



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:26 AM UTC

PDB ID : 3QPE / pdb_00003qpe
Title : Crystal structure of Galacturonate Dehydratase from GEOBACILLUS SP.
complexed with D-Galacturonate and 5-keto-4-deoxy-D-Galacturonate
Authors : Fedorov, A.A.; Fedorov, E.V.; Mills-Groninger, F.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2011-02-12
Resolution : 1.80 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

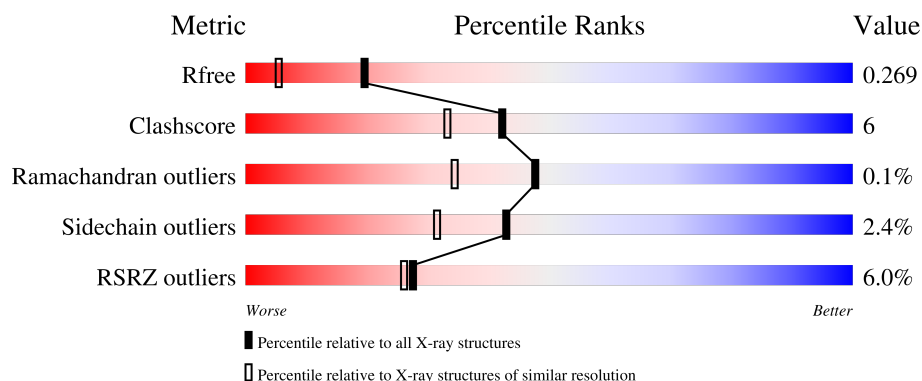
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	392	4% 86% 11% ..
1	B	392	11% 79% 15% 5%
1	C	392	6% 82% 13% ..
1	D	392	3% 87% 10% ..

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	GOL	C	395	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12829 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	2	0
			3053	1930	536	577	10			
1	B	371	Total	C	N	O	S	0	0	0
			2936	1860	512	554	10			
1	C	376	Total	C	N	O	S	0	2	0
			2989	1892	520	567	10			
1	D	385	Total	C	N	O	S	0	0	0
			3033	1919	531	573	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP D3EID5
A	2	SER	-	expression tag	UNP D3EID5
A	3	LEU	-	expression tag	UNP D3EID5
A	385	GLU	-	expression tag	UNP D3EID5
A	386	GLY	-	expression tag	UNP D3EID5
A	387	HIS	-	expression tag	UNP D3EID5
A	388	HIS	-	expression tag	UNP D3EID5
A	389	HIS	-	expression tag	UNP D3EID5
A	390	HIS	-	expression tag	UNP D3EID5
A	391	HIS	-	expression tag	UNP D3EID5
A	392	HIS	-	expression tag	UNP D3EID5
B	1	MET	-	expression tag	UNP D3EID5
B	2	SER	-	expression tag	UNP D3EID5
B	3	LEU	-	expression tag	UNP D3EID5
B	385	GLU	-	expression tag	UNP D3EID5
B	386	GLY	-	expression tag	UNP D3EID5
B	387	HIS	-	expression tag	UNP D3EID5
B	388	HIS	-	expression tag	UNP D3EID5
B	389	HIS	-	expression tag	UNP D3EID5
B	390	HIS	-	expression tag	UNP D3EID5
B	391	HIS	-	expression tag	UNP D3EID5

