



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:52 AM EDT

PDB ID : 7MC9  
Title : X-RAY STRUCTURE OF PEDV PAPAIN-LIKE PROTEASE 2 bound to UB-PA  
Authors : Durie, I.A.; Dzimianski, J.V.; Daczkowski, C.M.; Pegan, S.D.  
Deposited on : 2021-04-01  
Resolution : 3.10 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

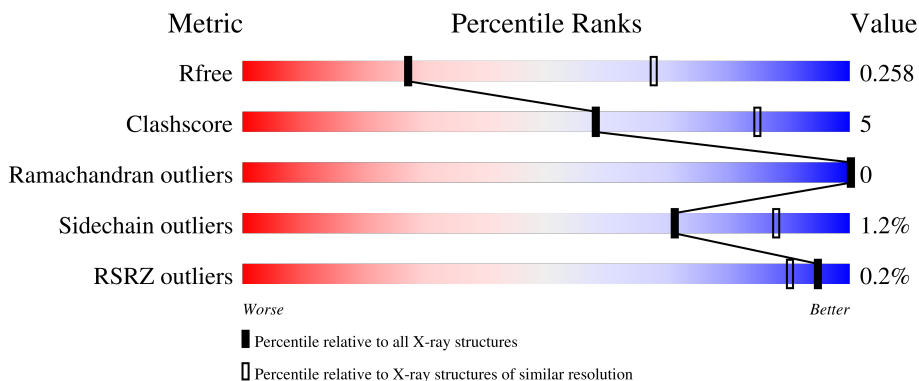
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	237	83% 15% .
1	C	237	81% 16% .
1	E	237	82% 14% ..
1	G	237	88% 9% .
1	I	237	88% 11% .

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Mol	Chain	Length	Quality of chain
1	K	237	 86% 13%
1	M	237	 87% 11%
1	O	237	 88% 11%
2	B	75	 93% 7%
2	D	75	 89% 11%
2	F	75	 80% 19%
2	H	75	 79% 20%
2	J	75	 89% 11%
2	L	75	 80% 20%
2	N	75	 79% 21%
2	P	75	 95% 5%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19153 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1790	1141	304	332	13	0	0	0
1	C	233	1790	1141	304	332	13	0	0	0
1	E	230	1771	1130	300	328	13	0	0	0
1	G	232	1786	1139	303	331	13	0	0	0
1	I	235	1802	1147	307	335	13	0	0	0
1	K	235	1802	1147	307	335	13	0	0	0
1	M	232	1783	1136	303	331	13	0	0	0
1	O	235	1802	1147	307	335	13	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3371	GLY	-	expression tag	UNP A0A0S3MQV7
A	3372	SER	-	expression tag	UNP A0A0S3MQV7
A	3373	HIS	-	expression tag	UNP A0A0S3MQV7
A	3374	MET	-	expression tag	UNP A0A0S3MQV7
C	1686	GLY	-	expression tag	UNP A0A0S3MQV7
C	1687	SER	-	expression tag	UNP A0A0S3MQV7
C	1688	HIS	-	expression tag	UNP A0A0S3MQV7
C	1689	MET	-	expression tag	UNP A0A0S3MQV7
E	1686	GLY	-	expression tag	UNP A0A0S3MQV7
E	1687	SER	-	expression tag	UNP A0A0S3MQV7
E	1688	HIS	-	expression tag	UNP A0A0S3MQV7
E	1689	MET	-	expression tag	UNP A0A0S3MQV7
G	1686	GLY	-	expression tag	UNP A0A0S3MQV7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1687	SER	-	expression tag	UNP A0A0S3MQV7
G	1688	HIS	-	expression tag	UNP A0A0S3MQV7
G	1689	MET	-	expression tag	UNP A0A0S3MQV7
I	1686	GLY	-	expression tag	UNP A0A0S3MQV7
I	1687	SER	-	expression tag	UNP A0A0S3MQV7
I	1688	HIS	-	expression tag	UNP A0A0S3MQV7
I	1689	MET	-	expression tag	UNP A0A0S3MQV7
K	1	GLY	-	expression tag	UNP A0A0S3MQV7
K	2	SER	-	expression tag	UNP A0A0S3MQV7
K	3	HIS	-	expression tag	UNP A0A0S3MQV7
K	4	MET	-	expression tag	UNP A0A0S3MQV7
M	1686	GLY	-	expression tag	UNP A0A0S3MQV7
M	1687	SER	-	expression tag	UNP A0A0S3MQV7
M	1688	HIS	-	expression tag	UNP A0A0S3MQV7
M	1689	MET	-	expression tag	UNP A0A0S3MQV7
O	1686	GLY	-	expression tag	UNP A0A0S3MQV7
O	1687	SER	-	expression tag	UNP A0A0S3MQV7
O	1688	HIS	-	expression tag	UNP A0A0S3MQV7
O	1689	MET	-	expression tag	UNP A0A0S3MQV7

