



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:24 AM UTC

PDB ID : 7PZZ / pdb_00007pzz
Title : Crystal structure of serine hydroxymethyltransferase, isoform 2 from *Arabidopsis thaliana* (SHM2)
Authors : Ruszkowski, M.; Sekula, B.
Deposited on : 2021-10-13
Resolution : 1.65 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

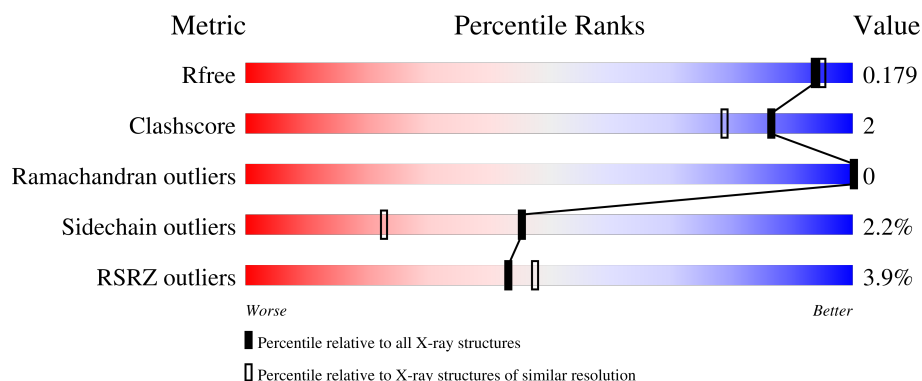
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	480	5% 92% 6% ..
1	B	480	4% 92% 6% .
1	C	480	3% 93% 5% .
1	D	480	3% 94% 5%

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
5	PEG	C	604	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17345 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 Serine hydroxymethyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	P	S	0	1	0
			3746	2377	639	711	1	18			
1	B	474	Total	C	N	O	P	S	0	1	0
			3740	2374	638	709	1	18			
1	C	473	Total	C	N	O	P	S	0	5	0
			3767	2388	644	716	1	18			
1	D	480	Total	C	N	O	P	S	0	4	0
			3816	2417	656	723	1	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	SER	-	expression tag	UNP Q94C74
A	39	ASN	-	expression tag	UNP Q94C74
A	40	ALA	-	expression tag	UNP Q94C74
B	38	SER	-	expression tag	UNP Q94C74
B	39	ASN	-	expression tag	UNP Q94C74
B	40	ALA	-	expression tag	UNP Q94C74
C	38	SER	-	expression tag	UNP Q94C74
C	39	ASN	-	expression tag	UNP Q94C74
C	40	ALA	-	expression tag	UNP Q94C74
D	38	SER	-	expression tag	UNP Q94C74
D	39	ASN	-	expression tag	UNP Q94C74
D	40	ALA	-	expression tag	UNP Q94C74

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



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

Continued on next page...

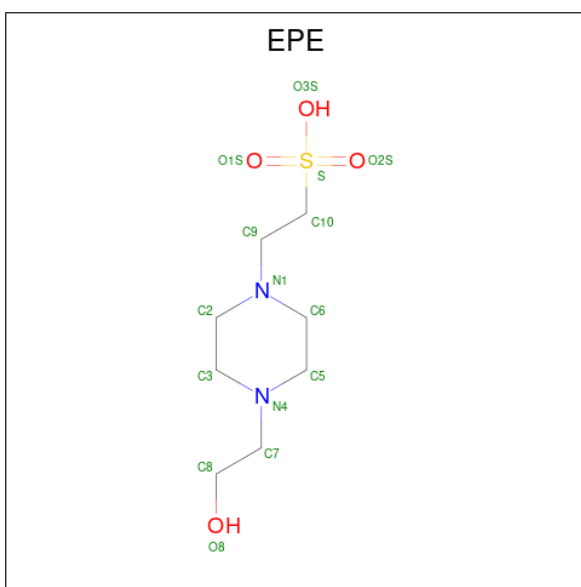
Continued from previous page...

