wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 10:43 PM EDT

PDB ID	:	4G0D
Title	:	Human collagenase 3 (MMP-13) full form with peptides from pro-domain
Authors	:	Stura, E.A.; Vera, L.; Visse, R.; Nagase, H.; Dive, V.
Deposited on	:	2012-07-09
Resolution	:	2.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

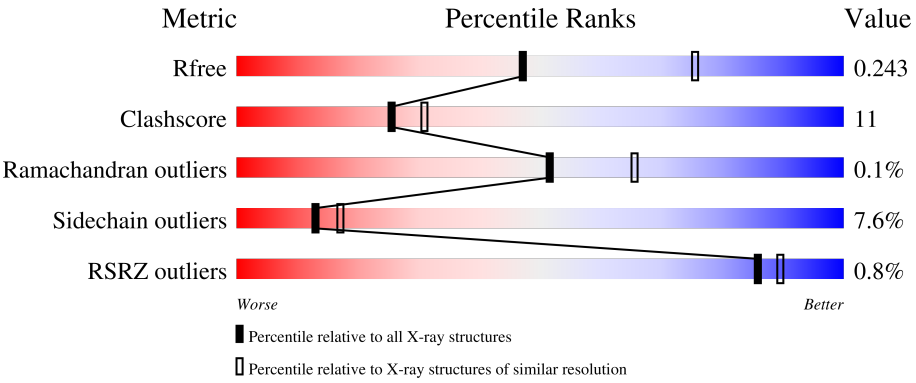
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	368	78% 21% ·
1	B	368	79% 18% ·
1	C	368	75% 23% ·
1	D	368	77% 20% ·
2	W	26	15% 42% 27% · 27%

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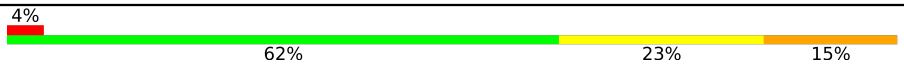
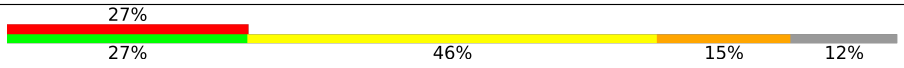
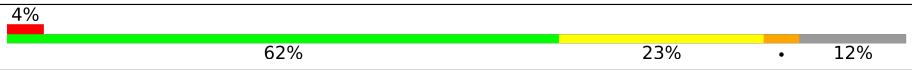
Mol	Chain	Length	Quality of chain
2	X	26	
2	Y	26	
2	Z	26	

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
5	CL	Y	101	-	-	X	-
5	CL	Z	101	-	-	X	-
6	PGO	D	516	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14137 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	5	0
			3042	1971	503	558	10			
1	B	368	Total	C	N	O	S	0	2	0
			3014	1957	497	550	10			
1	C	368	Total	C	N	O	S	0	9	0
			3078	1992	508	568	10			
1	D	368	Total	C	N	O	S	0	3	0
			3021	1960	497	554	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	GLU	engineered mutation	UNP P45452
B	223	ALA	GLU	engineered mutation	UNP P45452
C	223	ALA	GLU	engineered mutation	UNP P45452
D	223	ALA	GLU	engineered mutation	UNP P45452

- Molecule 2 is a protein called Collagenase 3, pro-domain peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	19	Total	C	N	O	0	0	0
			171	108	28	35			
2	X	26	Total	C	N	O	0	0	0
			220	135	35	50			
2	Y	23	Total	C	N	O	0	0	0
			204	127	32	45			
2	Z	23	Total	C	N	O	0	0	0
			204	127	32	45			

