



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2016 – 03:23 PM EDT

PDB ID : 5I43  
Title : Crystal structure of the catalytic domain of MMP-12 in complex with a selective sugar-conjugated triazole-linked carboxylate chelator water-soluble inhibitor (DC32).  
Authors : Stura, E.A.; Rosalia, L.; Cuffaro, D.; Tepshi, L.; Ciccone, L.; Rossello, A.  
Deposited on : 2016-02-11  
Resolution : 1.95 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

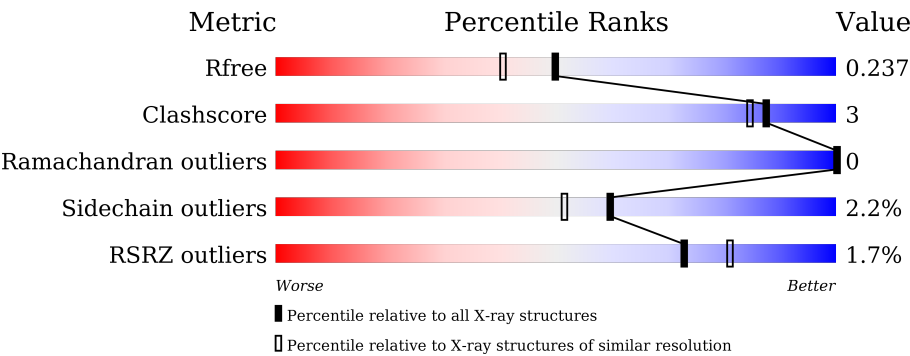
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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. 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	159	<div><div>3%</div><div><div></div><div>89%</div><div>9%</div><div>..</div></div></div>
1	B	159	<div><div>%</div><div><div></div><div>94%</div><div>5%</div><div>.</div></div></div>
1	C	159	<div><div>%</div><div><div></div><div>94%</div><div>5%</div><div>..</div></div></div>
1	D	159	<div><div>2%</div><div><div></div><div>94%</div><div>.</div><div>..</div></div></div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	67M	A	306	-	-	-	X
4	67M	B	301	-	-	-	X
4	67M	C	301	-	-	-	X
4	67M	D	301	-	-	-	X
5	EDO	A	307	-	-	-	X
5	EDO	A	308	-	-	-	X
5	EDO	A	310	-	-	-	X
5	EDO	A	312	-	-	-	X
5	EDO	A	315	-	-	-	X
5	EDO	B	307	-	-	-	X
5	EDO	D	309	-	-	-	X
5	EDO	D	310	-	-	-	X
5	EDO	D	311	-	-	-	X
7	PGO	D	313	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6013 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 Macrophage metalloelastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	1	0
			1245	793	220	229	3			
1	B	159	Total	C	N	O	S	0	2	0
			1260	801	220	235	4			
1	C	158	Total	C	N	O	S	0	3	0
			1268	807	226	232	3			
1	D	158	Total	C	N	O	S	0	3	0
			1262	803	221	235	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	MET	-	initiating methionine	UNP P39900
A	171	ASP	PHE	engineered mutation	UNP P39900
A	219	GLN	GLU	engineered mutation	UNP P39900
B	105	MET	-	initiating methionine	UNP P39900
B	171	ASP	PHE	engineered mutation	UNP P39900
B	219	GLN	GLU	engineered mutation	UNP P39900
C	105	MET	-	initiating methionine	UNP P39900
C	171	ASP	PHE	engineered mutation	UNP P39900
C	219	GLN	GLU	engineered mutation	UNP P39900
D	105	MET	-	initiating methionine	UNP P39900
D	171	ASP	PHE	engineered mutation	UNP P39900
D	219	GLN	GLU	engineered mutation	UNP P39900

