



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 4WW8 / pdb_00004ww8
Title : Crystal structure of human carbonic anhydrase isozyme XII with 4-Propylthiobenzenesulfonamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2014-11-10
Resolution : 1.42 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

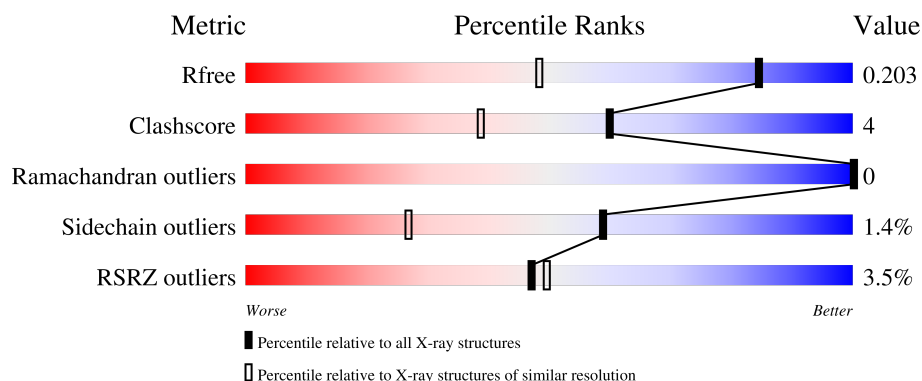
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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 $\leq 5\%$. 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	263	 3% 86% 13% .
1	B	263	 2% 83% 15% ..
1	C	263	 6% 89% 10% .
1	D	263	 3% 86% 12% .

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
3	EDO	B	305[A]	-	-	X	-
3	EDO	B	305[B]	-	-	X	-
3	EDO	B	306	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9594 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	12	0
			2171	1382	367	414	8			
1	B	261	Total	C	N	O	S	0	9	0
			2162	1375	366	413	8			
1	C	261	Total	C	N	O	S	0	5	0
			2093	1336	353	396	8			
1	D	260	Total	C	N	O	S	0	7	0
			2140	1359	360	414	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

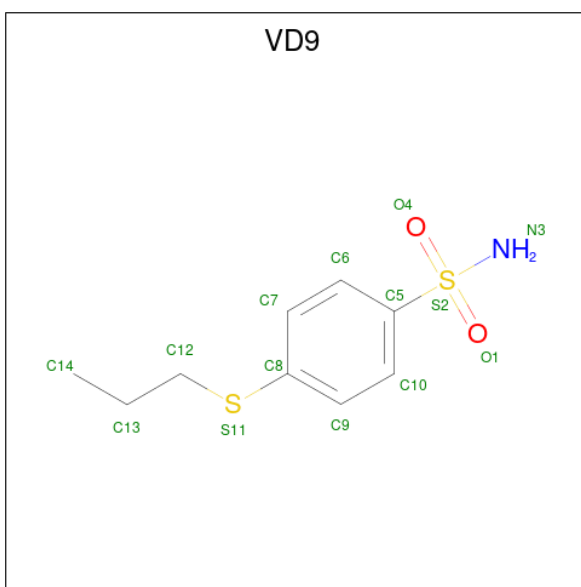
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	1
			8	4	4		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 4-(propylsulfanyl)benzenesulfonamide (CCD ID: VD9) (formula: C₉H₁₃NO₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			14	9	1	2	2		
4	B	1	Total	C	N	O	S	0	0
			14	9	1	2	2		
4	C	1	Total	C	N	O	S	0	0
			14	9	1	2	2		
4	D	1	Total	C	N	O	S	0	0
			14	9	1	2	2		

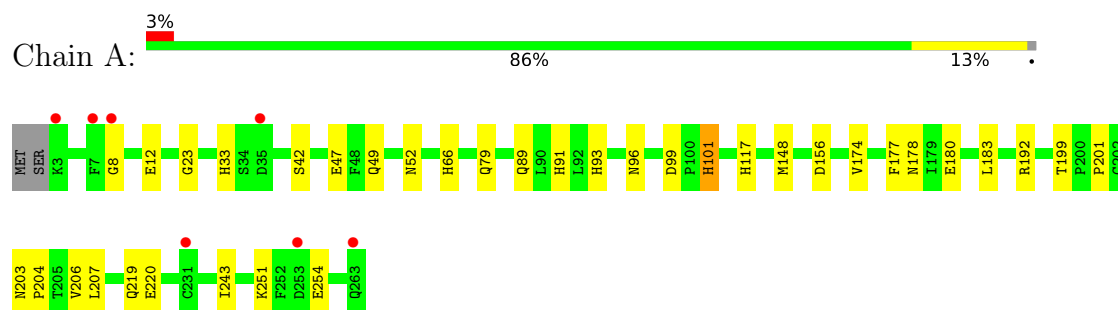
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	219	Total	O	0	0
			219	219		
5	B	260	Total	O	0	0
			260	260		
5	C	187	Total	O	0	0
			187	187		
5	D	246	Total	O	0	0
			246	246		