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

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

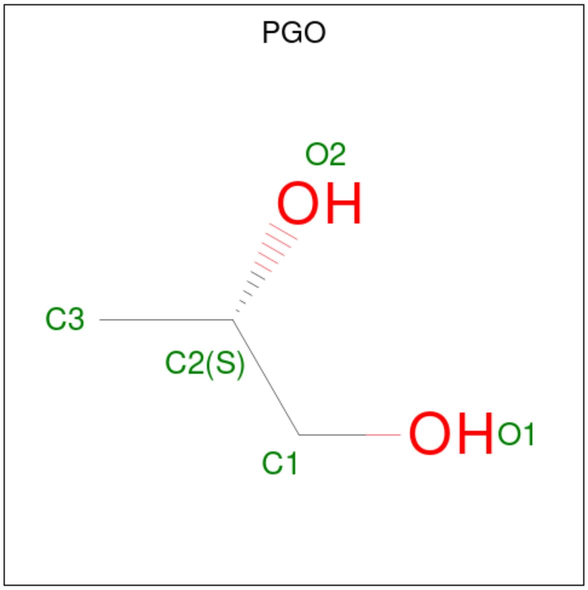
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Ca 5 5	0	0
4	B	6	Total Ca 6 6	0	0
4	C	7	Total Ca 7 7	0	0
4	D	5	Total Ca 5 5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0
5	D	2	Total Cl 2 2	0	0
5	Y	1	Total Cl 1 1	0	0
5	Z	1	Total Cl 1 1	0	0

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	B	1	Total C O 5 3 2	0	0
6	B	1	Total C O 5 3 2	0	0
6	B	1	Total C O 5 3 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 5 3 2	0	0
6	B	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	C	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0

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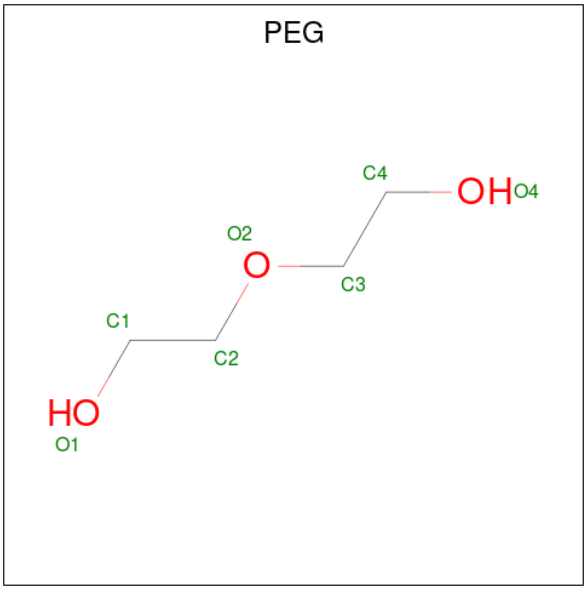
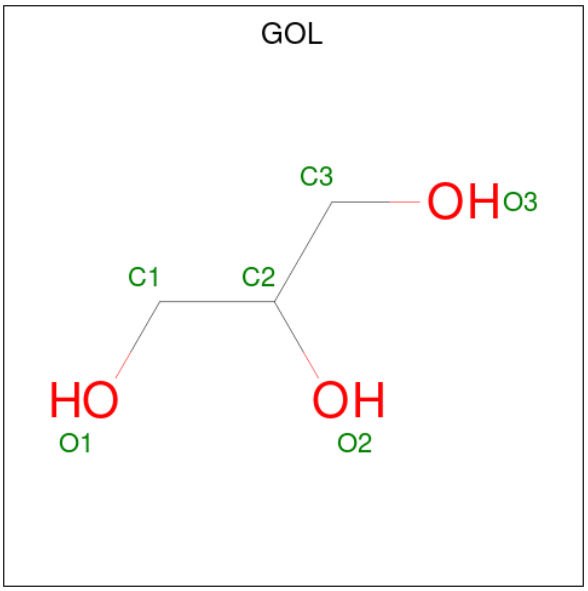
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0
6	D	1	Total C O 5 3 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	222	Total O 222 222	0	0
9	B	222	Total O 222 222	0	0
9	C	192	Total O 192 192	0	0
9	D	208	Total O 208 208	0	0
9	W	9	Total O 9 9	0	0
9	X	17	Total O 17 17	0	0
9	Y	8	Total O 8 8	0	0