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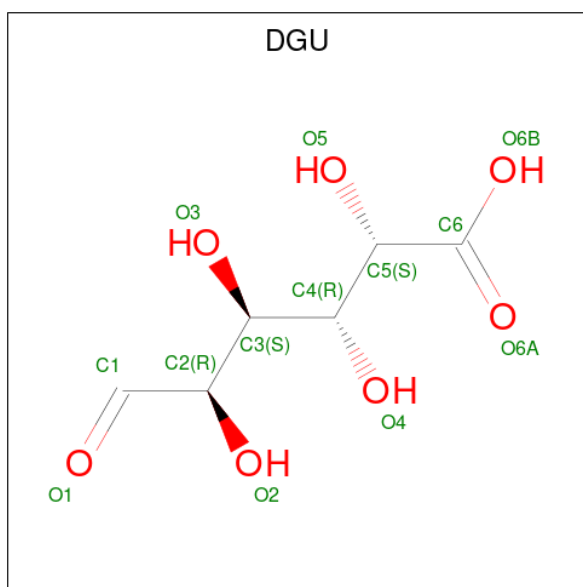
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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP D3EID5
C	1	MET	-	expression tag	UNP D3EID5
C	2	SER	-	expression tag	UNP D3EID5
C	3	LEU	-	expression tag	UNP D3EID5
C	385	GLU	-	expression tag	UNP D3EID5
C	386	GLY	-	expression tag	UNP D3EID5
C	387	HIS	-	expression tag	UNP D3EID5
C	388	HIS	-	expression tag	UNP D3EID5
C	389	HIS	-	expression tag	UNP D3EID5
C	390	HIS	-	expression tag	UNP D3EID5
C	391	HIS	-	expression tag	UNP D3EID5
C	392	HIS	-	expression tag	UNP D3EID5
D	1	MET	-	expression tag	UNP D3EID5
D	2	SER	-	expression tag	UNP D3EID5
D	3	LEU	-	expression tag	UNP D3EID5
D	385	GLU	-	expression tag	UNP D3EID5
D	386	GLY	-	expression tag	UNP D3EID5
D	387	HIS	-	expression tag	UNP D3EID5
D	388	HIS	-	expression tag	UNP D3EID5
D	389	HIS	-	expression tag	UNP D3EID5
D	390	HIS	-	expression tag	UNP D3EID5
D	391	HIS	-	expression tag	UNP D3EID5
D	392	HIS	-	expression tag	UNP D3EID5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

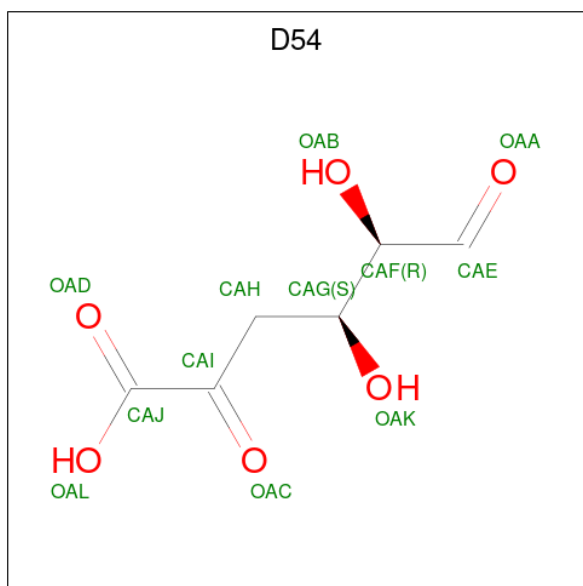
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is D-galacturonic acid (CCD ID: DGU) (formula: C₆H₁₀O₇).



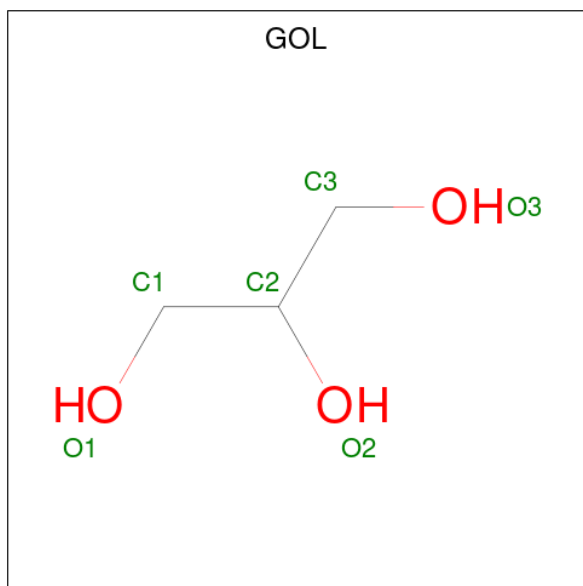
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 4-deoxy-L-threo-hex-5-ulosuronic acid (CCD ID: D54) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