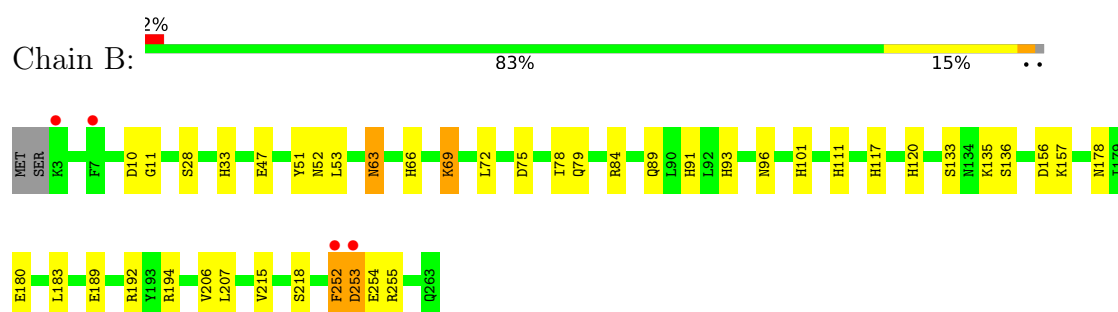
3 Residue-property plots [i](#)

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.

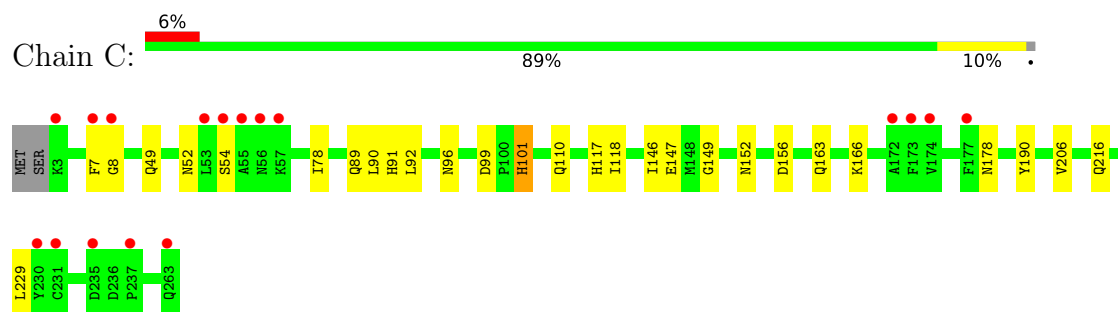
- Molecule 1: Carbonic anhydrase 12



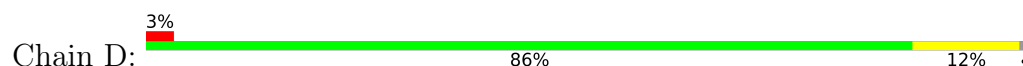
- Molecule 1: Carbonic anhydrase 12

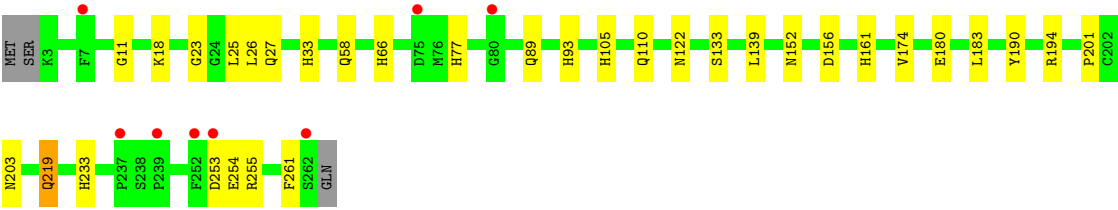


- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.31Å 74.26Å 91.57Å 90.00° 108.66° 90.00°	Depositor
Resolution (Å)	56.42 – 1.42 56.42 – 1.42	Depositor EDS
% Data completeness (in resolution range)	95.7 (56.42-1.42) 95.7 (56.42-1.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.172 , 0.205 0.170 , 0.203	Depositor DCC
R_{free} test set	17544 reflections (9.49%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9594	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 43.45 % 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 1.7593e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: VD9, EDO, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.53	16/2237 (0.7%)	1.32	8/3048 (0.3%)
1	B	1.68	21/2227 (0.9%)	1.37	10/3031 (0.3%)
1	C	1.51	10/2156 (0.5%)	1.27	4/2937 (0.1%)
1	D	1.64	21/2203 (1.0%)	1.38	3/3001 (0.1%)
All	All	1.59	68/8823 (0.8%)	1.34	25/12017 (0.2%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	HIS	ND1-CE1	9.02	1.41	1.32
1	D	93	HIS	ND1-CE1	8.69	1.41	1.32
1	C	146	ILE	N-CA	8.37	1.56	1.46
1	B	111	HIS	ND1-CE1	7.95	1.40	1.32
1	A	91	HIS	ND1-CE1	7.83	1.40	1.32
1	C	117	HIS	ND1-CE1	7.78	1.40	1.32
1	A	174	VAL	N-CA	-7.53	1.39	1.46
1	B	96	ASN	C-O	-7.41	1.17	1.24