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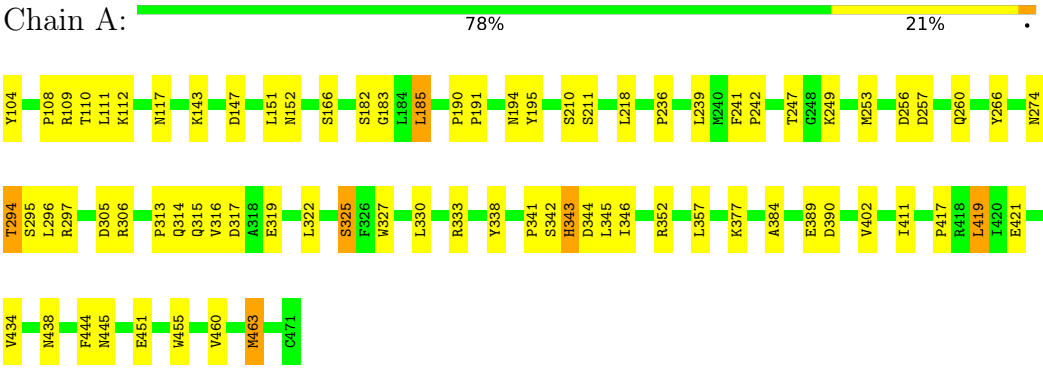
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	Z	18	Total	O	0	0
			18	18		

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.

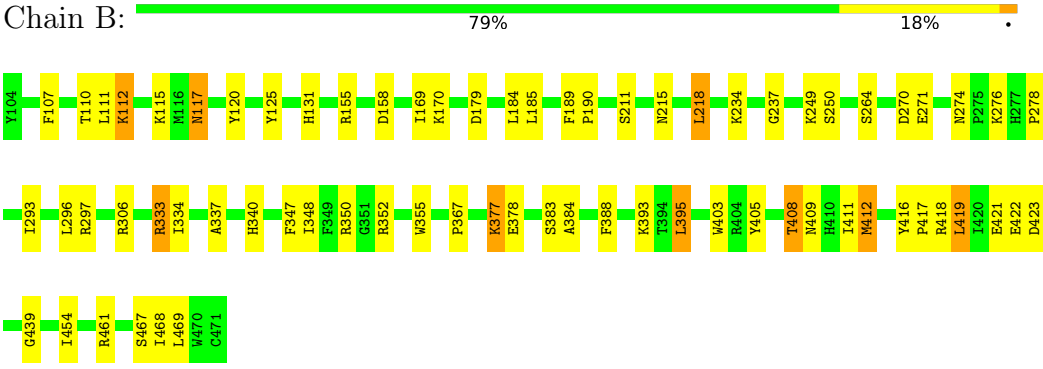
- Molecule 1: Collagenase 3

Chain A:



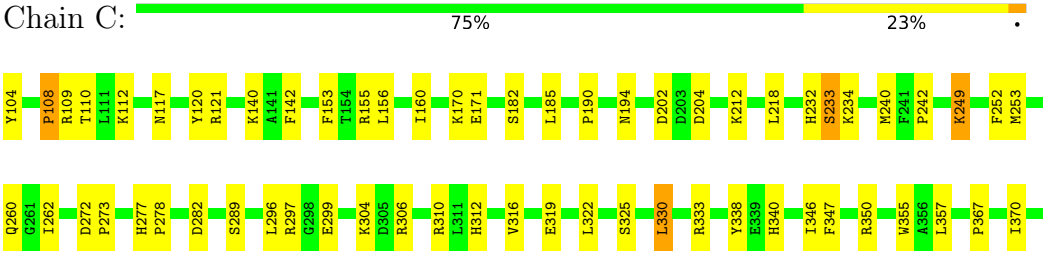
- Molecule 1: Collagenase 3

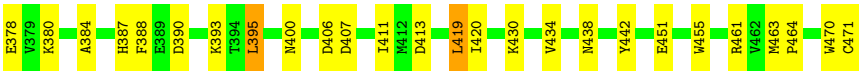
Chain B:



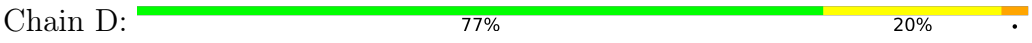
- Molecule 1: Collagenase 3

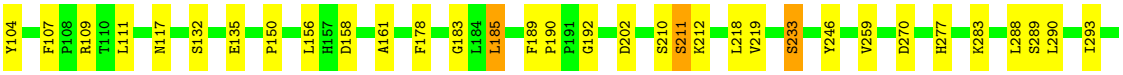
Chain C:

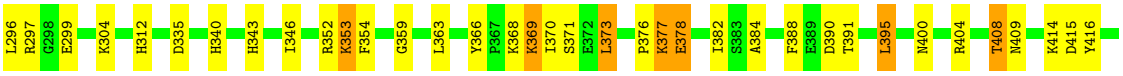


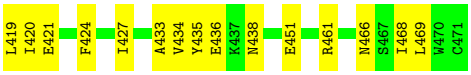


• Molecule 1: Collagenase 3

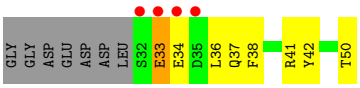




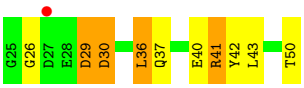




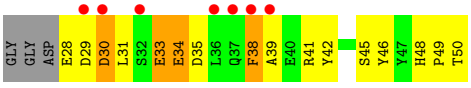
• Molecule 2: Collagenase 3, pro-domain peptide



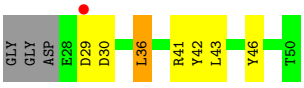
• Molecule 2: Collagenase 3, pro-domain peptide



• Molecule 2: Collagenase 3, pro-domain peptide



• Molecule 2: Collagenase 3, pro-domain peptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.26Å 105.90Å 101.18Å 90.00° 102.11° 90.00°	Depositor
Resolution (Å)	49.50 – 2.54 49.50 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.50-2.54) 99.7 (49.50-2.54)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.169 , 0.241 0.176 , 0.243	Depositor DCC
R_{free} test set	3444 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 20.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.407 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14137	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PGO, CL, ZN, PEG, CA

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	0.43	0/3147	0.59	0/4274
1	B	0.44	0/3119	0.58	0/4236
1	C	0.44	0/3182	0.58	0/4320
1	D	0.43	0/3125	0.59	0/4245
2	W	0.36	0/176	0.62	0/236
2	X	0.40	0/225	0.65	0/302
2	Y	0.35	0/209	0.58	0/281
2	Z	0.40	0/209	0.58	0/281
All	All	0.43	0/13392	0.58	0/18175

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

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	3042	0	2884	68	0
1	B	3014	0	2869	50	0
1	C	3078	0	2916	73	0
1	D	3021	0	2874	54	0
2	W	171	0	149	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	220	0	184	10	0
2	Y	204	0	174	31	0
2	Z	204	0	174	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	5	0	0	0	0
4	B	6	0	0	0	0
4	C	7	0	0	0	0
4	D	5	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	Y	1	0	0	2	0
5	Z	1	0	0	2	0
6	A	55	0	88	10	0
6	B	25	0	40	0	0
6	C	55	0	88	14	0
6	D	55	0	88	15	0
7	A	7	0	10	0	0
7	B	21	0	30	4	0
8	B	12	0	16	2	0
8	C	18	0	24	2	0
9	A	222	0	0	11	0
9	B	222	0	0	8	0
9	C	192	0	0	4	0
9	D	208	0	0	4	0
9	W	9	0	0	0	0
9	X	17	0	0	1	0
9	Y	8	0	0	2	0
9	Z	18	0	0	1	0
All	All	14137	0	12608	274	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 11.

The worst 5 of 274 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:Y:33:GLU:OE2	2:Y:33:GLU:HA	1.49	1.11
1:A:109:ARG:HD3	2:W:38:PHE:CE2	1.87	1.09
9:C:715:HOH:O	5:Y:101:CL:CL	2.27	0.88
9:D:714:HOH:O	5:Z:101:CL:CL	2.31	0.86
1:A:109:ARG:O	1:A:110:THR:HG22	1.78	0.83

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	371/368 (101%)	353 (95%)	15 (4%)	3 (1%)	19	27
1	B	368/368 (100%)	354 (96%)	14 (4%)	0	100	100
1	C	375/368 (102%)	362 (96%)	13 (4%)	0	100	100
1	D	369/368 (100%)	346 (94%)	23 (6%)	0	100	100
2	W	17/26 (65%)	16 (94%)	1 (6%)	0	100	100
2	X	24/26 (92%)	22 (92%)	2 (8%)	0	100	100
2	Y	21/26 (81%)	19 (90%)	2 (10%)	0	100	100
2	Z	21/26 (81%)	19 (90%)	2 (10%)	0	100	100
All	All	1566/1576 (99%)	1491 (95%)	72 (5%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343[A]	HIS
1	A	343[B]	HIS
1	A	341	PRO