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

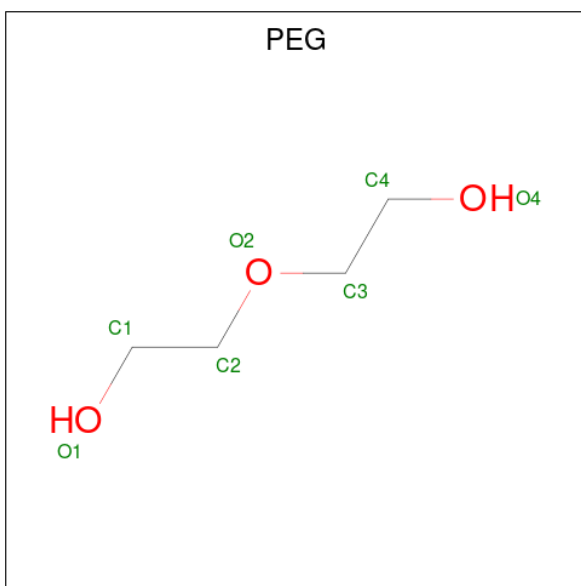
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

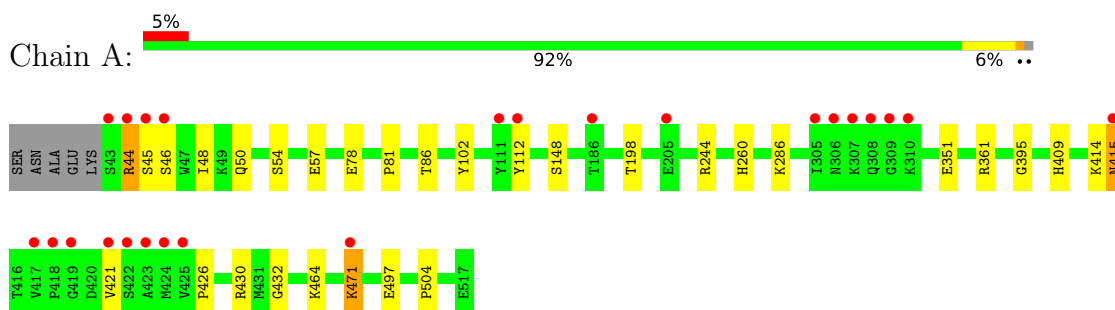
- Molecule 7 is water.

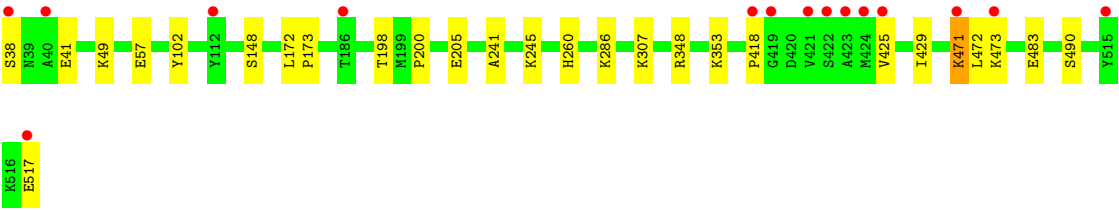
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	531	Total	O	0	0
			531	531		
7	B	495	Total	O	0	0
			495	495		
7	C	573	Total	O	0	0
			573	573		
7	D	517	Total	O	0	0
			517	517		

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: Serine hydroxymethyltransferase 2, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.20Å 131.24Å 151.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.84 – 1.65 53.84 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.84-1.65) 99.7 (53.84-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.158 , 0.178 0.160 , 0.179	Depositor DCC
R_{free} test set	1238 reflections (0.45%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17345	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: CL, EPE, LLP, SO4, EDO, PEG

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	0.34	0/3795	0.54	0/5119
1	B	0.33	0/3789	0.53	0/5111
1	C	0.37	0/3815	0.57	0/5143
1	D	0.33	0/3865	0.54	0/5210
All	All	0.34	0/15264	0.55	0/20583

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3746	0	3742	18	0
1	B	3740	0	3737	19	0
1	C	3767	0	3756	15	0
1	D	3816	0	3812	14	0
2	A	24	0	36	1	0
2	B	28	0	42	3	0
2	C	32	0	48	0	0
2	D	28	0	42	2	0
3	A	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	15	0	17	0	0
5	C	7	0	10	4	0
5	D	7	0	10	0	0
6	C	15	0	0	0	0
7	A	531	0	0	5	0
7	B	495	0	0	5	0
7	C	573	0	0	7	0
7	D	517	0	0	3	0
All	All	17345	0	15252	64	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 2.