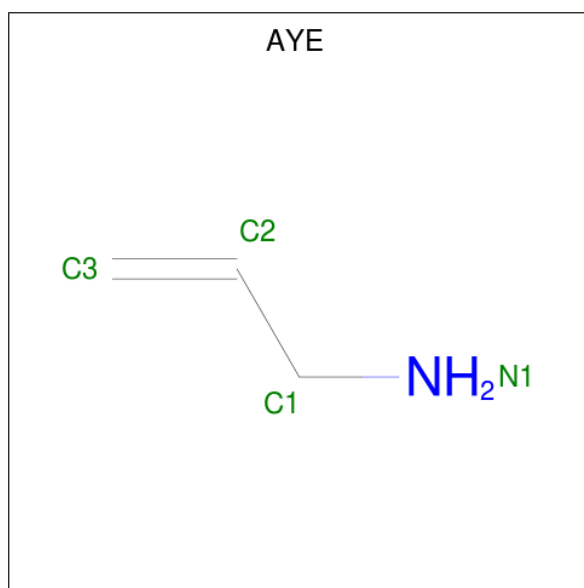
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	D	75	Total	C	N	O	S	0	0	0
			593	372	104	116	1			
2	F	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	H	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	J	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	L	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	N	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	P	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Zn 3	0	0
3	C	1	Total 1	Zn 1	0	0
3	E	3	Total 3	Zn 3	0	0
3	G	2	Total 2	Zn 2	0	0
3	I	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	M	2	Total 2	Zn 2	0	0
3	O	1	Total 1	Zn 1	0	0

- Molecule 4 is prop-2-en-1-amine (three-letter code: AYE) (formula: C<sub>3</sub>H<sub>7</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 4	C 3	N 1	0	0
4	D	1	Total 4	C 3	N 1	0	0
4	F	1	Total 4	C 3	N 1	0	0
4	H	1	Total 4	C 3	N 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	N	0	0
			4	3	1		
4	L	1	Total	C	N	0	0
			4	3	1		
4	N	1	Total	C	N	0	0
			4	3	1		
4	P	1	Total	C	N	0	0
			4	3	1		


- Molecule 5 is water.

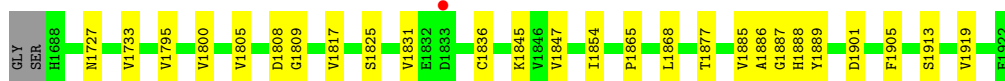
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total	O	0	0
			3	3		
5	D	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		
5	I	1	Total	O	0	0
			1	1		
5	K	1	Total	O	0	0
			1	1		






