



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:44 AM GMT

PDB ID : 1O7J
Title : ATOMIC RESOLUTION STRUCTURE OF ERWINIA CHRYSANTHEMI
L-ASPARAGINASE
Authors : Lubkowski, J.; Dauter, M.; Aghaiypour, K.; Wlodawer, A.; Dauter, Z.
Deposited on : 2002-11-07
Resolution : 1.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

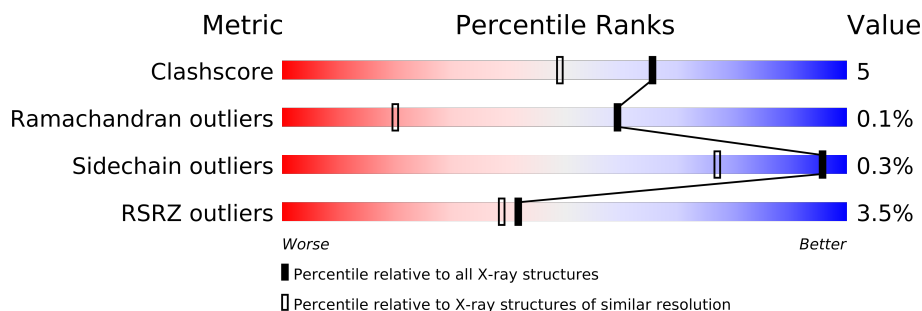
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.00 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))
Clashscore	79885	1028 (1.10-0.90)
Ramachandran outliers	78287	1056 (1.12-0.88)
Sidechain outliers	78261	1055 (1.12-0.88)
RSRZ outliers	66119	1007 (1.12-0.88)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	
1	C	327	
1	D	327	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	1329	-	X
2	SO4	C	1329	-	X
2	SO4	D	1329	-	X
3	GOL	A	1330	-	X
3	GOL	D	1330	-	X
4	EDO	A	1331	-	X
4	EDO	A	1332	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	A	1333	-	X
4	EDO	A	1334	-	X
4	EDO	A	1335	-	X
4	EDO	B	1331	-	X
4	EDO	B	1332	-	X
4	EDO	D	1331	-	X
4	EDO	D	1332	-	X
4	EDO	D	1333	-	X
4	EDO	D	1334	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20944 atoms, of which 9378 are hydrogens and 0 are deuterium.

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 L-ASPARAGINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	H	N	O	S	28	20	0
			4862	1600	2326	445	480	11			
1	B	325	Total	C	H	N	O	S	47	18	0
			4881	1585	2366	436	484	10			
1	C	325	Total	C	H	N	O	S	36	17	0
			4871	1586	2348	450	478	9			
1	D	325	Total	C	H	N	O	S	80	21	0
			4879	1600	2338	446	486	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ILE	LEU	VARIANT	UNP P06608
A	178	ARG	LYS	VARIANT	UNP P06608
A	267	LEU	MET	VARIANT	UNP P06608
A	274	MET	ILE	VARIANT	UNP P06608
B	156	ILE	LEU	VARIANT	UNP P06608
B	178	ARG	LYS	VARIANT	UNP P06608
B	267	LEU	MET	VARIANT	UNP P06608
B	274	MET	ILE	VARIANT	UNP P06608
C	156	ILE	LEU	VARIANT	UNP P06608
C	178	ARG	LYS	VARIANT	UNP P06608
C	267	LEU	MET	VARIANT	UNP P06608
C	274	MET	ILE	VARIANT	UNP P06608
D	156	ILE	LEU	VARIANT	UNP P06608
D	178	ARG	LYS	VARIANT	UNP P06608
D	267	LEU	MET	VARIANT	UNP P06608
D	274	MET	ILE	VARIANT	UNP P06608

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



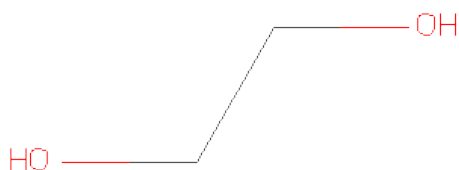
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 5 is water.