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	327/322 (102%)	312 (95%)	15 (5%)	27 36
1	B	324/322 (101%)	297 (92%)	27 (8%)	11 14
1	C	331/322 (103%)	309 (93%)	22 (7%)	16 22
1	D	325/322 (101%)	299 (92%)	26 (8%)	12 15
2	W	18/23 (78%)	14 (78%)	4 (22%)	1 1
2	X	23/23 (100%)	19 (83%)	4 (17%)	2 2
2	Y	22/23 (96%)	17 (77%)	5 (23%)	1 0
2	Z	22/23 (96%)	19 (86%)	3 (14%)	3 3
All	All	1392/1380 (101%)	1286 (92%)	106 (8%)	13 17

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	375	LEU
1	D	340	HIS
2	Y	33	GLU
1	C	407	ASP
1	D	158	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	D	343	HIS
1	D	438	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 86 ligands modelled in this entry, 39 are monoatomic - leaving 47 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	$\#\|Z\| > 2$
7	PEG	A	520	-	6,6,6	0.47	0	5,5,5	0.24	0
6	PGO	C	517	-	3,4,4	0.35	0	1,4,4	0.16	0
6	PGO	B	517	-	3,4,4	0.39	0	1,4,4	0.34	0
6	PGO	D	512	-	3,4,4	0.39	0	1,4,4	0.05	0
6	PGO	A	516	-	3,4,4	0.44	0	1,4,4	0.24	0
6	PGO	C	519	-	3,4,4	0.29	0	1,4,4	0.41	0
6	PGO	D	520	-	3,4,4	0.40	0	1,4,4	0.12	0
6	PGO	C	518	-	3,4,4	0.46	0	1,4,4	0.09	0
6	PGO	D	517	-	3,4,4	0.28	0	1,4,4	0.17	0
7	PEG	B	511	-	6,6,6	0.58	0	5,5,5	0.25	0
6	PGO	B	518	-	3,4,4	0.43	0	1,4,4	0.21	0
7	PEG	B	513	-	6,6,6	0.50	0	5,5,5	0.29	0
6	PGO	C	515	-	3,4,4	0.39	0	1,4,4	0.05	0
6	PGO	A	509	-	3,4,4	0.43	0	1,4,4	0.14	0
6	PGO	A	517	-	3,4,4	0.23	0	1,4,4	0.22	0
8	GOL	B	512	-	5,5,5	0.35	0	5,5,5	0.83	0
6	PGO	B	519	-	3,4,4	0.32	0	1,4,4	0.17	0
6	PGO	C	514	-	3,4,4	0.52	0	1,4,4	0.58	0
6	PGO	D	516	-	3,4,4	0.48	0	1,4,4	0.10	0
6	PGO	B	515	-	3,4,4	0.38	0	1,4,4	0.03	0
6	PGO	D	515	-	3,4,4	0.40	0	1,4,4	0.50	0
6	PGO	C	520	-	3,4,4	0.47	0	1,4,4	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PGO	C	521	-	3,4,4	0.29	0	1,4,4	0.09	0
6	PGO	D	511	-	3,4,4	0.41	0	1,4,4	0.47	0
6	PGO	D	513	-	3,4,4	0.23	0	1,4,4	0.48	0
6	PGO	A	512	-	3,4,4	0.30	0	1,4,4	0.08	0
6	PGO	A	510	-	3,4,4	0.29	0	1,4,4	0.06	0
7	PEG	B	514	-	6,6,6	0.52	0	5,5,5	0.22	0
6	PGO	A	518	-	3,4,4	0.27	0	1,4,4	0.09	0
6	PGO	C	523	-	3,4,4	0.35	0	1,4,4	0.02	0
6	PGO	A	511	-	3,4,4	0.34	0	1,4,4	0.26	0
6	PGO	A	515	-	3,4,4	0.42	0	1,4,4	0.10	0
