



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:44 AM UTC

PDB ID : 1O7J / pdb_00001o7j
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 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

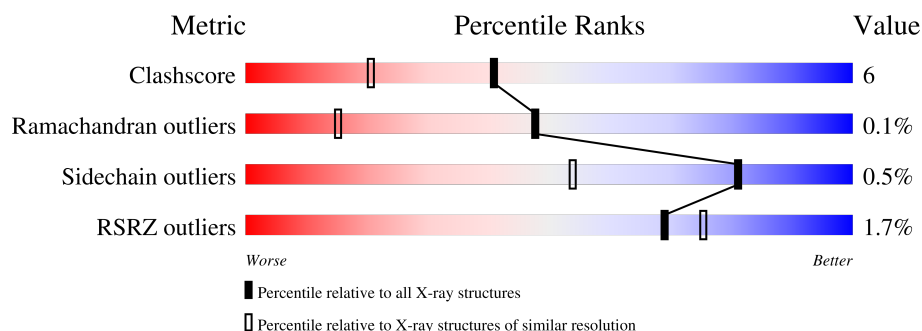
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 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	190562	1411 (1.04-0.96)
Ramachandran outliers	187476	1347 (1.04-0.96)
Sidechain outliers	187428	1348 (1.04-0.96)
RSRZ outliers	180081	1355 (1.04-0.96)

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 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	327	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	327	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	327	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>..</div> </div> </div>
1	D	327	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	1335	-	-	X	-
4	EDO	B	1331	-	-	X	-
4	EDO	B	1332	-	-	X	-
4	EDO	D	1331	-	-	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 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 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 (CCD ID: SO4) (formula: O₄S).



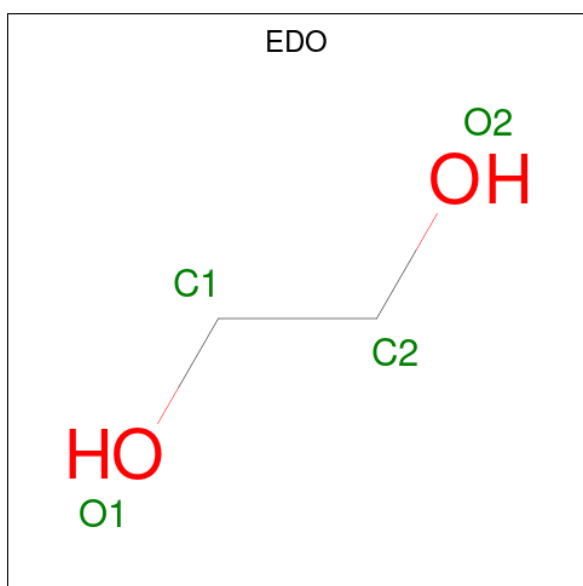
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	0	0
			3	2	1		
4	A	1	Total	C	O	0	0
			3	2	1		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			3	2	1		
4	D	1	Total	C	O	0	0
			3	2	1		
4	D	1	Total	C	O	0	0
			3	2	1		
4	D	1	Total	C	O	0	0
			4	2	2		

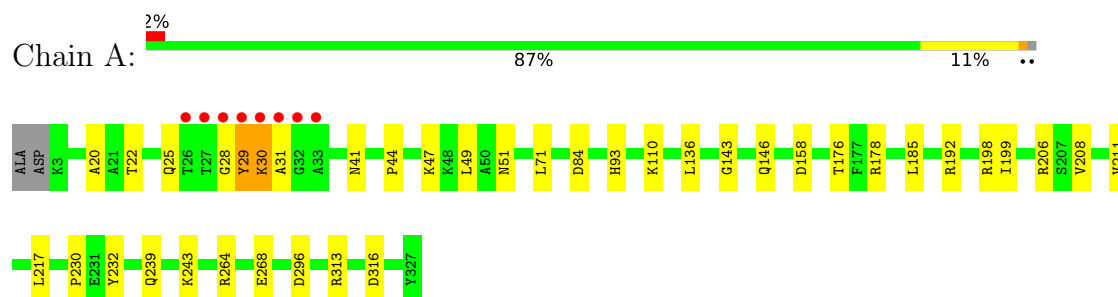
- Molecule 5 is water.