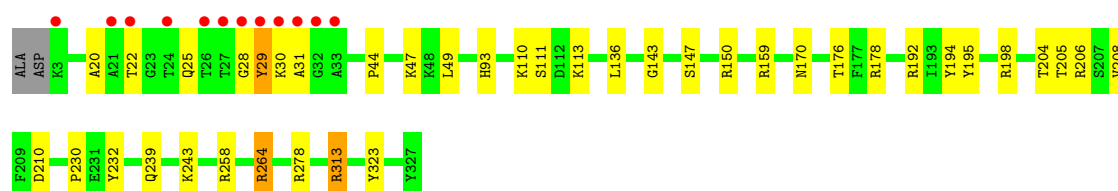
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	348	Total O 348 348	0	0
5	B	310	Total O 310 310	0	0
5	C	355	Total O 355 355	0	0
5	D	347	Total O 347 347	0	0

3 Residue-property plots

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.

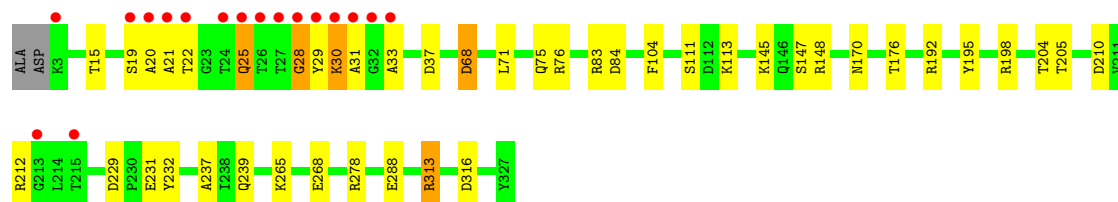
• Molecule 1: L-ASPARAGINASE

Chain A: 



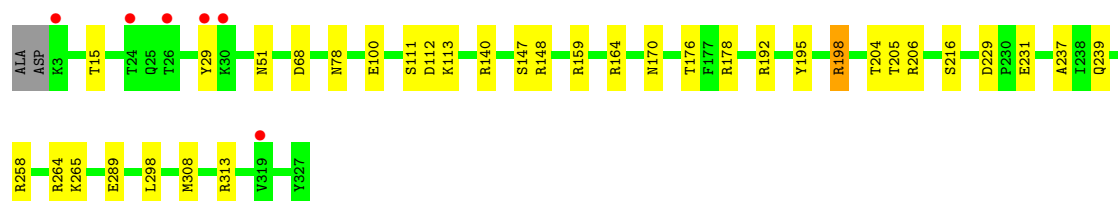
• Molecule 1: L-ASPARAGINASE

Chain B: 



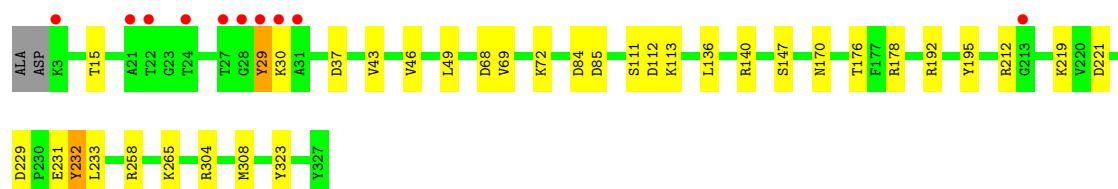
• Molecule 1: L-ASPARAGINASE

Chain C: 



• Molecule 1: L-ASPARAGINASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.38Å 90.35Å 127.59Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	10.00 – 1.00 24.76 – 1.00	Depositor EDS
% Data completeness (in resolution range)	85.6 (10.00-1.00) 82.3 (24.76-1.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 1.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.110 , 0.128 0.128 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	9.0	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 55.9	EDS
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 559622 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	20944	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	0.74	0/2653	1.27	24/3594 (0.7%)
1	B	0.75	0/2636	1.25	27/3574 (0.8%)
1	C	0.72	1/2636 (0.0%)	1.29	26/3571 (0.7%)
1	D	0.72	0/2662	1.17	26/3606 (0.7%)
All	All	0.74	1/10587 (0.0%)	1.24	103/14345 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	SER	CB-OG	-5.50	1.35	1.42