1	B	63	ASN	CA-C	-7.40	1.43	1.52
1	A	93	HIS	N-CA	7.12	1.54	1.45
1	C	96	ASN	N-CA	7.11	1.52	1.46
1	A	101	HIS	CA-C	-6.92	1.44	1.53
1	D	105	HIS	ND1-CE1	6.90	1.39	1.32
1	D	190	TYR	CA-C	-6.87	1.44	1.52
1	D	33	HIS	CG-CD2	6.72	1.43	1.35
1	A	33	HIS	CA-C	-6.64	1.44	1.52
1	B	120	HIS	CE1-NE2	6.48	1.39	1.32
1	A	206	VAL	CA-C	-6.47	1.45	1.52
1	B	218	SER	CA-C	-6.40	1.44	1.53
1	B	117	HIS	CE1-NE2	6.34	1.38	1.32
1	A	23	GLY	CA-C	-6.23	1.45	1.51
1	D	33	HIS	CG-ND1	-6.10	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	HIS	CG-CD2	6.07	1.42	1.35
1	A	220	GLU	N-CA	-6.06	1.39	1.46
1	D	233	HIS	ND1-CE1	6.04	1.38	1.32
1	B	93	HIS	CA-C	-5.98	1.45	1.52
1	B	91	HIS	CG-CD2	5.91	1.42	1.35
1	A	204	PRO	N-CA	-5.90	1.43	1.47
1	B	189	GLU	C-O	5.86	1.30	1.24
1	B	194	ARG	CA-C	-5.82	1.45	1.52
1	B	11	GLY	N-CA	5.81	1.52	1.45
1	A	117	HIS	CA-C	-5.80	1.45	1.52
1	C	91	HIS	ND1-CE1	5.73	1.38	1.32
1	D	161	HIS	ND1-CE1	5.65	1.38	1.32
1	B	101	HIS	ND1-CE1	5.59	1.38	1.32
1	A	243	ILE	C-O	5.56	1.29	1.23
1	B	53	LEU	CA-C	5.55	1.59	1.52
1	D	11	GLY	N-CA	5.55	1.51	1.45
1	B	111	HIS	CG-CD2	5.48	1.41	1.35
1	B	136	SER	C-O	-5.47	1.17	1.23
1	C	118	ILE	C-O	5.46	1.30	1.24
1	D	194	ARG	CA-C	-5.41	1.46	1.52
1	B	253	ASP	CA-C	5.39	1.59	1.52
1	D	174	VAL	CA-C	5.38	1.57	1.52
1	D	27	GLN	N-CA	5.38	1.52	1.45
1	C	190	TYR	C-O	-5.37	1.17	1.23
1	B	135	LYS	N-CA	5.36	1.52	1.45
1	A	96	ASN	N-CA	5.32	1.51	1.46
1	D	139	LEU	N-CA	5.32	1.52	1.45
1	C	152	ASN	CA-CB	5.31	1.60	1.53
1	D	66	HIS	ND1-CE1	5.27	1.37	1.32
1	D	93	HIS	CD2-NE2	5.26	1.43	1.37
1	A	117	HIS	ND1-CE1	5.22	1.37	1.32