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

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

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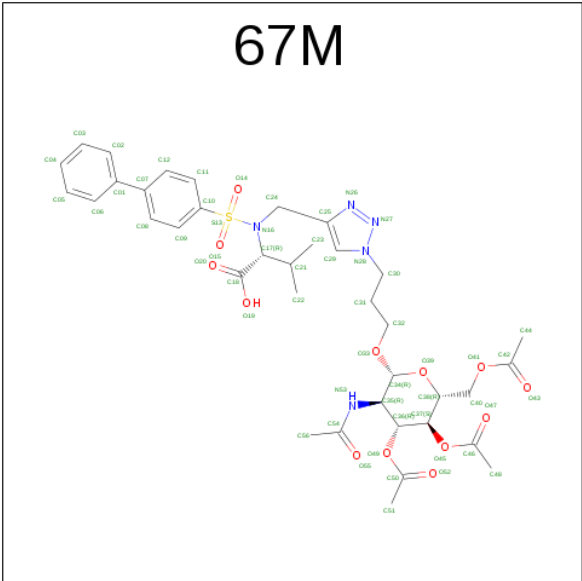
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is (2R)-2-[(1-{3-[(2R,3R,4R,5S,6R)-3-(acetylamino)-4,5-bis(acetyloxy)-6-[(acetyloxy)methyl]tetrahydro-2H-pyran-2-yl}oxy)propyl]-1H-1,2,3-triazol-4-yl)methyl](biphenyl-4-ylsulfonyl)amino]-3-methylbutanoic acid (non-preferred name) (three-letter code: 67M) (formula: C<sub>37</sub>H<sub>47</sub>N<sub>5</sub>O<sub>13</sub>S).



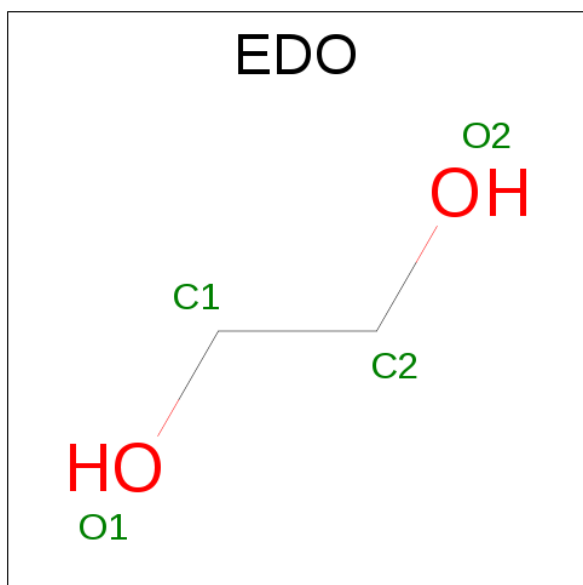
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			56	37	5	13	1		
4	B	1	Total	C	N	O	S	0	0
			56	37	5	13	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			56	37	5	13	1		
4	D	1	Total	C	N	O	S	0	0
			56	37	5	13	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



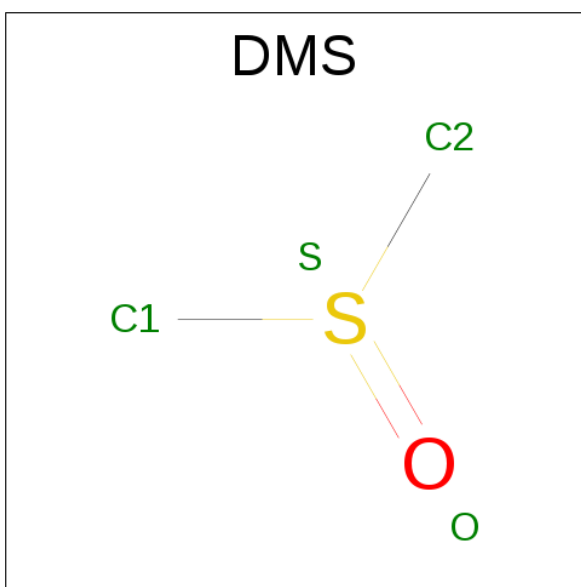
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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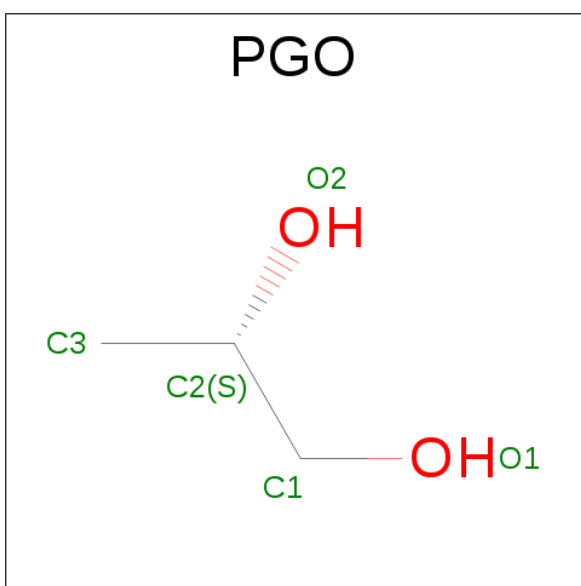
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0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

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula:  $C_3H_8O_2$ ).



