



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:34 AM UTC

PDB ID : 6NN5 / pdb_00006nn5
Title : The structure of human liver pyruvate kinase, hLPYK-W527H
Authors : McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on : 2019-01-14
Resolution : 2.26 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

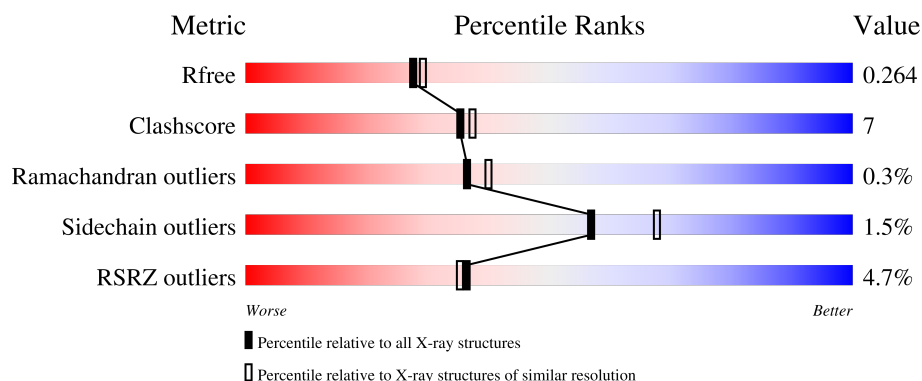
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	543	3% 65% 11% 23%
1	B	543	3% 63% 13% 23%
1	C	543	4% 63% 12% 24%
1	D	543	4% 64% 12% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26076 atoms, of which 13067 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 Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	417	Total	C	H	N	O	S	0	0	0
			6413	1995	3232	579	589	18			
1	B	417	Total	C	H	N	O	S	0	0	0
			6419	1996	3236	581	588	18			
1	C	413	Total	C	H	N	O	S	0	0	0
			6337	1968	3197	574	580	18			
1	D	420	Total	C	H	N	O	S	0	0	0
			6446	2007	3249	581	591	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	527	HIS	TRP	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	527	HIS	TRP	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	527	HIS	TRP	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	527	HIS	TRP	engineered mutation	UNP P30613

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			13	3	7	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			13	3	7	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is water.

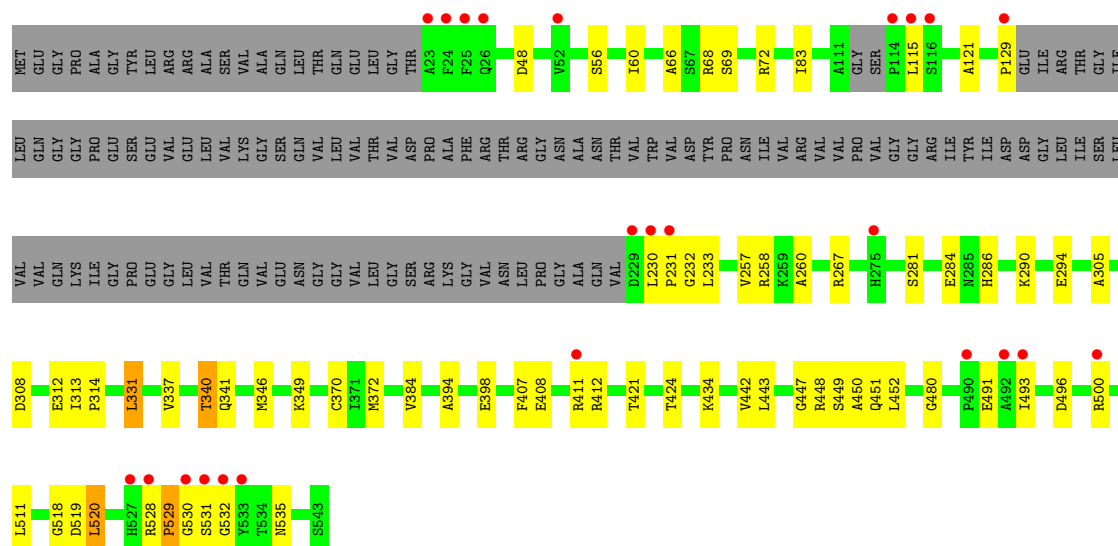
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	52	Total	O	0	0
			52	52		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	37	Total	O	0	0
			37	37		
4	D	56	Total	O	0	0
			56	56		

Chain C: 4% 63% 12% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.01Å 204.62Å 112.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.18 – 2.26 54.18 – 2.26	Depositor EDS
% Data completeness (in resolution range)	64.8 (54.18-2.26) 64.8 (54.18-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.225 , 0.264 0.227 , 0.264	Depositor DCC
R_{free} test set	4183 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26076	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 44.42 % 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 1.5294e-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: GOL, 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	0.54	0/3231	0.72	0/4365
