Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2021 – 10:06 PM EST

PDB ID	:	6XSZ
Title	:	The structure of the M60 catalytic domain from Clostridium perfringens ZmpC
Authors	:	Pluvinage, B.; Boraston, A.B.
Deposited on	:	2020-07-16
Resolution	:	2.25 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 following versions of software and data (see references ⓘ) were used in the production of this report:

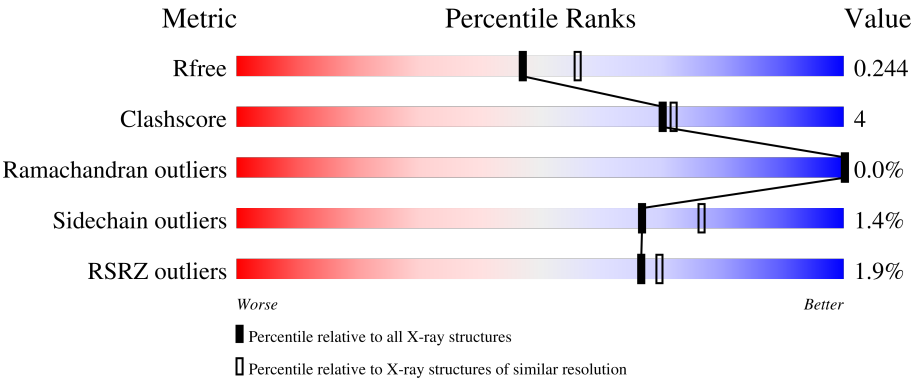
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	531	88% 8%
1	B	531	90% 5%
1	C	531	87% 8%
1	D	531	86% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17134 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 ZmpC Glycopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	1	0
			4039	2543	670	814	12			
1	B	509	Total	C	N	O	S	0	1	0
			4024	2537	669	806	12			
1	C	509	Total	C	N	O	S	0	3	0
			4042	2546	676	808	12			
1	D	510	Total	C	N	O	S	0	2	0
			3993	2517	669	795	12			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	MET	-	initiating methionine	UNP F8UNJ8
A	470	GLY	-	expression tag	UNP F8UNJ8
A	471	SER	-	expression tag	UNP F8UNJ8
A	472	SER	-	expression tag	UNP F8UNJ8
A	473	HIS	-	expression tag	UNP F8UNJ8
A	474	HIS	-	expression tag	UNP F8UNJ8
A	475	HIS	-	expression tag	UNP F8UNJ8
A	476	HIS	-	expression tag	UNP F8UNJ8
A	477	HIS	-	expression tag	UNP F8UNJ8
A	478	HIS	-	expression tag	UNP F8UNJ8
A	479	SER	-	expression tag	UNP F8UNJ8
A	480	SER	-	expression tag	UNP F8UNJ8
A	481	GLY	-	expression tag	UNP F8UNJ8
A	482	LEU	-	expression tag	UNP F8UNJ8
A	483	VAL	-	expression tag	UNP F8UNJ8
A	484	PRO	-	expression tag	UNP F8UNJ8
A	485	ARG	-	expression tag	UNP F8UNJ8
A	486	GLY	-	expression tag	UNP F8UNJ8
A	487	SER	-	expression tag	UNP F8UNJ8
A	488	HIS	-	expression tag	UNP F8UNJ8
A	489	MET	-	expression tag	UNP F8UNJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ALA	-	expression tag	UNP F8UNJ8
A	491	SER	-	expression tag	UNP F8UNJ8
B	469	MET	-	initiating methionine	UNP F8UNJ8
B	470	GLY	-	expression tag	UNP F8UNJ8
B	471	SER	-	expression tag	UNP F8UNJ8
B	472	SER	-	expression tag	UNP F8UNJ8
B	473	HIS	-	expression tag	UNP F8UNJ8
B	474	HIS	-	expression tag	UNP F8UNJ8
B	475	HIS	-	expression tag	UNP F8UNJ8
B	476	HIS	-	expression tag	UNP F8UNJ8
B	477	HIS	-	expression tag	UNP F8UNJ8
B	478	HIS	-	expression tag	UNP F8UNJ8
B	479	SER	-	expression tag	UNP F8UNJ8
B	480	SER	-	expression tag	UNP F8UNJ8
B	481	GLY	-	expression tag	UNP F8UNJ8
B	482	LEU	-	expression tag	UNP F8UNJ8
B	483	VAL	-	expression tag	UNP F8UNJ8
B	484	PRO	-	expression tag	UNP F8UNJ8
B	485	ARG	-	expression tag	UNP F8UNJ8
B	486	GLY	-	expression tag	UNP F8UNJ8
B	487	SER	-	expression tag	UNP F8UNJ8
B	488	HIS	-	expression tag	UNP F8UNJ8
B	489	MET	-	expression tag	UNP F8UNJ8
B	490	ALA	-	expression tag	UNP F8UNJ8
B	491	SER	-	expression tag	UNP F8UNJ8
C	469	MET	-	initiating methionine	UNP F8UNJ8
C	470	GLY	-	expression tag	UNP F8UNJ8
C	471	SER	-	expression tag	UNP F8UNJ8
C	472	SER	-	expression tag	UNP F8UNJ8
C	473	HIS	-	expression tag	UNP F8UNJ8
C	474	HIS	-	expression tag	UNP F8UNJ8
C	475	HIS	-	expression tag	UNP F8UNJ8
C	476	HIS	-	expression tag	UNP F8UNJ8
C	477	HIS	-	expression tag	UNP F8UNJ8
C	478	HIS	-	expression tag	UNP F8UNJ8
C	479	SER	-	expression tag	UNP F8UNJ8
C	480	SER	-	expression tag	UNP F8UNJ8
C	481	GLY	-	expression tag	UNP F8UNJ8
C	482	LEU	-	expression tag	UNP F8UNJ8
C	483	VAL	-	expression tag	UNP F8UNJ8
C	484	PRO	-	expression tag	UNP F8UNJ8
C	485	ARG	-	expression tag	UNP F8UNJ8

