



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:04 AM UTC

PDB ID : 8QAW / pdb_00008qaw
Title : Medicago truncatula HSN5 (IGPD) in complex with MN, IMD, EDO, FMT, GOL and TRS
Authors : Witek, W.; Ruszkowski, M.
Deposited on : 2023-08-23
Resolution : 1.55 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

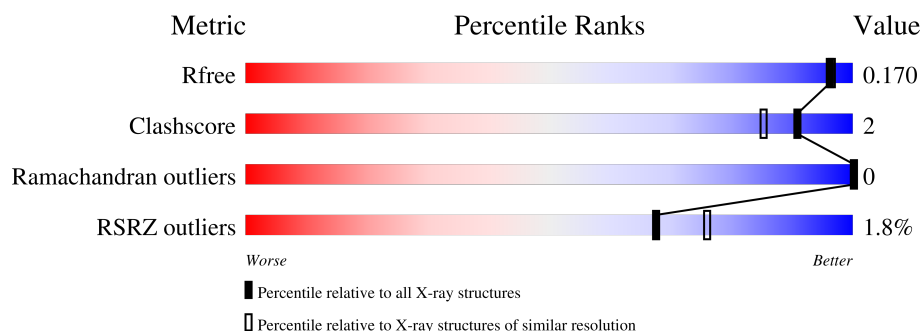
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	206	% 84% 5% 10%
1	B	206	% 87% • 10%
1	C	206	2% 88% • 10%
1	D	206	2% 86% • 10%
1	E	206	% 87% • 11%
1	F	206	2% 88% • 10%

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Mol	Chain	Length	Quality of chain
1	G	206	% 85% 5% 10%
1	H	206	2% 88% • 10%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13098 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 Imidazoleglycerol-phosphate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	2	0
			1448	901	268	276	3			
1	B	185	Total	C	N	O	S	0	0	0
			1435	893	265	274	3			
1	C	185	Total	C	N	O	S	0	2	0
			1448	901	268	276	3			
1	D	185	Total	C	N	O	S	0	1	0
			1441	897	266	275	3			
1	E	184	Total	C	N	O	S	0	1	0
			1431	892	263	273	3			
1	F	185	Total	C	N	O	S	0	0	0
			1435	893	265	274	3			
1	G	185	Total	C	N	O	S	0	0	0
			1435	893	265	274	3			
1	H	185	Total	C	N	O	S	0	0	0
			1435	893	265	274	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	PRO	-	expression tag	UNP I3SDM5
B	70	PRO	-	expression tag	UNP I3SDM5
C	70	PRO	-	expression tag	UNP I3SDM5
D	70	PRO	-	expression tag	UNP I3SDM5
E	70	PRO	-	expression tag	UNP I3SDM5
F	70	PRO	-	expression tag	UNP I3SDM5
G	70	PRO	-	expression tag	UNP I3SDM5
H	70	PRO	-	expression tag	UNP I3SDM5

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		
2	E	1	Total	C	N	0	0
			5	3	2		
2	F	1	Total	C	N	0	0
			5	3	2		
2	G	1	Total	C	N	0	0
			5	3	2		
2	H	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	G	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

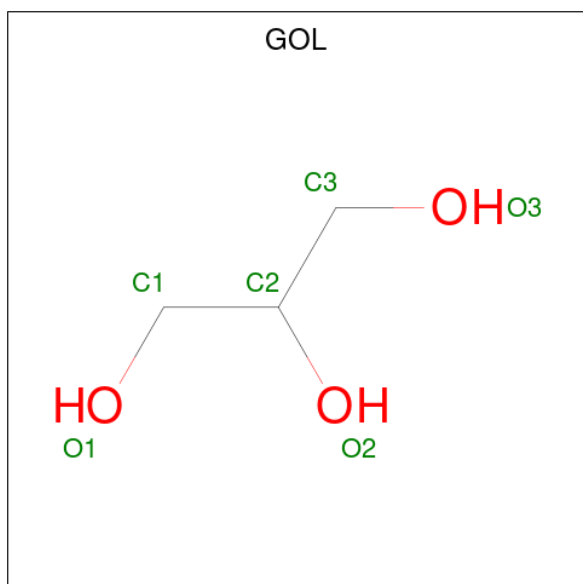
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mn 2 2	0	0
5	B	2	Total Mn 2 2	0	0