1	B	0.67	4/3233 (0.1%)	0.73	0/4367
1	C	0.55	0/3189	0.72	0/4311
1	D	0.77	10/3249 (0.3%)	0.78	2/4391 (0.0%)
All	All	0.64	14/12902 (0.1%)	0.74	2/17434 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	436	CYS	C-O	-11.31	1.10	1.23
1	D	530	GLY	C-O	-9.51	1.11	1.23
1	B	435	CYS	C-O	-9.16	1.11	1.24
1	D	520	LEU	C-O	-9.10	1.13	1.23
1	B	437	ALA	C-O	-8.36	1.13	1.23
1	D	531	SER	C-O	-8.06	1.13	1.23
1	D	531	SER	CA-C	-7.60	1.42	1.53
1	D	531	SER	C-N	-7.28	1.22	1.33
1	D	532	GLY	C-O	-6.87	1.14	1.23
1	D	529	PRO	C-O	-6.54	1.15	1.24
1	D	518	GLY	C-O	-5.52	1.16	1.24
1	D	519	ASP	CG-OD1	-5.42	1.15	1.25
1	D	519	ASP	CG-OD2	-5.18	1.15	1.25
1	B	438	ALA	C-O	-5.14	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	530	GLY	N-CA-C	5.08	125.23	113.18
1	D	331	LEU	CA-CB-CG	-5.03	98.69	116.30

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	3181	3232	3229	45	0
1	B	3183	3236	3234	54	0
1	C	3140	3197	3197	58	0
1	D	3197	3249	3248	44	0
2	A	24	31	32	1	0
2	B	12	15	16	0	0
2	C	18	23	24	3	0
2	D	18	24	24	0	0
3	A	12	18	17	1	0
3	B	8	12	12	3	0
3	C	12	18	17	6	0
3	D	8	12	12	1	0
4	A	51	0	0	1	0
4	B	52	0	0	5	0
4	C	37	0	0	2	0
4	D	56	0	0	1	0
All	All	13009	13067	13062	191	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 7.

All (191) 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:A:421:THR:HG23	1:A:534:THR:HG22	1.27	1.14
1:C:278:LYS:HE3	3:C:606:EDO:H21	1.39	1.01
1:B:421:THR:HG23	1:B:534:THR:HG22	1.50	0.92
1:C:421:THR:HG23	1:C:534:THR:HG22	1.53	0.90
1:B:108:GLU:HB2	4:B:713:HOH:O	1.77	0.85
1:C:527:HIS:HA	1:C:536:ILE:HD11	1.61	0.82
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:GLY:CA	1:D:258:ARG:HH22	1.99	0.74
1:C:422:GLU:OE2	1:C:455:ARG:NH1	2.20	0.74
1:C:68:ARG:NH2	1:C:95:TYR:O	2.22	0.72
1:C:421:THR:HG23	1:C:534:THR:CG2	2.20	0.71
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.72	0.70
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.74	0.70
1:C:522:ILE:HG23	1:C:537:MET:HE3	1.72	0.69
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.76	0.68
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.75	0.68
1:B:267:ARG:HE	3:B:604:EDO:H12	1.59	0.67
1:A:421:THR:HG23	1:A:534:THR:CG2	2.17	0.66
1:B:74:LYS:HE3	1:B:109:SER:OG	1.97	0.64
1:A:30:LEU:O	1:A:34:MET:HE3	1.98	0.64
1:B:339:ALA:HB1	1:B:372:MET:HE2	1.80	0.63
1:C:449:SER:OG	1:C:534:THR:HG21	1.98	0.63
1:B:267:ARG:HE	3:B:604:EDO:C1	2.12	0.62
