS:O	1:D:441:LYS:HD3	1.94	0.67
1:A:385:MET:CE	1:A:388:LEU:HD23	2.24	0.67
1:B:345:MET:HE1	1:B:348:LEU:HD23	1.77	0.66
1:D:453:MET:HE3	1:D:453:MET:HA	1.77	0.66
1:A:371:LEU:HB3	1:A:385:MET:HE3	1.76	0.66
1:C:34:ILE:HD11	1:C:163:LEU:HD12	1.77	0.66
1:C:235:GLU:HG2	4:C:1733:HOH:O	1.96	0.66
1:A:180:ASN:HD22	1:A:182:GLU:HG2	1.61	0.65
1:C:257:VAL:HG23	1:C:287:GLN:HB3	1.78	0.65
1:A:114:ILE:HD11	1:A:137:LEU:HB3	1.79	0.65
1:D:465:ASN:ND2	1:D:481:LYS:HE2	2.13	0.64
1:D:180:ASN:HD21	1:D:182:GLU:CG	2.11	0.64
1:C:467:SER:OG	1:C:479:LYS:HB2	1.98	0.64
1:C:345:MET:CE	1:C:349:LEU:HD11	2.25	0.64
1:C:439:THR:OG1	1:C:442:GLU:HG3	1.98	0.63
1:C:521:ILE:HB	1:C:524:GLU:CG	2.29	0.63
1:C:247:MET:CE	1:C:286:VAL:HG11	2.29	0.62
1:C:76:SER:HB3	1:C:160:ARG:HD2	1.81	0.62
1:C:434:VAL:HG12	1:C:517:ASN:HA	1.79	0.62
1:B:76:SER:HB3	1:B:160:ARG:HD2	1.81	0.62
1:D:345:MET:CE	1:D:349:LEU:HG	2.29	0.62
1:A:247:MET:HE3	1:A:309:MET:CE	2.30	0.62
1:C:247:MET:HE2	1:C:286:VAL:CG1	2.29	0.62
1:D:453:MET:HA	1:D:453:MET:CE	2.28	0.62
1:D:453:MET:HB2	1:D:461:PRO:HD3	1.81	0.62
1:A:493:MET:HE2	1:A:509:LEU:HD11	1.81	0.61
1:A:257:VAL:HG23	1:A:287:GLN:HB3	1.82	0.61
1:C:521:ILE:HB	1:C:524:GLU:HG3	1.83	0.61
1:B:257:VAL:HG23	1:B:287:GLN:HB3	1.81	0.60
1:D:257:VAL:HG23	1:D:287:GLN:HB3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:486:ASP:OD2	1:A:489:LYS:HE3	2.02	0.60
1:B:180:ASN:OD1	1:B:182:GLU:HG2	2.03	0.59
1:A:453:MET:HB2	1:A:461:PRO:HD3	1.85	0.59
1:A:322:LYS:HE3	1:A:332:ARG:CZ	2.31	0.58
1:A:157:LEU:HD13	1:A:164:LYS:HE3	1.85	0.58
1:D:276:LYS:HE2	4:D:1815:HOH:O	2.04	0.58
1:A:434:VAL:HG12	1:A:517:ASN:HA	1.86	0.57
1:D:385:MET:HE2	1:D:389:ILE:HG13	1.85	0.56
1:A:385:MET:HE2	1:A:385:MET:HA	1.87	0.56
1:A:345:MET:CE	1:A:349:LEU:HG	2.32	0.56
1:C:322:LYS:HD2	1:C:332:ARG:HG3	1.88	0.55
1:A:371:LEU:HD13	1:A:385:MET:HE1	1.88	0.55
1:D:400:ASP:O	1:D:481:LYS:HE3	2.07	0.55
1:A:401:PHE:CE1	1:A:493:MET:HB3	2.41	0.55
1:B:453:MET:HB2	1:B:461:PRO:HD3	1.88	0.55
1:B:194:ASP:O	1:B:198:LEU:HD22	2.06	0.55
1:D:155:TRP:CE3	1:D:199:VAL:HG13	2.41	0.55
1:C:322:LYS:HE3	1:C:330:SER:CB	2.31	0.55
1:C:247:MET:CE	1:C:286:VAL:CG1	2.85	0.55
1:C:368:ASN:ND2	1:C:538:VAL:HG22	2.18	0.54
1:A:114:ILE:CD1	1:A:137:LEU:HB3	2.38	0.54