1	B	28	SER	CA-C	-5.20	1.46	1.52
1	D	18	LYS	N-CA	5.18	1.52	1.46
1	D	122	ASN	N-CA	5.17	1.53	1.46
1	D	23	GLY	C-O	5.17	1.28	1.24
1	D	261	PHE	C-O	-5.15	1.17	1.23
1	D	161	HIS	CE1-NE2	5.12	1.37	1.32
1	B	66	HIS	CG-CD2	-5.12	1.30	1.35
1	A	49	GLN	CA-C	-5.12	1.46	1.52
1	A	66	HIS	ND1-CE1	5.11	1.37	1.32
1	C	101	HIS	ND1-CE1	5.11	1.37	1.32
1	A	251	LYS	C-O	5.08	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	HIS	ND1-CE1	5.05	1.37	1.32
1	D	77	HIS	ND1-CE1	5.04	1.37	1.32
1	D	152	ASN	N-CA	-5.03	1.40	1.46
1	C	49	GLN	N-CA	5.02	1.52	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	THR	O-C-N	7.30	127.24	121.55
1	A	8	GLY	CA-C-N	7.22	126.85	119.56
1	A	8	GLY	C-N-CA	7.22	126.85	119.56
1	D	77	HIS	O-C-N	6.16	130.27	123.25
1	D	77	HIS	CA-C-O	-5.98	114.87	121.33
1	A	12	GLU	N-CA-C	5.87	118.46	111.71
1	B	157	LYS	N-CA-C	-5.79	105.48	112.54
1	A	177	PHE	CA-C-O	-5.52	115.33	121.51
1	A	199	THR	CA-C-N	-5.44	114.78	120.38
1	A	199	THR	C-N-CA	-5.44	114.78	120.38
1	B	69	LYS	CG-CD-CE	-5.44	98.80	111.30
1	B	72	LEU	O-C-N	5.39	126.80	121.57
1	B	28	SER	O-C-N	-5.38	116.78	121.35
1	C	206	VAL	N-CA-C	5.32	115.75	107.99
1	D	133	SER	N-CA-C	5.29	117.79	111.71
1	B	111	HIS	CB-CA-C	-5.24	100.67	109.53
1	B	194	ARG	CA-C-O	5.21	126.26	120.43
1	B	10	ASP	O-C-N	5.19	128.73	122.35
1	B	133	SER	CA-C-N	-5.17	114.36	122.79
1	B	133	SER	C-N-CA	-5.17	114.36	122.79
1	C	92	LEU	CA-C-O	5.08	127.39	121.44
1	C	78	ILE	CB-CA-C	-5.08	103.82	110.98
1	A	49	GLN	O-C-N	-5.06	116.78	123.21
1	B	206	VAL	N-CA-C	5.02	115.20	108.17
1	C	229	LEU	N-CA-C	5.02	117.92	109.95