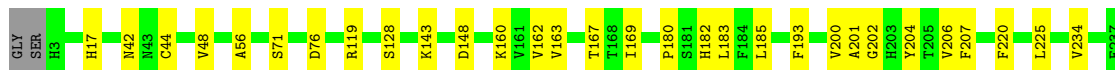
- Molecule 1: 3C-like proteinase

Chain I:  88% 11%



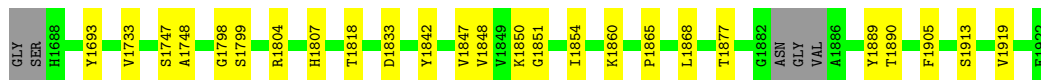
- Molecule 1: 3C-like proteinase

Chain K:  86% 13%




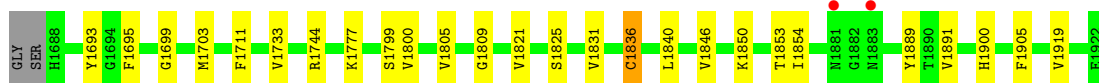
- Molecule 1: 3C-like proteinase

Chain M:  87% 11%



- Molecule 1: 3C-like proteinase

Chain O:  88% 11%

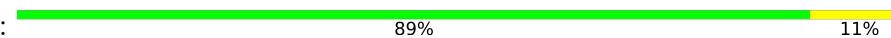


- Molecule 2: Ubiquitin

Chain B:  93% 7%




- Molecule 2: Ubiquitin

Chain D:  89% 11%




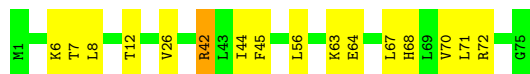
- Molecule 2: Ubiquitin

Chain F:  80% 19%




- Molecule 2: Ubiquitin

Chain H:  79% 20%




- Molecule 2: Ubiquitin

Chain J:  89% 11%




- Molecule 2: Ubiquitin

Chain L:  80% 20%



- Molecule 2: Ubiquitin

Chain N:  79% 21%



- Molecule 2: Ubiquitin

Chain P:  95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.14Å 136.87Å 193.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.10 49.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.07-3.10) 97.3 (49.07-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.200 , 0.257 0.201 , 0.258	Depositor DCC
$R_{free}$ test set	2352 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 26.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: AYE, ZN

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	0.24	0/1835	0.42	0/2500
1	C	0.24	0/1835	0.42	0/2500
1	E	0.24	0/1816	0.42	0/2474
1	G	0.24	0/1831	0.42	0/2495
1	I	0.24	0/1848	0.42	0/2519
1	K	0.25	0/1848	0.43	0/2519
1	M	0.24	0/1828	0.42	0/2490
1	O	0.24	0/1848	0.41	0/2519
2	B	0.23	0/603	0.42	0/811
2	D	0.24	0/599	0.44	0/805
2	F	0.23	0/603	0.44	0/811
2	H	0.23	0/603	0.43	0/811
2	J	0.24	0/603	0.42	0/811
2	L	0.23	0/603	0.43	0/811
2	N	0.23	0/603	0.42	0/811
2	P	0.24	0/603	0.43	0/811
All	All	0.24	0/19509	0.42	0/26498

There are no bond length outliers.

There are no bond angle outliers.

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	1790	0	1733	19	0
1	C	1790	0	1734	23	0
1	E	1771	0	1716	21	0
1	G	1786	0	1732	15	0
1	I	1802	0	1743	14	0
1	K	1802	0	1743	23	0
1	M	1783	0	1724	14	0
1	O	1802	0	1743	16	0
2	B	597	0	626	2	0
2	D	593	0	616	4	0
2	F	597	0	626	9	0
2	H	597	0	626	10	0
2	J	597	0	626	4	0
2	L	597	0	626	11	0
2	N	597	0	626	10	0
2	P	597	0	626	2	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
3	E	3	0	0	0	0
3	G	2	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	2	0	0	0	0
3	O	1	0	0	0	0
4	B	4	0	4	3	0
4	D	4	0	4	1	0
4	F	4	0	1	2	0
4	H	4	0	2	0	0
4	J	4	0	3	2	0
4	L	4	0	5	1	0
4	N	4	0	4	0	0
4	P	4	0	4	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
All	All	19153	0	18893	183	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 5.