3:A:607:EDO:H11	4:A:723:HOH:O	1.98	0.62
1:C:520:LEU:HD23	1:C:540:LEU:O	2.00	0.62
1:D:232:GLY:HA3	1:D:258:ARG:HH22	1.64	0.62
1:D:491:GLU:OE2	1:D:500:ARG:NH1	2.32	0.61
1:C:339:ALA:HB1	1:C:372:MET:HE2	1.83	0.61
1:B:416:LEU:HD23	1:B:416:LEU:N	2.16	0.61
1:B:28:GLN:HG2	1:B:30:LEU:HD13	1.83	0.60
1:C:97:ALA:HB1	3:C:604:EDO:H12	1.84	0.60
1:B:130:GLU:HG3	1:B:132:ARG:HH12	1.66	0.60
1:C:305:ALA:HB1	2:C:603:GOL:H12	1.84	0.59
1:D:511:LEU:HD13	1:D:511:LEU:O	2.03	0.59
1:A:419:ASP:HB3	1:A:422:GLU:HB3	1.84	0.58
1:A:234:SER:O	1:A:238:VAL:HG23	2.03	0.58
1:B:127:LYS:O	1:B:130:GLU:HG2	2.03	0.57
1:B:435:CYS:HB2	1:B:520:LEU:HD12	1.87	0.57
1:A:304:VAL:HG22	1:A:325:MET:HE3	1.86	0.57
1:B:130:GLU:HB2	1:B:132:ARG:HH22	1.71	0.56
1:A:523:VAL:HG21	1:A:540:LEU:HD13	1.88	0.55
1:B:130:GLU:OE2	1:B:256:PHE:HE2	1.89	0.55
1:D:115:LEU:HB2	1:D:511:LEU:HD11	1.89	0.54
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.88	0.54
1:D:257:VAL:HG21	1:D:281:SER:HB3	1.90	0.54
1:B:72:ARG:O	1:B:76:MET:HG3	2.07	0.54
1:B:130:GLU:OE2	1:B:256:PHE:CE2	2.61	0.54
1:B:38:PHE:O	1:B:41:HIS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:O	1:A:420:PRO:HD3	2.08	0.53
1:C:230:LEU:HD12	1:C:231:PRO:HD3	1.91	0.53
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.89	0.53
1:D:260:ALA:HB2	1:D:294:GLU:HG2	1.91	0.53
1:A:528:ARG:HH21	1:A:528:ARG:HG3	1.73	0.52
1:C:76:MET:HE2	1:C:387:VAL:HG21	1.92	0.52
1:C:73:LEU:HA	1:C:76:MET:HG3	1.90	0.52
1:B:30:LEU:O	1:B:34:MET:HG2	2.10	0.52
1:C:527:HIS:HA	1:C:536:ILE:CD1	2.36	0.52
1:A:494:TRP:CD1	1:A:529:PRO:HB3	2.45	0.52
1:C:445:THR:H	2:C:602:GOL:H11	1.75	0.52
1:C:230:LEU:HD12	1:C:231:PRO:CD	2.39	0.51
1:B:128:GLY:O	1:B:130:GLU:N	2.43	0.51
1:B:117:TYR:N	4:B:704:HOH:O	2.43	0.51
1:A:257:VAL:HG21	1:A:281:SER:HB3	1.93	0.51
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.93	0.51
1:B:28:GLN:CG	1:B:30:LEU:HD13	2.41	0.50
1:D:267:ARG:NH1	4:D:702:HOH:O	2.39	0.50
1:D:286:HIS:CE1	1:D:290:LYS:HG3	2.46	0.50
1:C:522:ILE:HG23	1:C:537:MET:CE	2.40	0.50
1:C:534:THR:O	1:C:534:THR:HG23	2.10	0.50
1:D:337:VAL:HG22	1:D:370:CYS:HB2	1.94	0.50
1:C:523:VAL:O	1:C:537:MET:HA	2.11	0.50
1:C:243:PHE:CE2	1:C:247:HIS:CE1	2.99	0.49
1:D:230:LEU:HD23	1:D:231:PRO:HD3	1.94	0.49
1:A:494:TRP:CZ3	1:A:527:HIS:O	2.65	0.49
1:A:523:VAL:O	1:A:537:MET:HA	2.11	0.49
1:A:250:ASP:C	1:A:251:ILE:HG13	2.37	0.49
1:D:346:MET:HA	1:D:349:LYS:O	2.12	0.49