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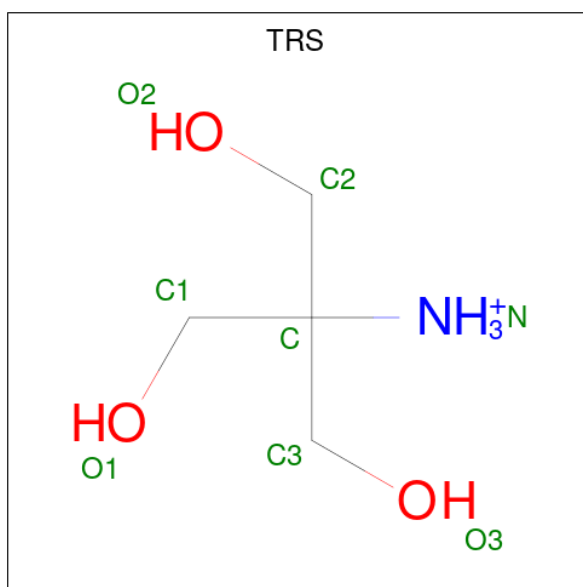
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mn	0	0
			2	2		
5	D	2	Total	Mn	0	0
			2	2		
5	E	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		
5	G	2	Total	Mn	0	0
			2	2		
5	H	2	Total	Mn	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		
9	B	1	Total	Na	0	0
			1	1		

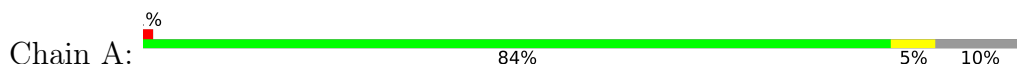
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	166	Total 166	O 166	0	0
10	B	187	Total 187	O 187	0	0
10	C	172	Total 172	O 172	0	0
10	D	168	Total 168	O 168	0	0
10	E	164	Total 164	O 164	0	0
10	F	155	Total 155	O 155	0	0
10	G	159	Total 159	O 159	0	0
10	H	164	Total 164	O 164	0	0

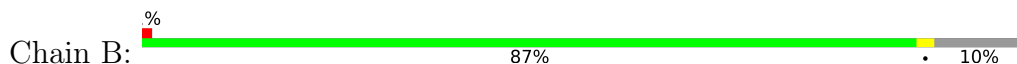
3 Residue-property plots [i](#)

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: Imidazoglycerol-phosphate dehydratase



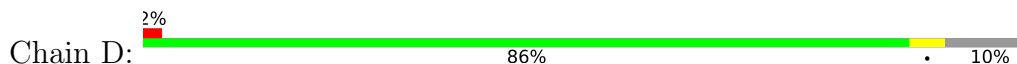
- Molecule 1: Imidazoglycerol-phosphate dehydratase



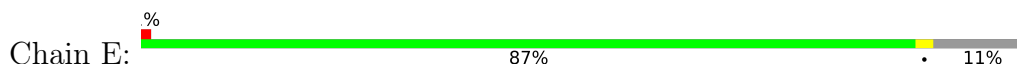
- Molecule 1: Imidazoglycerol-phosphate dehydratase



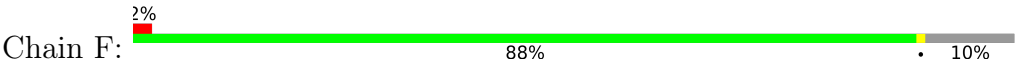
- Molecule 1: Imidazoglycerol-phosphate dehydratase