6	PGO	C	516	-	3,4,4	0.34	0	1,4,4	0.04	0
6	PGO	D	519	-	3,4,4	0.31	0	1,4,4	0.15	0
6	PGO	A	513	-	3,4,4	0.29	0	1,4,4	0.04	0
8	GOL	C	512	-	5,5,5	0.35	0	5,5,5	0.84	0
6	PGO	A	514	-	3,4,4	0.44	0	1,4,4	0.42	0
8	GOL	C	522	-	5,5,5	0.30	0	5,5,5	0.36	0
6	PGO	D	510	-	3,4,4	0.20	0	1,4,4	0.09	0
6	PGO	C	524	-	3,4,4	0.25	0	1,4,4	0.12	0
6	PGO	D	518	-	3,4,4	0.47	0	1,4,4	0.15	0
8	GOL	B	516	-	5,5,5	0.41	0	5,5,5	0.49	0
6	PGO	C	511	-	3,4,4	0.15	0	1,4,4	0.34	0
6	PGO	B	520	-	3,4,4	0.31	0	1,4,4	0.20	0
6	PGO	D	514	-	3,4,4	0.26	0	1,4,4	0.04	0
8	GOL	C	513	-	5,5,5	0.32	0	5,5,5	0.52	0
6	PGO	A	519	-	3,4,4	0.23	0	1,4,4	0.56	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
7	PEG	A	520	-	-	1/4/4/4	-
6	PGO	C	517	-	-	0/2/2/2	-
6	PGO	B	517	-	-	0/2/2/2	-
6	PGO	D	512	-	-	0/2/2/2	-
6	PGO	A	516	-	-	0/2/2/2	-
6	PGO	C	519	-	-	0/2/2/2	-
6	PGO	D	520	-	-	0/2/2/2	-
6	PGO	C	518	-	-	2/2/2/2	-
6	PGO	D	517	-	-	2/2/2/2	-
7	PEG	B	511	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGO	B	518	-	-	1/2/2/2	-
7	PEG	B	513	-	-	3/4/4/4	-
6	PGO	C	515	-	-	0/2/2/2	-
6	PGO	A	509	-	-	0/2/2/2	-
6	PGO	A	517	-	-	0/2/2/2	-
8	GOL	B	512	-	-	2/4/4/4	-
6	PGO	B	519	-	-	0/2/2/2	-
6	PGO	C	514	-	-	2/2/2/2	-
6	PGO	D	516	-	-	1/2/2/2	-
6	PGO	B	515	-	-	2/2/2/2	-
6	PGO	D	515	-	-	0/2/2/2	-
6	PGO	C	520	-	-	2/2/2/2	-
6	PGO	C	521	-	-	0/2/2/2	-
6	PGO	D	511	-	-	0/2/2/2	-
6	PGO	D	513	-	-	2/2/2/2	-
6	PGO	A	512	-	-	2/2/2/2	-
6	PGO	A	510	-	-	2/2/2/2	-
7	PEG	B	514	-	-	0/4/4/4	-
6	PGO	A	518	-	-	2/2/2/2	-
6	PGO	C	523	-	-	0/2/2/2	-
6	PGO	A	511	-	-	2/2/2/2	-
6	PGO	A	515	-	-	0/2/2/2	-
6	PGO	C	516	-	-	0/2/2/2	-
6	PGO	D	519	-	-	0/2/2/2	-
6	PGO	A	513	-	-	0/2/2/2	-
8	GOL	C	512	-	-	4/4/4/4	-
6	PGO	A	514	-	-	0/2/2/2	-
8	GOL	C	522	-	-	2/4/4/4	-
6	PGO	D	510	-	-	0/2/2/2	-
6	PGO	C	524	-	-	2/2/2/2	-
6	PGO	D	518	-	-	0/2/2/2	-
8	GOL	B	516	-	-	1/4/4/4	-
6	PGO	C	511	-	-	0/2/2/2	-
6	PGO	B	520	-	-	0/2/2/2	-
6	PGO	D	514	-	-	0/2/2/2	-
8	GOL	C	513	-	-	0/4/4/4	-
6	PGO	A	519	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	510	PGO	O1-C1-C2-C3
6	A	510	PGO	O1-C1-C2-O2
6	A	512	PGO	O1-C1-C2-O2
6	A	519	PGO	O1-C1-C2-C3
6	A	519	PGO	O1-C1-C2-O2

There are no ring outliers.