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.94	0.49
1:A:421:THR:HA	1:A:534:THR:O	2.12	0.49
1:A:290:LYS:NZ	1:D:48:ASP:OD2	2.46	0.49
1:B:130:GLU:HG3	1:B:132:ARG:NH1	2.28	0.48
1:B:336:VAL:HG13	1:B:368:ALA:HA	1.94	0.48
1:B:405:GLN:O	1:B:409:GLU:HG3	2.14	0.48
1:C:251:ILE:HD13	1:C:477:LEU:HD21	1.95	0.48
1:B:27:GLN:OE1	1:B:52:VAL:HG21	2.14	0.48
1:A:432:ALA:HB1	1:A:437:ALA:HB3	1.95	0.47
1:C:291:ARG:NH2	1:C:294:GLU:OE2	2.44	0.47
1:D:313:ILE:O	1:D:314:PRO:C	2.56	0.47
1:B:534:THR:O	1:B:534:THR:CG2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:O	1:A:31:PRO:HD3	2.15	0.47
1:D:411:ARG:HG3	1:D:412:ARG:N	2.28	0.47
1:C:101:ALA:HB2	3:C:604:EDO:H21	1.97	0.47
1:B:346:MET:HA	1:B:349:LYS:O	2.14	0.47
1:A:339:ALA:HB1	1:A:372:MET:HE2	1.97	0.46
1:C:257:VAL:HG21	1:C:281:SER:HB3	1.98	0.46
1:C:278:LYS:CE	3:C:606:EDO:H21	2.28	0.46
1:D:394:ALA:O	1:D:398:GLU:HG3	2.15	0.46
1:A:449:SER:HB3	1:A:534:THR:HG21	1.97	0.46
1:B:56:SER:HB2	1:B:480:GLY:CA	2.43	0.46
1:D:424:THR:OG1	1:D:535:ASN:HA	2.16	0.46
1:B:24:PHE:HD2	1:B:25:PHE:CD1	2.34	0.46
1:B:127:LYS:O	1:B:130:GLU:CG	2.64	0.46
1:C:449:SER:CB	1:C:534:THR:HG21	2.46	0.46
1:B:534:THR:O	1:B:534:THR:HG23	2.15	0.46
1:A:435:CYS:HB3	1:C:423:VAL:HG21	1.98	0.45
1:C:76:MET:HE2	1:C:76:MET:HB3	1.86	0.45
1:C:233:LEU:HD21	1:C:241:LEU:CD1	2.47	0.45
1:D:232:GLY:HA2	1:D:258:ARG:HH22	1.78	0.45
1:A:494:TRP:CE3	1:A:529:PRO:HD3	2.52	0.45
1:C:486:TYR:HD1	1:C:504:PHE:CD2	2.35	0.45
1:B:259:LYS:HD2	1:B:291:ARG:HH12	1.82	0.45
1:C:422:GLU:HG3	4:C:733:HOH:O	2.16	0.45
1:A:452:LEU:O	1:A:455:ARG:HG2	2.17	0.45
1:B:335:PRO:HB3	1:B:477:LEU:O	2.17	0.44
1:D:442:VAL:O	1:D:442:VAL:HG13	2.16	0.44
1:A:423:VAL:HG12	1:C:431:ALA:HB1	1.99	0.44
1:A:74:LYS:HE3	1:A:109:SER:OG	2.17	0.44
1:C:278:LYS:HE3	3:C:606:EDO:C2	2.29	0.44
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.99	0.44
1:A:287:GLU:HG2	1:A:291:ARG:HD3	2.00	0.44
1:A:506:ILE:HG23	1:A:542:ILE:HD12	2.00	0.44
1:D:69:SER:OG	1:D:72:ARG:HB2	2.17	0.44
1:A:290:LYS:CE	1:D:48:ASP:OD2	2.65	0.44
1:A:408:GLU:OE2	1:C:408:GLU:OE1	2.35	0.44
1:C:335:PRO:HB3	1:C:477:LEU:O	2.18	0.44
1:A:72:ARG:O	1:A:76:MET:HG3	2.17	0.44
1:B:374:SER:O	1:B:375:GLY:C	2.61	0.43
1:C:333:GLY:HA2	1:C:455:ARG:HB2	2.00	0.43
1:A:430:GLU:OE2	1:C:430:GLU:OE2	2.36	0.43
1:B:117:TYR:HA	4:B:714:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:603:GOL:H32	1:C:411:ARG:HH22	1.83	0.43
1:B:291:ARG:NH2	1:B:294:GLU:OE2	2.52	0.43