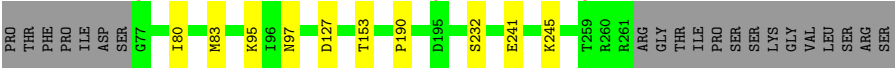
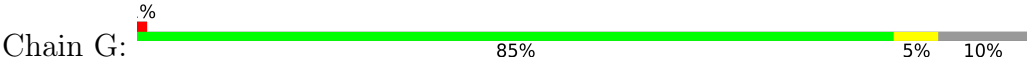
- Molecule 1: Imidazoglycerol-phosphate dehydratase



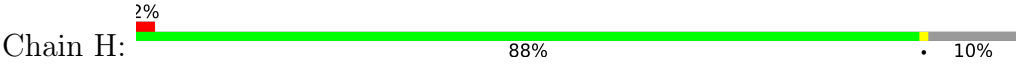
- Molecule 1: Imidazoglycerol-phosphate dehydratase



• Molecule 1: Imidazoglycerol-phosphate dehydratase



• Molecule 1: Imidazoglycerol-phosphate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	137.68Å 137.68Å 265.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.06 – 1.55 58.06 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.06-1.55) 99.9 (58.06-1.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.129 , 0.161 (Not available) , 0.170	Depositor DCC
R_{free} test set	1089 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13098	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: NA, IMD, FMT, GOL, MN, EDO, TRS, CL

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	0.25	0/1479	0.51	0/2001
1	B	0.23	0/1462	0.49	0/1978
1	C	0.23	0/1479	0.48	0/2001
1	D	0.24	0/1471	0.48	0/1990
1	E	0.24	0/1462	0.48	0/1979
1	F	0.22	0/1462	0.47	0/1978
1	G	0.22	0/1462	0.48	0/1978
1	H	0.23	0/1462	0.47	0/1978
All	All	0.23	0/11739	0.48	0/15883