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

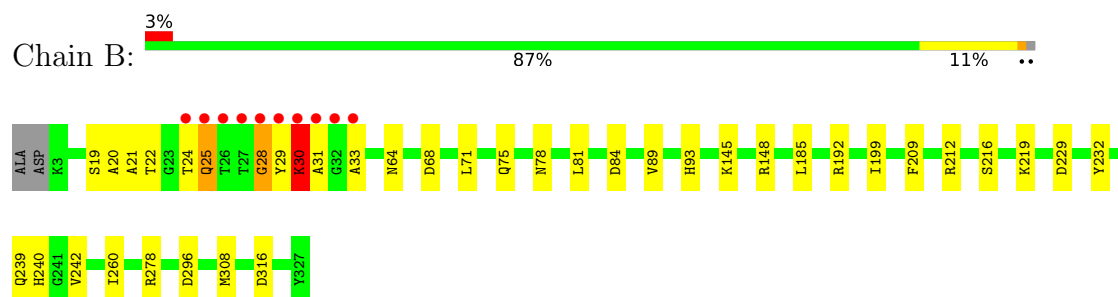
3 Residue-property plots [i](#)

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.

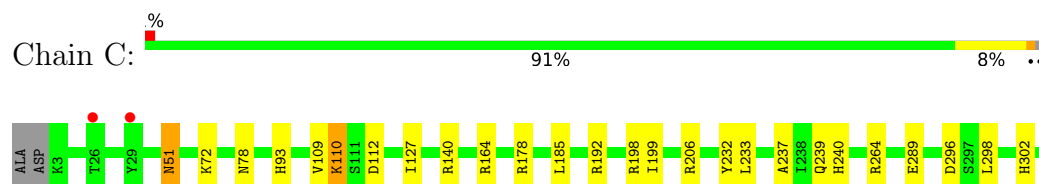
• Molecule 1: L-ASPARAGINASE



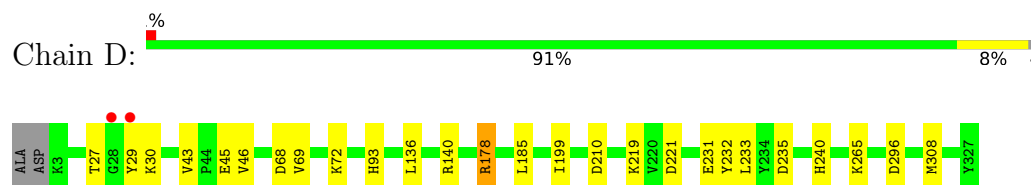
• Molecule 1: L-ASPARAGINASE



• Molecule 1: L-ASPARAGINASE



• Molecule 1: L-ASPARAGINASE



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 10.00 – 1.00	Depositor EDS
% Data completeness (in resolution range)	85.6 (10.00-1.00) 82.1 (10.00-1.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.110 , 0.128 0.110 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.51 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.99	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.