All (64) 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:172:LEU:H	5:C:604:PEG:H12	1.53	0.72
1:C:424:MET:SD	7:C:1041:HOH:O	2.52	0.68
1:D:471:LYS:HE2	1:D:472:LEU:H	1.64	0.63
1:C:172:LEU:N	5:C:604:PEG:H12	2.17	0.60
1:D:348[A]:ARG:NH1	7:D:703:HOH:O	2.36	0.58
1:A:44:ARG:NH1	1:A:45:SER:OG	2.38	0.57
1:D:205:GLU:HB3	1:D:418:PRO:HB3	1.86	0.56
1:C:493:ARG:NH2	7:C:708:HOH:O	2.39	0.55
1:D:418:PRO:HG2	7:D:714:HOH:O	2.09	0.53
1:A:50:GLN:NE2	7:A:702:HOH:O	2.36	0.52
1:B:198:THR:HB	2:B:607:EDO:H22	1.92	0.51
1:A:415:ASN:OD1	1:A:430:ARG:NH2	2.40	0.50
1:B:244:ARG:NH2	7:B:708:HOH:O	2.35	0.49
1:C:44:ARG:O	1:C:48:ILE:HG12	2.12	0.49
1:D:471:LYS:HG3	1:D:473:LYS:HZ3	1.77	0.49
1:C:171:ASP:HA	5:C:604:PEG:H12	1.94	0.49
1:A:414:LYS:HD3	1:A:426:PRO:HG3	1.94	0.48
1:C:289:ARG:NH2	7:C:713:HOH:O	2.45	0.48
1:D:200:PRO:HA	2:D:606:EDO:H11	1.96	0.48
1:A:54:SER:OG	1:A:57:GLU:HG3	2.13	0.47
1:C:78:GLU:HG3	7:C:727:HOH:O	2.15	0.47
1:B:328:LEU:HD22	2:B:601:EDO:H22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:NH1	3:A:607:CL:CL	2.86	0.46
1:D:38:SER:HB3	1:D:41:GLU:OE1	2.15	0.46
1:D:471:LYS:HA	1:D:471:LYS:HD2	1.71	0.46
1:B:471:LYS:HA	1:B:471:LYS:HD2	1.68	0.46
1:C:244:ARG:NH2	7:C:704:HOH:O	2.29	0.46
1:B:154:PHE:CD1	2:B:601:EDO:H11	2.51	0.45
1:A:409:HIS:ND1	1:A:497:GLU:OE2	2.49	0.45
1:C:392:LYS:HE2	1:C:417:VAL:HG23	1.99	0.45
1:D:353:LYS:NZ	7:D:718:HOH:O	2.50	0.45
5:C:604:PEG:H22	5:C:604:PEG:H42	1.58	0.45
1:B:74:TRP:NE1	1:B:510:LYS:HE2	2.32	0.44
1:A:504:PRO:HG2	1:B:48:ILE:HD13	1.98	0.44
1:B:458:LYS:NZ	7:B:721:HOH:O	2.50	0.44
1:B:110:ARG:HB3	7:B:712:HOH:O	2.17	0.44
1:A:48:ILE:HD13	1:B:504:PRO:HG2	2.01	0.43
1:B:311:GLU:HG3	1:B:313:MET:H	1.83	0.43
1:A:198:THR:HB	2:A:603:EDO:H11	2.00	0.43
1:A:244:ARG:NH2	7:A:719:HOH:O	2.52	0.42
1:A:395:GLY:O	1:A:464:LYS:NZ	2.48	0.42
1:A:112:TYR:HD1	7:A:723:HOH:O	2.01	0.42
1:B:517:GLU:OXT	7:B:701:HOH:O	2.22	0.42
1:B:476:VAL:HA	1:B:479:MET:HE2	2.01	0.42
1:D:172:LEU:HB3	1:D:173:PRO:HD3	2.01	0.42
1:D:241:ALA:O	1:D:245:LYS:HG2	2.20	0.42
1:A:361:ARG:NH2	7:A:718:HOH:O	2.52	0.42
1:A:81:PRO:HB3	1:A:432:GLY:HA3	2.02	0.41
1:A:351:GLU:CD	1:B:50:GLN:HE22	2.28	0.41
1:C:174:HIS:HB3	1:C:203:LEU:HG	2.02	0.41
1:C:57:GLU:OE1	7:C:701:HOH:O	2.22	0.41
1:B:74:TRP:HE1	1:B:510:LYS:HE2	1.86	0.41
1:D:198:THR:HB	2:D:606:EDO:H22	2.02	0.41
1:D:49:LYS:NZ	1:D:57:GLU:OE2	2.54	0.41
1:A:78:GLU:HG3	7:A:703:HOH:O	2.21	0.41
1:B:81:PRO:HG3	1:B:430:ARG:HG2	2.03	0.41
1:B:310:LYS:HD2	1:B:310:LYS:HA	1.84	0.41
1:C:494:GLU:HG2	7:C:836:HOH:O	2.20	0.41
1:A:471:LYS:HA	1:A:471:LYS:HD2	1.73	0.40
1:B:111:TYR:N	7:B:712:HOH:O	2.49	0.40
1:B:174:HIS:HB3	1:B:203:LEU:HG	2.04	0.40
1:C:413:ASN:HB3	1:C:430:ARG:HB3	2.03	0.40
1:D:245:LYS:HA	1:D:245:LYS:HD3	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASN:HD21	1:C:310:LYS:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	473/480 (98%)	459 (97%)	14 (3%)	0	100	100
1	B	472/480 (98%)	459 (97%)	13 (3%)	0	100	100
1	C	473/480 (98%)	461 (98%)	12 (2%)	0	100	100
1	D	481/480 (100%)	470 (98%)	11 (2%)	0	100	100
All	All	1899/1920 (99%)	1849 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	397/400 (99%)	388 (98%)	9 (2%)	44	21
1	B	396/400 (99%)	388 (98%)	8 (2%)	48	26
1	C	400/400 (100%)	392 (98%)	8 (2%)	48	26
1	D	404/400 (101%)	394 (98%)	10 (2%)	42	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1597/1600 (100%)	1562 (98%)	35 (2%)	45 23