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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	143	Total	O	0	2
			145	145		
8	B	139	Total	O	0	1
			140	140		
8	C	146	Total	O	0	1
			147	147		
8	D	167	Total	O	0	5
			172	172		

### 3 Residue-property plots [i](#)

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: Macrophage metalloelastase



- Molecule 1: Macrophage metalloelastase



- Molecule 1: Macrophage metalloelastase



- Molecule 1: Macrophage metalloelastase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.03Å 63.66Å 79.03Å 90.00° 103.03° 90.00°	Depositor
Resolution (Å)	44.56 – 1.95 44.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.56-1.95) 99.8 (44.56-1.95)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.200 , 0.233 0.210 , 0.237	Depositor DCC
$R_{free}$ test set	2264 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.6126e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PGO, CA, EDO, 67M, DMS

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	1.04	0/1282	0.98	4/1736 (0.2%)
1	B	1.02	0/1296	0.95	0/1752
1	C	1.13	2/1306 (0.2%)	0.97	3/1768 (0.2%)
1	D	1.06	1/1299 (0.1%)	0.95	1/1759 (0.1%)
All	All	1.06	3/5183 (0.1%)	0.96	8/7015 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	GLY	C-O	5.37	1.32	1.23
1	D	199	GLU	CD-OE1	5.35	1.31	1.25
1	C	128	GLU	CD-OE1	5.08	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	244	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	135	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	129	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	124	ASP	CB-CG-OD1	5.56	123.31	118.30
1	C	129	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	209	GLY	N-CA-C	-5.17	100.18	113.10
1	A	135	ARG	NE-CZ-NH1	5.13	122.87	120.30

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	1245	0	1179	11	0
1	B	1260	0	1184	4	0
1	C	1268	0	1199	5	0
1	D	1262	0	1190	6	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	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	56	0	0	1	0
4	B	56	0	0	0	0
4	C	56	0	0	0	0
4	D	56	0	0	0	0
5	A	40	0	60	1	0
5	B	20	0	30	0	0
5	C	8	0	12	0	0
5	D	24	0	36	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
7	B	5	0	8	0	0
7	C	20	0	32	0	0
7	D	5	0	8	0	0
8	A	145	0	0	7	0
8	B	140	0	0	1	0
8	C	147	0	0	1	1
8	D	172	0	0	6	1
All	All	6013	0	4950	27	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 3.

All (27) 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:D:106:GLY:N	8:D:401:HOH:O	2.00	0.92
1:D:222:HIS:CD2	8:D:428[B]:HOH:O	2.23	0.91
1:A:165[A]:ARG:NH1	8:A:401:HOH:O	2.09	0.86
1:A:172:HIS:NE2	8:A:402:HOH:O	2.13	0.80
1:D:222:HIS:HD2	8:D:428[B]:HOH:O	1.61	0.78
1:C:256[A]:ARG:HH11	1:C:256[A]:ARG:HG3	1.58	0.69
1:A:206:HIS:CG	1:A:207:SER:N	2.65	0.65
1:A:206:HIS:CG	1:A:207:SER:H	2.19	0.60
1:C:206[A]:HIS:ND1	8:C:402:HOH:O	2.32	0.58
1:C:241[B]:LYS:NZ	8:D:557[B]:HOH:O	2.38	0.56
1:B:259:GLN:O	1:B:263[B]:GLY:N	2.42	0.53
1:A:222:HIS:CD2	8:A:436:HOH:O	2.63	0.50
1:B:253:ASP:OD1	1:B:256:ARG:NH1	2.44	0.49
1:C:252:ALA:HB1	1:C:256[A]:ARG:NH1	2.31	0.46
1:A:109:TRP:HA	5:A:309:EDO:H12	1.98	0.45
1:D:241[A]:LYS:HE3	8:D:526:HOH:O	2.17	0.45
1:D:249:ARG:NH2	8:D:409:HOH:O	2.49	0.44
1:C:241[B]:LYS:HB3	1:C:241[B]:LYS:NZ	2.32	0.44
1:A:127:ARG:NH2	8:A:416:HOH:O	2.51	0.44
1:A:172:HIS:CD2	8:A:402:HOH:O	2.67	0.44
1:B:140:VAL:HG22	8:B:517:HOH:O	2.17	0.43
1:A:206:HIS:CE1	1:A:208:GLY:H	2.38	0.42
4:A:306:67M:C54	4:A:306:67M:O52	2.67	0.42
1:B:241:LYS:HB2	1:B:241:LYS:HE2	1.82	0.41
1:A:127:ARG:HD2	8:A:416:HOH:O	2.21	0.41
1:D:122:THR:HA	1:D:199:GLU:OE1	2.21	0.41
1:A:245:ILE:HB	8:A:442:HOH:O	2.21	0.41