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4, GOL

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	0.91	1/2653 (0.0%)	1.25	19/3594 (0.5%)
1	B	0.92	0/2636	1.31	23/3574 (0.6%)
1	C	0.90	1/2636 (0.0%)	1.19	11/3571 (0.3%)
1	D	0.89	1/2662 (0.0%)	1.19	11/3606 (0.3%)
All	All	0.90	3/10587 (0.0%)	1.24	64/14345 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	308	MET	SD-CE	-9.42	1.55	1.79
1	C	308	MET	SD-CE	-6.01	1.64	1.79
1	A	31	ALA	C-O	5.47	1.30	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	CD-NE-CZ	10.57	139.20	124.40
1	A	93	HIS	CA-CB-CG	8.99	122.79	113.80
1	B	28	GLY	CA-C-N	8.96	136.64	121.86
1	B	28	GLY	C-N-CA	8.96	136.64	121.86
1	A	198	ARG	NE-CZ-NH1	8.25	129.75	121.50
1	A	178	ARG	CD-NE-CZ	-8.20	112.93	124.40
1	A	41	ASN	CA-CB-CG	-7.84	104.75	112.60
1	C	206[A]	ARG	CD-NE-CZ	7.42	134.79	124.40
1	C	206[B]	ARG	CD-NE-CZ	7.42	134.79	124.40
1	C	51[A]	ASN	OD1-CG-ND2	7.23	129.83	122.60
1	C	51[B]	ASN	OD1-CG-ND2	7.23	129.83	122.60
1	D	235	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	30	LYS	CA-C-O	-7.16	112.89	120.40
1	B	93	HIS	CA-CB-CG	7.07	120.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ARG	CD-NE-CZ	-7.04	114.55	124.40
1	D	178	ARG	CD-NE-CZ	-6.96	114.66	124.40
1	D	93	HIS	CA-CB-CG	6.88	120.68	113.80
1	B	31	ALA	O-C-N	-6.88	114.47	122.93
1	B	71[A]	LEU	CB-CA-C	6.84	121.61	110.88
1	B	71[B]	LEU	CB-CA-C	6.84	121.61	110.88
1	A	51	ASN	OD1-CG-ND2	6.73	129.33	122.60
1	C	192	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	C	93	HIS	CA-CB-CG	6.71	120.51	113.80
1	C	308	MET	CG-SD-CE	-6.59	86.41	100.90
1	A	31	ALA	N-CA-C	-6.48	100.89	110.48
1	A	84	ASP	CA-CB-CG	-6.37	106.23	112.60
1	B	24	THR	CA-C-O	6.35	126.70	119.27
1	D	296	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	296	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	316[A]	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	316[B]	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	64	ASN	CA-CB-CG	-6.23	106.37	112.60
1	D	140	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	A	198	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	D	240	HIS	CA-CB-CG	-6.13	107.67	113.80
1	A	146	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	B	192	ARG	CD-NE-CZ	6.05	132.87	124.40
1	A	316	ASP	CA-CB-CG	5.99	118.58	112.60
1	D	210	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	29	TYR	CA-CB-CG	-5.91	103.27	113.90
1	D	29	TYR	CA-CB-CG	-5.74	103.57	113.90
1	A	146	GLN	CB-CG-CD	5.74	122.35	112.60
1	A	158	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	296	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	229	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	209[A]	PHE	N-CA-C	-5.62	100.64	109.25
1	B	209[B]	PHE	N-CA-C	-5.62	100.64	109.25
1	B	240	HIS	CG-CD2-NE2	-5.62	101.58	107.20
1	B	308[A]	MET	CB-CA-C	5.61	119.69	110.88
1	B	308[B]	MET	CB-CA-C	5.61	119.69	110.88
1	B	296	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	240	HIS	CE1-NE2-CD2	5.58	114.58	109.00
1	B	278	ARG	NE-CZ-NH2	5.56	124.21	119.20
1	A	31	ALA	O-C-N	-5.55	116.69	122.96
1	D	45	GLU	CA-C-O	-5.55	113.99	120.20
1	D	27	THR	O-C-N	-5.54	116.84	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	C	240	HIS	CA-CB-CG	-5.37	108.43	113.80
1	A	30	LYS	N-CA-C	5.23	117.15	108.20
1	B	192	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	D	140	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	A	176	THR	N-CA-C	5.06	117.53	111.71
1	C	72	LYS	CG-CD-CE	5.03	122.88	111.30
1	A	192	ARG	CD-NE-CZ	5.00	131.41	124.40

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	2536	2326	2582	39	2
1	B	2515	2366	2540	31	3
1	C	2523	2348	2571	22	0
1	D	2541	2338	2575	42	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	8	0	0
3	D	6	0	8	0	0
4	A	16	0	14	14	0
4	B	10	0	10	8	0
4	D	13	0	12	21	0
5	A	348	0	0	9	4
5	B	310	0	0	8	5
5	C	355	0	0	8	2
5	D	347	0	0	7	3
All	All	11566	9378	10320	133	11

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 6.