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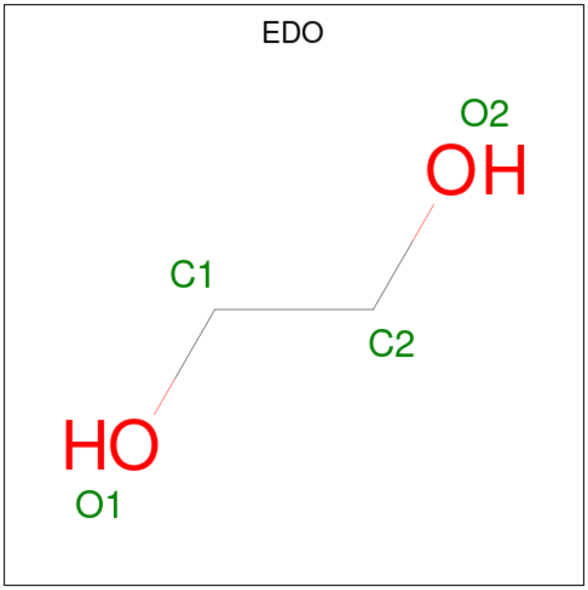
Chain	Residue	Modelled	Actual	Comment	Reference
C	486	GLY	-	expression tag	UNP F8UNJ8
C	487	SER	-	expression tag	UNP F8UNJ8
C	488	HIS	-	expression tag	UNP F8UNJ8
C	489	MET	-	expression tag	UNP F8UNJ8
C	490	ALA	-	expression tag	UNP F8UNJ8
C	491	SER	-	expression tag	UNP F8UNJ8
D	469	MET	-	initiating methionine	UNP F8UNJ8
D	470	GLY	-	expression tag	UNP F8UNJ8
D	471	SER	-	expression tag	UNP F8UNJ8
D	472	SER	-	expression tag	UNP F8UNJ8
D	473	HIS	-	expression tag	UNP F8UNJ8
D	474	HIS	-	expression tag	UNP F8UNJ8
D	475	HIS	-	expression tag	UNP F8UNJ8
D	476	HIS	-	expression tag	UNP F8UNJ8
D	477	HIS	-	expression tag	UNP F8UNJ8
D	478	HIS	-	expression tag	UNP F8UNJ8
D	479	SER	-	expression tag	UNP F8UNJ8
D	480	SER	-	expression tag	UNP F8UNJ8
D	481	GLY	-	expression tag	UNP F8UNJ8
D	482	LEU	-	expression tag	UNP F8UNJ8
D	483	VAL	-	expression tag	UNP F8UNJ8
D	484	PRO	-	expression tag	UNP F8UNJ8
D	485	ARG	-	expression tag	UNP F8UNJ8
D	486	GLY	-	expression tag	UNP F8UNJ8
D	487	SER	-	expression tag	UNP F8UNJ8
D	488	HIS	-	expression tag	UNP F8UNJ8
D	489	MET	-	expression tag	UNP F8UNJ8
D	490	ALA	-	expression tag	UNP F8UNJ8
D	491	SER	-	expression tag	UNP F8UNJ8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 4 is water.