1:C:34:ILE:HD11	1:C:163:LEU:CD1	2.38	0.54
1:A:200:ILE:HG22	1:A:204:GLN:HE21	1.71	0.54
1:C:508:ARG:HD2	1:C:510:ASP:OD1	2.06	0.54
1:B:453:MET:HE3	1:B:453:MET:HA	1.90	0.54
1:B:385:MET:HE3	1:B:388:LEU:HB3	1.90	0.54
1:D:180:ASN:ND2	1:D:182:GLU:CG	2.72	0.53
1:C:414:GLU:OE1	1:C:414:GLU:HA	2.09	0.53
1:A:91:GLU:CD	1:A:91:GLU:H	2.11	0.53
1:B:57:ALA:HA	1:B:345:MET:HG2	1.91	0.53
1:B:432:VAL:HG12	1:B:521:ILE:HD13	1.91	0.52
1:B:178:ILE:HB	3:B:1603:A12:H3'	1.91	0.52
1:C:510:ASP:HA	1:C:515:TYR:CD2	2.44	0.52
1:D:400:ASP:HA	1:D:481:LYS:HE3	1.91	0.52
1:C:350:SER:HB2	1:C:351:PRO:HD3	1.92	0.52
1:C:345:MET:HE2	1:C:349:LEU:HG	1.90	0.52
1:B:385:MET:HE3	1:B:388:LEU:HD23	1.90	0.52
1:A:77:VAL:O	1:A:160:ARG:NH1	2.42	0.52
1:A:486:ASP:HB3	1:A:489:LYS:HD2	1.91	0.52
1:C:496:LEU:HD13	4:C:1660:HOH:O	2.10	0.52
1:A:241:PRO:HB2	1:A:244:SER:HB3	1.91	0.52
1:A:161:GLN:HG3	4:A:1724:HOH:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:ASN:HB2	4:A:1821:HOH:O	2.10	0.52
1:A:247:MET:HE1	1:A:286:VAL:HG11	1.92	0.51
1:C:453:MET:HB2	1:C:461:PRO:HD3	1.91	0.51
1:B:511:ASN:HD21	1:B:512:LYS:HE2	1.75	0.51
1:C:441:LYS:HE2	1:C:445:ASP:OD2	2.11	0.51
1:A:321:LYS:HB3	1:A:335:TYR:CZ	2.46	0.51
1:A:179:GLY:O	1:A:181:PRO:HD3	2.10	0.51
1:A:98:GLU:N	1:A:99:PRO:HD2	2.26	0.51
1:B:453:MET:CE	1:B:453:MET:HA	2.41	0.51
1:C:191:LYS:HD2	1:C:194:ASP:OD2	2.11	0.50
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.75	0.50
1:C:57:ALA:HA	1:C:345:MET:HG2	1.92	0.50
1:A:151:LEU:HD11	1:A:187:ILE:HG12	1.93	0.50
1:C:420:TYR:CD1	1:C:527:LYS:HD3	2.47	0.50
1:A:26:TYR:CE1	1:A:304:ASN:HA	2.47	0.50
1:C:60:LYS:HE3	1:C:64:ASP:OD2	2.12	0.49
1:B:510:ASP:HA	1:B:515:TYR:CD2	2.47	0.49
1:C:98:GLU:N	1:C:99:PRO:HD2	2.27	0.49
1:B:401:PHE:CE2	1:B:493:MET:HE3	2.46	0.49
1:D:300:PHE:HB3	1:D:307:MET:CE	2.43	0.49
1:D:403:VAL:CG1	1:D:493:MET:HE1	2.42	0.49
1:C:202:GLU:OE2	1:C:206:THR:CG2	2.61	0.49
1:D:480:ILE:HG12	1:D:485:VAL:HG22	1.95	0.49
1:B:326:GLU:HG2	1:C:306:GLU:OE2	2.13	0.48
1:C:90:PRO:HD3	1:C:425:LYS:HD2	1.94	0.48
1:C:410:ARG:HD2	4:C:1843:HOH:O	2.13	0.48
1:D:467:SER:OG	1:D:479:LYS:HB2	2.13	0.48
1:D:508:ARG:HD2	1:D:510:ASP:OD1	2.14	0.48
1:D:511:ASN:ND2	1:D:511:ASN:H	2.12	0.48
1:A:57:ALA:HA	1:A:345:MET:HG2	1.96	0.48
1:B:385:MET:CE	1:B:388:LEU:HD23	2.43	0.48