All (133) 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:78:ASN:ND2	5:C:2097:HOH:O	1.65	1.29
1:B:19:SER:O	1:B:30:LYS:HE2	1.34	1.27
1:B:75[A]:GLN:HG3	5:B:2073:HOH:O	1.30	1.26
2:B:1329:SO4:O3	5:B:2307:HOH:O	1.63	1.13
1:D:72:LYS:HZ1	4:D:1334:EDO:H22	1.08	1.07
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:NZ	4:D:1334:EDO:H22	1.80	0.97
1:A:243:LYS:HZ3	4:A:1334:EDO:H11	1.31	0.95
1:D:72:LYS:HZ3	4:D:1331:EDO:C2	1.78	0.95
1:B:212:ARG:HH11	4:B:1332:EDO:H11	1.29	0.94
1:D:72:LYS:NZ	4:D:1331:EDO:C2	2.32	0.92
1:D:72:LYS:HZ1	4:D:1334:EDO:C2	1.82	0.91
1:B:20:ALA:HB2	1:B:29:TYR:HB3	1.52	0.90
1:D:72:LYS:CE	4:D:1333:EDO:C1	2.49	0.90
1:D:72:LYS:CE	4:D:1333:EDO:H11	2.01	0.90
1:B:19:SER:O	1:B:30:LYS:CE	2.20	0.89
1:A:49:LEU:HD11	1:A:136[B]:LEU:CD1	2.04	0.88
1:D:72:LYS:HE3	4:D:1333:EDO:H11	1.58	0.85
1:D:46[A]:VAL:CG1	1:D:136[A]:LEU:HD23	2.07	0.85
1:D:232[B]:TYR:HD2	5:D:2278:HOH:O	1.62	0.82
1:B:78:ASN:HB3	4:B:1332:EDO:H12	1.61	0.81
1:D:46[A]:VAL:HG13	1:D:136[A]:LEU:HD23	1.60	0.81
1:A:49:LEU:CD1	1:A:136[B]:LEU:HD12	2.10	0.81
1:B:75[A]:GLN:CG	5:B:2073:HOH:O	2.00	0.81
1:D:72:LYS:NZ	4:D:1334:EDO:C2	2.41	0.80
1:C:232:TYR:CE1	1:C:233[B]:LEU:HD13	2.19	0.77
1:D:68[B]:ASP:OD1	5:D:2081:HOH:O	2.01	0.77
1:A:239[A]:GLN:HG3	5:A:2273:HOH:O	1.85	0.77
1:D:72:LYS:HE2	4:D:1333:EDO:O1	1.87	0.74
1:A:49:LEU:HD11	1:A:136[B]:LEU:HD11	1.69	0.73
1:D:69:VAL:HG22	4:D:1331:EDO:H11	1.71	0.72
1:A:49:LEU:HD11	1:A:136[B]:LEU:HD12	1.70	0.72
2:D:1329:SO4:O1	5:D:2344:HOH:O	2.09	0.70
1:D:232[B]:TYR:CD2	5:D:2278:HOH:O	2.40	0.69
1:A:264[B]:ARG:NH2	5:A:2284:HOH:O	2.23	0.69
1:D:233:LEU:HD12	5:D:2263:HOH:O	1.92	0.69
1:D:72:LYS:CE	4:D:1333:EDO:O1	2.41	0.69
1:D:72:LYS:HE2	4:D:1333:EDO:C1	2.21	0.68
1:B:212:ARG:NH1	4:B:1332:EDO:H11	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:HD2	4:B:1331:EDO:H11	1.77	0.67
1:B:68:ASP:OD1	5:B:2065:HOH:O	2.13	0.66
1:B:75[B]:GLN:HE22	4:B:1331:EDO:H12	1.61	0.66