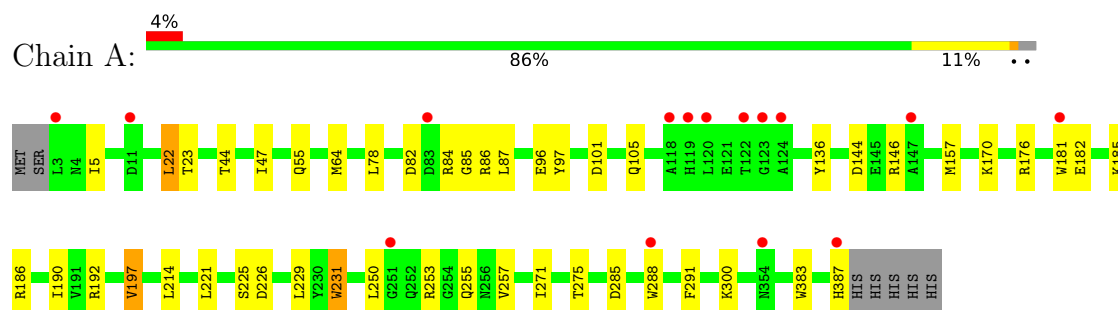
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	249	Total	O	0	0
			249	249		
6	B	129	Total	O	0	0
			129	129		
6	C	145	Total	O	0	0
			145	145		
6	D	232	Total	O	0	0
			232	232		

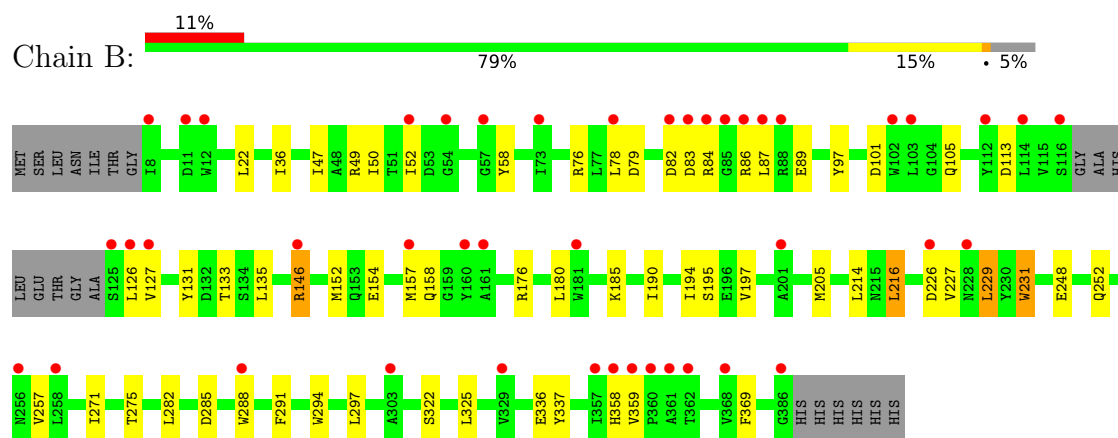
3 Residue-property plots [i](#)

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.

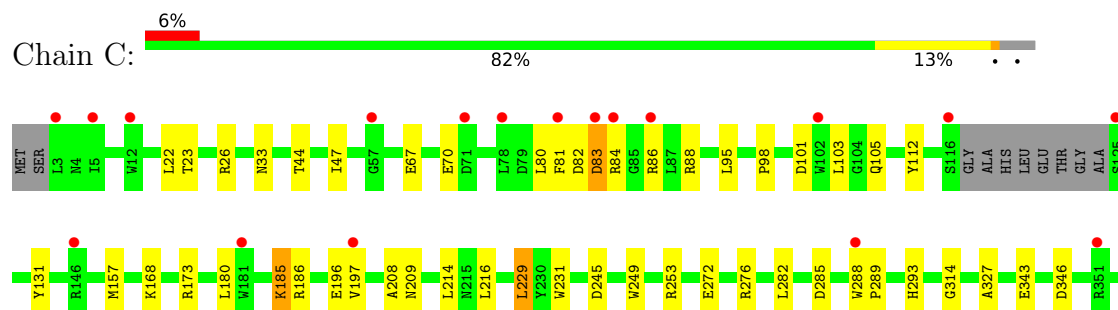
- Molecule 1: Mandelate racemase/muconate lactonizing protein

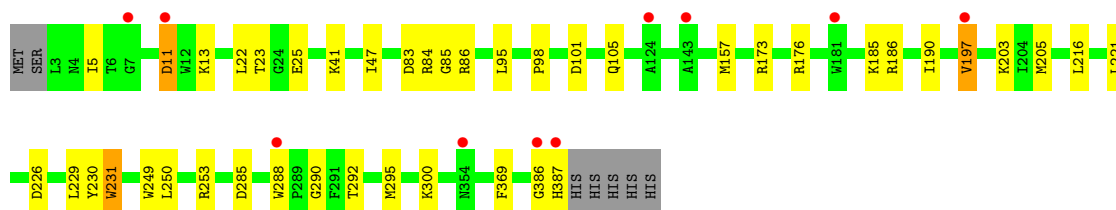


- Molecule 1: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.02Å 66.27Å 154.61Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	39.03 – 1.80 39.03 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.03-1.80) 99.4 (39.03-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.79Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.221 , 0.270 0.221 , 0.269	Depositor DCC
R_{free} test set	7389 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtrriage
Anisotropy	0.507	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12829	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.84 % 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 2.9428e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D54, MG, GOL, DGU