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)
8:C:459:HOH:O	8:D:507:HOH:O[2_657]	2.13	0.07

## 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	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	B	158/159 (99%)	153 (97%)	5 (3%)	0	100	100
1	C	159/159 (100%)	152 (96%)	7 (4%)	0	100	100
1	D	159/159 (100%)	151 (95%)	8 (5%)	0	100	100
All	All	632/636 (99%)	609 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	128/128 (100%)	124 (97%)	4 (3%)	47	34
1	B	129/128 (101%)	125 (97%)	4 (3%)	47	34
1	C	130/128 (102%)	127 (98%)	3 (2%)	58	50
1	D	130/128 (102%)	129 (99%)	1 (1%)	86	85
All	All	517/512 (101%)	505 (98%)	12 (2%)	60	50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	142	SER
1	A	206	HIS
1	A	253	ASP
1	B	122	THR
1	B	183	HIS
1	B	241	LYS
1	B	249	ARG
1	C	191	ILE
1	C	241[A]	LYS

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Mol	Chain	Res	Type
1	C	241[B]	LYS
1	D	108	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 55 ligands modelled in this entry, 20 are monoatomic - leaving 35 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	67M	A	306	2	52,59,59	2.18	9 (17%)	70,83,83	2.25	24 (34%)
5	EDO	A	307	-	3,3,3	0.84	0	2,2,2	0.63	0
5	EDO	A	308	-	3,3,3	0.34	0	2,2,2	0.26	0
5	EDO	A	309	-	3,3,3	0.55	0	2,2,2	0.04	0
5	EDO	A	310	-	3,3,3	0.46	0	2,2,2	0.06	0
5	EDO	A	311	-	3,3,3	0.49	0	2,2,2	0.16	0
5	EDO	A	312	-	3,3,3	0.47	0	2,2,2	0.41	0
5	EDO	A	313	-	3,3,3	0.48	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	314	-	3,3,3	0.34	0	2,2,2	0.59	0
5	EDO	A	315	-	3,3,3	0.75	0	2,2,2	0.32	0
5	EDO	A	316	-	3,3,3	0.30	0	2,2,2	0.12	0
4	67M	B	301	2	52,59,59	2.27	12 (23%)	70,83,83	2.23	21 (30%)
5	EDO	B	307	-	3,3,3	0.57	0	2,2,2	0.28	0
5	EDO	B	308	-	3,3,3	0.71	0	2,2,2	0.21	0
5	EDO	B	309	-	3,3,3	0.50	0	2,2,2	0.11	0
5	EDO	B	310	-	3,3,3	0.50	0	2,2,2	0.07	0
5	EDO	B	311	-	3,3,3	0.61	0	2,2,2	0.25	0
6	DMS	B	312	-	3,3,3	0.43	0	3,3,3	0.71	0
7	PGO	B	313	-	4,4,4	0.88	0	2,4,4	0.86	0
4	67M	C	301	2	52,59,59	2.29	10 (19%)	70,83,83	2.30	22 (31%)
5	EDO	C	307	-	3,3,3	0.89	0	2,2,2	0.15	0
5	EDO	C	308	-	3,3,3	0.61	0	2,2,2	0.29	0
6	DMS	C	309	-	3,3,3	0.62	0	3,3,3	0.36	0
7	PGO	C	310	-	4,4,4	0.42	0	2,4,4	0.63	0
7	PGO	C	311	-	4,4,4	0.66	0	2,4,4	0.90	0
7	PGO	C	312	-	4,4,4	0.40	0	2,4,4	0.49	0
7	PGO	C	313	-	4,4,4	0.53	0	2,4,4	0.26	0
4	67M	D	301	2	52,59,59	2.19	11 (21%)	70,83,83	2.39	24 (34%)
5	EDO	D	307	-	3,3,3	0.64	0	2,2,2	0.81	0
5	EDO	D	308	-	3,3,3	0.41	0	2,2,2	0.65	0
5	EDO	D	309	-	3,3,3	0.46	0	2,2,2	0.40	0
5	EDO	D	310	-	3,3,3	0.23	0	2,2,2	1.10	0
5	EDO	D	311	-	3,3,3	0.53	0	2,2,2	0.20	0
5	EDO	D	312	-	3,3,3	0.45	0	2,2,2	0.16	0
7	PGO	D	313	-	4,4,4	0.42	0	2,4,4	1.23	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	67M	A	306	2	-	0/51/76/76	0/4/4/4