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	2171	0	2027	11	0
1	B	2162	0	2038	45	0
1	C	2093	0	1959	9	0
1	D	2140	0	2008	7	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	12	0	18	0	0
3	B	28	0	42	14	0
3	C	8	0	12	0	0
3	D	8	0	12	0	0
4	A	14	0	12	0	0
4	B	14	0	12	0	0
4	C	14	0	12	0	0
4	D	14	0	12	0	0
5	A	219	0	0	2	0
5	B	260	0	0	9	0
5	C	187	0	0	0	0
5	D	246	0	0	0	0
All	All	9594	0	8164	72	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 4.

All (72) 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)
3:B:306:EDO:H11	5:B:622:HOH:O	1.42	1.15
1:B:252[A]:PHE:CZ	1:B:255:ARG:HB3	2.02	0.95
1:B:69:LYS:NZ	3:B:305[B]:EDO:H12	1.82	0.93
1:A:148[A]:MET:SD	1:A:219:GLN:HB3	2.13	0.87
1:B:215:VAL:HG12	3:B:306:EDO:H12	1.58	0.85
1:B:255:ARG:CD	5:B:595:HOH:O	2.23	0.85
1:B:69:LYS:NZ	3:B:305[A]:EDO:H11	1.94	0.82
1:B:252[A]:PHE:CZ	1:B:255:ARG:CB	2.63	0.81
1:B:252[A]:PHE:CE1	1:B:255:ARG:HB2	2.16	0.79
1:B:69:LYS:HZ2	3:B:305[B]:EDO:H12	1.46	0.78
1:B:252[A]:PHE:CE1	1:B:255:ARG:CB	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:HIS:HE1	1:B:252[B]:PHE:CZ	2.07	0.73
1:B:69:LYS:HZ2	3:B:305[A]:EDO:H11	1.51	0.72
1:A:201:PRO:HG2	1:A:203[B]:ASN:OD1	1.91	0.71
3:B:306:EDO:H22	5:B:493:HOH:O	1.90	0.70
1:B:69:LYS:HZ3	3:B:305[B]:EDO:H12	1.58	0.69
1:B:252[A]:PHE:CD1	1:B:255:ARG:HB2	2.27	0.69
1:B:69:LYS:NZ	3:B:305[B]:EDO:C1	2.57	0.68
1:B:84[B]:ARG:HD2	5:B:647:HOH:O	1.94	0.68
1:D:201:PRO:HG2	1:D:203[B]:ASN:OD1	1.93	0.67
1:B:33:HIS:HE1	1:B:252[B]:PHE:CE1	2.13	0.67
1:B:252[A]:PHE:O	1:B:254:GLU:N	2.30	0.64
1:A:148[A]:MET:SD	1:A:219:GLN:CB	2.85	0.64
1:B:252[A]:PHE:CD2	1:B:255:ARG:O	2.51	0.64
1:B:33:HIS:CE1	1:B:252[B]:PHE:CZ	2.88	0.61
1:B:69:LYS:HZ3	3:B:305[B]:EDO:C1	2.12	0.61
1:A:148[B]:MET:HE3	5:A:492:HOH:O	2.01	0.61
1:C:7:PHE:CD1	1:C:8:GLY:N	2.69	0.59
1:B:75:ASP:OD2	5:B:623:HOH:O	2.17	0.58
1:B:255:ARG:CG	5:B:595:HOH:O	2.50	0.57
1:C:163:GLN:OE1	1:C:166:LYS:HD2	2.04	0.57
1:B:69:LYS:HZ3	3:B:305[A]:EDO:H11	1.70	0.57
1:B:255:ARG:HG2	5:B:595:HOH:O	2.05	0.56
1:B:252[A]:PHE:CE2	1:B:255:ARG:C	2.84	0.56
1:B:255:ARG:HD2	5:B:595:HOH:O	1.94	0.55
1:B:252[A]:PHE:CE1	1:B:255:ARG:NE	2.75	0.55