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	NE-CZ-NH1	18.91	129.75	120.30
1	C	198[A]	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	C	198[B]	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	C	192	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	A	198	ARG	NE-CZ-NH2	-13.24	113.68	120.30
1	B	192	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	A	198	ARG	CD-NE-CZ	11.15	139.20	123.60
1	D	140	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	B	198	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	B	37	ASP	CB-CG-OD1	9.40	126.76	118.30
1	C	313[A]	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	C	313[B]	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	192	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	C	140	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	C	308	MET	CG-SD-CE	-8.62	86.41	100.20
1	B	76	ARG	NE-CZ-NH2	-8.45	116.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	148	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	68	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	178	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	D	37	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	68	ASP	CB-CG-OD1	8.04	125.53	118.30
1	C	206[A]	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	206[B]	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	206[A]	ARG	CD-NE-CZ	7.99	134.79	123.60
1	C	206[B]	ARG	CD-NE-CZ	7.99	134.79	123.60
1	C	178[A]	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	178[B]	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	278	ARG	NE-CZ-NH2	7.81	124.21	120.30
1	A	323	TYR	CB-CG-CD1	7.70	125.62	121.00
1	A	178	ARG	CD-NE-CZ	-7.62	112.93	123.60
1	B	288	GLU	OE1-CD-OE2	7.59	132.40	123.30
1	A	264[A]	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	264[B]	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	C	229	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	29	TYR	CZ-CE2-CD2	7.24	126.31	119.80
1	B	313	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	159	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	D	178	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	229	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	323	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C	198[A]	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	C	198[B]	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	A	159	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	104	PHE	CB-CG-CD1	6.63	125.44	120.80
1	D	112	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	192	ARG	CD-NE-CZ	6.62	132.87	123.60
1	B	148	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	178	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	148	ARG	CD-NE-CZ	-6.47	114.55	123.60
1	D	178	ARG	CD-NE-CZ	-6.39	114.66	123.60
1	A	313[A]	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	313[B]	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	192[A]	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	192[B]	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	278	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	84	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	D	192[A]	ARG	NE-CZ-NH2	-6.27	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	192[B]	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	150	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	304	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	178[A]	ARG	CD-NE-CZ	-6.17	114.96	123.60