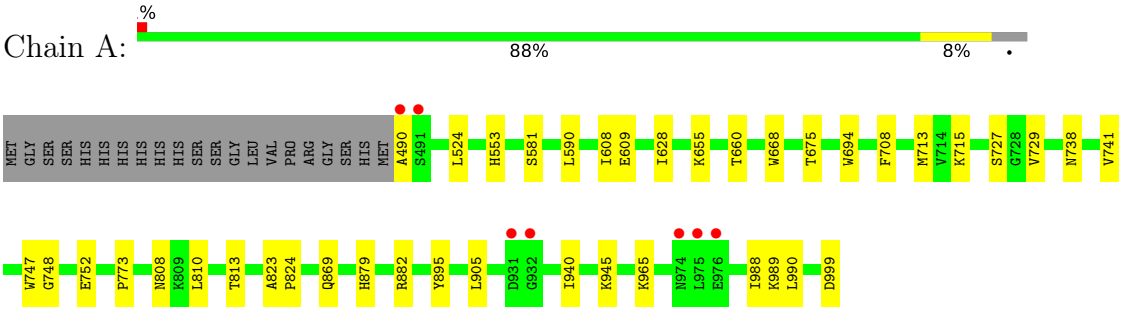
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	265	Total O 265 265	0	0
4	B	225	Total O 225 225	0	0
4	C	232	Total O 232 232	0	0
4	D	218	Total O 218 218	0	0

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.

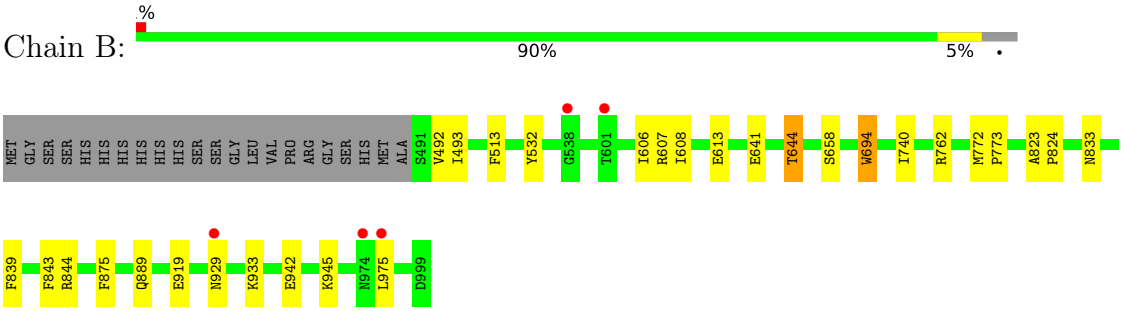
• Molecule 1: ZmpC Glycopeptidase

Chain A:



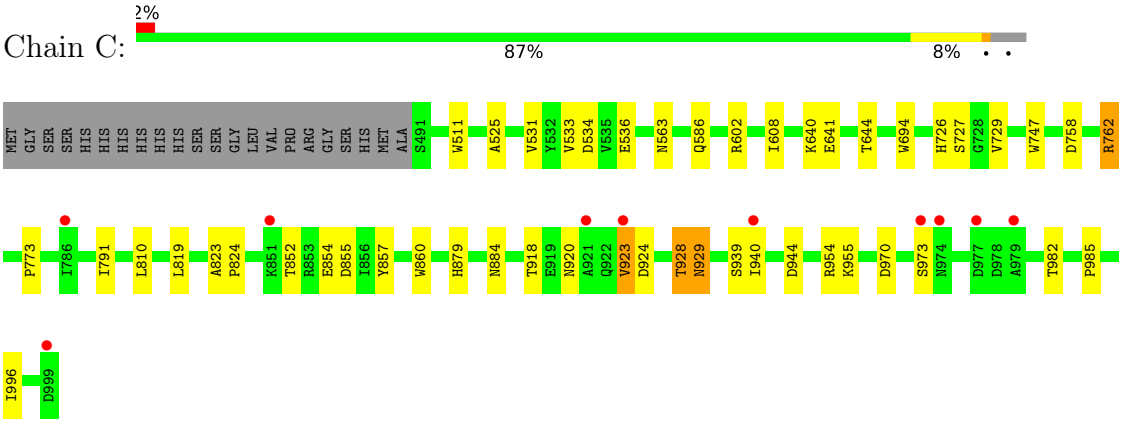
• Molecule 1: ZmpC Glycopeptidase

Chain B:



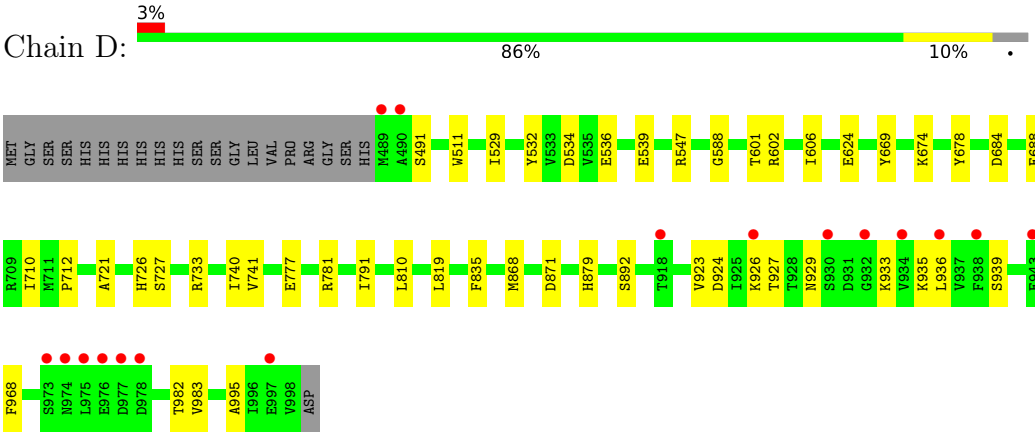
• Molecule 1: ZmpC Glycopeptidase

Chain C:



• Molecule 1: ZmpC Glycopeptidase

Chain D:


3%
86%
10%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M489 A490 S491 W511 I529 Y532 V533 D534 V535 E536 E539 R547 G588 T601 R602 I606 E624 Y669 K674 Y678 D684 E688 W694 F708
R709 I710 M711 P712 A721 H726 S727 R733 I740 V741 E777 R781 I791 L810 L819 F835 M868 D871 H879 S892 T918 V923 D924 I925 K926 T927 T928 N929 S930 D931 G932 K933 V934 K935 L936 V937 F938 S939 E943 E952 I963
F968 S973 N974 L975 E976 D977 D978 T982 V983 A995 I996 E997 V998 ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.69Å 99.99Å 118.59Å 90.00° 95.95° 90.00°	Depositor
Resolution (Å)	38.98 – 2.25 38.95 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.9 (38.98-2.25) 95.9 (38.95-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.244 0.201 , 0.244	Depositor DCC
R_{free} test set	5723 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17134	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: ZN, EDO

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	0.27	0/4125	0.57	0/5602
1	B	0.27	0/4110	0.56	0/5583
1	C	0.27	0/4128	0.59	0/5605
1	D	0.27	0/4079	0.58	0/5543
All	All	0.27	0/16442	0.57	0/22333

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	4039	0	3805	30	0
1	B	4024	0	3800	17	0
1	C	4042	0	3807	36	0
1	D	3993	0	3707	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	36	1	0
3	C	16	0	24	0	0
3	D	32	0	48	1	0
4	A	265	0	0	2	1
4	B	225	0	0	2	0
4	C	232	0	0	1	0
4	D	218	0	0	1	1
All	All	17134	0	15257	113	1

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 4.