1:A:243:LYS:NZ	4:A:1335:EDO:C1	2.59	0.65
1:A:49:LEU:CD1	1:A:136[B]:LEU:CD1	2.71	0.65
1:D:46[A]:VAL:HG13	1:D:136[A]:LEU:CD2	2.26	0.65
1:A:49:LEU:HD12	1:A:136[B]:LEU:HD12	1.79	0.64
1:A:243:LYS:HZ3	4:A:1333:EDO:C2	2.11	0.64
1:A:243:LYS:HZ2	4:A:1335:EDO:C1	2.10	0.64
1:B:20:ALA:HB2	1:B:29:TYR:CB	2.25	0.64
1:B:185:LEU:HD21	1:B:199[B]:ILE:HG23	1.80	0.64
1:B:260[B]:ILE:HD11	5:B:2271:HOH:O	1.97	0.64
1:C:198[A]:ARG:NH2	5:C:2233:HOH:O	1.66	0.63
1:B:21:ALA:HB3	1:B:25:GLN:OE1	1.98	0.63
1:B:22:THR:OG1	1:B:25:GLN:HG2	1.99	0.62
1:B:232[B]:TYR:OH	1:D:219[B]:LYS:HE3	2.00	0.62
1:C:239:GLN:NE2	5:C:2278:HOH:O	2.33	0.61
1:A:243:LYS:NZ	4:A:1335:EDO:H12	2.14	0.61
1:A:28:GLY:HA3	5:A:2020:HOH:O	1.99	0.61
1:C:185:LEU:HD21	1:C:199[B]:ILE:HG23	1.82	0.60
1:D:46[A]:VAL:HG12	1:D:136[A]:LEU:HD23	1.82	0.60
1:B:145:LYS:HG2	5:B:2139:HOH:O	2.02	0.59
1:A:22:THR:HG23	1:A:25[A]:GLN:HE21	1.67	0.59
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:B:30:LYS:O	1:B:30:LYS:CG	2.51	0.59
1:A:208[B]:VAL:HG22	1:A:313[B]:ARG:NH1	2.17	0.58
1:C:264[A]:ARG:NH2	5:C:2292:HOH:O	2.35	0.58
1:A:243:LYS:HD2	4:A:1335:EDO:H11	1.85	0.58
1:B:75[B]:GLN:HE22	4:B:1330:EDO:H11	1.68	0.58
1:A:232[B]:TYR:HD2	5:A:2265:HOH:O	1.88	0.57
1:D:185:LEU:HD21	1:D:199[B]:ILE:HG23	1.87	0.57
1:D:233:LEU:CD1	5:D:2263:HOH:O	2.50	0.57
4:A:1335:EDO:H22	5:A:2348:HOH:O	2.05	0.56
1:D:72:LYS:HZ1	4:D:1333:EDO:C2	2.18	0.56
1:D:72:LYS:HZ2	4:D:1331:EDO:C2	2.17	0.56
1:D:231[A]:GLU:OE2	1:D:265:LYS:CE	2.54	0.55
1:A:71[B]:LEU:HG	1:A:217:LEU:HD21	1.88	0.55
1:C:289:GLU:HG3	5:C:2311:HOH:O	2.06	0.55
1:D:72:LYS:HE2	4:D:1333:EDO:H11	1.79	0.54
1:D:72:LYS:NZ	4:D:1334:EDO:O2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LYS:NZ	4:D:1333:EDO:O1	2.42	0.53
1:A:30:LYS:O	1:A:30:LYS:HG3	2.09	0.53
1:A:208[B]:VAL:HG22	1:A:313[B]:ARG:CZ	2.40	0.52
1:A:243:LYS:NZ	4:A:1335:EDO:H11	2.26	0.51
1:A:185:LEU:HD21	1:A:199[B]:ILE:HG23	1.92	0.51