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	46	SER
1	A	86	THR
1	A	102	TYR
1	A	148	SER
1	A	260	HIS
1	A	415	ASN
1	A	421	VAL
1	A	471	LYS
1	B	86	THR
1	B	102	TYR
1	B	148	SER
1	B	215	LEU
1	B	238	TYR
1	B	260	HIS
1	B	468	GLN
1	B	471	LYS
1	C	44	ARG
1	C	86	THR
1	C	102	TYR
1	C	148	SER
1	C	260	HIS
1	C	312	VAL
1	C	494	GLU
1	C	517	GLU
1	D	102	TYR
1	D	148	SER
1	D	260	HIS
1	D	307	LYS
1	D	425	VAL
1	D	429	ILE
1	D	471	LYS
1	D	483	GLU
1	D	490	SER
1	D	517	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	346	GLN
1	A	468	GLN
1	A	502	GLN
1	B	214	GLN
1	B	250	GLN
1	B	358	GLN
1	B	413	ASN
1	C	134	GLN
1	C	308	GLN
1	C	409	HIS
1	C	468	GLN
1	D	214	GLN
1	D	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	B	286	1	23,24,25	1.52	4 (17%)	25,32,34	1.88	5 (20%)
1	LLP	C	286	1	23,24,25	1.56	5 (21%)	25,32,34	2.10	7 (28%)
1	LLP	A	286	1	23,24,25	1.40	5 (21%)	25,32,34	1.94	5 (20%)
1	LLP	D	286	1	23,24,25	1.50	5 (21%)	25,32,34	1.75	5 (20%)