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	1448	0	1413	7	0
1	B	1435	0	1402	3	0
1	C	1448	0	1413	6	0
1	D	1441	0	1410	6	0
1	E	1431	0	1396	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1435	0	1402	3	0
1	G	1435	0	1402	7	0
1	H	1435	0	1402	2	0
2	A	5	0	5	0	0
2	B	5	0	5	1	0
2	C	5	0	5	0	0
2	D	5	0	5	0	0
2	E	5	0	5	0	0
2	F	5	0	5	0	0
2	G	5	0	5	0	0
2	H	5	0	5	0	0
3	A	3	0	1	0	0
3	B	9	0	3	0	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
3	E	6	0	2	0	0
3	F	3	0	1	0	0
3	G	3	0	1	0	0
3	H	3	0	1	0	0
4	A	12	0	18	1	0
4	B	12	0	18	0	0
4	C	20	0	30	2	0
4	D	24	0	36	2	0
4	E	16	0	24	2	0
4	F	12	0	18	0	0
4	G	12	0	18	2	0
4	H	16	0	24	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	6	0	8	1	0
7	A	8	0	12	0	0
7	B	8	0	12	0	0
7	D	8	0	12	0	0
7	G	8	0	12	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	166	0	0	1	0
10	B	187	0	0	0	0
10	C	172	0	0	4	0
10	D	168	0	0	0	0
10	E	164	0	0	1	0
10	F	155	0	0	1	0
10	G	159	0	0	0	0
10	H	164	0	0	0	0
All	All	13098	0	11533	39	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 (39) 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:F:88:LYS:H	1:F:88:LYS:HZ3	1.17	0.89
1:C:84:LYS:CG	10:C:424:HOH:O	2.41	0.68
1:C:84:LYS:HG3	10:C:424:HOH:O	1.97	0.63
1:E:230:GLN:HE21	4:E:307:EDO:H22	1.66	0.60
1:D:230:GLN:HG2	4:D:310:EDO:H12	1.86	0.58
1:G:80:ILE:HG21	1:G:95:LYS:HE3	1.87	0.56
1:F:88:LYS:H	1:F:88:LYS:NZ	1.99	0.56
1:A:162:ARG:HD3	4:A:306:EDO:H22	1.89	0.55
1:E:205:LYS:NZ	10:E:401:HOH:O	2.26	0.54
1:G:97:ASN:HB3	1:G:127:ASP:HB2	1.90	0.53
1:E:97:ASN:HB3	1:E:127:ASP:HB2	1.91	0.52
1:A:83:MET:HG2	1:A:150:ALA:HB1	1.93	0.50
1:D:83:MET:HE3	1:D:153:THR:HG21	1.92	0.50
1:C:84:LYS:HE3	10:C:424:HOH:O	2.11	0.49
1:A:85:ARG:NH2	10:A:407:HOH:O	2.46	0.48
1:C:84:LYS:CE	10:C:424:HOH:O	2.62	0.48
1:E:230:GLN:HE21	4:E:307:EDO:C2	2.25	0.48
1:B:97:ASN:HB3	1:B:127:ASP:HB2	1.96	0.47
1:D:97:ASN:HB3	1:D:127:ASP:HB2	1.95	0.47
1:D:80:ILE:HG21	1:D:95:LYS:HE3	1.97	0.46
1:C:97:ASN:HB3	1:C:127:ASP:HB2	1.98	0.46
1:H:97:ASN:HB3	1:H:127:ASP:HB2	1.98	0.46
1:A:97:ASN:HB3	1:A:127:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:ARG:HD3	4:H:307:EDO:H22	1.98	0.45
1:G:190:PRO:HB2	4:G:307:EDO:H22	1.98	0.45
1:F:97:ASN:HB3	1:F:127:ASP:HB2	1.98	0.44
1:A:123:HIS:NE2	6:A:308:GOL:H2	2.32	0.44
1:G:241:GLU:HG2	1:G:245:LYS:HE3	1.99	0.44
1:A:241:GLU:HG2	1:A:245:LYS:HE3	2.00	0.44
4:C:303:EDO:H21	10:F:417:HOH:O	2.16	0.44
1:G:83:MET:HE3	1:G:153:THR:HG21	1.99	0.43
1:G:83:MET:HE3	1:G:153:THR:CG2	2.48	0.43
1:C:162:ARG:HD3	4:C:307:EDO:H22	2.00	0.42
1:B:83:MET:HE3	1:B:153:THR:CG2	2.50	0.42
1:D:83:MET:HE3	1:D:153:THR:CG2	2.50	0.41
1:D:162:ARG:HD3	4:D:309:EDO:H22	2.01	0.41
1:B:145:GLU:OE1	2:B:301:IMD:H4	2.20	0.41