1:C:112:ASP:OD1	5:C:2147:HOH:O	2.19	0.51
1:C:178[B]:ARG:HH22	1:D:178:ARG:NH2	2.09	0.51
1:A:208[B]:VAL:CG2	1:A:313[B]:ARG:CZ	2.89	0.50
1:A:71[B]:LEU:HD21	1:A:211:VAL:HB	1.93	0.50
1:A:20:ALA:HB2	1:A:29:TYR:HB3	1.93	0.50
1:D:69:VAL:CG2	4:D:1331:EDO:H11	2.41	0.49
1:A:110:LYS:NZ	5:A:2125:HOH:O	2.47	0.48
1:A:44:PRO:O	1:A:47:LYS:HG2	2.13	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:A:243:LYS:HZ2	4:A:1335:EDO:H12	1.75	0.47
1:D:43:VAL:O	1:D:46[A]:VAL:HG22	2.15	0.47
1:A:243:LYS:CD	4:A:1335:EDO:H11	2.45	0.46
1:D:68[B]:ASP:CG	5:D:2081:HOH:O	2.57	0.46
1:C:164:ARG:NH2	1:C:298[B]:LEU:CD2	2.79	0.46
1:D:231[A]:GLU:OE2	1:D:265:LYS:HE2	2.16	0.45
1:A:232[A]:TYR:OH	1:C:237:ALA:HA	2.17	0.45
1:B:22:THR:OG1	1:B:25:GLN:CG	2.65	0.45
1:B:22:THR:H	1:B:25:GLN:HG3	1.82	0.45
1:A:243:LYS:NZ	4:A:1331:EDO:H12	2.31	0.44
1:D:72:LYS:NZ	4:D:1333:EDO:C1	2.80	0.44
1:A:22:THR:HG23	1:A:25[A]:GLN:NE2	2.30	0.44
1:A:22:THR:OG1	1:A:25[A]:GLN:HG3	2.17	0.44
1:A:143:GLY:HA3	5:A:2158:HOH:O	2.17	0.44
1:A:243:LYS:NZ	4:A:1334:EDO:H11	2.17	0.44
1:B:30:LYS:O	1:B:30:LYS:HG2	2.18	0.43
1:C:298[B]:LEU:HD12	1:C:302[B]:HIS:HB3	2.00	0.43
1:B:30:LYS:HG3	1:B:33:ALA:HB2	2.00	0.43
1:B:232[B]:TYR:OH	1:D:219[B]:LYS:CE	2.66	0.43
1:B:232[B]:TYR:HD2	5:B:2232:HOH:O	2.01	0.43
1:D:72:LYS:HE3	4:D:1333:EDO:C1	2.28	0.43
1:C:164:ARG:CZ	1:C:298[B]:LEU:HD21	2.49	0.42
1:A:239[A]:GLN:NE2	5:A:2271:HOH:O	2.52	0.42
1:C:109:VAL:C	1:C:110:LYS:HD3	2.45	0.42
1:C:198[A]:ARG:NE	5:C:2233:HOH:O	2.50	0.42
1:A:230:PRO:HB2	1:A:232[A]:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:O	1:D:43:VAL:HG23	2.19	0.41
1:A:243:LYS:HZ3	4:A:1335:EDO:H12	1.84	0.41
1:B:212:ARG:HH11	4:B:1331:EDO:H11	1.85	0.41
4:B:1331:EDO:H11	4:B:1332:EDO:H11	1.89	0.41
1:C:127:ILE:HD13	1:D:136[A]:LEU:CD1	2.50	0.40
1:C:178[B]:ARG:HH11	1:C:178[B]:ARG:HD3	1.69	0.40
1:B:81:LEU:HD21	1:B:89[B]:VAL:HG13	2.03	0.40
1:B:219[A]:LYS:HG2	1:B:242:VAL:HG12	2.04	0.40