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
1	LLP	B	286	1	-	5/16/17/19	0/1/1/1
1	LLP	C	286	1	-	5/16/17/19	0/1/1/1
1	LLP	A	286	1	-	5/16/17/19	0/1/1/1
1	LLP	D	286	1	-	5/16/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	LLP	C4-C4'	3.52	1.54	1.46
1	D	286	LLP	C4-C4'	3.39	1.53	1.46
1	B	286	LLP	C4-C4'	3.12	1.53	1.46
1	B	286	LLP	C4-C5	-3.10	1.37	1.42
1	C	286	LLP	C3-C2	-3.04	1.37	1.41
1	A	286	LLP	C4-C4'	3.02	1.53	1.46
1	B	286	LLP	C3-C2	-2.92	1.37	1.41
1	C	286	LLP	C4-C5	-2.91	1.37	1.42
1	C	286	LLP	C4-C3	-2.72	1.36	1.41
1	D	286	LLP	C4-C5	-2.70	1.38	1.42
1	D	286	LLP	C2'-C2	2.64	1.54	1.50
1	A	286	LLP	C4-C3	-2.62	1.36	1.41
1	A	286	LLP	C4-C5	-2.51	1.38	1.42
1	A	286	LLP	C2'-C2	2.38	1.54	1.50
1	C	286	LLP	C2'-C2	2.37	1.54	1.50
1	B	286	LLP	C2'-C2	2.34	1.54	1.50
1	A	286	LLP	C3-C2	-2.23	1.38	1.41
1	D	286	LLP	C4-C3	-2.09	1.37	1.41
1	D	286	LLP	C3-C2	-2.07	1.38	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	LLP	OP4-C5'-C5	5.89	120.39	109.36
1	B	286	LLP	OP4-C5'-C5	5.55	119.76	109.36
1	A	286	LLP	OP4-C5'-C5	5.33	119.35	109.36
1	D	286	LLP	OP4-C5'-C5	4.77	118.30	109.36
1	D	286	LLP	CE-NZ-C4'	4.48	133.06	118.72
1	C	286	LLP	CE-NZ-C4'	4.37	132.72	118.72
1	A	286	LLP	C4-C3-C2	4.28	122.55	120.14
1	A	286	LLP	CE-NZ-C4'	4.07	131.75	118.72
1	B	286	LLP	CE-NZ-C4'	3.98	131.47	118.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	LLP	C4-C3-C2	3.35	122.03	120.14
1	A	286	LLP	C4-C4'-NZ	-3.28	108.88	124.04
1	B	286	LLP	C4-C4'-NZ	-3.28	108.91	124.04
1	D	286	LLP	C4-C4'-NZ	-3.26	108.98	124.04
1	C	286	LLP	C4-C4'-NZ	-3.17	109.40	124.04
1	A	286	LLP	C5'-C5-C6	-2.63	115.07	119.36
1	B	286	LLP	C5'-C5-C6	-2.53	115.24	119.36
1	C	286	LLP	OP4-P-OP1	-2.39	99.99	106.44
1	D	286	LLP	C4-C3-C2	2.32	121.45	120.14
1	B	286	LLP	C4-C3-C2	2.26	121.41	120.14
1	C	286	LLP	C5-C6-N1	-2.18	120.29	123.83
1	C	286	LLP	C3-C2-N1	-2.18	118.22	120.96
1	D	286	LLP	C2'-C2-C3	2.05	123.19	120.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	286	LLP	O-C-CA-CB
1	B	286	LLP	O-C-CA-CB
1	C	286	LLP	O-C-CA-CB
1	D	286	LLP	O-C-CA-CB
1	C	286	LLP	CG-CD-CE-NZ
1	A	286	LLP	CG-CD-CE-NZ
1	B	286	LLP	CG-CD-CE-NZ
1	D	286	LLP	CG-CD-CE-NZ
1	C	286	LLP	C3-C4-C4'-NZ
1	A	286	LLP	C3-C4-C4'-NZ
1	B	286	LLP	C3-C4-C4'-NZ
1	B	286	LLP	CD-CE-NZ-C4'
1	C	286	LLP	CD-CE-NZ-C4'
1	C	286	LLP	C5-C4-C4'-NZ
1	A	286	LLP	CD-CE-NZ-C4'
1	D	286	LLP	CD-CE-NZ-C4'
1	B	286	LLP	C5-C4-C4'-NZ
1	D	286	LLP	C3-C4-C4'-NZ
1	A	286	LLP	C5-C4-C4'-NZ
1	D	286	LLP	C5-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 4 are monoatomic - leaving 34 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EPE	B	602	-	15,15,15	0.79	1 (6%)	19,20,20	1.60	3 (15%)