All (113) 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:762:ARG:HH11	1:C:762:ARG:HG2	1.25	0.98
1:A:713:MET:CE	1:A:715:LYS:HE2	1.95	0.97
1:A:713:MET:HE2	1:A:715:LYS:HE2	1.53	0.90
1:C:762:ARG:O	1:C:762:ARG:HG2	1.72	0.90
1:A:713:MET:HE2	1:A:715:LYS:CE	2.06	0.86
1:C:918:THR:HG22	1:C:944:ASP:OD2	1.85	0.76
1:A:668:TRP:CE3	1:A:741:VAL:HG12	2.22	0.74
1:A:965:LYS:HE3	4:A:1273:HOH:O	1.86	0.74
1:D:534:ASP:OD1	1:D:602[A]:ARG:NH2	2.22	0.72
1:A:713:MET:HE3	1:A:715:LYS:HE2	1.70	0.71
1:C:923:VAL:HG21	1:C:985:PRO:CG	2.22	0.69
1:C:854:GLU:HG2	4:C:1113:HOH:O	1.92	0.69
1:C:762:ARG:O	1:C:762:ARG:CG	2.41	0.68
1:C:923:VAL:HG23	1:C:996:ILE:CD1	2.24	0.68
1:B:833:ASN:HB2	4:B:1312:HOH:O	1.95	0.66
1:D:684:ASP:O	1:D:688[B]:GLU:HG3	1.96	0.65
1:C:923:VAL:HG23	1:C:996:ILE:HD11	1.79	0.64
1:B:694:TRP:O	1:B:844:ARG:NH2	2.27	0.64
1:C:536[A]:GLU:OE1	1:C:536[A]:GLU:HA	2.00	0.62
1:A:668:TRP:CE3	1:A:741:VAL:CG1	2.82	0.62
1:C:923:VAL:HG21	1:C:985:PRO:HG3	1.82	0.61
1:C:918:THR:HG23	1:C:920:ASN:H	1.66	0.61
1:D:708:PHE:HE1	1:D:710:ILE:HG12	1.66	0.60
1:A:808:ASN:O	1:A:882:ARG:NH2	2.34	0.60
1:D:678:TYR:OH	3:D:1008:EDO:H11	2.01	0.59
1:C:923:VAL:HG21	1:C:985:PRO:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:923:VAL:HG13	1:C:940:ILE:HD12	1.86	0.58
1:C:923:VAL:HG13	1:C:940:ILE:CD1	2.34	0.58
1:C:954:ARG:HB2	1:C:982:THR:HB	1.86	0.57
1:D:927:THR:HA	1:D:935:LYS:O	2.05	0.56
1:A:713:MET:HE2	1:A:715:LYS:HE3	1.85	0.55
1:A:660:THR:HG21	1:A:741:VAL:HG23	1.88	0.54
1:C:791:ILE:CD1	1:C:819:LEU:HB2	2.38	0.54
1:D:868:MET:HA	1:D:868:MET:HE2	1.89	0.54
1:D:791:ILE:CD1	1:D:819:LEU:HB2	2.38	0.54
1:A:490:ALA:HB2	1:A:609:GLU:HG2	1.89	0.53
1:A:988:ILE:O	3:A:1006:EDO:H21	2.09	0.52
1:D:511:TRP:O	1:D:727:SER:HA	2.10	0.52
1:D:953:ILE:HD13	1:D:968:PHE:CG	2.45	0.52
1:B:492:VAL:HG22	1:B:607:ARG:HG3	1.91	0.52
1:A:713:MET:CE	1:A:729:VAL:HG11	2.40	0.51
1:B:641:GLU:HB3	1:B:644:THR:HG23	1.93	0.51
1:A:628:ILE:HD11	1:A:675:THR:HG22	1.93	0.51
1:B:606:ILE:HD13	1:B:608:ILE:HD11	1.91	0.50
1:D:923:VAL:HG12	1:D:924:ASP:N	2.26	0.50
1:D:708:PHE:CE1	1:D:710:ILE:HG12	2.46	0.50
1:D:777:GLU:HG2	1:D:781:ARG:HD3	1.94	0.50
1:C:810:LEU:HA	1:C:879:HIS:O	2.11	0.49
1:C:534:ASP:OD1	1:C:602[A]:ARG:NH2	2.46	0.49
1:D:674:LYS:HE2	1:D:678:TYR:CE1	2.47	0.49
1:B:823:ALA:N	1:B:824:PRO:HD2	2.27	0.49
1:C:533:VAL:O	1:C:563:ASN:O	2.30	0.49
1:C:747:TRP:CE3	1:C:773:PRO:HB2	2.48	0.48
1:A:823:ALA:N	1:A:824:PRO:HD2	2.29	0.48
1:C:928:THR:HG22	1:C:929:ASN:H	1.79	0.48
1:D:721:ALA:O	1:D:733:ARG:NH1	2.47	0.48
1:D:547:ARG:O	1:D:588:GLY:HA3	2.14	0.47