1:G:232:SER:HA	4:G:306:EDO:H21	2.03	0.41
1:A:80:ILE:HG21	1:A:95:LYS:HE3	2.03	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	185/206 (90%)	177 (96%)	8 (4%)	0	100	100
1	B	183/206 (89%)	176 (96%)	7 (4%)	0	100	100
1	C	185/206 (90%)	179 (97%)	6 (3%)	0	100	100
1	D	184/206 (89%)	177 (96%)	7 (4%)	0	100	100
1	E	183/206 (89%)	176 (96%)	7 (4%)	0	100	100
1	F	183/206 (89%)	177 (97%)	6 (3%)	0	100	100
1	G	183/206 (89%)	176 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	183/206 (89%)	176 (96%)	7 (4%)	0	100	100
All	All	1469/1648 (89%)	1414 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 20 are monoatomic - leaving 55 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	EDO	C	308	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	H	305	-	3,3,3	0.42	0	2,2,2	0.56	0
4	EDO	F	306	-	3,3,3	0.42	0	2,2,2	0.53	0
3	FMT	B	303	-	2,2,2	0.71	0	1,1,1	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IMD	F	301	-	5,5,5	0.67	0	5,5,5	0.38	0
4	EDO	H	306	-	3,3,3	0.43	0	2,2,2	0.46	0
3	FMT	B	306	-	2,2,2	0.75	0	1,1,1	0.28	0
4	EDO	D	307	-	3,3,3	0.44	0	2,2,2	0.36	0
2	IMD	E	301	-	5,5,5	0.67	0	5,5,5	0.43	0
3	FMT	G	302	5	2,2,2	0.65	0	1,1,1	0.20	0
4	EDO	G	307	-	3,3,3	0.42	0	2,2,2	0.61	0
6	GOL	A	308	-	5,5,5	0.59	0	5,5,5	0.38	0
3	FMT	H	302	5	2,2,2	0.69	0	1,1,1	0.25	0
3	FMT	E	303	-	2,2,2	0.73	0	1,1,1	0.25	0
4	EDO	B	307	-	3,3,3	0.45	0	2,2,2	0.34	0
7	TRS	B	310	-	7,7,7	0.55	0	9,9,9	0.37	0
4	EDO	A	306	-	3,3,3	0.41	0	2,2,2	0.46	0
4	EDO	C	307	-	3,3,3	0.45	0	2,2,2	0.27	0
2	IMD	C	301	-	5,5,5	0.66	0	5,5,5	0.43	0
4	EDO	B	309	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	E	307	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	B	308	-	3,3,3	0.43	0	2,2,2	0.47	0
4	EDO	C	309	-	3,3,3	0.43	0	2,2,2	0.37	0
7	TRS	D	311	-	7,7,7	0.56	0	9,9,9	0.41	0
2	IMD	H	301	-	5,5,5	0.66	0	5,5,5	0.42	0
4	EDO	F	307	-	3,3,3	0.42	0	2,2,2	0.36	0
3	FMT	A	302	5	2,2,2	0.68	0	1,1,1	0.25	0
4	EDO	D	308	-	3,3,3	0.42	0	2,2,2	0.59	0
4	EDO	G	305	-	3,3,3	0.42	0	2,2,2	0.34	0
7	TRS	A	309	-	7,7,7	0.56	0	9,9,9	0.45	0
4	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.28	0
4	EDO	E	308	-	3,3,3	0.44	0	2,2,2	0.27	0
2	IMD	A	301	-	5,5,5	0.65	0	5,5,5	0.53	0
2	IMD	D	302	-	5,5,5	0.66	0	5,5,5	0.44	0
2	IMD	G	301	-	5,5,5	0.68	0	5,5,5	0.41	0
4	EDO	H	308	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	E	309	-	3,3,3	0.44	0	2,2,2	0.36	0
3	FMT	F	302	5	2,2,2	0.68	0	1,1,1	0.22	0
3	FMT	C	302	5	2,2,2	0.65	0	1,1,1	0.14	0
4	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	D	301	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	F	305	-	3,3,3	0.42	0	2,2,2	0.33	0
4	EDO	D	309	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	G	306	-	3,3,3	0.44	0	2,2,2	0.39	0