2	EDO	B	603	-	3,3,3	0.40	0	2,2,2	0.49	0
2	EDO	C	606	-	3,3,3	0.53	0	2,2,2	0.32	0
2	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.42	0
2	EDO	B	601	-	3,3,3	0.27	0	2,2,2	0.43	0
2	EDO	B	605	-	3,3,3	0.41	0	2,2,2	0.47	0
2	EDO	B	607	-	3,3,3	0.67	0	2,2,2	0.43	0
2	EDO	A	605	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	B	604	-	3,3,3	0.43	0	2,2,2	0.70	0
2	EDO	D	603	-	3,3,3	0.43	0	2,2,2	0.14	0
5	PEG	C	604	-	6,6,6	0.12	0	5,5,5	0.26	0
2	EDO	C	602	-	3,3,3	0.53	0	2,2,2	0.15	0
2	EDO	D	601	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	C	609	-	3,3,3	0.50	0	2,2,2	0.41	0
2	EDO	C	607	-	3,3,3	0.48	0	2,2,2	0.47	0
2	EDO	D	604	-	3,3,3	0.49	0	2,2,2	0.14	0
2	EDO	D	606	-	3,3,3	0.46	0	2,2,2	0.55	0
2	EDO	C	601	-	3,3,3	0.47	0	2,2,2	0.39	0
2	EDO	C	605	-	3,3,3	0.43	0	2,2,2	0.25	0
2	EDO	D	602	-	3,3,3	0.38	0	2,2,2	0.43	0
2	EDO	B	609	-	3,3,3	0.49	0	2,2,2	0.22	0
5	PEG	D	605	-	6,6,6	0.15	0	5,5,5	0.16	0
2	EDO	A	604	-	3,3,3	0.45	0	2,2,2	0.42	0
2	EDO	B	606	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	601	-	3,3,3	0.41	0	2,2,2	0.48	0
2	EDO	C	608	-	3,3,3	0.47	0	2,2,2	0.37	0
6	SO4	C	610	-	4,4,4	0.24	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	603	-	3,3,3	0.55	0	2,2,2	0.44	0
2	EDO	A	606	-	3,3,3	0.38	0	2,2,2	0.48	0
2	EDO	D	607	-	3,3,3	0.45	0	2,2,2	0.57	0
6	SO4	C	611	-	4,4,4	0.33	0	6,6,6	0.39	0
6	SO4	C	612	-	4,4,4	0.22	0	6,6,6	0.15	0
2	EDO	C	603	-	3,3,3	0.44	0	2,2,2	0.65	0
2	EDO	D	608	-	3,3,3	0.44	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	B	602	-	-	4/9/19/19	0/1/1/1
2	EDO	B	603	-	-	1/1/1/1	-
2	EDO	C	606	-	-	1/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	B	605	-	-	1/1/1/1	-
2	EDO	B	607	-	-	1/1/1/1	-
2	EDO	A	605	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
5	PEG	C	604	-	-	4/4/4/4	-
2	EDO	C	602	-	-	0/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	C	609	-	-	0/1/1/1	-
2	EDO	C	607	-	-	0/1/1/1	-
2	EDO	D	604	-	-	0/1/1/1	-
2	EDO	D	606	-	-	0/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	C	605	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
2	EDO	B	609	-	-	0/1/1/1	-
5	PEG	D	605	-	-	1/4/4/4	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	B	606	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	C	608	-	-	1/1/1/1	-
2	EDO	A	603	-	-	1/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	607	-	-	0/1/1/1	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	D	608	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	EPE	C10-S	2.62	1.81	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	EPE	C5-N4-C3	4.52	118.58	108.84
4	B	602	EPE	C7-N4-C5	2.38	117.58	111.24