1	C	178[B]	ARG	CD-NE-CZ	-6.17	114.96	123.60
1	D	229	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	258	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	159	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	71[A]	LEU	CB-CA-C	6.01	121.61	110.20
1	B	71[B]	LEU	CB-CA-C	6.01	121.61	110.20
1	B	28	GLY	C-N-CA	5.98	136.64	121.70
1	D	140	ARG	NH1-CZ-NH2	5.92	125.92	119.40
1	A	29	TYR	CG-CD2-CE2	-5.87	116.60	121.30
1	A	210	ASP	CB-CG-OD1	5.68	123.41	118.30
1	D	258	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	192	ARG	CD-NE-CZ	5.58	131.41	123.60
1	B	231[A]	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	B	231[B]	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	B	83	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	212[A]	ARG	C-N-CA	5.50	133.86	122.30
1	D	212[B]	ARG	C-N-CA	5.50	133.86	122.30
1	C	192	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	29	TYR	CG-CD1-CE1	-5.47	116.93	121.30
1	A	93	HIS	CA-CB-CG	5.40	122.79	113.60
1	C	148	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	229	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	D	308	MET	CG-SD-CE	-5.38	91.59	100.20
1	C	68	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	31	ALA	CA-C-N	5.35	126.90	116.20
1	A	29	TYR	CA-CB-CG	-5.33	103.27	113.40
1	D	232[A]	TYR	CB-CG-CD1	5.31	124.18	121.00
1	D	232[B]	TYR	CB-CG-CD1	5.31	124.18	121.00
1	D	229	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	258	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	112	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	D	29	TYR	CA-CB-CG	-5.17	103.57	113.40
1	B	316[A]	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	316[B]	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	31	ALA	O-C-N	-5.14	114.47	123.20
1	A	194	TYR	CB-CG-CD1	5.11	124.07	121.00
1	B	210[A]	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	210[B]	ASP	CB-CG-OD2	-5.09	113.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	323	TYR	CB-CG-CD1	5.08	124.05	121.00
1	D	323	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	D	85	ASP	CB-CG-OD2	-5.03	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2536	2326	0	23	1
1	B	2515	2366	0	27	1
1	C	2523	2348	0	20	0
1	D	2541	2338	0	32	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	6	0	0	0	0
3	D	6	0	0	0	0
4	A	16	0	0	4	0
4	B	10	0	0	1	0
4	D	13	0	0	14	0
5	A	348	0	0	6	4
5	B	310	0	0	5	5
5	C	355	0	0	8	2
5	D	347	0	0	5	3
All	All	11566	9378	0	100	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (100) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:78:ASN:ND2	5:C:2097:HOH:O	1.65	1.29
1:D:72:LYS:HZ2	4:D:1331:EDO:C2	1.44	1.28
1:B:19:SER:O	1:B:30:LYS:HE2	1.35	1.26
1:C:198[A]:ARG:NH2	5:C:2233:HOH:O	1.66	1.23
2:B:1329:SO4:O3	5:B:2307:HOH:O	1.63	1.13
1:B:75[A]:GLN:CG	5:B:2073:HOH:O	2.00	1.09
1:B:239:GLN:HG3	5:B:2233:HOH:O	1.53	1.06
1:C:51[A]:ASN:OD1	5:C:2066:HOH:O	1.76	1.02
1:D:72:LYS:HZ1	4:D:1334:EDO:C2	1.75	1.00
1:C:147:SER:HG	1:C:195:TYR:HH	1.12	0.97
1:B:147:SER:HG	1:B:195:TYR:HH	1.13	0.94
1:C:15:THR:HG1	1:C:29:TYR:HH	1.06	0.93
1:D:147:SER:HG	1:D:195:TYR:HH	1.15	0.93
1:D:72:LYS:NZ	4:D:1331:EDO:C2	2.32	0.92
1:A:147:SER:HG	1:A:195:TYR:HH	1.14	0.92
1:D:15:THR:HG1	1:D:29:TYR:HH	1.04	0.91
1:D:72:LYS:CE	4:D:1333:EDO:C1	2.49	0.90
1:B:15:THR:HG1	1:B:29:TYR:HH	1.13	0.90
1:B:19:SER:O	1:B:30:LYS:CE	2.20	0.89
1:A:243:LYS:HZ1	4:A:1335:EDO:C1	1.86	0.88