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	0.48	0/3124	0.77	1/4234 (0.0%)
1	B	0.39	0/3004	0.77	2/4070 (0.0%)
1	C	0.42	0/3057	0.77	0/4142
1	D	0.47	0/3104	0.79	1/4208 (0.0%)
All	All	0.44	0/12289	0.78	4/16654 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	N-CA-C	-6.80	105.06	113.15
1	B	36	ILE	N-CA-C	5.42	115.14	108.53
1	D	290	GLY	N-CA-C	5.10	119.31	112.17
1	A	231	TRP	N-CA-C	5.02	116.70	109.07

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	3053	0	2942	26	0
1	B	2936	0	2832	42	0
1	C	2989	0	2880	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3033	0	2925	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	13	0	0	1	0
4	B	12	0	7	0	0
4	C	12	0	7	1	0
4	D	12	0	7	0	0
5	C	6	0	8	4	0
6	A	249	0	0	3	0
6	B	129	0	0	0	0
6	C	145	0	0	0	0
6	D	232	0	0	1	0
All	All	12829	0	11608	148	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 6.

All (148) 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:26:ARG:HH22	5:C:395:GOL:H12	1.16	1.09
1:D:22:LEU:HD22	1:D:47:ILE:HD12	1.47	0.94
1:C:26:ARG:HH22	5:C:395:GOL:C1	1.83	0.91
1:B:22:LEU:HD22	1:B:47:ILE:HD12	1.58	0.85
1:B:82:ASP:HB2	1:B:86:ARG:H	1.40	0.84
1:C:26:ARG:NH2	5:C:395:GOL:H12	1.95	0.81
1:C:22:LEU:HD22	1:C:47:ILE:HD12	1.61	0.80
1:A:84:ARG:HD3	1:A:86:ARG:HH21	1.49	0.78
1:D:84:ARG:HD3	1:D:86:ARG:HH21	1.50	0.76
1:A:157:MET:SD	1:A:197:VAL:HG13	2.30	0.71
1:D:5:ILE:HD13	1:D:85:GLY:HA2	1.74	0.69
1:D:22:LEU:HD22	1:D:47:ILE:CD1	2.24	0.68
1:C:82:ASP:C	1:C:84:ARG:H	2.02	0.68
1:A:5:ILE:HD13	1:A:85:GLY:HA2	1.76	0.67
1:D:292:THR:HA	1:D:295:MET:HE2	1.77	0.67
1:D:157:MET:SD	1:D:197:VAL:HG13	2.37	0.64
1:B:101:ASP:O	1:B:105:GLN:HG2	1.97	0.63
1:D:173:ARG:HD3	1:D:186:ARG:HG2	1.81	0.63
1:B:82:ASP:C	1:B:84:ARG:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:HD3	1:B:86:ARG:HH21	1.65	0.62
1:D:47:ILE:HD13	1:D:369:PHE:CE1	2.35	0.61
1:B:127:VAL:HG22	1:B:358:HIS:CD2	2.35	0.61
1:C:84:ARG:HD3	1:C:86:ARG:HH21	1.66	0.61
1:B:82:ASP:HB3	1:B:84:ARG:H	1.65	0.61
1:B:285:ASP:HB3	1:B:288:TRP:O	2.01	0.60
1:D:47:ILE:CD1	1:D:369:PHE:CE1	2.85	0.60
1:D:221:LEU:HD13	1:D:250:LEU:HD21	1.83	0.60
1:D:84:ARG:HD3	1:D:86:ARG:NH2	2.17	0.59
1:C:214:LEU:HD23	1:D:176:ARG:HG3	1.84	0.59
1:B:135:LEU:HD13	1:B:194:ILE:HD13	1.86	0.58
1:C:285:ASP:HB3	1:C:288:TRP:O	2.04	0.57
1:C:101:ASP:O	1:C:105:GLN:HG2	2.04	0.57
1:C:249:TRP:O	1:C:253:ARG:HG3	2.04	0.57
1:D:386:GLY:C	1:D:387:HIS:CG	2.82	0.57
1:A:55:GLN:HB2	6:A:592:HOH:O	2.05	0.56
1:D:25:GLU:OE1	1:D:41:LYS:HE3	2.06	0.55
1:B:146:ARG:HH11	1:B:146:ARG:HB2	1.71	0.55