5	EDO	A	307	-	-	0/1/1/1	0/0/0/0
5	EDO	A	308	-	-	0/1/1/1	0/0/0/0
5	EDO	A	309	-	-	0/1/1/1	0/0/0/0
5	EDO	A	310	-	-	0/1/1/1	0/0/0/0
5	EDO	A	311	-	-	0/1/1/1	0/0/0/0
5	EDO	A	312	-	-	0/1/1/1	0/0/0/0
5	EDO	A	313	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	314	-	-	0/1/1/1	0/0/0/0
5	EDO	A	315	-	-	0/1/1/1	0/0/0/0
5	EDO	A	316	-	-	0/1/1/1	0/0/0/0
4	67M	B	301	2	-	0/51/76/76	0/4/4/4
5	EDO	B	307	-	-	0/1/1/1	0/0/0/0
5	EDO	B	308	-	-	0/1/1/1	0/0/0/0
5	EDO	B	309	-	-	0/1/1/1	0/0/0/0
5	EDO	B	310	-	-	0/1/1/1	0/0/0/0
5	EDO	B	311	-	-	0/1/1/1	0/0/0/0
6	DMS	B	312	-	-	0/0/0/0	0/0/0/0
7	PGO	B	313	-	-	0/2/2/2	0/0/0/0
4	67M	C	301	2	-	0/51/76/76	0/4/4/4
5	EDO	C	307	-	-	0/1/1/1	0/0/0/0
5	EDO	C	308	-	-	0/1/1/1	0/0/0/0
6	DMS	C	309	-	-	0/0/0/0	0/0/0/0
7	PGO	C	310	-	-	0/2/2/2	0/0/0/0
7	PGO	C	311	-	-	0/2/2/2	0/0/0/0
7	PGO	C	312	-	-	0/2/2/2	0/0/0/0
7	PGO	C	313	-	-	0/2/2/2	0/0/0/0
4	67M	D	301	2	-	0/51/76/76	0/4/4/4
5	EDO	D	307	-	-	0/1/1/1	0/0/0/0
5	EDO	D	308	-	-	0/1/1/1	0/0/0/0
5	EDO	D	309	-	-	0/1/1/1	0/0/0/0
5	EDO	D	310	-	-	0/1/1/1	0/0/0/0
5	EDO	D	311	-	-	0/1/1/1	0/0/0/0
5	EDO	D	312	-	-	0/1/1/1	0/0/0/0
7	PGO	D	313	-	-	0/2/2/2	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	67M	C10-S13	-8.72	1.63	1.76
4	B	301	67M	C10-S13	-8.56	1.64	1.76
4	A	306	67M	C10-S13	-8.12	1.64	1.76
4	D	301	67M	C10-S13	-7.82	1.65	1.76
4	B	301	67M	S13-N16	-5.49	1.54	1.63
4	A	306	67M	S13-N16	-5.20	1.55	1.63
4	D	301	67M	S13-N16	-5.03	1.55	1.63
4	C	301	67M	S13-N16	-3.98	1.57	1.63
4	D	301	67M	C29-N28	-2.91	1.32	1.35
4	C	301	67M	O14-S13	-2.49	1.40	1.43
4	A	306	67M	C12-C07	2.02	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	67M	N27-N28	2.05	1.38	1.34
4	D	301	67M	O41-C42	2.11	1.44	1.33
4	B	301	67M	O33-C34	2.13	1.44	1.40
4	B	301	67M	N27-N28	2.15	1.38	1.34
4	D	301	67M	C11-C10	2.36	1.42	1.38
4	B	301	67M	O41-C42	2.40	1.45	1.33
4	B	301	67M	C09-C08	2.48	1.43	1.38
4	C	301	67M	C09-C08	2.49	1.43	1.38
4	B	301	67M	C03-C02	2.56	1.43	1.38
4	C	301	67M	O41-C42	2.68	1.47	1.33
4	A	306	67M	C11-C10	2.69	1.43	1.38
4	B	301	67M	C37-C36	2.72	1.58	1.52
4	D	301	67M	O33-C34	2.79	1.45	1.40
4	A	306	67M	N27-N28	2.83	1.39	1.34
4	A	306	67M	O41-C42	2.90	1.48	1.33
4	D	301	67M	C03-C02	3.24	1.45	1.38
4	B	301	67M	O15-S13	3.63	1.48	1.43
4	C	301	67M	N27-N28	3.67	1.41	1.34
4	C	301	67M	C25-N26	3.98	1.38	1.34
4	B	301	67M	N26-N27	4.65	1.40	1.34
4	A	306	67M	N26-N27	4.81	1.41	1.34
4	D	301	67M	O49-C50	5.18	1.47	1.35
4	A	306	67M	O49-C50	5.30	1.47	1.35
4	D	301	67M	N26-N27	5.34	1.41	1.34
4	C	301	67M	O45-C46	5.35	1.47	1.35
4	B	301	67M	O49-C50	5.68	1.48	1.35
4	D	301	67M	O45-C46	5.73	1.48	1.35
4	C	301	67M	O49-C50	5.75	1.48	1.35
4	B	301	67M	O45-C46	5.76	1.48	1.35
4	C	301	67M	N26-N27	6.26	1.43	1.34
4	A	306	67M	O45-C46	6.30	1.49	1.35