1:C:357:LYS:O	1:C:361:GLU:HG3	2.14	0.48
1:D:132:TRP:O	1:D:134:LYS:HE2	2.14	0.47
1:A:438:MET:CE	1:A:493:MET:HG2	2.44	0.47
1:D:385:MET:HE1	1:D:388:LEU:HD23	1.95	0.47
1:C:401:PHE:HE2	1:C:493:MET:HE3	1.78	0.47
1:C:401:PHE:CE2	1:C:493:MET:HE3	2.49	0.47
1:D:197:LYS:HE3	4:D:1713:HOH:O	2.13	0.47
1:A:372:GLU:CD	1:A:377:LYS:HG3	2.35	0.47
1:A:277:PRO:HB3	1:A:286:VAL:HG12	1.97	0.46
1:B:403:VAL:CG1	1:B:493:MET:HE1	2.45	0.46
1:D:159:LYS:HD3	1:D:159:LYS:HA	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:401:PHE:CZ	1:A:493:MET:HB3	2.51	0.46
1:A:160:ARG:NH2	4:A:1861:HOH:O	2.42	0.46
1:C:157:LEU:HD11	1:C:207:GLU:HG3	1.98	0.46
1:D:128:GLN:HE22	1:D:131:LYS:HD3	1.81	0.46
1:A:359:GLN:O	1:A:362:VAL:HG12	2.15	0.46
1:B:201:GLN:O	1:B:205:GLN:HG3	2.16	0.45
1:D:106:LEU:HD21	1:D:344:GLN:HG2	1.99	0.45
1:D:441:LYS:HD3	1:D:441:LYS:C	2.35	0.45
1:C:401:PHE:CZ	1:C:493:MET:HB2	2.52	0.45
1:A:180:ASN:ND2	1:A:182:GLU:CG	2.77	0.45
1:A:468:PHE:C	1:A:468:PHE:CD1	2.89	0.45
1:B:98:GLU:N	1:B:99:PRO:HD2	2.30	0.45
1:B:446:TYR:HE2	1:B:493:MET:HE1	1.82	0.45
1:B:322:LYS:HE2	1:B:332:ARG:NH2	2.32	0.45
1:D:241:PRO:HB2	1:D:244:SER:HB3	1.97	0.45
1:D:496:LEU:CD1	4:D:1735:HOH:O	2.63	0.45
1:D:496:LEU:HD12	4:D:1735:HOH:O	2.17	0.45
1:C:534:SER:OG	1:C:535:PRO:HA	2.17	0.45
1:B:322:LYS:CE	1:B:332:ARG:NH2	2.80	0.45
1:B:511:ASN:C	1:B:511:ASN:HD22	2.19	0.45
1:D:401:PHE:CE2	1:D:493:MET:HE3	2.52	0.45
1:D:468:PHE:CD1	1:D:468:PHE:C	2.90	0.44
1:A:200:ILE:O	1:A:204:GLN:HG3	2.17	0.44
1:A:191:LYS:HE2	4:A:1711:HOH:O	2.16	0.44
1:D:125:VAL:O	1:D:129:GLN:HG3	2.17	0.44
1:D:345:MET:CE	1:D:348:LEU:HB3	2.47	0.44
1:C:432:VAL:HG12	1:C:521:ILE:HD13	2.00	0.44
1:C:480:ILE:HG12	1:C:485:VAL:HG22	1.99	0.44
1:C:401:PHE:CE2	1:C:493:MET:CE	3.01	0.43
1:D:98:GLU:N	1:D:99:PRO:HD2	2.32	0.43
1:C:321:LYS:HB3	1:C:335:TYR:CZ	2.52	0.43
1:D:345:MET:HE2	1:D:345:MET:O	2.18	0.43
1:C:423:VAL:HG13	1:C:526:LEU:HD23	2.00	0.43
1:C:392:ALA:HA	1:C:529:TYR:CD2	2.53	0.43
1:A:145:LYS:HG2	1:A:188:GLU:HB3	2.00	0.43
1:A:91:GLU:OE2	1:A:421:LYS:HE3	2.18	0.43
1:B:468:PHE:C	1:B:468:PHE:CD1	2.92	0.43
1:C:438:MET:HG3	1:C:443:VAL:HG23	2.01	0.43
1:A:327:ASP:OD1	1:A:327:ASP:O	2.36	0.43
1:B:321:LYS:HB3	1:B:335:TYR:CZ	2.54	0.43
1:D:322:LYS:HE2	1:D:330:SER:OG	2.19	0.43