1:C:47:ILE:CD1	1:C:369:PHE:CE1	2.90	0.55
1:A:176:ARG:HG3	1:B:214:LEU:HD23	1.88	0.55
1:D:249:TRP:CZ2	1:D:253:ARG:HD2	2.42	0.54
1:A:185:LYS:HE3	6:A:517:HOH:O	2.07	0.54
3:A:401:DGU:C1	3:A:401:DGU:O4	2.56	0.54
1:C:157:MET:SD	1:C:197:VAL:HG13	2.47	0.54
1:A:181:TRP:CH2	1:A:185:LYS:HD3	2.43	0.54
1:C:173:ARG:HD3	1:C:186:ARG:HG2	1.89	0.54
1:A:23:THR:HG22	1:A:44:THR:HG22	1.90	0.53
1:B:195:SER:HB2	1:B:227:VAL:HG13	1.91	0.53
1:A:253:ARG:HG3	6:A:492:HOH:O	2.08	0.52
1:B:47:ILE:HD13	1:B:369:PHE:CE1	2.44	0.52
1:B:282:LEU:HD22	1:B:282:LEU:N	2.24	0.52
1:B:76:ARG:HB2	1:B:79:ASP:OD2	2.11	0.51
1:C:84:ARG:CD	1:C:86:ARG:HH21	2.23	0.51
1:C:23:THR:HG22	1:C:44:THR:HG22	1.92	0.51
1:C:84:ARG:HD3	1:C:86:ARG:NH2	2.24	0.51
1:D:47:ILE:CD1	1:D:369:PHE:HE1	2.24	0.50
1:D:249:TRP:O	1:D:253:ARG:HG3	2.11	0.50
1:C:82:ASP:C	1:C:84:ARG:N	2.69	0.50
1:A:101:ASP:O	1:A:105:GLN:HG2	2.12	0.50
1:C:82:ASP:OD2	1:C:86:ARG:HB2	2.11	0.50
1:D:95:LEU:C	1:D:98:PRO:HD2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ASP:HB3	1:D:288:TRP:O	2.11	0.50
1:B:82:ASP:OD2	1:B:86:ARG:HB2	2.12	0.50
1:B:84:ARG:CD	1:B:86:ARG:HH21	2.24	0.49
1:A:285:ASP:HB3	1:A:288:TRP:O	2.12	0.49
1:D:288:TRP:O	1:D:288:TRP:CE3	2.66	0.49
1:C:81:PHE:HZ	1:C:103:LEU:HD11	1.77	0.49
1:C:180:LEU:HD22	1:D:216:LEU:HG	1.94	0.49
1:B:231:TRP:CD1	1:B:231:TRP:C	2.91	0.49
4:C:401:D54:HAE	4:C:401:D54:HAH	1.57	0.48
1:C:314:GLY:HA2	5:C:395:GOL:H11	1.95	0.48
1:B:205:MET:HG2	1:B:231:TRP:CG	2.49	0.48
1:C:84:ARG:NE	1:C:86:ARG:HH21	2.12	0.48
1:C:289:PRO:HB2	1:C:293:HIS:CG	2.49	0.48
1:D:5:ILE:CD1	1:D:85:GLY:HA2	2.44	0.48
1:C:82:ASP:O	1:C:84:ARG:N	2.43	0.47
1:C:81:PHE:CZ	1:C:103:LEU:HD11	2.49	0.47
1:C:370:ASP:HB3	1:C:373:LEU:HB3	1.94	0.47
1:B:248:GLU:O	1:B:252:GLN:HG2	2.15	0.47
1:C:272[A]:GLU:HG2	1:C:276:ARG:NH1	2.29	0.47
1:C:95:LEU:C	1:C:98:PRO:HD2	2.39	0.47
1:B:22:LEU:HD22	1:B:47:ILE:CD1	2.36	0.47
1:B:146:ARG:HB2	1:B:146:ARG:NH1	2.30	0.47
1:B:205:MET:HG2	1:B:231:TRP:CD2	2.49	0.47
1:B:50:ILE:HD13	1:B:52:ILE:HD11	1.97	0.47
1:A:22:LEU:HD22	1:A:47:ILE:HG13	1.97	0.47
1:B:82:ASP:C	1:B:84:ARG:N	2.72	0.47
1:B:157:MET:SD	1:B:197:VAL:HG13	2.55	0.46
1:D:205:MET:HG2	1:D:231:TRP:CG	2.51	0.46
1:A:181:TRP:CE3	1:A:182[A]:GLU:HG3	2.50	0.46
1:C:33:ASN:OD1	1:C:33:ASN:C	2.58	0.46
1:A:186:ARG:O	1:A:190:ILE:HG12	2.15	0.46
1:B:271:ILE:O	1:B:275:THR:HG23	2.16	0.45
1:C:180:LEU:HD11	1:C:216:LEU:HD11	1.99	0.45
1:B:49:ARG:HD3	1:B:58:TYR:CZ	2.52	0.45
1:C:249:TRP:CE2	1:C:253:ARG:HD2	2.52	0.45
1:D:186:ARG:O	1:D:190:ILE:HG12	2.16	0.45
1:B:229:LEU:HB3	1:B:257:VAL:HG22	1.99	0.45