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	67M	O15-S13-O14	-6.69	108.00	119.47
4	C	301	67M	N26-N27-N28	-6.18	102.66	107.31
4	B	301	67M	O15-S13-O14	-5.24	110.50	119.47
4	D	301	67M	O55-C54-C56	-5.23	112.45	122.07
4	D	301	67M	N26-N27-N28	-5.19	103.40	107.31
4	C	301	67M	C31-C30-N28	-4.30	103.82	112.39
4	D	301	67M	O15-S13-C10	-4.12	102.81	108.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	67M	O15-S13-O14	-3.89	112.81	119.47
4	B	301	67M	C34-C35-N53	-3.56	104.30	111.01
4	A	306	67M	O45-C46-O47	-3.42	115.97	122.92
4	A	306	67M	N26-N27-N28	-3.39	104.76	107.31
4	D	301	67M	O14-S13-C10	-3.19	103.97	108.01
4	D	301	67M	C36-C35-N53	-3.16	105.66	111.06
4	C	301	67M	O55-C54-C56	-3.06	116.43	122.07
4	A	306	67M	O15-S13-O14	-3.05	114.24	119.47
4	C	301	67M	O49-C50-O52	-3.00	116.82	122.92
4	B	301	67M	C11-C10-C09	-2.86	116.64	120.42
4	A	306	67M	C37-C36-C35	-2.85	104.70	110.26
4	B	301	67M	C29-C25-N26	-2.79	106.93	111.42
4	C	301	67M	C34-C35-C36	-2.76	104.94	110.16
4	A	306	67M	C23-C21-C17	-2.74	107.54	110.62
4	A	306	67M	C34-C35-C36	-2.70	105.05	110.16
4	D	301	67M	O45-C46-O47	-2.68	117.48	122.92
4	D	301	67M	C29-C25-N26	-2.66	107.15	111.42
4	C	301	67M	O45-C46-O47	-2.59	117.65	122.92
4	A	306	67M	O15-S13-C10	-2.55	104.79	108.01
4	D	301	67M	C10-S13-N16	-2.50	103.19	107.40
4	C	301	67M	C37-O45-C46	-2.45	113.88	117.71
4	A	306	67M	C29-C25-N26	-2.43	107.50	111.42
4	B	301	67M	O55-C54-C56	-2.39	117.67	122.07
4	B	301	67M	O39-C38-C40	-2.34	101.78	106.61
4	A	306	67M	C31-C30-N28	-2.30	107.79	112.39
4	C	301	67M	C03-C02-C01	-2.21	117.66	120.56
4	C	301	67M	O39-C34-O33	-2.10	104.95	109.99
4	A	306	67M	C36-O49-C50	-2.08	114.46	117.71
4	A	306	67M	C11-C10-C09	-2.08	117.67	120.42
4	D	301	67M	O33-C32-C31	-2.06	103.71	109.63
4	B	301	67M	O45-C46-O47	-2.03	118.80	122.92
4	B	301	67M	C05-C06-C01	2.01	123.20	120.56
4	A	306	67M	O39-C34-O33	2.17	115.20	109.99
4	A	306	67M	O45-C37-C38	2.17	112.43	108.14
4	C	301	67M	C11-C10-S13	2.32	122.22	119.79
4	D	301	67M	C37-O45-C46	2.33	121.35	117.71
4	C	301	67M	C08-C09-C10	2.33	121.98	119.49
4	B	301	67M	C11-C10-S13	2.35	122.25	119.79
4	D	301	67M	C40-C38-C37	2.37	119.06	113.33