1:A:247:MET:CE	1:A:309:MET:CE	2.95	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:155:TRP:CD1	1:D:155:TRP:C	2.91	0.43
1:C:43:HIS:CE1	1:C:84:ASP:HB3	2.54	0.43
1:B:345:MET:HE3	1:B:348:LEU:HB3	2.01	0.42
1:D:145:LYS:HB2	1:D:186:ASP:OD1	2.18	0.42
1:D:321:LYS:HB3	1:D:335:TYR:CZ	2.54	0.42
1:B:194:ASP:O	1:B:198:LEU:CD2	2.68	0.42
1:C:127:ARG:O	1:C:131:LYS:HG3	2.19	0.42
1:A:493:MET:HE2	1:A:509:LEU:CD1	2.48	0.42
1:A:106:LEU:HD21	1:A:344:GLN:HG2	2.00	0.42
1:C:385:MET:CE	1:C:389:ILE:HG13	2.50	0.42
1:D:26:TYR:CE1	1:D:304:ASN:HA	2.55	0.42
1:A:326:GLU:C	1:A:328:GLY:N	2.73	0.42
1:C:521:ILE:HB	1:C:524:GLU:HG2	2.01	0.42
1:D:300:PHE:HB3	1:D:307:MET:HE2	2.00	0.42
1:B:241:PRO:HB2	1:B:244:SER:HB3	2.00	0.42
1:A:468:PHE:CG	1:A:475:LEU:HD22	2.55	0.42
1:C:453:MET:HE2	1:C:453:MET:HB3	1.84	0.41
1:A:448:THR:O	1:A:452:GLN:HG2	2.20	0.41
1:D:180:ASN:ND2	1:D:182:GLU:HG2	2.34	0.41
1:D:326:GLU:O	1:D:328:GLY:N	2.53	0.41
1:C:403:VAL:CG2	1:C:493:MET:HE1	2.50	0.41
1:A:332:ARG:HG2	1:A:332:ARG:NH1	2.36	0.41
1:B:368:ASN:ND2	1:B:537:ASP:HA	2.35	0.41
1:B:528:ALA:HA	1:B:531:GLN:HE21	1.86	0.41
1:D:385:MET:CE	1:D:389:ILE:HG13	2.50	0.41
1:A:114:ILE:HD11	1:A:137:LEU:CB	2.49	0.41
1:B:54:TYR:HB2	1:B:55:GLY:H	1.59	0.41
1:B:329:LYS:HG2	1:B:330:SER:N	2.35	0.41
1:C:106:LEU:HD23	1:C:345:MET:SD	2.61	0.41
1:D:511:ASN:HD22	1:D:511:ASN:H	1.69	0.41
1:D:326:GLU:C	1:D:328:GLY:H	2.24	0.41
1:C:542:GLU:HA	1:C:543:PRO:HD3	1.88	0.41
1:C:151:LEU:HD11	1:C:187:ILE:HG12	2.03	0.41
1:D:76:SER:HB3	1:D:160:ARG:HD2	2.02	0.41
1:B:357:LYS:HA	4:B:1797:HOH:O	2.20	0.40
1:D:223:ASN:HB2	1:D:263:ASN:HB3	2.03	0.40
1:D:405:SER:HB3	1:D:458:GLY:O	2.22	0.40
1:A:32:TYR:O	1:A:301:GLU:HA	2.20	0.40
1:B:260:ALA:HB2	1:B:266:GLN:HA	2.03	0.40
1:A:322:LYS:CE	1:A:332:ARG:NH2	2.72	0.40
1:A:438:MET:HE1	1:A:493:MET:HG2	2.03	0.40
1:A:503:GLY:HA2	4:A:1846:HOH:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:434:VAL:HG12	1:B:517:ASN:HA	2.04	0.40
1:C:435:TYR:CE1	1:C:516:VAL:HB	2.57	0.40
1:D:87:THR:HA	1:D:93:ASP:OD1	2.21	0.40
1:B:403:VAL:HG22	1:B:404:MET:N	2.36	0.40
1:A:326:GLU:C	1:A:328:GLY:H	2.25	0.40
1:A:94:LEU:HD11	1:A:360:LEU:HD11	2.02	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	523/525 (100%)	504 (96%)	17 (3%)	2 (0%)	43	24