7	TRS	G	308	-	7,7,7	0.53	0	9,9,9	0.31	0
4	EDO	D	310	-	3,3,3	0.42	0	2,2,2	0.25	0
4	EDO	H	307	-	3,3,3	0.42	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IMD	B	301	-	5,5,5	0.67	0	5,5,5	0.47	0
4	EDO	D	304	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	C	306	-	3,3,3	0.44	0	2,2,2	0.40	0
3	FMT	E	302	5	2,2,2	0.65	0	1,1,1	0.24	0
4	EDO	A	307	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	E	306	-	3,3,3	0.43	0	2,2,2	0.39	0
3	FMT	D	303	5	2,2,2	0.67	0	1,1,1	0.18	0
3	FMT	B	302	5	2,2,2	0.69	0	1,1,1	0.26	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	EDO	C	308	-	-	0/1/1/1	-
4	EDO	H	305	-	-	1/1/1/1	-
4	EDO	F	306	-	-	1/1/1/1	-
2	IMD	F	301	-	-	-	0/1/1/1
4	EDO	H	306	-	-	1/1/1/1	-
4	EDO	D	307	-	-	0/1/1/1	-
2	IMD	E	301	-	-	-	0/1/1/1
4	EDO	G	307	-	-	1/1/1/1	-
6	GOL	A	308	-	-	3/4/4/4	-
4	EDO	B	307	-	-	1/1/1/1	-
7	TRS	B	310	-	-	3/9/9/9	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	C	307	-	-	1/1/1/1	-
4	EDO	B	309	-	-	1/1/1/1	-
2	IMD	C	301	-	-	-	0/1/1/1
4	EDO	E	307	-	-	1/1/1/1	-
4	EDO	B	308	-	-	0/1/1/1	-
4	EDO	C	309	-	-	0/1/1/1	-
7	TRS	D	311	-	-	0/9/9/9	-
2	IMD	H	301	-	-	-	0/1/1/1
4	EDO	F	307	-	-	0/1/1/1	-
4	EDO	D	308	-	-	1/1/1/1	-
4	EDO	G	305	-	-	0/1/1/1	-
7	TRS	A	309	-	-	4/9/9/9	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	E	308	-	-	0/1/1/1	-
2	IMD	A	301	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	D	302	-	-	-	0/1/1/1
2	IMD	G	301	-	-	-	0/1/1/1
4	EDO	H	308	-	-	0/1/1/1	-
4	EDO	E	309	-	-	0/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	F	305	-	-	0/1/1/1	-
4	EDO	D	309	-	-	1/1/1/1	-
4	EDO	G	306	-	-	1/1/1/1	-
7	TRS	G	308	-	-	8/9/9/9	-
4	EDO	D	310	-	-	0/1/1/1	-
4	EDO	H	307	-	-	1/1/1/1	-
2	IMD	B	301	-	-	-	0/1/1/1
4	EDO	D	304	-	-	1/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	E	306	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	308	GOL	O2-C2-C3-O3
7	B	310	TRS	C1-C-C2-O2
7	B	310	TRS	C3-C-C2-O2
6	A	308	GOL	C1-C2-C3-O3
4	E	307	EDO	O1-C1-C2-O2
4	D	308	EDO	O1-C1-C2-O2
4	D	309	EDO	O1-C1-C2-O2
7	B	310	TRS	N-C-C2-O2
7	G	308	TRS	N-C-C1-O1
7	G	308	TRS	C1-C-C2-O2
7	G	308	TRS	C3-C-C2-O2
7	G	308	TRS	N-C-C3-O3
7	G	308	TRS	C3-C-C1-O1
7	G	308	TRS	C1-C-C3-O3
7	G	308	TRS	C2-C-C3-O3
4	B	307	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	G	308	TRS	N-C-C2-O2
6	A	308	GOL	O1-C1-C2-C3
4	G	306	EDO	O1-C1-C2-O2
4	H	306	EDO	O1-C1-C2-O2
7	A	309	TRS	C3-C-C1-O1
7	A	309	TRS	C1-C-C2-O2
4	A	306	EDO	O1-C1-C2-O2
4	B	309	EDO	O1-C1-C2-O2
4	C	306	EDO	O1-C1-C2-O2
4	C	307	EDO	O1-C1-C2-O2
4	D	304	EDO	O1-C1-C2-O2
4	F	306	EDO	O1-C1-C2-O2
4	G	307	EDO	O1-C1-C2-O2
4	H	305	EDO	O1-C1-C2-O2
4	H	307	EDO	O1-C1-C2-O2
7	A	309	TRS	N-C-C1-O1
7	A	309	TRS	N-C-C2-O2