4	B	301	67M	O41-C42-C44	2.39	122.90	112.37
4	A	306	67M	C08-C09-C10	2.45	122.10	119.49
4	D	301	67M	C36-O49-C50	2.46	121.56	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	67M	C40-O41-C42	2.48	123.34	117.12
4	D	301	67M	C34-O39-C38	2.51	118.67	113.74
4	A	306	67M	O14-S13-C10	2.61	111.31	108.01
4	B	301	67M	O15-S13-C10	2.62	111.32	108.01
4	B	301	67M	C36-C37-C38	2.62	116.29	110.58
4	C	301	67M	C23-C21-C17	2.67	113.63	110.62
4	C	301	67M	C36-C37-C38	2.69	116.42	110.58
4	C	301	67M	C25-C24-N16	2.85	117.21	112.56
4	C	301	67M	O14-S13-N16	3.12	113.50	106.97
4	B	301	67M	O14-S13-C10	3.13	111.96	108.01
4	B	301	67M	O39-C38-C37	3.13	116.45	109.78
4	B	301	67M	C40-O41-C42	3.19	125.10	117.12
4	D	301	67M	O15-S13-N16	3.29	113.84	106.97
4	C	301	67M	O39-C38-C40	3.34	113.50	106.61
4	D	301	67M	C11-C10-S13	3.36	123.31	119.79
4	A	306	67M	O45-C37-C36	3.37	114.92	108.21
4	A	306	67M	C11-C10-S13	3.48	123.45	119.79
4	D	301	67M	O49-C50-C51	3.66	118.06	111.09
4	D	301	67M	C22-C21-C17	3.68	114.77	110.62
4	A	306	67M	O14-S13-N16	3.77	114.86	106.97
4	A	306	67M	C36-C35-N53	3.78	117.53	111.06
4	C	301	67M	O14-S13-C10	3.92	112.96	108.01
4	B	301	67M	O49-C50-C51	4.15	118.99	111.09
4	C	301	67M	C34-C35-N53	4.15	118.83	111.01
4	D	301	67M	C34-C35-N53	4.19	118.90	111.01
4	B	301	67M	O49-C36-C37	4.21	116.62	108.21
4	A	306	67M	C40-O41-C42	4.50	128.40	117.12
4	D	301	67M	C35-N53-C54	4.57	135.23	123.21
4	A	306	67M	O49-C36-C37	4.58	117.36	108.21
4	A	306	67M	C22-C21-C17	4.59	115.78	110.62
4	C	301	67M	O49-C50-C51	4.62	119.89	111.09
4	C	301	67M	O45-C46-C48	4.82	120.26	111.09
4	A	306	67M	O49-C50-C51	4.87	120.36	111.09
4	B	301	67M	O45-C46-C48	4.89	120.40	111.09
4	C	301	67M	O41-C40-C38	4.90	119.11	108.47
4	D	301	67M	O14-S13-N16	5.22	117.88	106.97
4	B	301	67M	C36-O49-C50	5.52	126.35	117.71
4	B	301	67M	C25-C24-N16	6.19	122.64	112.56
4	B	301	67M	C36-C35-N53	6.32	121.87	111.06
4	D	301	67M	O45-C46-C48	6.34	123.15	111.09
4	D	301	67M	C56-C54-N53	6.37	128.31	116.10
4	A	306	67M	O45-C46-C48	7.97	126.26	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	67M	1	0
5	A	309	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	262:TYR	C	263[B]:GLY	N	3.38