1	B	523/525 (100%)	503 (96%)	18 (3%)	2 (0%)	43	24
1	C	523/525 (100%)	504 (96%)	18 (3%)	1 (0%)	56	38
1	D	523/525 (100%)	503 (96%)	18 (3%)	2 (0%)	43	24
All	All	2092/2100 (100%)	2014 (96%)	71 (3%)	7 (0%)	50	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ASP
1	C	87	THR
1	D	87	THR
1	A	87	THR
1	B	87	THR
1	A	289	HIS
1	B	289	HIS

### 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	433/433 (100%)	427 (99%)	6 (1%)	78	68
1	B	433/433 (100%)	430 (99%)	3 (1%)	91	87
1	C	433/433 (100%)	432 (100%)	1 (0%)	96	95
1	D	433/433 (100%)	425 (98%)	8 (2%)	71	57
All	All	1732/1732 (100%)	1714 (99%)	18 (1%)	85	80

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	188	GLU
1	A	360	LEU
1	A	385	MET
1	A	477	ASP
1	A	493	MET
1	B	188	GLU
1	B	428	PRO
1	B	511	ASN
1	C	428	PRO
1	D	94	LEU
1	D	118	GLU
1	D	330	SER
1	D	360	LEU
1	D	428	PRO
1	D	441	LYS
1	D	452	GLN
1	D	511	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	180	ASN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	531	GLN
1	B	354	ASN
1	B	511	ASN
1	B	531	GLN
1	C	204	GLN
1	C	266	GLN
1	C	368	ASN
1	D	128	GLN
1	D	180	ASN
1	D	201	GLN
1	D	204	GLN
1	D	205	GLN
1	D	452	GLN
1	D	511	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
3	A12	A	1602	2	29,29,29	1.32	5 (17%)	45,45,45	0.88	2 (4%)
3	A12	B	1603	2	29,29,29	1.59	5 (17%)	45,45,45	0.77	0
3	A12	C	1604	2	29,29,29	1.20	3 (10%)	45,45,45	0.82	1 (2%)
3	A12	D	1605	2	29,29,29	1.42	4 (13%)	45,45,45	0.83	1 (2%)

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
3	A12	A	1602	2	-	0/16/32/32	0/1/3/3
3	A12	B	1603	2	-	0/16/32/32	0/1/3/3
3	A12	C	1604	2	-	0/16/32/32	0/1/3/3
3	A12	D	1605	2	-	0/16/32/32	0/1/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1603	A12	PB-C3A	-5.22	1.75	1.79
3	D	1605	A12	PB-O3B	-4.22	1.46	1.54
3	A	1602	A12	PB-C3A	-3.69	1.76	1.79
3	B	1603	A12	PA-O2A	-3.67	1.47	1.56
3	C	1604	A12	PB-O2B	-3.56	1.47	1.54
3	B	1603	A12	PB-O3B	-3.48	1.47	1.54
3	D	1605	A12	PB-O2B	-3.36	1.48	1.54
3	D	1605	A12	PA-O2A	-3.33	1.48	1.56
3	C	1604	A12	PA-O2A	-3.05	1.48	1.56
3	A	1602	A12	PA-O2A	-3.03	1.48	1.56
3	D	1605	A12	PB-C3A	-2.98	1.77	1.79
3	A	1602	A12	PB-O3B	-2.87	1.49	1.54
3	B	1603	A12	PB-O2B	-2.64	1.49	1.54
3	C	1604	A12	PB-C3A	-2.48	1.77	1.79