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	307	EDO	1	0
6	A	308	GOL	1	0
4	A	306	EDO	1	0
4	C	307	EDO	1	0
4	E	307	EDO	2	0
4	C	303	EDO	1	0
4	D	309	EDO	1	0
4	G	306	EDO	1	0
4	D	310	EDO	1	0
4	H	307	EDO	1	0
2	B	301	IMD	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	185/206 (89%)	-0.28	2 (1%) 78 84	13, 24, 41, 64	2 (1%)
1	B	185/206 (89%)	-0.23	3 (1%) 70 78	20, 26, 47, 56	0
1	C	185/206 (89%)	-0.23	4 (2%) 62 71	14, 25, 45, 61	2 (1%)
1	D	185/206 (89%)	-0.22	4 (2%) 62 71	19, 26, 47, 59	1 (0%)
1	E	184/206 (89%)	-0.18	3 (1%) 70 78	19, 27, 49, 61	1 (0%)
1	F	185/206 (89%)	-0.15	4 (2%) 62 71	21, 27, 49, 65	0
1	G	185/206 (89%)	-0.22	3 (1%) 70 78	20, 27, 49, 59	0
1	H	185/206 (89%)	-0.17	4 (2%) 62 71	20, 28, 49, 64	0
All	All	1479/1648 (89%)	-0.21	27 (1%) 67 76	13, 26, 48, 65	6 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	259	THR	3.1
1	D	195	ASP	2.8
1	E	195	ASP	2.8
1	E	259	THR	2.7
1	G	77	GLY	2.6
1	C	195	ASP	2.6
1	B	83	MET	2.4
1	H	261	ARG	2.4
1	F	85	ARG	2.4
1	D	84	LYS	2.3
1	B	259	THR	2.3
1	E	77	GLY	2.3
1	H	259	THR	2.3
1	A	129[A]	HIS	2.2
1	F	195	ASP	2.2
1	H	195	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	83	MET	2.2
1	C	88	LYS	2.2
1	C	261	ARG	2.2
1	D	77	GLY	2.1
1	B	261	ARG	2.1
1	C	259	THR	2.1
1	G	259	THR	2.1
1	A	261	ARG	2.1
1	G	195	ASP	2.1
1	F	84	LYS	2.0
1	F	88	LYS	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
7	TRS	D	311	8/8	0.74	0.21	58,60,62,62	8
7	TRS	G	308	8/8	0.74	0.20	61,62,63,64	0
6	GOL	A	308	6/6	0.80	0.16	54,59,60,61	0
4	EDO	E	307	4/4	0.83	0.16	57,59,62,62	0
4	EDO	C	306	4/4	0.83	0.18	52,54,56,56	0
7	TRS	A	309	8/8	0.84	0.17	70,71,72,72	8
4	EDO	F	306	4/4	0.85	0.16	50,52,55,55	0
4	EDO	D	308	4/4	0.86	0.16	49,52,52,53	0
4	EDO	H	306	4/4	0.86	0.17	53,55,55,56	0
3	FMT	B	303	3/3	0.86	0.13	48,48,50,52	0
7	TRS	B	310	8/8	0.87	0.17	67,68,70,71	0
4	EDO	C	309	4/4	0.87	0.15	56,57,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	E	308	4/4	0.87	0.15	67,68,69,69	0
4	EDO	C	308	4/4	0.88	0.17	63,63,64,64	0
4	EDO	D	309	4/4	0.88	0.13	39,42,42,43	0
4	EDO	G	307	4/4	0.88	0.21	60,60,60,62	0
4	EDO	H	305	4/4	0.88	0.14	46,48,51,53	0
4	EDO	A	307	4/4	0.88	0.15	61,63,64,66	0
4	EDO	A	306	4/4	0.89	0.15	47,48,49,50	0
4	EDO	G	306	4/4	0.89	0.15	56,61,64,66	0
4	EDO	C	307	4/4	0.91	0.12	38,42,46,48	0