1:B:252[B]:PHE:HD1	5:B:541:HOH:O	1.90	0.54
1:D:180[A]:GLU:HG3	1:D:183:LEU:HD12	1.89	0.54
1:B:252[A]:PHE:CE2	1:B:255:ARG:O	2.63	0.52
1:B:252[A]:PHE:CE1	1:B:255:ARG:CD	2.93	0.51
1:B:252[A]:PHE:CZ	1:B:255:ARG:HB2	2.39	0.50
1:B:69:LYS:HD3	3:B:305[A]:EDO:H12	1.95	0.48
1:A:47:GLU:HB2	1:A:79:GLN:HB3	1.95	0.47
1:A:219:GLN:NE2	5:A:401:HOH:O	2.35	0.46
1:B:252[A]:PHE:CE1	1:B:255:ARG:HD2	2.50	0.46
1:D:26:LEU:HD22	1:D:255:ARG:HD3	1.98	0.46
1:B:252[A]:PHE:CD1	1:B:255:ARG:NE	2.84	0.45
1:D:253:ASP:O	1:D:254:GLU:HB2	2.15	0.45
1:B:252[A]:PHE:CE1	1:B:255:ARG:HB3	2.44	0.45
1:A:99:ASP:OD1	1:A:101:HIS:HD2	2.00	0.45
1:B:51:TYR:OH	1:B:78[B]:ILE:HD11	2.16	0.45
1:C:52:ASN:HA	1:C:178:ASN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:CG1	3:B:306:EDO:H12	2.39	0.44
1:A:254[B]:GLU:HA	1:A:254[B]:GLU:OE1	2.18	0.44
1:B:180:GLU:HG3	1:B:183:LEU:HD12	1.99	0.44
1:B:47:GLU:HB2	1:B:79:GLN:HB3	2.00	0.44
1:B:52:ASN:HA	1:B:178:ASN:HA	1.99	0.44
1:B:192:ARG:HD2	1:B:207:LEU:HD11	2.00	0.43
1:A:180:GLU:HG3	1:A:183:LEU:HD12	2.01	0.42
1:B:69:LYS:HZ3	3:B:305[A]:EDO:C1	2.25	0.42
1:B:253:ASP:O	1:B:254:GLU:HB2	2.18	0.42
1:C:99:ASP:OD1	1:C:101:HIS:HD2	2.02	0.42
1:D:219[A]:GLN:CD	1:D:219[A]:GLN:O	2.62	0.42
1:C:110:GLN:NE2	1:D:110[A]:GLN:NE2	2.67	0.42
1:A:192:ARG:HD2	1:A:207:LEU:HD11	2.02	0.42
1:A:52:ASN:HA	1:A:178:ASN:HA	2.02	0.42
1:C:90:LEU:C	1:C:90:LEU:HD12	2.44	0.42
1:C:147:GLU:O	1:C:216:GLN:HA	2.20	0.42
1:C:149:GLY:HA3	1:C:216:GLN:OE1	2.21	0.41
1:B:252[A]:PHE:CE2	1:B:255:ARG:CB	3.03	0.40
1:C:8:GLY:HA2	1:D:25:LEU:HD21	2.02	0.40
1:B:63:ASN:OD1	1:B:63:ASN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/263 (103%)	266 (98%)	4 (2%)	0	100	100
1	B	268/263 (102%)	261 (97%)	7 (3%)	0	100	100
1	C	264/263 (100%)	254 (96%)	10 (4%)	0	100	100
1	D	265/263 (101%)	256 (97%)	9 (3%)	0	100	100
All	All	1067/1052 (101%)	1037 (97%)	30 (3%)	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	237/235 (101%)	234 (99%)	3 (1%)	61	29
1	B	240/235 (102%)	236 (98%)	4 (2%)	53	20
1	C	226/235 (96%)	223 (99%)	3 (1%)	61	29
1	D	237/235 (101%)	232 (98%)	5 (2%)	47	14
All	All	940/940 (100%)	925 (98%)	15 (2%)	59	22