1:C:249:TRP:CZ2	1:C:253:ARG:HD2	2.52	0.45
1:D:47:ILE:HD11	1:D:369:PHE:HE1	1.82	0.44
1:D:203:LYS:HD3	1:D:230:TYR:CD1	2.52	0.44
1:A:214:LEU:HD23	1:B:176:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LYS:HE2	1:D:185:LYS:HB3	1.41	0.44
1:A:82:ASP:OD2	1:A:86:ARG:HB2	2.18	0.44
1:A:97:TYR:CZ	1:A:291:PHE:HB2	2.52	0.44
1:D:47:ILE:HD11	1:D:369:PHE:CE1	2.53	0.44
1:A:221:LEU:HD13	1:A:250:LEU:HD21	2.00	0.44
1:D:249:TRP:CE2	1:D:253:ARG:HD2	2.53	0.44
1:A:64:MET:HE3	1:A:383:TRP:CH2	2.52	0.44
1:B:154:GLU:O	1:B:158:GLN:HG3	2.19	0.43
1:D:11:ASP:O	1:D:13:LYS:HG3	2.18	0.43
1:D:23:THR:HG23	6:D:477:HOH:O	2.18	0.43
1:A:181:TRP:HE3	1:A:182[A]:GLU:HG3	1.83	0.43
1:C:112:TYR:HB2	1:C:327:ALA:CB	2.49	0.43
1:C:272[A]:GLU:CG	1:C:276:ARG:HH12	2.32	0.43
1:D:101:ASP:O	1:D:105:GLN:HG2	2.19	0.43
1:D:226:ASP:OD1	1:D:226:ASP:N	2.44	0.43
1:C:245:ASP:OD1	1:C:245:ASP:C	2.61	0.43
1:B:205:MET:HG2	1:B:231:TRP:CD1	2.54	0.43
1:B:294:TRP:CZ3	1:B:297:LEU:HD23	2.54	0.43
1:C:47:ILE:HD13	1:C:369:PHE:CE1	2.54	0.43
1:C:346:ASP:OD1	1:C:346:ASP:C	2.62	0.43
1:B:282:LEU:N	1:B:282:LEU:CD2	2.83	0.42
1:D:231:TRP:C	1:D:231:TRP:CD1	2.98	0.42
1:C:70:GLU:HG2	1:C:385:GLU:OE1	2.18	0.42
1:B:180:LEU:HD11	1:B:216:LEU:HD11	2.02	0.42
1:C:80:LEU:O	1:C:88:ARG:HG3	2.19	0.42
1:A:255:GLN:HG2	1:A:257:VAL:HG23	2.00	0.42
1:C:282:LEU:N	1:C:282:LEU:HD22	2.35	0.42
1:A:144:ASP:OD1	1:A:146:ARG:HB2	2.19	0.42
1:B:131:TYR:CE1	1:B:336:GLU:HG3	2.55	0.42
1:B:133:THR:HG22	1:B:337:TYR:O	2.20	0.42
1:A:136:TYR:CZ	1:A:170:LYS:HE2	2.55	0.42
1:C:67:GLU:O	1:C:70:GLU:HB2	2.20	0.41
1:C:229:LEU:HD12	1:C:229:LEU:HA	1.89	0.41
1:B:152:MET:HG3	1:B:190:ILE:HD12	2.03	0.41
1:C:22:LEU:CD2	1:C:47:ILE:HD12	2.43	0.41
1:C:185:LYS:HB3	1:C:185:LYS:HE2	1.85	0.41
1:B:97:TYR:CZ	1:B:291:PHE:HB2	2.56	0.41
1:B:322:SER:O	1:B:325:LEU:HB3	2.20	0.41
1:B:205:MET:HG2	1:B:231:TRP:CE2	2.56	0.41
1:C:131:TYR:CE1	1:C:168:LYS:HE2	2.55	0.41
1:C:208:ALA:O	1:C:209:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:MET:SD	1:D:197:VAL:CG1	3.07	0.40
1:A:87:LEU:CD2	1:A:96:GLU:HA	2.51	0.40
1:A:271:ILE:O	1:A:275:THR:HG23	2.21	0.40
1:B:126:LEU:HB3	1:B:359:VAL:HB	2.03	0.40
1:A:192[B]:ARG:NH2	1:A:226:ASP:OD1	2.55	0.40
1:C:23:THR:O	1:C:343:GLU:HG2	2.21	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	385/392 (98%)	381 (99%)	4 (1%)	0	100	100
1	B	367/392 (94%)	355 (97%)	12 (3%)	0	100	100
1	C	374/392 (95%)	366 (98%)	7 (2%)	1 (0%)	36	25
1	D	383/392 (98%)	376 (98%)	7 (2%)	0	100	100
All	All	1509/1568 (96%)	1478 (98%)	30 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	83	ASP