1:C:762:ARG:NH1	1:C:762:ARG:HG2	2.03	0.47
1:C:791:ILE:HD13	1:C:819:LEU:HB2	1.97	0.47
1:A:553:HIS:CE1	1:D:601:THR:HG22	2.51	0.46
1:A:668:TRP:CZ3	1:A:741:VAL:HG12	2.50	0.46
1:B:942:GLU:HA	1:B:945:LYS:HE3	1.97	0.46
1:D:982:THR:HG23	1:D:995:ALA:HB1	1.97	0.46
1:D:871:ASP:OD2	1:D:892:SER:HB3	2.15	0.46
1:C:857:TYR:O	1:C:860:TRP:HB2	2.16	0.46
1:C:641:GLU:HB3	1:C:644:THR:HG22	1.98	0.46
1:A:989:LYS:HA	3:A:1006:EDO:H11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:GLU:HB3	1:D:539:GLU:CD	2.37	0.45
1:A:747:TRP:CE3	1:A:773:PRO:HB2	2.51	0.45
1:A:655:LYS:HE3	1:A:708:PHE:CE2	2.52	0.45
1:D:791:ILE:HD13	1:D:819:LEU:HB2	1.99	0.45
1:B:658:SER:HB3	1:B:740:ILE:CG2	2.47	0.44
1:D:952:GLU:O	1:D:983:VAL:HA	2.17	0.44
1:B:929:ASN:HB2	1:B:975:LEU:HD21	1.99	0.44
1:A:905:LEU:HG	1:A:990:LEU:HD11	1.98	0.44
1:C:852:THR:HG23	1:C:855:ASP:H	1.82	0.44
1:A:738:ASN:ND2	3:A:1002:EDO:H11	2.33	0.44
1:D:810:LEU:HA	1:D:879:HIS:O	2.18	0.44
1:D:835:PHE:HA	1:D:868:MET:HE1	2.00	0.44
1:D:669:TYR:CZ	1:D:741:VAL:HG23	2.53	0.44
1:D:712:PRO:HB2	1:D:740:ILE:HG23	1.99	0.43
1:B:772:MET:HB3	1:B:773:PRO:CD	2.48	0.43
1:B:839:PHE:CZ	1:B:843:PHE:HE2	2.36	0.43
1:C:823:ALA:N	1:C:824:PRO:HD2	2.33	0.43
1:C:536[A]:GLU:HG2	1:C:602[A]:ARG:HG2	2.01	0.43
1:B:513:PHE:CD1	1:B:513:PHE:N	2.85	0.43
1:C:726:HIS:O	1:C:729:VAL:HB	2.19	0.43
1:B:493:ILE:HB	1:B:606:ILE:HD11	2.01	0.42
1:C:525:ALA:HB2	1:C:586:GLN:HB3	2.01	0.42
1:A:713:MET:HE2	1:A:729:VAL:HG11	2.01	0.42
1:B:493:ILE:HB	1:B:606:ILE:CD1	2.49	0.42
1:C:955:LYS:HE2	1:C:970:ASP:OD2	2.20	0.42
1:A:748:GLY:O	1:A:752:GLU:HG2	2.20	0.42
1:A:940:ILE:HG23	1:A:945:LYS:HG3	2.02	0.42
1:C:970:ASP:OD2	1:C:973:SER:HB3	2.19	0.42
1:D:674:LYS:HE2	1:D:678:TYR:CD1	2.55	0.41
1:D:939:SER:CB	4:D:1284:HOH:O	2.67	0.41
4:A:1121:HOH:O	1:C:640:LYS:HE2	2.20	0.41
1:A:810:LEU:HA	1:A:879:HIS:O	2.20	0.41
1:A:869:GLN:HG2	1:A:895:TYR:CE1	2.55	0.41
1:C:511:TRP:O	1:C:727:SER:HA	2.21	0.41
1:A:999:ASP:N	1:A:999:ASP:OD2	2.54	0.41
1:D:926:LYS:O	1:D:936:LEU:HA	2.20	0.41
1:D:532:TYR:O	1:D:606:ILE:HA	2.21	0.41
1:A:590:LEU:HD13	1:A:608:ILE:HD11	2.02	0.41
1:B:919:GLU:HG2	4:B:1197:HOH:O	2.20	0.41
1:D:929:ASN:HA	1:D:933:LYS:O	2.21	0.41
1:B:875:PHE:HB2	3:B:1004:EDO:H22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:VAL:HG22	1:C:608:ILE:HG12	2.02	0.40
1:A:628:ILE:CD1	1:A:675:THR:HG22	2.50	0.40
1:B:532:TYR:O	1:B:606:ILE:HA	2.21	0.40
1:D:606:ILE:C	1:D:606:ILE:HD12	2.42	0.40
1:C:923:VAL:HA	1:C:939:SER:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1307:HOH:O	4:D:1144:HOH:O[2_745]	2.19	0.01