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	89	GLN
1	A	156	ASP
1	B	89	GLN
1	B	156	ASP
1	B	252[A]	PHE
1	B	252[B]	PHE
1	C	54	SER
1	C	89	GLN
1	C	156	ASP
1	D	58	GLN
1	D	89	GLN
1	D	156	ASP
1	D	219[A]	GLN
1	D	219[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	77	HIS

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	111	HIS
1	A	250	GLN
1	B	13	ASN
1	B	33	HIS
1	B	79	GLN
1	B	96	ASN
1	B	110	GLN
1	B	111	HIS
1	B	244	ASN
1	B	250	GLN
1	C	13	ASN
1	C	77	HIS
1	C	110	GLN
1	C	233	HIS
1	C	250	GLN
1	C	263	GLN
1	D	13	ASN
1	D	49	GLN
1	D	79	GLN
1	D	250	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	B	304	-	3,3,3	1.13	0	2,2,2	1.09	0
3	EDO	C	302	-	3,3,3	0.67	0	2,2,2	0.43	0
3	EDO	B	306	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	A	302	-	3,3,3	0.60	0	2,2,2	0.74	0
3	EDO	B	305[B]	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	B	307	-	3,3,3	0.26	0	2,2,2	1.01	0
4	VD9	A	305	2	14,14,14	1.46	2 (14%)	19,19,19	2.44	8 (42%)
4	VD9	B	308	2	14,14,14	1.81	6 (42%)	19,19,19	2.81	9 (47%)
4	VD9	C	304	2	14,14,14	1.68	2 (14%)	19,19,19	2.39	7 (36%)
4	VD9	D	304	2	14,14,14	1.17	1 (7%)	19,19,19	2.26	5 (26%)
3	EDO	B	302	-	3,3,3	0.69	0	2,2,2	0.28	0
3	EDO	D	303	-	3,3,3	0.85	0	2,2,2	0.15	0
3	EDO	A	303	-	3,3,3	0.69	0	2,2,2	0.61	0
3	EDO	D	302	-	3,3,3	0.56	0	2,2,2	0.33	0
3	EDO	B	305[A]	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	B	303	-	3,3,3	0.86	0	2,2,2	0.54	0
3	EDO	A	304	-	3,3,3	0.93	0	2,2,2	0.38	0
3	EDO	C	303	-	3,3,3	0.93	0	2,2,2	0.23	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
3	EDO	B	304	-	-	0/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	B	306	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	305[B]	-	-	0/1/1/1	-
3	EDO	B	307	-	-	1/1/1/1	-
4	VD9	A	305	2	-	3/10/10/10	0/1/1/1
4	VD9	B	308	2	-	2/10/10/10	0/1/1/1
4	VD9	C	304	2	-	3/10/10/10	0/1/1/1
4	VD9	D	304	2	-	2/10/10/10	0/1/1/1
3	EDO	B	302	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	B	305[A]	-	-	0/1/1/1	-
3	EDO	B	303	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	C	303	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	VD9	O4-S2	4.40	1.51	1.43
4	A	305	VD9	O1-S2	3.78	1.50	1.43
4	B	308	VD9	C10-C5	3.22	1.43	1.38
4	B	308	VD9	C7-C8	-3.02	1.33	1.39
4	D	304	VD9	C5-S2	3.00	1.81	1.77
4	C	304	VD9	C8-S11	2.89	1.82	1.76
4	B	308	VD9	C6-C7	2.67	1.43	1.38
4	B	308	VD9	C9-C8	-2.38	1.34	1.39
4	B	308	VD9	C8-S11	2.24	1.81	1.76
4	B	308	VD9	C6-C5	2.10	1.42	1.38
4	A	305	VD9	O4-S2	2.08	1.47	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	308	VD9	C7-C8-C9	6.70	129.74	118.85
4	C	304	VD9	O1-S2-O4	-5.60	110.18	118.80
4	A	305	VD9	C6-C7-C8	-5.33	114.34	120.48
4	D	304	VD9	C7-C8-C9	5.09	127.13	118.85
4	B	308	VD9	C10-C9-C8	-4.77	114.98	120.48
4	B	308	VD9	O4-S2-N3	4.62	114.02	107.35
4	D	304	VD9	C10-C9-C8	-4.62	115.16	120.48
4	D	304	VD9	C6-C7-C8	-4.45	115.35	120.48
4	B	308	VD9	C6-C7-C8	-4.08	115.77	120.48
4	A	305	VD9	C7-C6-C5	4.01	123.34	119.44
4	A	305	VD9	C7-C8-C9	3.98	125.31	118.85
4	C	304	VD9	C6-C7-C8	-3.78	116.12	120.48
4	A	305	VD9	C10-C9-C8	-3.67	116.25	120.48
4	C	304	VD9	C9-C10-C5	-3.60	115.94	119.44
4	C	304	VD9	O1-S2-N3	3.29	112.09	107.35
4	B	308	VD9	C10-C5-S2	3.25	124.14	119.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	VD9	O1-S2-O4	-3.08	114.05	118.80
4	D	304	VD9	O1-S2-C5	-2.84	104.14	107.35
4	C	304	VD9	C12-S11-C8	-2.79	98.85	104.03
4	B	308	VD9	O4-S2-C5	-2.77	104.22	107.35
4	C	304	VD9	C7-C8-S11	-2.70	109.68	120.68
4	A	305	VD9	O4-S2-N3	2.59	111.09	107.35
4	B	308	VD9	C9-C8-S11	-2.58	110.17	120.68
4	B	308	VD9	C6-C5-C10	-2.55	117.14	120.47
4	B	308	VD9	C9-C10-C5	2.43	121.81	119.44
4	D	304	VD9	O1-S2-N3	2.32	110.69	107.35
4	C	304	VD9	C7-C8-C9	2.27	122.53	118.85
4	A	305	VD9	C9-C10-C5	2.18	121.56	119.44
4	A	305	VD9	O4-S2-C5	-2.04	105.04	107.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	VD9	C6-C5-S2-O4
4	C	304	VD9	C10-C5-S2-O4
4	C	304	VD9	C6-C5-S2-O4
4	A	305	VD9	C10-C5-S2-O4
3	B	307	EDO	O1-C1-C2-O2
4	D	304	VD9	C10-C5-S2-O4
4	B	308	VD9	C10-C5-S2-O4
3	A	303	EDO	O1-C1-C2-O2
4	B	308	VD9	C6-C5-S2-O4
4	D	304	VD9	C6-C5-S2-O4
3	B	303	EDO	O1-C1-C2-O2
4	C	304	VD9	C10-C5-S2-N3
4	A	305	VD9	C6-C5-S2-N3