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	311/316 (98%)	303 (97%)	8 (3%)	40	28
1	B	300/316 (95%)	290 (97%)	10 (3%)	33	21
1	C	306/316 (97%)	301 (98%)	5 (2%)	55	47
1	D	309/316 (98%)	303 (98%)	6 (2%)	50	41
All	All	1226/1264 (97%)	1197 (98%)	29 (2%)	43	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	78	LEU
1	A	197	VAL
1	A	225	SER
1	A	229	LEU
1	A	231	TRP
1	A	300	LYS
1	A	387	HIS
1	B	78	LEU
1	B	87	LEU
1	B	89	GLU
1	B	113	ASP
1	B	146	ARG
1	B	185	LYS
1	B	216	LEU
1	B	226	ASP
1	B	229	LEU
1	B	231	TRP
1	C	83	ASP
1	C	185	LYS
1	C	196	GLU
1	C	229	LEU
1	C	231	TRP
1	D	11	ASP
1	D	83	ASP
1	D	197	VAL
1	D	229	LEU
1	D	231	TRP
1	D	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	B	177	HIS
1	B	293	HIS
1	B	358	HIS
1	C	209	ASN
1	D	105	GLN
1	D	209	ASN

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 ⓘ

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
5	GOL	C	395	-	5,5,5	0.34	0	5,5,5	0.31	0
4	D54	D	401	2	9,11,11	1.41	2 (22%)	9,14,14	1.65	2 (22%)
4	D54	B	401	2	9,11,11	1.08	0	9,14,14	1.23	1 (11%)
4	D54	C	401	2	9,11,11	1.21	1 (11%)	9,14,14	1.45	1 (11%)
3	DGU	A	401	2	11,12,12	0.99	0	14,16,16	0.94	1 (7%)

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
5	GOL	C	395	-	-	4/4/4/4	-
4	D54	D	401	2	-	1/13/14/14	-
4	D54	B	401	2	-	4/13/14/14	-
4	D54	C	401	2	-	3/13/14/14	-
3	DGU	A	401	2	-	5/17/18/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	D54	CAH-CAI	2.25	1.55	1.51
4	D	401	D54	CAI-CAJ	2.15	1.56	1.53
4	C	401	D54	OAD-CAJ	2.07	1.27	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	D54	OAD-CAJ-CAI	-3.69	117.22	121.81
4	D	401	D54	OAD-CAJ-CAI	-2.98	118.10	121.81
4	D	401	D54	CAH-CAI-CAJ	2.56	120.46	115.89
4	B	401	D54	OAD-CAJ-CAI	-2.53	118.67	121.81
3	A	401	DGU	O6A-C6-C5	-2.05	116.16	121.62