27 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	519	PGO	3	0
6	D	520	PGO	1	0
6	C	518	PGO	1	0
6	D	517	PGO	1	0
7	B	513	PEG	1	0
6	A	517	PGO	1	0
8	B	512	GOL	1	0
6	C	514	PGO	1	0
6	D	516	PGO	6	0
6	D	515	PGO	1	0
6	C	520	PGO	2	0
6	C	521	PGO	1	0
6	D	513	PGO	3	0
6	A	512	PGO	1	0
6	A	510	PGO	1	0
7	B	514	PEG	3	0
6	A	515	PGO	1	0
6	C	516	PGO	3	0
6	A	513	PGO	2	0
8	C	512	GOL	2	0
6	A	514	PGO	3	0
6	D	510	PGO	2	0
6	C	524	PGO	1	0
8	B	516	GOL	1	0
6	C	511	PGO	3	0
6	D	514	PGO	1	0
6	A	519	PGO	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, 95^{th} 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	368/368 (100%)	-0.61	0 100 100	9, 25, 47, 59	0
1	B	368/368 (100%)	-0.54	0 100 100	9, 23, 56, 71	0
1	C	368/368 (100%)	-0.62	0 100 100	9, 25, 48, 61	0
1	D	368/368 (100%)	-0.55	0 100 100	10, 24, 56, 68	0
2	W	19/26 (73%)	0.58	4 (21%) 1 0	18, 54, 93, 96	0
2	X	26/26 (100%)	0.15	1 (3%) 40 47	15, 44, 83, 85	0
2	Y	23/26 (88%)	1.03	7 (30%) 0 0	19, 64, 96, 105	0
2	Z	23/26 (88%)	-0.17	1 (4%) 35 42	15, 38, 62, 79	0
All	All	1563/1576 (99%)	-0.52	13 (0%) 86 89	9, 25, 56, 105	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	29	ASP	3.5
2	W	32	SER	3.4
2	W	34	GLU	3.3
2	Y	30	ASP	3.2
2	Y	32	SER	3.1