3	A	1602	A12	PB-O2B	-2.47	1.49	1.54
3	B	1603	A12	PA-C3A	-2.14	1.77	1.79
3	A	1602	A12	PA-C3A	-2.09	1.78	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1602	A12	O5'-PA-O1A	-2.44	108.12	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	D	1605	A12	O5'-PA-C3A	2.21	109.46	103.97
3	C	1604	A12	O5'-PA-O1A	-2.08	109.02	114.21
3	A	1602	A12	O5'-PA-C3A	2.01	108.97	103.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	525/525 (100%)	0.06	14 (2%) 52 48	21, 34, 52, 65	0
1	B	525/525 (100%)	-0.00	13 (2%) 54 52	18, 31, 50, 62	0
1	C	525/525 (100%)	-0.06	6 (1%) 77 76	18, 31, 50, 58	0
1	D	525/525 (100%)	-0.00	19 (3%) 41 38	18, 32, 49, 63	0
All	All	2100/2100 (100%)	-0.00	52 (2%) 54 52	18, 32, 51, 65	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	ALA	5.9
1	D	328	GLY	5.8
1	A	327	ASP	4.8
1	D	324	THR	4.6
1	A	328	GLY	4.2
1	D	330	SER	4.0
1	D	327	ASP	3.8
1	B	474	LYS	3.8
1	B	359	GLN	3.7
1	D	325	TRP	3.7
1	B	489	LYS	3.6
1	A	471	LYS	3.5
1	D	162	ASP	3.3
1	A	329	LYS	3.2
1	A	472	ASP	3.2
1	A	324	THR	3.1
1	D	513	PRO	3.1
1	D	329	LYS	3.1
1	B	357	LYS	3.1
1	D	26	TYR	3.0
1	B	471	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	472	ASP	2.8
1	A	326	GLU	2.6
1	B	249	VAL	2.6
1	D	29	ASP	2.6
1	C	328	GLY	2.6
1	C	324	THR	2.5
1	C	359	GLN	2.5
1	B	473	GLY	2.4
1	D	323	VAL	2.4
1	B	356	GLY	2.4
1	A	178	ILE	2.3
1	D	268	ASP	2.3
1	B	488	ALA	2.3
1	B	550	GLN	2.3
1	A	185	THR	2.3
1	A	358	ALA	2.3
1	D	182	GLU	2.3
1	D	516	VAL	2.3
1	C	356	GLY	2.2
1	C	326	GLU	2.2
1	D	249	VAL	2.2
1	D	474	LYS	2.1
1	D	32	TYR	2.1
1	A	249	VAL	2.1
1	D	261	ALA	2.1
1	A	473	GLY	2.1
1	A	161	GLN	2.1
1	C	535	PRO	2.1
1	A	474	LYS	2.0
1	D	185	THR	2.0
1	B	328	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	A12	D	1605	27/27	0.10	0.30	27,36,42,44	0
3	A12	C	1604	27/27	0.07	-0.59	23,27,32,34	0
3	A12	A	1602	27/27	0.09	-0.79	25,28,37,38	0
3	A12	B	1603	27/27	0.06	-1.21	25,28,32,35	0
2	MN	D	600	1/1	0.08	-1.23	22,22,22,22	0
2	MN	C	600	1/1	0.09	-1.54	20,20,20,20	0
2	MN	A	601	1/1	0.08	-1.70	46,46,46,46	0
2	MN	B	601	1/1	0.07	-1.98	45,45,45,45	0
2	MN	B	600	1/1	0.06	-2.01	24,24,24,24	0
2	MN	A	600	1/1	0.07	-2.39	26,26,26,26	0
2	MN	D	601	1/1	0.04	-3.36	36,36,36,36	0
2	MN	C	601	1/1	0.02	-8.39	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.