1:A:49:LEU:HD13	1:A:136[B]:LEU:CD1	2.04	0.88
1:B:20:ALA:HB3	1:B:29:TYR:HB3	1.57	0.87
1:D:72:LYS:NZ	4:D:1334:EDO:C2	2.41	0.83
1:D:68[B]:ASP:OD1	5:D:2081:HOH:O	2.01	0.77
1:A:243:LYS:HZ2	4:A:1333:EDO:C2	1.99	0.75
1:D:232[B]:TYR:CD2	5:D:2278:HOH:O	2.40	0.74
1:D:72:LYS:HE2	4:D:1333:EDO:O1	1.87	0.73
1:B:170:ASN:H	1:B:176:THR:HG1	1.37	0.73
1:A:264[B]:ARG:NH2	5:A:2284:HOH:O	2.23	0.70
2:D:1329:SO4:O1	5:D:2344:HOH:O	2.09	0.70
1:D:170:ASN:H	1:D:176:THR:HG1	1.38	0.70
1:D:233:LEU:HD11	5:D:2263:HOH:O	1.92	0.70
1:C:170:ASN:H	1:C:176:THR:HG1	1.40	0.69
1:A:170:ASN:H	1:A:176:THR:HG1	1.40	0.69
1:D:72:LYS:CE	4:D:1333:EDO:O1	2.41	0.69
1:A:49:LEU:CD1	1:A:136[B]:LEU:CD1	2.71	0.68
1:D:111:SER:HG	1:D:113:LYS:H	1.39	0.68
1:C:111:SER:HG	1:C:113:LYS:H	1.41	0.68
1:A:111:SER:HG	1:A:113:LYS:H	1.40	0.67
1:B:111:SER:HG	1:B:113:LYS:H	1.41	0.67
1:D:72:LYS:HE2	4:D:1333:EDO:C1	2.22	0.66
1:B:68:ASP:OD1	5:B:2065:HOH:O	2.13	0.66
1:A:243:LYS:NZ	4:A:1335:EDO:C1	2.59	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:ALA:HB3	1:B:29:TYR:CB	2.28	0.63
1:C:204:THR:HG1	1:C:205:THR:H	1.46	0.63
1:B:21:ALA:HB3	1:B:25:GLN:OE1	1.99	0.62
1:C:239:GLN:NE2	5:C:2278:HOH:O	2.33	0.61
1:B:22:THR:OG1	1:B:25:GLN:HG2	2.00	0.61
1:D:72:LYS:HE3	4:D:1333:EDO:C1	2.30	0.61
1:A:28:GLY:HA2	5:A:2020:HOH:O	1.99	0.61
1:B:145:LYS:HG2	5:B:2139:HOH:O	2.01	0.60
1:B:232[B]:TYR:OH	1:D:221:ASP:OD2	2.18	0.59
1:D:231[A]:GLU:OE2	1:D:265:LYS:NZ	2.35	0.59
1:D:72:LYS:HZ3	4:D:1333:EDO:C2	2.15	0.59
1:B:30:LYS:O	1:B:30:LYS:CG	2.51	0.59
1:C:264[A]:ARG:NH2	5:C:2292:HOH:O	2.35	0.58
1:D:233:LEU:CD1	5:D:2263:HOH:O	2.50	0.57
1:A:204:THR:HG1	1:A:205:THR:H	1.52	0.56
1:C:289:GLU:HG3	5:C:2311:HOH:O	2.05	0.56
1:B:204:THR:HG1	1:B:205:THR:H	1.52	0.56
1:D:231[A]:GLU:OE2	1:D:265:LYS:CE	2.54	0.55
1:A:30:LYS:O	1:A:30:LYS:HG3	2.08	0.53
1:D:72:LYS:NZ	4:D:1333:EDO:O1	2.42	0.53
1:C:112:ASP:OD1	5:C:2147:HOH:O	2.19	0.51
1:B:265:LYS:NZ	1:B:268:GLU:OE1	2.44	0.51
1:A:278[B]:ARG:NH2	1:C:100:GLU:OE2	2.44	0.51
1:A:208[B]:VAL:CG2	1:A:313[B]:ARG:CZ	2.89	0.50
1:B:212:ARG:HH11	4:B:1332:EDO:C1	2.25	0.50
1:C:231:GLU:OE2	1:C:265:LYS:NZ	2.47	0.48
1:A:44:PRO:O	1:A:47:LYS:HG2	2.12	0.48
1:A:110:LYS:NZ	5:A:2125:HOH:O	2.47	0.48
1:A:232[A]:TYR:OH	1:C:237:ALA:HA	2.14	0.48
1:C:164:ARG:CZ	1:C:298[B]:LEU:CD2	2.92	0.48
4:A:1335:EDO:C2	5:A:2348:HOH:O	2.62	0.47
1:D:46[A]:VAL:CG1	1:D:136[A]:LEU:CD2	2.92	0.47
1:B:170:ASN:N	1:B:176:THR:HG1	2.10	0.46
1:D:72:LYS:HZ3	4:D:1333:EDO:C1	2.29	0.46
1:C:164:ARG:NH2	1:C:298[B]:LEU:CD2	2.79	0.46
1:A:22:THR:HG22	1:A:25[A]:GLN:NE2	2.31	0.45
1:D:231[A]:GLU:OE2	1:D:265:LYS:HE2	2.17	0.45
1:B:22:THR:OG1	1:B:25:GLN:CG	2.65	0.45
1:B:30:LYS:HG3	1:B:33:ALA:HB3	1.99	0.45
1:C:170:ASN:N	1:C:176:THR:HG1	2.10	0.45
1:A:20:ALA:HB2	1:A:29:TYR:HB3	1.98	0.44
1:D:72:LYS:NZ	4:D:1333:EDO:C1	2.80	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:GLY:HA2	5:A:2158:HOH:O	2.17	0.44
1:B:232[B]:TYR:OH	1:D:219[B]:LYS:CE	2.66	0.43
1:B:30:LYS:O	1:B:30:LYS:HG2	2.18	0.43
1:D:170:ASN:N	1:D:176:THR:HG1	2.10	0.43
1:B:237:ALA:HA	1:D:232[A]:TYR:OH	2.19	0.42
1:C:198[A]:ARG:NE	5:C:2233:HOH:O	2.50	0.42
1:A:239[A]:GLN:NE2	5:A:2271:HOH:O	2.52	0.42
1:D:43:VAL:HG21	1:D:43:VAL:O	2.20	0.42
1:D:69:VAL:HG23	4:D:1331:EDO:C1	2.50	0.41
1:D:49:LEU:HD13	1:D:136[B]:LEU:CD1	2.50	0.41
1:A:230:PRO:HB2	1:A:232[A]:TYR:CD2	2.56	0.41
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.86	0.41
1:A:170:ASN:N	1:A:176:THR:HG1	2.12	0.40
1:B:22:THR:H	1:B:25:GLN:HG3	1.87	0.40