All (183) 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:1796:PRO:HD2	1:M:1818:THR:HG21	1.67	0.76
1:K:148:ASP:OD1	2:L:68:HIS:NE2	2.21	0.73
2:J:7:THR:HG23	2:J:69:LEU:HD23	1.71	0.72
1:C:1889:TYR:HB2	4:D:101:AYE:H3A	1.72	0.70
1:K:200:VAL:HG23	1:K:201:ALA:H	1.57	0.69
1:I:1887:GLY:O	4:J:101:AYE:N1	2.29	0.66
2:H:8:LEU:HD21	2:H:71:LEU:HD13	1.78	0.66
1:M:1860:LYS:HD2	2:N:8:LEU:HB2	1.79	0.63
1:E:1827:LEU:HD11	1:E:1862:VAL:HG21	1.81	0.63
1:E:1825:SER:HB2	1:E:1831:VAL:HG13	1.80	0.62
1:G:1825:SER:HB2	1:G:1831:VAL:HG13	1.81	0.61
1:C:1865:PRO:HD2	1:C:1868:LEU:HD12	1.84	0.60
1:O:1854:ILE:HG12	1:O:1919:VAL:HG22	1.83	0.60
1:K:207:PHE:HE2	1:K:225:LEU:HB2	1.66	0.59
1:E:1806:THR:HG21	1:E:1836:CYS:HB2	1.85	0.59
1:I:1854:ILE:HG12	1:I:1919:VAL:HG22	1.83	0.58
1:K:44:CYS:HB2	1:K:204:TYR:HB2	1.85	0.58
1:K:202:GLY:H	2:L:75:GLY:HA2	1.67	0.58
1:I:1727:ASN:HA	4:J:101:AYE:H3	1.84	0.58
1:A:3561:THR:HG22	1:A:3576:VAL:HG22	1.84	0.58
2:F:7:THR:HG22	2:F:11:LYS:O	2.04	0.57
1:M:1865:PRO:HD2	1:M:1868:LEU:HD12	1.86	0.57
1:K:71:SER:HB3	1:K:76:ASP:HB3	1.85	0.57
2:P:63:LYS:HG2	2:P:64:GLU:HG3	1.86	0.57
2:F:44:ILE:HB	2:F:68:HIS:HB2	1.85	0.57
1:M:1804:ARG:NH2	1:M:1833:ASP:OD2	2.37	0.57
2:H:42:ARG:HG3	2:H:70:VAL:HG23	1.87	0.57
1:K:42:ASN:HA	4:L:101:AYE:H3A	1.87	0.56
1:G:1818:THR:HG21	1:I:1795:VAL:HG13	1.88	0.56
2:H:26:VAL:HG21	2:H:56:LEU:HD21	1.88	0.56
1:O:1800:VAL:HG23	1:O:1853:THR:HG21	1.88	0.55
1:C:1733:VAL:HG11	1:C:1889:TYR:HB3	1.89	0.55
1:E:1800:VAL:HG13	1:E:1846:VAL:HG13	1.89	0.55
1:K:160:LYS:HE2	1:K:162:VAL:HG12	1.88	0.55
1:M:1847:VAL:HG23	1:M:1848:VAL:HG23	1.89	0.55
1:A:3550:PRO:HD2	1:A:3553:LEU:HD12	1.88	0.54
1:M:1854:ILE:HG12	1:M:1919:VAL:HG22	1.89	0.54
1:A:3521:CYS:HB2	1:A:3522:PRO:HD2	1.88	0.54
1:G:1854:ILE:HG12	1:G:1919:VAL:HG22	1.90	0.54
2:L:63:LYS:HG3	2:L:64:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:VAL:HG21	2:D:56:LEU:HD21	1.90	0.54
1:I:1845:LYS:HE2	1:I:1847:VAL:HG12	1.89	0.54
2:L:1:MET:HB2	2:L:63:LYS:HD3	1.89	0.54
2:N:5:VAL:HG21	2:N:30:ILE:HD11	1.90	0.54
1:I:1885:VAL:HG12	1:I:1886:ALA:H	1.73	0.53
2:P:60:ASN:OD1	2:P:62:GLN:NE2	2.42	0.53
2:F:45:PHE:HB3	2:F:50:LEU:HD21	1.91	0.53
1:A:3575:THR:OG1	1:A:3585:HIS:O	2.22	0.53
2:F:42:ARG:HG3	2:F:70:VAL:HG23	1.92	0.52
1:G:1898:MET:HB2	1:G:1905:PHE:CZ	2.45	0.52
1:A:3415:TRP:CE2	1:A:3466:SER:HB3	2.45	0.52
2:J:23:ILE:HD12	2:J:50:LEU:HD13	1.92	0.51
1:C:1905:PHE:HD2	1:E:1905:PHE:HD2	1.58	0.51
1:I:1825:SER:HB2	1:I:1831:VAL:HG13	1.93	0.51
1:G:1877:THR:OG1	1:G:1890:THR:OG1	2.25	0.51
1:M:1877:THR:OG1	1:M:1890:THR:OG1	2.29	0.51
1:O:1733:VAL:HG11	1:O:1889:TYR:HB3	1.93	0.51
1:O:1733:VAL:HG12	1:O:1891:VAL:HG23	1.92	0.51
2:B:45:PHE:HB2	2:B:67:LEU:HD22	1.93	0.50
1:C:1827:LEU:HD11	1:C:1862:VAL:HG21	1.94	0.50
1:E:1733:VAL:HG11	1:E:1889:TYR:HB3	1.93	0.50
1:C:1712:PRO:HB2	1:C:1723:LYS:HD2	1.93	0.49
1:C:1796:PRO:HG3	1:C:1820:PRO:HD3	1.94	0.49
1:G:1896:THR:HG1	1:G:1905:PHE:HZ	1.57	0.49
2:L:56:LEU:HG	2:L:61:ILE:HD12	1.94	0.49
2:N:42:ARG:HB3	2:N:49:GLN:HE22	1.78	0.49
2:H:6:LYS:HD3	2:H:12:THR:HB	1.95	0.48
2:N:42:ARG:HB2	2:N:70:VAL:HG23	1.95	0.48
1:A:3414:CYS:HB3	4:B:101:AYE:H3A	1.50	0.48
1:C:1800:VAL:HG13	1:C:1846:VAL:HG13	1.96	0.48
2:N:63:LYS:HG2	2:N:64:GLU:HG3	1.95	0.48
1:A:3418:VAL:HG11	1:A:3574:TYR:HB3	1.94	0.48
2:H:45:PHE:HB2	2:H:67:LEU:HD22	1.96	0.48
1:G:1812:CYS:SG	1:G:1813:SER:N	2.86	0.48
2:H:7:THR:HG22	2:H:8:LEU:H	1.79	0.47
2:H:44:ILE:HG13	2:H:68:HIS:HB2	1.96	0.47
1:K:119:ARG:HB3	1:K:128:SER:HB3	1.95	0.47
1:C:1901:ASP:O	1:C:1904:VAL:HG22	2.14	0.47
1:K:48:VAL:HG11	1:K:204:TYR:HB3	1.97	0.47
1:C:1877:THR:OG1	1:C:1890:THR:OG1	2.26	0.47