## 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	157/159 (98%)	-0.07	4 (2%) 61 71	13, 23, 46, 66	0
1	B	159/159 (100%)	-0.01	2 (1%) 79 86	14, 23, 42, 88	1 (0%)
1	C	158/159 (99%)	-0.12	2 (1%) 79 86	12, 20, 40, 72	0
1	D	158/159 (99%)	-0.08	3 (1%) 70 78	11, 21, 45, 68	0
All	All	632/636 (99%)	-0.07	11 (1%) 73 81	11, 22, 43, 88	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263[A]	GLY	5.6
1	C	106	GLY	4.3
1	A	107	PRO	4.2
1	A	113	TYR	4.2
1	D	263	GLY	3.2
1	B	105	MET	2.8
1	D	113	TYR	2.7
1	D	107	PRO	2.7
1	C	110	ARG	2.5
1	A	207	SER	2.4
1	A	206	HIS	2.2

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	A	307	4/4	0.41	0.21	18.84	46,47,49,55	0
5	EDO	A	315	4/4	0.65	0.18	5.95	41,41,44,47	0
4	67M	B	301	56/56	0.90	0.23	5.47	19,75,129,138	0
5	EDO	A	308	4/4	0.86	0.18	4.86	55,55,57,59	0
5	EDO	A	312	4/4	0.89	0.17	4.68	37,43,45,49	0
7	PGO	D	313	5/5	0.79	0.20	4.57	58,59,59,63	0
4	67M	A	306	56/56	0.88	0.21	3.97	21,51,102,108	0
4	67M	C	301	56/56	0.87	0.23	3.85	18,50,103,115	0
5	EDO	D	311	4/4	0.87	0.14	3.19	37,43,45,49	0
5	EDO	D	309	4/4	0.76	0.29	3.03	76,77,78,79	0
5	EDO	B	307	4/4	0.86	0.15	2.45	34,41,43,43	0
5	EDO	A	310	4/4	0.84	0.17	2.42	48,53,60,62	0
5	EDO	D	310	4/4	0.87	0.19	2.37	37,41,43,44	0
4	67M	D	301	56/56	0.88	0.21	2.33	22,45,94,109	0
5	EDO	C	307	4/4	0.83	0.12	1.83	28,29,29,29	0
7	PGO	B	313	5/5	0.74	0.18	1.30	50,51,52,54	0
5	EDO	A	316	4/4	0.92	0.16	1.15	36,40,44,49	0
7	PGO	C	311	5/5	0.87	0.20	1.11	45,47,47,50	0
5	EDO	B	311	4/4	0.89	0.16	1.07	27,33,39,46	0
5	EDO	B	308	4/4	0.83	0.15	1.01	39,44,47,51	0
7	PGO	C	313	5/5	0.79	0.19	0.92	40,41,46,52	0
5	EDO	A	309	4/4	0.85	0.17	0.81	39,42,45,47	0
7	PGO	C	310	5/5	0.94	0.12	0.75	53,54,57,60	0
5	EDO	A	314	4/4	0.92	0.12	0.33	38,38,40,42	0
5	EDO	D	312	4/4	0.90	0.13	0.12	39,39,40,42	0
5	EDO	A	311	4/4	0.87	0.14	0.04	52,53,56,59	0
5	EDO	C	308	4/4	0.84	0.13	0.02	47,48,49,53	0
5	EDO	B	309	4/4	0.86	0.13	-0.09	53,58,59,61	0
5	EDO	A	313	4/4	0.89	0.09	-1.42	49,50,50,50	0
3	CA	A	303	1/1	0.99	0.05	-1.79	19,19,19,19	0
2	ZN	B	303	1/1	1.00	0.06	-1.88	18,18,18,18	0
3	CA	B	304	1/1	1.00	0.03	-2.07	21,21,21,21	0
3	CA	A	304	1/1	1.00	0.06	-2.22	16,16,16,16	0
3	CA	B	305	1/1	0.99	0.04	-2.23	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	306	1/1	1.00	0.07	-2.33	19,19,19,19	0
2	ZN	C	303	1/1	1.00	0.05	-2.37	16,16,16,16	0
3	CA	C	304	1/1	0.99	0.05	-2.79	16,16,16,16	0
2	ZN	D	303	1/1	1.00	0.06	-3.10	17,17,17,17	0
2	ZN	A	302	1/1	1.00	0.07	-3.27	17,17,17,17	0
3	CA	D	305	1/1	1.00	0.07	-3.38	16,16,16,16	0
3	CA	C	306	1/1	0.99	0.04	-3.88	16,16,16,16	0
3	CA	D	306	1/1	1.00	0.04	-4.31	16,16,16,16	0
3	CA	D	304	1/1	1.00	0.03	-4.55	17,17,17,17	0
3	CA	A	305	1/1	0.99	0.03	-4.57	16,16,16,16	0
3	CA	C	305	1/1	1.00	0.04	-6.08	16,16,16,16	0
6	DMS	C	309	4/4	0.89	0.23	-	61,64,64,65	0
7	PGO	C	312	5/5	0.87	0.14	-	56,56,58,60	0
5	EDO	D	308	4/4	0.73	0.25	-	47,57,64,77	0
6	DMS	B	312	4/4	0.51	0.21	-	61,64,69,80	0
5	EDO	B	310	4/4	0.88	0.14	-	51,53,53,57	0
2	ZN	B	302	1/1	1.00	0.03	-	20,20,20,20	0
2	ZN	A	301	1/1	1.00	0.03	-	17,17,17,17	0
2	ZN	C	302	1/1	1.00	0.03	-	16,16,16,16	0
2	ZN	D	302	1/1	1.00	0.03	-	16,16,16,16	0
5	EDO	D	307	4/4	0.83	0.17	-	37,39,47,54	0

## 6.5 Other polymers

There are no such residues in this entry.