All (9) 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	Distance(Å)	Clash(Å)
5:B:2211:HOH:O	5:B:2212:HOH:O[2_655]	1.32	0.88
5:A:2107:HOH:O	5:C:2253:HOH:O[4_556]	1.35	0.85
5:B:2250:HOH:O	5:D:2243:HOH:O[4_545]	1.56	0.64
5:A:2222:HOH:O	5:B:2083:HOH:O[3_455]	1.73	0.47
5:A:2004:HOH:O	5:C:2039:HOH:O[3_555]	1.77	0.43
1:A:206:ARG:NH2	1:B:84:ASP:O[3_455]	1.81	0.39
5:B:2080:HOH:O	5:D:2241:HOH:O[3_545]	1.99	0.21
5:A:2222:HOH:O	5:B:2019:HOH:O[3_455]	2.02	0.18
5:D:2098:HOH:O	5:D:2251:HOH:O[2_555]	2.13	0.07

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	343/327 (105%)	335 (98%)	8 (2%)	0	100 100
1	B	341/327 (104%)	328 (96%)	12 (4%)	1 (0%)	50 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	340/327 (104%)	333 (98%)	7 (2%)	0	100	100
1	D	344/327 (105%)	337 (98%)	7 (2%)	0	100	100
All	All	1368/1308 (105%)	1333 (97%)	34 (2%)	1 (0%)	59	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLY

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	282/264 (107%)	282 (100%)	0	100	100
1	B	280/264 (106%)	278 (99%)	2 (1%)	91	66
1	C	279/264 (106%)	279 (100%)	0	100	100
1	D	282/264 (107%)	281 (100%)	1 (0%)	95	76
All	All	1123/1056 (106%)	1120 (100%)	3 (0%)	96	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	GLN
1	B	30	LYS
1	D	30	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	GLN
1	B	180	ASN
1	B	191	ASN
1	C	78	ASN
1	C	239	GLN

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Mol	Chain	Res	Type
1	D	239	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

22 ligands are modelled in this entry.

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$
2	SO4	A	1328	-	4,4,4	0.57	0	6,6,6	0.30	0
2	SO4	A	1329	-	4,4,4	1.60	2 (50%)	6,6,6	1.27	1 (16%)
3	GOL	A	1330	-	5,5,5	0.67	0	5,5,5	0.43	0
4	EDO	A	1331	4	2,2,3	3.36	1 (50%)	0,1,2	0.00	-
4	EDO	A	1332	4	2,2,3	4.68	1 (50%)	0,1,2	0.00	-
4	EDO	A	1333	4	2,2,3	10.78	1 (50%)	0,1,2	0.00	-
4	EDO	A	1334	4	2,2,3	13.11	1 (50%)	0,1,2	0.00	-
4	EDO	A	1335	4	3,3,3	0.65	0	2,2,2	0.26	0
2	SO4	B	1328	-	4,4,4	0.87	0	6,6,6	0.34	0
2	SO4	B	1329	-	4,4,4	2.36	2 (50%)	6,6,6	1.54	1 (16%)
4	EDO	B	1330	4	2,2,3	3.17	1 (50%)	0,1,2	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1331	4	2,2,3	1.54	1 (50%)	0,1,2	0.00	-
4	EDO	B	1332	4	3,3,3	0.65	0	2,2,2	0.30	0
2	SO4	C	1328	-	4,4,4	0.39	0	6,6,6	0.23	0
2	SO4	C	1329	-	4,4,4	0.87	0	6,6,6	0.60	0
2	SO4	D	1328	-	4,4,4	0.71	0	6,6,6	0.29	0
2	SO4	D	1329	-	4,4,4	1.52	1 (25%)	6,6,6	0.67	0
3	GOL	D	1330	-	5,5,5	0.40	0	5,5,5	1.12	1 (20%)
4	EDO	D	1331	4	2,2,3	2.89	1 (50%)	0,1,2	0.00	-
4	EDO	D	1332	4	2,2,3	8.56	1 (50%)	0,1,2	0.00	-
4	EDO	D	1333	4	2,2,3	3.60	1 (50%)	0,1,2	0.00	-
4	EDO	D	1334	4	3,3,3	0.69	0	2,2,2	0.48	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
2	SO4	A	1328	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1329	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1330	-	-	0/4/4/4	0/0/0/0
4	EDO	A	1331	4	-	0/0/0/1	0/0/0/0
4	EDO	A	1332	4	-	0/0/0/1	0/0/0/0
4	EDO	A	1333	4	-	0/0/0/1	0/0/0/0
4	EDO	A	1334	4	-	0/0/0/1	0/0/0/0
4	EDO	A	1335	4	-	0/1/1/1	0/0/0/0
2	SO4	B	1328	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1329	-	-	0/0/0/0	0/0/0/0
4	EDO	B	1330	4	-	0/0/0/1	0/0/0/0
4	EDO	B	1331	4	-	0/0/0/1	0/0/0/0
4	EDO	B	1332	4	-	0/1/1/1	0/0/0/0
2	SO4	C	1328	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1329	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1328	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1329	-	-	0/0/0/0	0/0/0/0
3	GOL	D	1330	-	-	0/4/4/4	0/0/0/0
4	EDO	D	1331	4	-	0/0/0/1	0/0/0/0
4	EDO	D	1332	4	-	0/0/0/1	0/0/0/0
4	EDO	D	1333	4	-	0/0/0/1	0/0/0/0
4	EDO	D	1334	4	-	0/1/1/1	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1334	EDO	C2-C1	-18.55	1.47	1.55
4	A	1333	EDO	C2-C1	-15.22	1.49	1.55
4	D	1332	EDO	C2-C1	-12.10	1.50	1.55
4	A	1332	EDO	C2-C1	-6.42	1.52	1.55
4	D	1333	EDO	C2-C1	-5.07	1.53	1.55
4	A	1331	EDO	C2-C1	-4.75	1.53	1.55
4	B	1330	EDO	C2-C1	-4.46	1.53	1.55
4	D	1331	EDO	C2-C1	-4.06	1.53	1.55
2	B	1329	SO4	O4-S	3.45	1.59	1.47
2	B	1329	SO4	O3-S	2.89	1.57	1.47
2	D	1329	SO4	O2-S	2.60	1.55	1.47
2	A	1329	SO4	O1-S	-2.30	1.39	1.47
4	B	1331	EDO	C2-C1	-2.12	1.54	1.55
2	A	1329	SO4	O2-S	2.06	1.53	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1329	SO4	O4-S-O3	-2.82	97.14	109.08
2	A	1329	SO4	O2-S-O1	2.67	118.37	109.53
3	D	1330	GOL	O2-C2-C3	2.16	118.07	108.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	325/327 (99%)	-0.14	12 (3%)	39 37	8, 12, 28, 46	5 (1%)
1	B	325/327 (99%)	-0.06	17 (5%)	26 25	8, 11, 27, 59	7 (2%)
1	C	325/327 (99%)	-0.20	6 (1%)	65 61	7, 11, 22, 40	4 (1%)
1	D	325/327 (99%)	-0.19	10 (3%)	47 44	7, 12, 24, 44	8 (2%)
All	All	1300/1308 (99%)	-0.15	45 (3%)	42 39	7, 12, 26, 59	24 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	THR	9.4
1	B	29	TYR	8.5
1	B	27	THR	8.4
1	B	30	LYS	8.3
1	A	26	THR	7.1
1	B	22	THR	6.7
1	A	29	TYR	6.2
1	B	28	GLY	6.0
1	B	24	THR	5.9
1	B	31	ALA	5.5
1	B	25	GLN	5.4
1	B	21	ALA	5.4
1	A	30	LYS	4.9
1	A	28	GLY	4.8
1	B	33	ALA	4.8
1	A	27	THR	4.8
1	A	31	ALA	4.5
1	D	28	GLY	4.2
1	A	22	THR	4.0
1	B	32	GLY	4.0
1	C	26	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	24	THR	3.7
1	D	29	TYR	3.5
1	D	21	ALA	3.1
1	B	20	ALA	2.9
1	D	27	THR	2.9
1	C	29	TYR	2.8
1	A	3	LYS	2.6
1	D	24	THR	2.6
1	D	30	LYS	2.6
1	A	24	THR	2.5
1	B	215	THR	2.5
1	B	3	LYS	2.4
1	A	32	GLY	2.4
1	D	3	LYS	2.3
1	D	22	THR	2.3
1	A	21	ALA	2.3
1	C	30	LYS	2.2
1	C	319	VAL	2.2
1	C	3	LYS	2.1
1	D	213[A]	GLY	2.1
1	A	33	ALA	2.1
1	B	213	GLY	2.1
1	B	19	SER	2.0
1	D	31	ALA	2.0