1:E:1729:CYS:H	4:F:101:AYE:C2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180:PRO:HD2	1:K:183:LEU:HD12	1.96	0.47
1:G:1877:THR:HG21	1:G:1913:SER:HB3	1.97	0.47
1:O:1836:CYS:N	1:O:1840:LEU:O	2.37	0.47
2:D:61:ILE:HG23	2:D:65:SER:HB2	1.97	0.47
2:F:56:LEU:HD22	2:F:61:ILE:HD12	1.97	0.47
1:A:3441:SER:HB3	1:A:3446:ASP:HB3	1.97	0.47
1:G:1733:VAL:HG12	1:G:1891:VAL:HG23	1.97	0.47
1:K:193:PHE:CE1	1:K:202:GLY:HA3	2.50	0.47
1:I:1865:PRO:HD2	1:I:1868:LEU:HD12	1.97	0.46
2:N:7:THR:HG22	2:N:8:LEU:H	1.80	0.46
1:G:1860:LYS:NZ	2:H:8:LEU:HB3	2.30	0.46
2:B:63:LYS:HG3	2:B:64:GLU:HG3	1.97	0.46
1:C:1814:LYS:HB2	1:M:1748:ALA:HB2	1.98	0.46
1:O:1800:VAL:HG13	1:O:1846:VAL:HG13	1.97	0.46
1:I:1877:THR:HG21	1:I:1913:SER:HB3	1.98	0.46
1:A:3384:GLY:O	1:A:3388:MET:HG3	2.16	0.46
1:G:1808:ASP:OD1	1:K:17:HIS:NE2	2.49	0.46
1:A:3398:SER:OG	1:A:3405:ARG:NH1	2.49	0.46
1:K:169:ILE:HG12	1:K:234:VAL:HG22	1.98	0.45
1:O:1850:LYS:HE3	1:O:1850:LYS:HB2	1.80	0.45
1:O:1825:SER:HB2	1:O:1831:VAL:HG22	1.98	0.45
1:C:1806:THR:HG21	1:C:1836:CYS:SG	2.57	0.45
1:K:56:ALA:HA	1:K:167:THR:HG21	1.98	0.45
2:N:8:LEU:HD12	2:N:9:THR:HG23	1.98	0.45
1:E:1713:SER:HB2	1:E:1720:ARG:HD2	1.99	0.45
1:E:1731:VAL:HG13	1:E:1769:LEU:HD12	1.99	0.45
1:A:3485:VAL:HG13	1:A:3531:VAL:HG13	1.99	0.45
1:C:1723:LYS:NZ	1:C:1903:ASP:OD2	2.50	0.45
1:C:1825:SER:HB2	1:C:1831:VAL:HG13	1.98	0.45
2:L:7:THR:HG22	2:L:8:LEU:H	1.82	0.45
1:E:1729:CYS:H	4:F:101:AYE:C3	2.30	0.45
2:F:45:PHE:HB2	2:F:67:LEU:HD22	1.99	0.45
1:I:1888:HIS:NE2	1:I:1901:ASP:OD1	2.42	0.45
1:M:1733:VAL:HG11	1:M:1889:TYR:HB3	1.98	0.44
1:O:1799:SER:N	1:O:1850:LYS:O	2.50	0.44
1:A:3572:GLY:O	4:B:101:AYE:N1	2.50	0.44
2:L:42:ARG:HG3	2:L:70:VAL:HG23	1.98	0.44
1:I:1733:VAL:HG11	1:I:1889:TYR:HB3	1.99	0.44
2:J:7:THR:HG22	2:J:8:LEU:N	2.32	0.44
1:A:3400:VAL:HG23	1:A:3405:ARG:NH2	2.33	0.44
1:C:1909:ASP:HB3	1:C:1912:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:42:ARG:HD2	2:L:49:GLN:HE22	1.83	0.44
1:K:207:PHE:CE2	1:K:225:LEU:HB2	2.50	0.43
1:O:1821:VAL:HG22	1:O:1854:ILE:HB	1.99	0.43
1:C:1769:LEU:HD21	1:C:1790:LEU:HD11	2.00	0.43
1:E:1804:ARG:O	1:E:1812:CYS:HA	2.18	0.43
2:H:8:LEU:H	2:H:8:LEU:HD12	1.83	0.43
1:K:162:VAL:HG23	1:K:163:VAL:HG23	2.00	0.43
2:N:43:LEU:HB3	2:N:50:LEU:HD12	2.00	0.43
1:O:1805:VAL:HG22	1:O:1809:GLY:HA2	2.01	0.43
1:A:3535:LYS:HD2	1:O:1744:ARG:HH22	1.84	0.43
1:E:1805:VAL:O	1:E:1843:ILE:N	2.51	0.43
1:C:1801:THR:HB	1:C:1848:VAL:HB	2.00	0.43
1:K:143:LYS:HG2	1:K:185:LEU:HD23	2.01	0.43
1:A:3510:SER:HB2	1:A:3516:VAL:HG13	2.00	0.43
2:N:45:PHE:HB2	2:N:67:LEU:HD22	2.01	0.43
1:O:1711:PHE:HE1	1:O:1777:LYS:HE3	1.83	0.43
1:A:3395:ALA:HB2	1:A:3448:ALA:HB2	2.00	0.43
1:A:3583:MET:HB2	1:A:3590:PHE:CE2	2.54	0.42
1:C:1730:TRP:HB3	2:D:75:GLY:HA3	2.01	0.42
1:E:1849:VAL:HG21	1:E:1920:VAL:HG11	2.01	0.42
1:M:1798:GLY:HA2	1:M:1851:GLY:HA3	2.01	0.42
1:E:1756:SER:HB3	1:E:1761:ASP:HB3	2.00	0.42
1:C:1805:VAL:HG22	1:C:1806:THR:H	1.83	0.42
2:L:15:LEU:HD22	2:L:29:LYS:HB3	2.02	0.42
1:E:1877:THR:OG1	1:E:1890:THR:OG1	2.35	0.42
1:K:193:PHE:HE1	1:K:202:GLY:HA3	1.85	0.42
1:I:1805:VAL:HG22	1:I:1809:GLY:HA2	2.02	0.42
2:L:56:LEU:HB3	2:L:61:ILE:HB	2.02	0.42
2:H:63:LYS:HG2	2:H:64:GLU:HG3	2.01	0.42
1:C:1845:LYS:HE2	1:C:1847:VAL:HG12	2.01	0.42
1:G:1796:PRO:HG3	1:G:1820:PRO:HD3	2.02	0.42
1:M:1877:THR:HG21	1:M:1913:SER:HB3	2.01	0.42
1:O:1891:VAL:HB	1:O:1900:HIS:HB2	2.01	0.42
1:A:3412:ASN:HA	4:B:101:AYE:H3	2.02	0.41
1:C:1736:LEU:HA	1:C:1739:GLN:HE21	1.85	0.41
1:E:1730:TRP:CD2	1:E:1781:SER:HB3	2.55	0.41
1:M:1693:TYR:O	1:M:1747:SER:OG	2.31	0.41
1:K:48:VAL:HG12	1:K:206:VAL:HG23	2.01	0.41