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	306	EDO	4	0
3	B	305[B]	EDO	5	0
3	B	305[A]	EDO	5	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, 95th 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	261/263 (99%)	-0.00	7 (2%) 56 59	6, 16, 30, 52	12 (4%)
1	B	261/263 (99%)	-0.13	4 (1%) 72 76	5, 13, 25, 44	9 (3%)
1	C	261/263 (99%)	0.42	17 (6%) 25 27	6, 20, 37, 50	5 (1%)
1	D	260/263 (98%)	-0.04	8 (3%) 51 54	6, 15, 28, 43	7 (2%)
All	All	1043/1052 (99%)	0.06	36 (3%) 47 49	5, 16, 31, 52	33 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252[A]	PHE	4.2
1	C	55	ALA	4.1
1	D	7	PHE	3.8
1	C	7	PHE	3.7
1	D	252	PHE	3.6
1	A	3[A]	LYS	3.5
1	B	7	PHE	3.4
1	B	253	ASP	3.4
1	C	8	GLY	3.3
1	C	57	LYS	3.3
1	C	56	ASN	3.3
1	C	3	LYS	3.2
1	D	262	SER	3.2
1	D	80	GLY	3.1
1	C	230	TYR	2.9
1	C	231[A]	CYS	2.9
1	D	253	ASP	2.9
1	A	263	GLN	2.8
1	A	8	GLY	2.8
1	A	7	PHE	2.5
1	D	237	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	3	LYS	2.5
1	C	173	PHE	2.4
1	D	75	ASP	2.4
1	C	263	GLN	2.4
1	C	235	ASP	2.3
1	C	54	SER	2.2
1	A	35	ASP	2.2
1	A	253	ASP	2.2
1	C	174	VAL	2.2
1	C	53	LEU	2.1
1	A	231	CYS	2.1
1	C	237	PRO	2.1
1	D	239	PRO	2.1
1	C	172	ALA	2.1
1	C	177	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 oligosaccharides 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, 95th 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	B	305[A]	4/4	0.67	0.16	19,23,24,24	4
3	EDO	B	305[B]	4/4	0.67	0.16	16,20,20,21	4
3	EDO	B	307	4/4	0.86	0.13	27,37,37,40	0
3	EDO	D	303	4/4	0.87	0.11	25,25,26,34	0
3	EDO	C	302	4/4	0.88	0.11	29,31,32,34	0
3	EDO	A	303	4/4	0.88	0.11	29,32,35,39	0
3	EDO	B	306	4/4	0.90	0.11	23,29,34,37	0
3	EDO	B	304	4/4	0.90	0.10	22,25,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	304	4/4	0.90	0.11	22,27,28,28	0
3	EDO	B	303	4/4	0.90	0.11	20,24,27,28	0
3	EDO	C	303	4/4	0.91	0.10	26,26,26,27	0
3	EDO	A	302	4/4	0.93	0.10	20,21,23,24	0
3	EDO	D	302	4/4	0.95	0.07	15,15,18,19	0
3	EDO	B	302	4/4	0.96	0.07	15,15,16,17	0
4	VD9	A	305	14/14	0.98	0.06	9,13,19,22	0
4	VD9	B	308	14/14	0.98	0.05	8,10,17,19	0
4	VD9	C	304	14/14	0.98	0.07	12,17,23,25	0
4	VD9	D	304	14/14	0.98	0.06	9,12,20,20	0
2	ZN	C	301	1/1	0.99	0.02	12,12,12,12	0
2	ZN	B	301	1/1	1.00	0.01	7,7,7,7	0
2	ZN	A	301	1/1	1.00	0.01	8,8,8,8	0
2	ZN	D	301	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.