1:D:284:GLU:OE2	1:D:308:ASP:OD2	2.37	0.43
1:B:540:LEU:HD23	1:B:541:SER:N	2.34	0.43
1:C:497:ASP:OD2	1:C:501:ARG:NH2	2.52	0.43
1:C:106:ALA:O	1:C:109:SER:OG	2.36	0.43
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.82	0.43
1:A:537:MET:CG	1:C:537:MET:HG2	2.49	0.43
1:D:129:PRO:HB3	1:D:230:LEU:HD13	2.01	0.43
1:B:253:PHE:HD1	1:B:280:ILE:HB	1.84	0.43
1:C:68:ARG:NH2	1:C:98:GLU:HB2	2.34	0.43
1:C:438:ALA:HB3	1:C:515:LEU:HD23	2.00	0.42
1:B:117:TYR:O	1:B:512:ARG:NH2	2.52	0.42
1:D:66:ALA:O	1:D:72:ARG:HG2	2.19	0.42
1:D:443:LEU:N	1:D:443:LEU:CD1	2.82	0.42
1:B:127:LYS:NZ	1:B:132:ARG:NH2	2.68	0.42
1:B:343:LEU:HD23	1:B:356:GLU:HB3	2.02	0.42
1:B:62:THR:HA	1:B:85:ARG:HB3	2.01	0.42
1:D:284:GLU:HG2	1:D:305:ALA:HB3	2.01	0.42
1:B:130:GLU:HB2	1:B:132:ARG:NH2	2.35	0.42
1:D:493:ILE:HB	1:D:496:ASP:OD2	2.18	0.42
1:B:494:TRP:CG	1:B:529:PRO:HG3	2.55	0.42
1:B:28:GLN:HA	4:B:720:HOH:O	2.19	0.42
1:B:234:SER:O	1:B:238:VAL:HG23	2.18	0.42
1:D:232:GLY:HA2	1:D:258:ARG:NH2	2.35	0.42
1:D:448:ARG:O	1:D:451:GLN:N	2.53	0.42
1:C:308:ASP:H	2:C:603:GOL:H11	1.85	0.42
1:C:424:THR:OG1	1:C:535:ASN:HA	2.19	0.42
1:B:279:ILE:HD12	3:B:604:EDO:H11	2.02	0.41
1:D:60:ILE:CG2	1:D:372:MET:HG3	2.48	0.41
1:D:408:GLU:O	1:D:412:ARG:HB2	2.20	0.41
1:D:448:ARG:O	1:D:449:SER:C	2.59	0.41
1:A:522:ILE:HD13	1:A:539:VAL:HG22	2.03	0.41
1:B:108:GLU:CB	4:B:713:HOH:O	2.50	0.41
1:B:509:GLY:O	1:B:514:PHE:N	2.52	0.41
1:C:97:ALA:HB1	3:C:604:EDO:C1	2.48	0.41
1:C:402:TYR:CE2	1:C:405:GLN:HB2	2.56	0.41
1:D:447:GLY:O	1:D:450:ALA:HB3	2.20	0.41
1:A:342:MET:O	1:A:343:LEU:HD23	2.20	0.41
1:A:494:TRP:HZ3	1:A:527:HIS:O	2.03	0.41
1:B:415:PRO:O	1:D:434:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PHE:CD1	1:B:243:PHE:C	2.99	0.41
1:C:346:MET:HA	1:C:349:LYS:O	2.20	0.41
1:A:404:ARG:HD3	1:C:412:ARG:CZ	2.51	0.41
1:A:404:ARG:HD3	1:C:412:ARG:NH2	2.36	0.41
1:A:494:TRP:O	1:A:497:ASP:N	2.53	0.41
1:A:534:THR:CG2	1:A:534:THR:O	2.68	0.41
1:A:538:ARG:HA	1:C:535:ASN:O	2.21	0.41
1:D:528:ARG:O	1:D:529:PRO:C	2.62	0.41
1:A:486:TYR:HD1	1:A:504:PHE:CD2	2.39	0.40
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.04	0.40
1:A:494:TRP:NE1	1:A:529:PRO:HB3	2.37	0.40
1:B:250:ASP:C	1:B:251:ILE:HG13	2.46	0.40
1:D:83:ILE:HG12	1:D:121:ALA:HB3	2.03	0.40
1:D:284:GLU:O	1:D:312:GLU:HG3	2.22	0.40
1:D:384:VAL:HG23	3:D:605:EDO:H22	2.03	0.40
1:D:407:PHE:CE2	1:D:411:ARG:NH1	2.89	0.40