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	509/531 (96%)	498 (98%)	11 (2%)	0	100	100
1	B	508/531 (96%)	498 (98%)	10 (2%)	0	100	100
1	C	510/531 (96%)	496 (97%)	14 (3%)	0	100	100
1	D	510/531 (96%)	492 (96%)	17 (3%)	1 (0%)	47	55
All	All	2037/2124 (96%)	1984 (97%)	52 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	726	HIS

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	433/464 (93%)	428 (99%)	5 (1%)	71 80
1	B	431/464 (93%)	425 (99%)	6 (1%)	67 76
1	C	430/464 (93%)	422 (98%)	8 (2%)	57 66
1	D	413/464 (89%)	409 (99%)	4 (1%)	76 84
All	All	1707/1856 (92%)	1684 (99%)	23 (1%)	67 79

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	LEU
1	A	581	SER
1	A	694	TRP
1	A	727	SER
1	A	813	THR
1	B	613	GLU
1	B	644	THR
1	B	694	TRP
1	B	762	ARG
1	B	889	GLN
1	B	933	LYS
1	C	694	TRP
1	C	758	ASP
1	C	762	ARG
1	C	884	ASN
1	C	923	VAL
1	C	924	ASP
1	C	928	THR
1	C	929	ASN
1	D	491	SER
1	D	529	ILE
1	D	624	GLU
1	D	694	TRP