4	EDO	D	310	4/4	0.91	0.12	53,55,57,59	0
4	EDO	F	307	4/4	0.91	0.16	45,48,53,55	0
4	EDO	B	308	4/4	0.91	0.12	48,50,51,51	0
4	EDO	H	308	4/4	0.92	0.11	61,63,63,64	0
2	IMD	B	301	5/5	0.92	0.12	50,52,54,54	0
4	EDO	D	304	4/4	0.92	0.14	58,58,58,60	0
2	IMD	H	301	5/5	0.92	0.14	58,58,60,61	0
4	EDO	F	305	4/4	0.92	0.12	42,43,45,45	0
4	EDO	B	309	4/4	0.92	0.11	38,42,44,44	0
4	EDO	E	306	4/4	0.93	0.12	47,51,52,53	0
2	IMD	A	301	5/5	0.93	0.10	36,37,39,40	0
2	IMD	D	302	5/5	0.93	0.12	55,55,56,56	0
4	EDO	H	307	4/4	0.93	0.10	39,40,42,43	0
4	EDO	E	309	4/4	0.93	0.13	45,49,52,53	0
4	EDO	D	307	4/4	0.93	0.11	60,62,63,65	0
2	IMD	E	301	5/5	0.93	0.12	55,56,57,58	0
2	IMD	F	301	5/5	0.93	0.13	56,57,57,57	0
4	EDO	G	305	4/4	0.93	0.12	42,45,46,46	0
4	EDO	B	307	4/4	0.93	0.12	53,54,55,56	0
4	EDO	C	303	4/4	0.94	0.12	51,55,59,60	0
3	FMT	B	306	3/3	0.94	0.15	55,55,56,57	0
3	FMT	E	303	3/3	0.94	0.10	50,50,53,56	0
4	EDO	A	303	4/4	0.94	0.12	48,51,53,54	0
2	IMD	G	301	5/5	0.94	0.12	60,61,61,61	0
4	EDO	D	301	4/4	0.94	0.10	43,43,47,48	0
8	CL	A	310	1/1	0.94	0.11	79,79,79,79	0
2	IMD	C	301	5/5	0.95	0.10	48,48,49,49	0
9	NA	A	311	1/1	0.96	0.14	40,40,40,40	0
8	CL	C	310	1/1	0.97	0.10	70,70,70,70	0
3	FMT	G	302	3/3	0.98	0.09	25,25,26,27	0
9	NA	B	311	1/1	0.98	0.17	37,37,37,37	0
3	FMT	C	302	3/3	0.99	0.04	23,23,23,24	0
3	FMT	H	302	3/3	0.99	0.03	26,26,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMT	D	303	3/3	0.99	0.03	24,24,24,25	0
3	FMT	E	302	3/3	0.99	0.04	25,25,26,26	0
3	FMT	B	302	3/3	0.99	0.05	22,22,23,23	0
3	FMT	F	302	3/3	0.99	0.06	25,25,25,27	0
5	MN	E	304	1/1	1.00	0.01	22,22,22,22	0
5	MN	E	305	1/1	1.00	0.01	22,22,22,22	0
5	MN	F	303	1/1	1.00	0.01	22,22,22,22	0
5	MN	F	304	1/1	1.00	0.02	25,25,25,25	0
5	MN	G	303	1/1	1.00	0.02	24,24,24,24	0
5	MN	G	304	1/1	1.00	0.01	22,22,22,22	0
5	MN	H	303	1/1	1.00	0.01	22,22,22,22	0
5	MN	H	304	1/1	1.00	0.01	23,23,23,23	0
3	FMT	A	302	3/3	1.00	0.02	23,23,23,23	0
5	MN	A	304	1/1	1.00	0.01	20,20,20,20	0
5	MN	A	305	1/1	1.00	0.01	21,21,21,21	0
5	MN	B	304	1/1	1.00	0.01	20,20,20,20	0
5	MN	B	305	1/1	1.00	0.02	24,24,24,24	0
5	MN	C	304	1/1	1.00	0.01	23,23,23,23	0
5	MN	C	305	1/1	1.00	0.02	20,20,20,20	0
5	MN	D	305	1/1	1.00	0.03	22,22,22,22	0
5	MN	D	306	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.