2:N:27:LYS:HB3	2:N:38:PRO:HB3	2.01	0.41
1:G:1769:LEU:HD23	1:G:1769:LEU:HA	1.94	0.41
1:M:1799:SER:N	1:M:1850:LYS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1699:GLY:O	1:O:1703:MET:HG3	2.20	0.41
1:G:1733:VAL:HG11	1:G:1889:TYR:HB3	2.02	0.41
2:J:45:PHE:HB2	2:J:67:LEU:HD22	2.01	0.41
1:A:3562:THR:HG21	1:A:3598:SER:HB3	2.03	0.41
1:E:1831:VAL:HG21	1:E:1858:VAL:HG21	2.01	0.41
1:I:1808:ASP:HB3	1:M:1807:HIS:NE2	2.35	0.41
1:C:1713:SER:HB2	1:C:1720:ARG:HD2	2.02	0.41
1:E:1804:ARG:HA	1:E:1843:ILE:O	2.21	0.41
2:F:63:LYS:HG2	2:F:64:GLU:HG3	2.03	0.41
1:K:148:ASP:O	2:L:66:THR:HG21	2.21	0.41
1:E:1890:THR:HG22	1:E:1901:ASP:HA	2.02	0.41
1:K:143:LYS:NZ	1:K:182:HIS:O	2.46	0.41
1:O:1693:TYR:HB3	1:O:1695:PHE:CE1	2.55	0.41
1:E:1866:SER:HB2	1:E:1910:LEU:HD23	2.02	0.40
1:I:1800:VAL:HG12	1:I:1817:VAL:HB	2.03	0.40
1:K:207:PHE:HD2	1:K:225:LEU:HD13	1.85	0.40
1:E:1833:ASP:OD2	2:F:68:HIS:NE2	2.54	0.40
2:F:41:GLN:HB2	2:F:69:LEU:HD11	2.03	0.40
2:D:37:PRO:HA	2:D:38:PRO:HD3	1.99	0.40
1:G:1801:THR:HB	1:G:1848:VAL:HB	2.04	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	229/237 (97%)	218 (95%)	11 (5%)	0	100	100
1	C	229/237 (97%)	223 (97%)	6 (3%)	0	100	100
1	E	226/237 (95%)	218 (96%)	8 (4%)	0	100	100
1	G	228/237 (96%)	221 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	233/237 (98%)	227 (97%)	6 (3%)	0	100	100
1	K	233/237 (98%)	223 (96%)	10 (4%)	0	100	100
1	M	228/237 (96%)	222 (97%)	6 (3%)	0	100	100
1	O	233/237 (98%)	229 (98%)	4 (2%)	0	100	100
2	B	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	D	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	F	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
2	H	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
2	J	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	L	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
2	N	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	P	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
All	All	2423/2496 (97%)	2353 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	200/202 (99%)	196 (98%)	4 (2%)	55	80
1	C	200/202 (99%)	196 (98%)	4 (2%)	55	80
1	E	198/202 (98%)	194 (98%)	4 (2%)	55	80
1	G	200/202 (99%)	199 (100%)	1 (0%)	88	94
1	I	201/202 (100%)	199 (99%)	2 (1%)	76	90
1	K	201/202 (100%)	200 (100%)	1 (0%)	88	94
1	M	199/202 (98%)	197 (99%)	2 (1%)	76	90
1	O	201/202 (100%)	199 (99%)	2 (1%)	76	90
2	B	68/68 (100%)	67 (98%)	1 (2%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	67/68 (98%)	66 (98%)	1 (2%)	65	85
2	F	68/68 (100%)	67 (98%)	1 (2%)	65	85
2	H	68/68 (100%)	66 (97%)	2 (3%)	42	72
2	J	68/68 (100%)	67 (98%)	1 (2%)	65	85
2	L	68/68 (100%)	68 (100%)	0	100	100
2	N	68/68 (100%)	68 (100%)	0	100	100
2	P	68/68 (100%)	68 (100%)	0	100	100
All	All	2143/2160 (99%)	2117 (99%)	26 (1%)	71	88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3375	ASP
1	A	3381	ASP
1	A	3556	LYS
1	A	3590	PHE
2	B	32	ASP
1	C	1729	CYS
1	C	1808	ASP
1	C	1881	ASN
1	C	1905	PHE
2	D	32	ASP
1	E	1696	ASP
1	E	1829	LEU
1	E	1833	ASP
1	E	1905	PHE
2	F	42	ARG
1	G	1905	PHE
2	H	42	ARG
2	H	72	ARG
1	I	1836	CYS
1	I	1905	PHE
2	J	32	ASP
1	K	220	PHE
1	M	1842	TYR
1	M	1905	PHE
1	O	1836	CYS
1	O	1905	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	$\# Z  > 2$
4	AYE	J	101	2,1	3,3,3	0.42	0	1,2,2	1.21	0
4	AYE	H	101	2,1	3,3,3	0.46	0	1,2,2	1.03	0
4	AYE	D	101	2,1	3,3,3	0.46	0	1,2,2	1.19	0
4	AYE	F	101	2,1	3,3,3	0.53	0	1,2,2	0.88	0
4	AYE	N	101	2,1	3,3,3	0.48	0	1,2,2	1.10	0
4	AYE	P	101	2,1	3,3,3	0.47	0	1,2,2	0.99	0
4	AYE	L	101	2,1	3,3,3	0.46	0	1,2,2	1.19	0
4	AYE	B	101	2,1	3,3,3	0.47	0	1,2,2	1.16	0