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 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	EDO	C	1005	-	3,3,3	0.07	0	2,2,2	0.05	0
3	EDO	A	1005	-	3,3,3	0.04	0	2,2,2	0.13	0
3	EDO	A	1004	-	3,3,3	0.09	0	2,2,2	0.22	0
3	EDO	C	1004	-	3,3,3	0.06	0	2,2,2	0.12	0
3	EDO	D	1006	-	3,3,3	0.04	0	2,2,2	0.21	0
3	EDO	C	1002	-	3,3,3	0.11	0	2,2,2	0.13	0
3	EDO	B	1003	-	3,3,3	0.11	0	2,2,2	0.35	0
3	EDO	A	1006	-	3,3,3	0.18	0	2,2,2	0.51	0
3	EDO	D	1004	-	3,3,3	0.10	0	2,2,2	0.18	0
3	EDO	D	1005	-	3,3,3	0.04	0	2,2,2	0.35	0
3	EDO	B	1005	-	3,3,3	0.10	0	2,2,2	0.20	0
3	EDO	B	1007	-	3,3,3	0.05	0	2,2,2	0.07	0
3	EDO	D	1003	-	3,3,3	0.11	0	2,2,2	0.14	0
3	EDO	C	1003	-	3,3,3	0.15	0	2,2,2	0.23	0
3	EDO	D	1007	-	3,3,3	0.08	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	1004	-	3,3,3	0.09	0	2,2,2	0.39	0
3	EDO	A	1002	-	3,3,3	0.16	0	2,2,2	0.15	0
3	EDO	D	1008	-	3,3,3	0.04	0	2,2,2	0.39	0
3	EDO	D	1009	-	3,3,3	0.07	0	2,2,2	0.10	0
3	EDO	D	1002	-	3,3,3	0.11	0	2,2,2	0.13	0
3	EDO	B	1006	-	3,3,3	0.10	0	2,2,2	0.39	0
3	EDO	B	1002	-	3,3,3	0.06	0	2,2,2	0.18	0
3	EDO	A	1003	-	3,3,3	0.08	0	2,2,2	0.12	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
3	EDO	C	1005	-	-	0/1/1/1	-
3	EDO	A	1005	-	-	1/1/1/1	-
3	EDO	A	1004	-	-	0/1/1/1	-
3	EDO	C	1004	-	-	0/1/1/1	-
3	EDO	D	1006	-	-	1/1/1/1	-
3	EDO	C	1002	-	-	0/1/1/1	-
3	EDO	B	1003	-	-	0/1/1/1	-
3	EDO	A	1006	-	-	1/1/1/1	-
3	EDO	D	1004	-	-	0/1/1/1	-
3	EDO	D	1005	-	-	1/1/1/1	-
3	EDO	B	1005	-	-	1/1/1/1	-
3	EDO	B	1007	-	-	0/1/1/1	-
3	EDO	D	1003	-	-	0/1/1/1	-
3	EDO	C	1003	-	-	0/1/1/1	-
3	EDO	D	1007	-	-	1/1/1/1	-
3	EDO	B	1004	-	-	1/1/1/1	-
3	EDO	A	1002	-	-	1/1/1/1	-
3	EDO	D	1008	-	-	1/1/1/1	-
3	EDO	D	1009	-	-	1/1/1/1	-
3	EDO	D	1002	-	-	0/1/1/1	-
3	EDO	B	1006	-	-	1/1/1/1	-
3	EDO	B	1002	-	-	0/1/1/1	-
3	EDO	A	1003	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1005	EDO	O1-C1-C2-O2
3	A	1002	EDO	O1-C1-C2-O2
3	D	1009	EDO	O1-C1-C2-O2
3	D	1006	EDO	O1-C1-C2-O2
3	B	1004	EDO	O1-C1-C2-O2
3	D	1008	EDO	O1-C1-C2-O2
3	D	1005	EDO	O1-C1-C2-O2
3	A	1006	EDO	O1-C1-C2-O2
3	D	1007	EDO	O1-C1-C2-O2
3	B	1006	EDO	O1-C1-C2-O2
3	A	1005	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1006	EDO	2	0
3	B	1004	EDO	1	0
3	A	1002	EDO	1	0
3	D	1008	EDO	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	510/531 (96%)	-0.30	7 (1%)	75 77	21, 31, 53, 78	0
1	B	509/531 (95%)	-0.19	5 (0%)	82 84	23, 35, 58, 77	0
1	C	509/531 (95%)	-0.14	10 (1%)	65 68	23, 36, 64, 89	0
1	D	510/531 (96%)	-0.10	17 (3%)	46 48	21, 34, 76, 102	0
All	All	2038/2124 (95%)	-0.19	39 (1%)	66 69	21, 34, 63, 102	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	974	ASN	4.5
1	D	930	SER	4.3
1	A	975	LEU	3.7
1	D	490	ALA	3.7
1	D	977	ASP	3.6
1	D	975	LEU	3.4
1	B	975	LEU	3.2
1	D	489	MET	3.2
1	D	936	LEU	3.1
1	D	918	THR	3.1
1	A	932	GLY	3.0
1	C	923	VAL	3.0
1	C	999	ASP	2.7
1	B	974	ASN	2.7
1	A	974	ASN	2.6
1	D	973	SER	2.6
1	D	934	VAL	2.6
1	B	929	ASN	2.5
1	A	931	ASP	2.5
1	C	940	ILE	2.4
1	D	997	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	973	SER	2.4
1	C	921	ALA	2.4
1	D	978	ASP	2.4
1	C	786	ILE	2.3
1	D	974	ASN	2.3
1	A	976	GLU	2.3
1	C	977	ASP	2.3
1	B	601	THR	2.3
1	A	490	ALA	2.2
1	C	979	ALA	2.2
1	D	932	GLY	2.2
1	D	926	LYS	2.2
1	D	943	GLU	2.1
1	D	976	GLU	2.1
1	B	538	GLY	2.1
1	A	491	SER	2.1
1	C	851	LYS	2.1
1	D	938	PHE	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 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
3	EDO	D	1005	4/4	0.80	0.21	49,52,53,56	0
3	EDO	D	1004	4/4	0.84	0.19	45,49,51,51	0
3	EDO	B	1007	4/4	0.84	0.24	47,51,56,65	0
3	EDO	D	1008	4/4	0.84	0.24	44,48,49,53	0
3	EDO	B	1006	4/4	0.88	0.19	38,38,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	1006	4/4	0.89	0.13	39,41,41,41	0
3	EDO	B	1004	4/4	0.89	0.18	45,46,46,46	0
3	EDO	C	1005	4/4	0.90	0.15	46,46,48,49	0
3	EDO	D	1007	4/4	0.91	0.24	42,44,44,48	0
3	EDO	B	1005	4/4	0.92	0.18	41,42,43,46	0
3	EDO	D	1002	4/4	0.92	0.17	41,42,43,43	0
3	EDO	A	1004	4/4	0.92	0.14	33,39,41,42	0
3	EDO	D	1006	4/4	0.93	0.13	45,46,47,48	0
3	EDO	B	1002	4/4	0.93	0.17	41,44,45,51	0
3	EDO	A	1003	4/4	0.93	0.19	49,49,51,54	0
3	EDO	B	1003	4/4	0.94	0.18	41,41,42,43	0
3	EDO	A	1002	4/4	0.95	0.12	38,41,41,43	0
3	EDO	D	1003	4/4	0.95	0.11	28,28,29,31	0
3	EDO	C	1003	4/4	0.95	0.29	34,35,38,41	0
3	EDO	C	1004	4/4	0.96	0.14	41,43,44,46	0
3	EDO	A	1005	4/4	0.96	0.17	32,32,33,36	0
3	EDO	C	1002	4/4	0.97	0.12	28,28,29,30	0
3	EDO	D	1009	4/4	0.99	0.15	32,33,33,37	0
2	ZN	C	1001	1/1	0.99	0.07	40,40,40,40	0
2	ZN	B	1001	1/1	0.99	0.06	41,41,41,41	0
2	ZN	D	1001	1/1	0.99	0.05	38,38,38,38	0
2	ZN	A	1001	1/1	0.99	0.07	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.