1:D:434:LYS:O	1:D:434:LYS:HG3	2.20	0.40
1:A:23:ALA:O	1:A:24:PHE:C	2.63	0.40
1:B:235:GLU:O	1:B:239:ARG:HG3	2.22	0.40
1:C:380:GLY:HA3	4:C:701:HOH:O	2.22	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	411/543 (76%)	402 (98%)	8 (2%)	1 (0%)	43	50
1	B	411/543 (76%)	404 (98%)	6 (2%)	1 (0%)	43	50
1	C	407/543 (75%)	403 (99%)	2 (0%)	2 (0%)	24	24
1	D	414/543 (76%)	403 (97%)	10 (2%)	1 (0%)	43	50
All	All	1643/2172 (76%)	1612 (98%)	26 (2%)	5 (0%)	36	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	C	415	PRO

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	333/433 (77%)	328 (98%)	5 (2%)	57	68
1	B	333/433 (77%)	326 (98%)	7 (2%)	47	58
1	C	329/433 (76%)	324 (98%)	5 (2%)	57	68
1	D	335/433 (77%)	332 (99%)	3 (1%)	70	79
All	All	1330/1732 (77%)	1310 (98%)	20 (2%)	57	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	109	SER
1	A	349	LYS
1	A	511	LEU
1	A	534	THR
1	B	71	GLU
1	B	235	GLU
1	B	313	ILE
1	B	331	LEU
1	B	422	GLU
1	B	516	ARG
1	B	534	THR
1	C	68	ARG
1	C	76	MET
1	C	233	LEU

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Mol	Chain	Res	Type
1	C	294	GLU
1	C	488	GLU
1	D	68	ARG
1	D	331	LEU
1	D	520	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	247	HIS
1	C	527	HIS
1	D	28	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](#)

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	EDO	B	604	-	3,3,3	0.40	0	2,2,2	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	602	-	5,5,5	1.14	0	5,5,5	1.16	1 (20%)
2	GOL	B	601	-	5,5,5	0.74	0	5,5,5	0.92	0
2	GOL	A	601	-	5,5,5	1.29	1 (20%)	5,5,5	1.17	0
2	GOL	C	603	-	5,5,5	1.17	0	5,5,5	0.66	0
3	EDO	A	607	-	3,3,3	0.84	0	2,2,2	0.36	0
2	GOL	C	601	-	5,5,5	0.84	0	5,5,5	1.56	1 (20%)
2	GOL	D	601	-	5,5,5	1.59	1 (20%)	5,5,5	0.79	0
2	GOL	A	602	-	5,5,5	1.00	0	5,5,5	0.60	0
3	EDO	A	606	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	A	605	-	3,3,3	0.35	0	2,2,2	0.47	0
2	GOL	C	602	-	5,5,5	1.12	1 (20%)	5,5,5	1.18	0
3	EDO	D	605	-	3,3,3	0.46	0	2,2,2	0.80	0
3	EDO	C	605	-	3,3,3	0.48	0	2,2,2	0.32	0
2	GOL	D	602	-	5,5,5	0.89	0	5,5,5	1.26	0
3	EDO	B	603	-	3,3,3	0.49	0	2,2,2	0.48	0
3	EDO	D	604	-	3,3,3	0.65	0	2,2,2	0.29	0
3	EDO	C	604	-	3,3,3	0.35	0	2,2,2	0.44	0
2	GOL	A	603	-	5,5,5	1.24	1 (20%)	5,5,5	1.02	0
2	GOL	A	604	-	5,5,5	1.04	0	5,5,5	0.58	0
2	GOL	D	603	-	5,5,5	0.82	0	5,5,5	0.76	0
3	EDO	C	606	-	3,3,3	0.82	0	2,2,2	1.33	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	604	-	-	1/1/1/1	-