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	D	1331	3/4	0.37	17.74	51,51,53,64	0
3	GOL	D	1330	6/6	0.16	11.77	12,24,27,28	0
4	EDO	D	1333	3/4	0.26	7.54	56,56,58,60	0
4	EDO	D	1334	4/4	0.21	6.38	59,60,61,61	0
4	EDO	D	1332	3/4	0.18	5.46	47,47,47,50	0
4	EDO	A	1331	3/4	0.13	5.35	28,28,37,46	0
4	EDO	A	1332	3/4	0.11	5.20	16,16,23,25	0
4	EDO	A	1335	4/4	0.22	4.25	28,38,39,43	0
4	EDO	A	1333	3/4	0.09	4.02	20,20,25,25	0
4	EDO	B	1332	4/4	0.15	3.90	20,23,31,57	0
2	SO4	B	1329	5/5	0.14	3.80	21,24,27,31	0
4	EDO	A	1334	3/4	0.12	3.30	24,24,29,29	0
2	SO4	D	1329	5/5	0.18	3.14	20,25,39,49	0
4	EDO	B	1331	3/4	0.14	3.08	20,20,26,28	0
2	SO4	C	1329	5/5	0.24	3.03	19,19,40,40	0
3	GOL	A	1330	6/6	0.08	2.36	11,13,15,16	0
4	EDO	B	1330	3/4	0.14	1.61	22,22,26,38	0
2	SO4	A	1329	5/5	0.14	0.24	19,27,51,52	0
2	SO4	B	1328	5/5	0.04	-0.43	9,9,10,11	0
2	SO4	A	1328	5/5	0.04	-0.49	8,9,10,11	0
2	SO4	D	1328	5/5	0.04	-0.60	8,9,10,11	0
2	SO4	C	1328	5/5	0.03	-0.74	9,9,10,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.