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
4	AYE	J	101	2,1	-	0/1/1/1	-
4	AYE	H	101	2,1	-	0/1/1/1	-
4	AYE	D	101	2,1	-	1/1/1/1	-
4	AYE	F	101	2,1	-	1/1/1/1	-
4	AYE	N	101	2,1	-	1/1/1/1	-
4	AYE	P	101	2,1	-	1/1/1/1	-
4	AYE	L	101	2,1	-	1/1/1/1	-
4	AYE	B	101	2,1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	101	AYE	N1-C1-C2-C3
4	D	101	AYE	N1-C1-C2-C3
4	F	101	AYE	N1-C1-C2-C3
4	L	101	AYE	N1-C1-C2-C3
4	N	101	AYE	N1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	101	AYE	2	0
4	D	101	AYE	1	0
4	F	101	AYE	2	0
4	L	101	AYE	1	0
4	B	101	AYE	3	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 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, 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	233/237 (98%)	-0.50	0 100 100	24, 43, 66, 89	0
1	C	233/237 (98%)	-0.48	0 100 100	23, 42, 63, 83	0
1	E	230/237 (97%)	-0.47	0 100 100	20, 43, 63, 76	0
1	G	232/237 (97%)	-0.45	0 100 100	24, 40, 62, 88	0
1	I	235/237 (99%)	-0.45	1 (0%) 92 84	25, 44, 63, 104	0
1	K	235/237 (99%)	-0.25	0 100 100	33, 57, 98, 116	0
1	M	232/237 (97%)	-0.41	0 100 100	29, 57, 85, 96	0
1	O	235/237 (99%)	-0.33	2 (0%) 84 69	32, 59, 81, 115	0
2	B	75/75 (100%)	-0.29	0 100 100	29, 57, 76, 84	0
2	D	75/75 (100%)	-0.34	0 100 100	29, 52, 72, 85	0
2	F	75/75 (100%)	-0.19	0 100 100	36, 63, 86, 91	0
2	H	75/75 (100%)	-0.45	0 100 100	33, 58, 79, 89	0
2	J	75/75 (100%)	-0.38	0 100 100	34, 59, 84, 93	0
2	L	75/75 (100%)	-0.10	1 (1%) 77 59	49, 85, 112, 121	0
2	N	75/75 (100%)	0.03	0 100 100	49, 77, 95, 108	0
2	P	75/75 (100%)	0.15	0 100 100	51, 83, 99, 108	0
All	All	2465/2496 (98%)	-0.36	4 (0%) 95 90	20, 52, 87, 121	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1883	ASN	2.5
2	L	8	LEU	2.3
1	I	1833	ASP	2.1
1	O	1881	ASN	2.1