All (11) 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)
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
1:B:216:SER:HG	1:B:216:SER:HG[2_655]	1.10	0.50
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
1:A:206:ARG:HH21	1:B:84:ASP:O[3_455]	1.31	0.29
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%)	36 12

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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%)	48	15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLY

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	282/264 (107%)	281 (100%)	1 (0%)	84	59
1	B	280/264 (106%)	278 (99%)	2 (1%)	76	46
1	C	279/264 (106%)	278 (100%)	1 (0%)	84	59
1	D	282/264 (107%)	281 (100%)	1 (0%)	84	59
All	All	1123/1056 (106%)	1118 (100%)	5 (0%)	81	59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	B	25	GLN
1	B	30	LYS
1	C	110	LYS
1	D	30	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN

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Mol	Chain	Res	Type
1	A	281	ASN
1	B	180	ASN
1	B	191	ASN
1	B	281	ASN
1	C	180	ASN
1	C	191	ASN
1	C	239	GLN
1	C	240	HIS
1	C	281	ASN
1	D	239	GLN

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 oligosaccharides 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	$\# Z > 2$
3	GOL	D	1330	-	5,5,5	0.50	0	5,5,5	1.11	1 (20%)
3	GOL	A	1330	-	5,5,5	0.72	0	5,5,5	0.46	0
4	EDO	A	1334	4	2,2,3	0.11	0	1,1,2	1.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	1329	-	4,4,4	0.88	0	6,6,6	1.64	3 (50%)
4	EDO	A	1335	4	3,3,3	0.54	0	2,2,2	0.26	0
2	SO4	A	1328	-	4,4,4	0.54	0	6,6,6	0.46	0
4	EDO	D	1331	4	2,2,3	0.53	0	1,1,2	0.14	0
2	SO4	C	1328	-	4,4,4	0.45	0	6,6,6	0.29	0
4	EDO	A	1331	4	2,2,3	0.48	0	1,1,2	0.18	0
2	SO4	B	1328	-	4,4,4	0.68	0	6,6,6	0.46	0
4	EDO	B	1330	4	2,2,3	0.51	0	1,1,2	0.06	0
4	EDO	B	1332	4	3,3,3	0.52	0	2,2,2	0.31	0
4	EDO	D	1332	4	2,2,3	0.29	0	1,1,2	0.63	0
2	SO4	D	1328	-	4,4,4	0.60	0	6,6,6	0.30	0
4	EDO	B	1331	4	2,2,3	0.58	0	1,1,2	0.01	0
4	EDO	D	1334	4	3,3,3	0.57	0	2,2,2	0.46	0
2	SO4	A	1329	-	4,4,4	0.88	0	6,6,6	1.19	1 (16%)
4	EDO	A	1332	4	2,2,3	0.66	0	1,1,2	0.34	0
4	EDO	D	1333	4	2,2,3	0.51	0	1,1,2	0.08	0
2	SO4	C	1329	-	4,4,4	0.21	0	6,6,6	0.53	0
4	EDO	A	1333	4	2,2,3	0.33	0	1,1,2	0.16	0
2	SO4	D	1329	-	4,4,4	1.04	0	6,6,6	0.99	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	GOL	D	1330	-	-	1/4/4/4	-
4	EDO	D	1334	4	-	1/1/1/1	-
3	GOL	A	1330	-	-	0/4/4/4	-
4	EDO	A	1335	4	-	1/1/1/1	-
4	EDO	B	1332	4	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1329	SO4	O4-S-O2	-2.47	96.63	109.56
2	A	1329	SO4	O3-S-O2	-2.45	96.73	109.56
3	D	1330	GOL	O2-C2-C3	2.15	118.07	109.18
2	B	1329	SO4	O3-S-O2	2.14	120.72	109.56
2	B	1329	SO4	O4-S-O3	-2.07	97.14	108.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1334	EDO	O1-C1-C2-O2
4	A	1335	EDO	O1-C1-C2-O2
3	D	1330	GOL	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1334	EDO	2	0
2	B	1329	SO4	1	0
4	A	1335	EDO	10	0
4	D	1331	EDO	5	0
4	A	1331	EDO	1	0
4	B	1330	EDO	1	0
4	B	1332	EDO	4	0
4	B	1331	EDO	4	0
4	D	1334	EDO	5	0
4	D	1333	EDO	11	0
4	A	1333	EDO	1	0
2	D	1329	SO4	1	0