4	B	602	EPE	C7-N4-C3	2.10	116.83	111.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	EPE	C9-C10-S-O1S
4	B	602	EPE	C9-C10-S-O3S
5	C	604	PEG	C4-C3-O2-C2
2	B	603	EDO	O1-C1-C2-O2
2	B	607	EDO	O1-C1-C2-O2
2	D	601	EDO	O1-C1-C2-O2
5	C	604	PEG	O2-C3-C4-O4
5	C	604	PEG	O1-C1-C2-O2
2	A	606	EDO	O1-C1-C2-O2
2	C	605	EDO	O1-C1-C2-O2
2	C	608	EDO	O1-C1-C2-O2
4	B	602	EPE	C9-C10-S-O2S
5	C	604	PEG	C1-C2-O2-C3
5	D	605	PEG	O2-C3-C4-O4
2	B	605	EDO	O1-C1-C2-O2
2	A	603	EDO	O1-C1-C2-O2
4	B	602	EPE	N4-C7-C8-O8
2	C	606	EDO	O1-C1-C2-O2
2	D	603	EDO	O1-C1-C2-O2
2	B	601	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	EDO	2	0
2	B	607	EDO	1	0
5	C	604	PEG	4	0
2	D	606	EDO	2	0
2	A	603	EDO	1	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	474/480 (98%)	-0.16	24 (5%)	33 37	9, 20, 57, 96	1 (0%)
1	B	473/480 (98%)	-0.10	19 (4%)	42 46	10, 22, 56, 88	1 (0%)
1	C	472/480 (98%)	-0.32	16 (3%)	48 52	8, 19, 40, 80	5 (1%)
1	D	479/480 (99%)	-0.17	15 (3%)	51 55	10, 21, 52, 95	4 (0%)
All	All	1898/1920 (98%)	-0.19	74 (3%)	43 48	8, 20, 52, 96	11 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	421	VAL	8.1
1	A	421	VAL	5.7
1	D	421	VAL	5.2
1	B	423	ALA	5.1
1	D	418	PRO	4.9
1	A	424	MET	4.7
1	A	418	PRO	4.6
1	B	112	TYR	4.5
1	A	44	ARG	4.5
1	D	425	VAL	4.4
1	D	423	ALA	4.3
1	A	112	TYR	4.3
1	B	421	VAL	4.3
1	D	424	MET	4.1
1	A	46	SER	4.0
1	C	43	SER	4.0
1	B	424	MET	4.0
1	B	46	SER	3.8
1	A	45	SER	3.7
1	B	425	VAL	3.7
1	B	111	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	423	ALA	3.6
1	A	309	GLY	3.5
1	A	419	GLY	3.5
1	A	43	SER	3.4
1	B	47	TRP	3.4
1	B	310	LYS	3.3
1	B	471	LYS	3.2
1	B	470	THR	3.2
1	A	310	LYS	3.2
1	A	425	VAL	3.2
1	C	424	MET	3.2
1	C	45	SER	3.2
1	A	417	VAL	3.2
1	B	44	ARG	3.1
1	D	38	SER	3.1
1	C	44	ARG	3.0
1	A	307	LYS	3.0
1	C	419	GLY	3.0
1	D	186	THR	3.0
1	D	517	GLU	3.0
1	A	305	ILE	3.0
1	D	112	TYR	2.9
1	C	307	LYS	2.9
1	A	205	GLU	2.9
1	D	419	GLY	2.8
1	D	515	TYR	2.8
1	D	471	LYS	2.8
1	C	415	ASN	2.7
1	B	409	HIS	2.7
1	A	306	ASN	2.6
1	A	471	LYS	2.6
1	D	422	SER	2.6
1	C	418	PRO	2.5
1	C	310	LYS	2.5
1	A	415	ASN	2.5
1	A	422	SER	2.5
1	A	308	GLN	2.5
1	D	473	LYS	2.3
1	C	305	ILE	2.3
1	C	409	HIS	2.2
1	C	308	GLN	2.2
1	B	418	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	422	SER	2.2
1	D	40	ALA	2.2
1	B	413	ASN	2.2
1	C	417	VAL	2.1
1	C	517	GLU	2.1
1	C	46	SER	2.1
1	A	111	TYR	2.1
1	B	468	GLN	2.1
1	B	469	GLY	2.1
1	A	186	THR	2.0
1	B	477	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	286	24/25	0.98	0.06	13,15,23,25	0
1	LLP	B	286	24/25	0.98	0.06	13,16,23,28	0
1	LLP	C	286	24/25	0.98	0.05	12,14,22,24	0
1	LLP	D	286	24/25	0.98	0.06	13,16,20,26	0