2	GOL	B	602	-	-	3/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
3	EDO	A	607	-	-	0/1/1/1	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	D	601	-	-	4/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
3	EDO	A	606	-	-	1/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
2	GOL	C	602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	605	-	-	0/1/1/1	-
3	EDO	C	605	-	-	0/1/1/1	-
2	GOL	D	602	-	-	4/4/4/4	-
3	EDO	B	603	-	-	1/1/1/1	-
3	EDO	D	604	-	-	0/1/1/1	-
3	EDO	C	604	-	-	1/1/1/1	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	A	604	-	-	4/4/4/4	-
2	GOL	D	603	-	-	1/4/4/4	-
3	EDO	C	606	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	GOL	C1-C2	2.14	1.59	1.51
2	C	602	GOL	O2-C2	-2.13	1.37	1.43
2	D	601	GOL	C1-C2	2.04	1.59	1.51
2	A	601	GOL	C3-C2	2.04	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	GOL	C3-C2-C1	-2.52	102.56	111.80
2	B	602	GOL	C3-C2-C1	-2.20	103.73	111.80

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	604	GOL	O1-C1-C2-C3
2	A	604	GOL	C1-C2-C3-O3
2	A	604	GOL	O2-C2-C3-O3
2	B	602	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	D	602	GOL	O1-C1-C2-C3
2	D	602	GOL	C1-C2-C3-O3
2	D	602	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
2	A	603	GOL	O2-C2-C3-O3
2	D	601	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	A	602	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	D	601	GOL	O1-C1-C2-C3
2	D	601	GOL	C1-C2-C3-O3
2	B	602	GOL	O2-C2-C3-O3
2	D	601	GOL	O2-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
2	D	602	GOL	O1-C1-C2-O2
3	C	604	EDO	O1-C1-C2-O2
2	A	604	GOL	O1-C1-C2-O2
2	C	602	GOL	O1-C1-C2-O2
3	A	606	EDO	O1-C1-C2-O2
2	B	602	GOL	O1-C1-C2-O2
2	D	603	GOL	O2-C2-C3-O3
3	A	605	EDO	O1-C1-C2-O2
3	C	606	EDO	O1-C1-C2-O2
3	B	603	EDO	O1-C1-C2-O2
3	B	604	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	EDO	3	0
2	C	603	GOL	2	0
3	A	607	EDO	1	0
2	C	602	GOL	1	0
3	D	605	EDO	1	0
3	C	604	EDO	3	0
2	A	603	GOL	1	0
3	C	606	EDO	3	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	417/543 (76%)	0.10	16 (3%) 44 44	23, 36, 64, 87	0
1	B	417/543 (76%)	0.15	17 (4%) 41 41	24, 37, 63, 87	0
1	C	413/543 (76%)	0.08	22 (5%) 32 30	21, 35, 66, 77	0
1	D	420/543 (77%)	0.06	24 (5%) 29 27	19, 34, 66, 82	0
All	All	1667/2172 (76%)	0.10	79 (4%) 36 35	19, 36, 65, 87	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	GLY	5.2