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%)	-0.69	8 (2%) 58 65	6, 13, 30, 57	25 (7%)
1	B	325/327 (99%)	-0.66	10 (3%) 51 58	5, 12, 31, 76	25 (7%)
1	C	325/327 (99%)	-0.79	2 (0%) 85 89	6, 12, 26, 51	21 (6%)
1	D	325/327 (99%)	-0.76	2 (0%) 85 89	5, 12, 27, 55	28 (8%)
All	All	1300/1308 (99%)	-0.72	22 (1%) 69 75	5, 12, 29, 76	99 (7%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	THR	5.8
1	B	29	TYR	5.3
1	A	26	THR	5.2
1	B	27	THR	5.2
1	A	29	TYR	4.8
1	B	30	LYS	4.3
1	B	28	GLY	4.2
1	A	31	ALA	3.9
1	B	31	ALA	3.6
1	A	28	GLY	3.4
1	D	28	GLY	3.2
1	B	33	ALA	3.1
1	A	27	THR	3.0
1	B	32	GLY	2.9
1	C	26	THR	2.8
1	D	29	TYR	2.7
1	A	30	LYS	2.5
1	B	24	THR	2.5
1	A	33	ALA	2.5
1	C	29	TYR	2.4
1	B	25	GLN	2.3
1	A	32	GLY	2.1

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(\AA^2)	Q<0.9
4	EDO	D	1333	3/4	0.53	0.18	56,56,58,60	0
4	EDO	D	1334	4/4	0.60	0.16	59,60,61,61	0
4	EDO	D	1332	3/4	0.74	0.17	47,47,47,50	0
4	EDO	D	1331	3/4	0.79	0.12	51,51,53,64	0
4	EDO	A	1331	3/4	0.86	0.10	28,28,37,46	0
4	EDO	A	1334	3/4	0.87	0.11	24,24,29,29	0
4	EDO	B	1332	4/4	0.90	0.10	20,23,31,57	0
3	GOL	D	1330	6/6	0.91	0.10	12,24,27,28	0
4	EDO	A	1333	3/4	0.91	0.09	20,20,25,25	0
4	EDO	A	1335	4/4	0.92	0.08	28,38,39,43	0
2	SO4	C	1329	5/5	0.92	0.13	19,19,40,40	0
2	SO4	A	1329	5/5	0.93	0.10	19,27,51,52	0
4	EDO	B	1330	3/4	0.94	0.06	22,22,26,38	0
4	EDO	A	1332	3/4	0.94	0.10	16,16,23,25	0
4	EDO	B	1331	3/4	0.95	0.06	20,20,26,28	0
2	SO4	D	1329	5/5	0.95	0.10	20,25,39,49	0
2	SO4	B	1329	5/5	0.95	0.10	21,24,27,31	0
3	GOL	A	1330	6/6	0.97	0.05	11,13,15,16	0
2	SO4	D	1328	5/5	1.00	0.02	8,9,10,11	0
2	SO4	A	1328	5/5	1.00	0.02	8,9,10,11	0
2	SO4	C	1328	5/5	1.00	0.02	9,9,10,11	0
2	SO4	B	1328	5/5	1.00	0.02	9,9,10,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.