## 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 monosaccharides 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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	K	301	1/1	0.81	0.08	88,88,88,88	0
3	ZN	G	2002	1/1	0.85	0.13	47,47,47,47	0
3	ZN	G	2001	1/1	0.90	0.14	82,82,82,82	0
4	AYE	F	101	4/4	0.93	0.21	61,64,66,67	0
4	AYE	J	101	4/4	0.94	0.17	55,63,66,67	0
4	AYE	P	101	4/4	0.94	0.12	64,65,76,77	0
3	ZN	E	2003	1/1	0.95	0.07	96,96,96,96	0
4	AYE	H	101	4/4	0.95	0.19	47,51,56,57	0
3	ZN	A	3702	1/1	0.96	0.11	53,53,53,53	0
4	AYE	L	101	4/4	0.96	0.15	62,65,66,68	0
4	AYE	N	101	4/4	0.96	0.20	67,74,79,86	0
4	AYE	B	101	4/4	0.96	0.14	42,50,51,58	0
3	ZN	C	2001	1/1	0.97	0.13	36,36,36,36	0
3	ZN	E	2001	1/1	0.97	0.07	68,68,68,68	0
3	ZN	A	3701	1/1	0.97	0.09	52,52,52,52	0
4	AYE	D	101	4/4	0.97	0.20	47,51,54,60	0
3	ZN	A	3703	1/1	0.97	0.14	140,140,140,140	0
3	ZN	M	2001	1/1	0.98	0.08	54,54,54,54	0
3	ZN	M	2002	1/1	0.98	0.10	55,55,55,55	0
3	ZN	O	2001	1/1	0.99	0.08	53,53,53,53	0
3	ZN	I	2001	1/1	0.99	0.10	55,55,55,55	0
3	ZN	E	2002	1/1	0.99	0.10	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.