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
4	EPE	B	602	15/15	0.76	0.16	46,54,72,74	0
5	PEG	D	605	7/7	0.78	0.17	44,51,52,53	0
2	EDO	D	608	4/4	0.79	0.17	36,36,40,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	C	604	7/7	0.81	0.15	16,18,20,22	7
2	EDO	A	603	4/4	0.83	0.20	18,22,25,32	0
2	EDO	B	605	4/4	0.83	0.15	30,31,34,44	0
6	SO4	C	611	5/5	0.83	0.12	29,31,47,50	0
2	EDO	C	602	4/4	0.84	0.16	31,32,37,41	0
2	EDO	D	607	4/4	0.85	0.15	24,32,38,40	0
2	EDO	B	607	4/4	0.85	0.19	23,25,28,31	0
2	EDO	C	607	4/4	0.85	0.14	36,38,40,42	0
2	EDO	B	601	4/4	0.86	0.24	25,25,27,32	0
2	EDO	B	609	4/4	0.86	0.20	26,32,35,46	0
2	EDO	D	606	4/4	0.86	0.17	22,22,27,30	0
6	SO4	C	612	5/5	0.86	0.12	40,44,57,60	0
2	EDO	D	601	4/4	0.87	0.13	25,29,30,37	0
6	SO4	C	610	5/5	0.87	0.11	38,46,59,63	0
2	EDO	B	606	4/4	0.87	0.13	36,39,42,45	0
2	EDO	C	601	4/4	0.87	0.12	30,32,40,40	0
2	EDO	D	604	4/4	0.88	0.15	26,28,34,40	0
2	EDO	C	603	4/4	0.88	0.11	27,30,34,35	0
2	EDO	C	608	4/4	0.89	0.12	31,32,38,46	0
2	EDO	A	605	4/4	0.89	0.10	35,36,44,46	0
2	EDO	C	605	4/4	0.89	0.12	37,38,40,51	0
2	EDO	A	604	4/4	0.89	0.18	25,33,34,45	0
2	EDO	C	609	4/4	0.91	0.12	29,35,39,41	0
2	EDO	B	603	4/4	0.91	0.10	25,26,26,33	0
2	EDO	A	602	4/4	0.92	0.08	27,31,34,38	0
2	EDO	A	606	4/4	0.93	0.12	27,30,31,37	0
2	EDO	D	602	4/4	0.93	0.10	23,24,25,27	0
2	EDO	C	606	4/4	0.94	0.12	25,26,28,31	0
2	EDO	D	603	4/4	0.94	0.10	29,31,35,35	0
2	EDO	B	604	4/4	0.95	0.10	19,22,30,36	0
2	EDO	A	601	4/4	0.96	0.08	22,24,29,30	0
3	CL	D	609	1/1	0.97	0.06	29,29,29,29	0
3	CL	B	608	1/1	0.98	0.07	27,27,27,27	0
3	CL	C	613	1/1	0.99	0.07	22,22,22,22	0
3	CL	A	607	1/1	0.99	0.09	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.