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 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^{th} 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
6	PGO	D	516	5/5	0.84	0.28	15,30,39,40	0
8	GOL	C	513	6/6	0.84	0.27	46,54,61,69	0
6	PGO	D	512	5/5	0.86	0.22	35,39,55,55	0
6	PGO	D	514	5/5	0.86	0.24	49,51,60,70	0
6	PGO	A	512	5/5	0.87	0.46	39,45,51,61	0
6	PGO	C	517	5/5	0.87	0.17	37,50,58,63	0
6	PGO	D	520	5/5	0.88	0.24	30,48,56,57	0
8	GOL	C	512	6/6	0.88	0.18	36,40,49,52	0
6	PGO	A	511	5/5	0.88	0.29	17,45,50,57	0
8	GOL	B	516	6/6	0.89	0.21	34,43,51,51	0
6	PGO	B	518	5/5	0.89	0.24	39,45,58,58	0
8	GOL	B	512	6/6	0.89	0.13	43,47,50,52	0
6	PGO	A	515	5/5	0.90	0.19	30,35,49,53	0
6	PGO	C	521	5/5	0.90	0.17	34,47,52,58	0
6	PGO	A	510	5/5	0.90	0.30	45,53,58,70	0
7	PEG	A	520	7/7	0.90	0.39	39,55,60,66	0
6	PGO	D	510	5/5	0.91	0.13	29,31,48,49	0
6	PGO	C	524	5/5	0.92	0.15	34,46,52,54	0
6	PGO	D	519	5/5	0.92	0.25	36,36,51,56	0
4	CA	D	507	1/1	0.93	0.14	54,54,54,54	0
6	PGO	C	518	5/5	0.93	0.32	32,35,42,55	0
6	PGO	C	519	5/5	0.93	0.17	19,24,36,38	0
6	PGO	B	515	5/5	0.93	0.24	35,36,50,57	0
6	PGO	D	518	5/5	0.93	0.21	24,42,46,59	0
4	CA	C	509	1/1	0.93	0.08	66,66,66,66	0
8	GOL	C	522	6/6	0.93	0.23	34,39,50,51	0
4	CA	D	504	1/1	0.94	0.04	31,31,31,31	0
4	CA	B	507	1/1	0.94	0.06	42,42,42,42	0
6	PGO	B	519	5/5	0.94	0.20	26,36,39,48	0
7	PEG	B	511	7/7	0.94	0.24	43,45,58,63	0
7	PEG	B	514	7/7	0.94	0.30	24,33,42,45	0
6	PGO	D	511	5/5	0.94	0.15	17,32,37,44	0
6	PGO	C	514	5/5	0.94	0.22	13,24,31,41	0
6	PGO	A	516	5/5	0.94	0.17	21,26,38,47	0
6	PGO	A	517	5/5	0.94	0.22	28,35,45,48	0
6	PGO	A	519	5/5	0.94	0.19	30,32,43,46	0
6	PGO	A	514	5/5	0.95	0.23	27,31,40,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PGO	C	520	5/5	0.95	0.38	30,34,40,51	0
6	PGO	A	518	5/5	0.95	0.14	34,41,45,53	0
6	PGO	C	523	5/5	0.95	0.18	36,50,58,64	0
6	PGO	B	520	5/5	0.95	0.20	24,27,29,33	0
6	PGO	C	511	5/5	0.95	0.33	35,37,50,50	0
6	PGO	A	509	5/5	0.95	0.20	41,44,50,54	0
6	PGO	C	516	5/5	0.95	0.34	39,40,55,61	0
4	CA	B	509	1/1	0.95	0.06	62,62,62,62	0
6	PGO	B	517	5/5	0.95	0.13	29,37,52,53	0
6	PGO	D	517	5/5	0.95	0.14	21,26,32,47	0
6	PGO	A	513	5/5	0.96	0.19	25,34,43,43	0
4	CA	C	510	1/1	0.96	0.09	56,56,56,56	0
6	PGO	D	513	5/5	0.96	0.14	42,49,50,52	0
7	PEG	B	513	7/7	0.96	0.27	31,36,46,50	0
6	PGO	C	515	5/5	0.96	0.09	26,31,34,43	0
6	PGO	D	515	5/5	0.97	0.12	23,23,34,46	0
4	CA	B	506	1/1	0.97	0.08	16,16,16,16	0
4	CA	C	503	1/1	0.97	0.04	46,46,46,46	0
5	CL	B	508	1/1	0.98	0.06	28,28,28,28	0
4	CA	C	505	1/1	0.98	0.06	30,30,30,30	0
4	CA	A	503	1/1	0.98	0.09	42,42,42,42	0
4	CA	A	505	1/1	0.98	0.07	31,31,31,31	0
4	CA	B	503	1/1	0.98	0.06	33,33,33,33	0
4	CA	D	505	1/1	0.98	0.08	20,20,20,20	0
4	CA	D	506	1/1	0.98	0.08	17,17,17,17	0
4	CA	B	505	1/1	0.98	0.08	22,22,22,22	0
5	CL	Z	101	1/1	0.99	0.09	32,32,32,32	0
4	CA	C	506	1/1	0.99	0.07	14,14,14,14	0
4	CA	C	507	1/1	0.99	0.04	39,39,39,39	0
4	CA	A	504	1/1	0.99	0.06	33,33,33,33	0
3	ZN	C	502	1/1	0.99	0.09	28,28,28,28	0
4	CA	D	503	1/1	0.99	0.10	18,18,18,18	0
4	CA	A	506	1/1	0.99	0.11	12,12,12,12	0
4	CA	A	507	1/1	0.99	0.04	34,34,34,34	0
3	ZN	A	502	1/1	0.99	0.08	25,25,25,25	0
4	CA	C	504	1/1	0.99	0.08	30,30,30,30	0
5	CL	A	508	1/1	0.99	0.07	14,14,14,14	0
4	CA	B	504	1/1	0.99	0.06	17,17,17,17	0
5	CL	B	510	1/1	0.99	0.08	34,34,34,34	0
5	CL	C	508	1/1	0.99	0.08	12,12,12,12	0
5	CL	D	508	1/1	0.99	0.04	38,38,38,38	0
5	CL	Y	101	1/1	0.99	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	501	1/1	1.00	0.09	14,14,14,14	0
3	ZN	D	502	1/1	1.00	0.08	18,18,18,18	0
3	ZN	B	501	1/1	1.00	0.09	13,13,13,13	0
3	ZN	B	502	1/1	1.00	0.07	18,18,18,18	0
3	ZN	C	501	1/1	1.00	0.10	19,19,19,19	0
3	ZN	A	501	1/1	1.00	0.10	17,17,17,17	0
5	CL	D	509	1/1	1.00	0.08	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.