1	B	23	ALA	5.0
1	D	114	PRO	4.8
1	C	232	GLY	4.7
1	D	528	ARG	4.6
1	D	23	ALA	4.3
1	D	531	SER	4.2
1	B	412	ARG	3.9
1	D	24	PHE	3.8
1	C	489	PRO	3.6
1	A	110	PHE	3.6
1	C	116	SER	3.5
1	C	30	LEU	3.5
1	C	527	HIS	3.4
1	B	110	PHE	3.4
1	A	20	LEU	3.3
1	C	242	ARG	3.3
1	B	493	ILE	3.2
1	D	492	ALA	3.1
1	A	18	GLN	3.1
1	A	490	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	542	ILE	3.0
1	D	116	SER	3.0
1	D	25	PHE	3.0
1	D	129	PRO	3.0
1	D	490	PRO	3.0
1	B	24	PHE	3.0
1	C	233	LEU	2.9
1	B	516	ARG	2.9
1	D	500	ARG	2.9
1	A	24	PHE	2.9
1	D	229	ASP	2.8
1	B	492	ALA	2.8
1	C	492	ALA	2.8
1	A	25	PHE	2.7
1	D	527	HIS	2.7
1	D	115	LEU	2.7
1	A	527	HIS	2.7
1	A	21	GLY	2.6
1	D	231	PRO	2.6
1	A	275	HIS	2.6
1	A	528	ARG	2.6
1	C	493	ILE	2.6
1	C	129	PRO	2.5
1	D	532	GLY	2.5
1	C	417	SER	2.5
1	B	487	ARG	2.5
1	A	129	PRO	2.5
1	C	490	PRO	2.5
1	A	22	THR	2.4
1	B	118	ARG	2.4
1	D	530	GLY	2.4
1	C	52	VAL	2.4
1	C	533	TYR	2.4
1	C	26	GLN	2.4
1	B	531	SER	2.4
1	D	533	TYR	2.3
1	B	275	HIS	2.3
1	A	297	GLU	2.3
1	D	493	ILE	2.3
1	D	411	ARG	2.3
1	B	26	GLN	2.2
1	B	133	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	26	GLN	2.2
1	C	517	VAL	2.2
1	C	511	LEU	2.2
1	C	27	GLN	2.2
1	A	531	SER	2.2
1	B	533	TYR	2.1
1	C	36	ASP	2.1
1	C	494	TRP	2.1
1	D	275	HIS	2.1
1	B	108	GLU	2.1
1	C	231	PRO	2.1
1	A	118	ARG	2.1
1	D	52	VAL	2.1
1	A	489	PRO	2.0
1	D	230	LEU	2.0
1	B	415	PRO	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
2	GOL	A	603	6/6	0.69	0.26	50,63,68,76	0
2	GOL	C	603	6/6	0.77	0.18	19,40,50,50	0
2	GOL	A	602	6/6	0.78	0.18	35,43,49,51	0
3	EDO	A	605	4/4	0.78	0.24	44,52,56,64	0
2	GOL	A	601	6/6	0.80	0.17	42,53,58,67	0
2	GOL	D	601	6/6	0.80	0.16	38,51,66,66	0
2	GOL	D	603	6/6	0.80	0.21	42,50,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	601	6/6	0.80	0.16	38,50,64,64	0
3	EDO	A	607	4/4	0.80	0.29	20,20,20,20	0
2	GOL	C	602	6/6	0.82	0.19	41,54,68,68	0
3	EDO	C	606	4/4	0.82	0.27	20,20,20,20	0
3	EDO	D	604	4/4	0.83	0.26	46,58,69,69	0
2	GOL	B	602	6/6	0.86	0.22	29,44,53,53	0
2	GOL	A	604	6/6	0.87	0.16	56,68,80,83	0
2	GOL	D	602	6/6	0.88	0.17	19,36,49,49	0
3	EDO	C	605	4/4	0.89	0.16	34,43,56,59	0
2	GOL	B	601	6/6	0.89	0.16	36,46,60,60	0
3	EDO	C	604	4/4	0.89	0.28	35,42,47,49	0
3	EDO	A	606	4/4	0.91	0.14	41,50,58,62	0
3	EDO	D	605	4/4	0.92	0.15	35,51,88,106	0
3	EDO	B	604	4/4	0.93	0.12	42,51,60,69	0
3	EDO	B	603	4/4	0.97	0.07	34,41,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.