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	DGU	O1-C1-C2-C3
4	B	401	D54	OAA-CAE-CAF-CAG
4	B	401	D54	OAB-CAF-CAG-CAH
4	B	401	D54	CAE-CAF-CAG-CAH
4	C	401	D54	OAA-CAE-CAF-CAG
4	C	401	D54	OAB-CAF-CAG-CAH
3	A	401	DGU	C4-C5-C6-O6B
3	A	401	DGU	C4-C5-C6-O6A
3	A	401	DGU	O5-C5-C6-O6A
5	C	395	GOL	O1-C1-C2-C3
5	C	395	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	395	GOL	O2-C2-C3-O3
3	A	401	DGU	O5-C5-C6-O6B
5	C	395	GOL	O1-C1-C2-O2
4	D	401	D54	OAB-CAF-CAG-CAH
4	B	401	D54	CAG-CAH-CAI-CAJ
4	C	401	D54	CAE-CAF-CAG-CAH

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	395	GOL	4	0
4	C	401	D54	1	0
3	A	401	DGU	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	385/392 (98%)	0.28	15 (3%) 43 43	14, 25, 41, 69	2 (0%)
1	B	371/392 (94%)	1.00	44 (11%) 9 7	23, 37, 56, 92	0
1	C	376/392 (95%)	0.69	22 (5%) 28 27	15, 33, 52, 77	2 (0%)
1	D	385/392 (98%)	0.28	10 (2%) 57 57	19, 27, 43, 63	0
All	All	1517/1568 (96%)	0.56	91 (5%) 27 26	14, 30, 52, 92	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	ALA	5.4
1	C	288	TRP	4.5
1	D	387	HIS	4.2
1	B	102	TRP	4.1
1	B	8	ILE	4.0
1	A	181	TRP	3.9
1	B	288	TRP	3.8
1	C	3	LEU	3.7
1	B	12	TRP	3.7
1	A	387	HIS	3.6
1	B	73	ILE	3.5
1	B	146	ARG	3.4
1	B	85	GLY	3.4
1	A	122	THR	3.2
1	C	181	TRP	3.2
1	C	197	VAL	3.2
1	B	86	ARG	3.2
1	A	120	LEU	3.1
1	B	362	THR	3.1
1	B	54	GLY	3.1
1	B	228	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	124	ALA	3.0
1	B	127	VAL	3.0
1	C	383	TRP	3.0
1	B	303	ALA	3.0
1	B	361	ALA	2.9
1	C	386	GLY	2.9
1	D	386	GLY	2.9
1	A	123	GLY	2.8
1	B	226	ASP	2.8
1	B	112	TYR	2.8
1	B	52	ILE	2.8
1	D	288	TRP	2.8
1	C	86	ARG	2.8
1	B	57	GLY	2.8
1	B	82	ASP	2.7
1	B	78	LEU	2.7
1	A	11	ASP	2.7
1	A	288	TRP	2.6
1	C	83	ASP	2.6
1	B	126	LEU	2.5
1	A	118	ALA	2.5
1	B	258	LEU	2.5
1	B	125	SER	2.5
1	B	359	VAL	2.5
1	B	386	GLY	2.5
1	C	5	ILE	2.5
1	C	378	ILE	2.5
1	D	181	TRP	2.4
1	B	87	LEU	2.4
1	C	351	ARG	2.4
1	C	12	TRP	2.4
1	B	160	TYR	2.4
1	B	11	ASP	2.4
1	B	368	VAL	2.4
1	A	147	ALA	2.3
1	B	83	ASP	2.3
1	B	357	ILE	2.3
1	A	3	LEU	2.3
1	B	114	LEU	2.3
1	C	81	PHE	2.3
1	B	329	VAL	2.3
1	D	143	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	379	ASN	2.3
1	B	157	MET	2.3
1	A	83	ASP	2.2
1	B	256	ASN	2.2
1	B	116	SER	2.2
1	B	161	ALA	2.2
1	B	103	LEU	2.2
1	A	119	HIS	2.2
1	B	360	PRO	2.2
1	B	201	ALA	2.1
1	B	84	ARG	2.1
1	C	84	ARG	2.1
1	A	251	GLY	2.1
1	C	57	GLY	2.1
1	A	354	ASN	2.1
1	D	354	ASN	2.1
1	C	78	LEU	2.1
1	C	116	SER	2.1
1	C	125	SER	2.1
1	B	88	ARG	2.1
1	D	7	GLY	2.1
1	C	102	TRP	2.1
1	D	11	ASP	2.0
1	C	146	ARG	2.0
1	B	181	TRP	2.0
1	C	71	ASP	2.0
1	D	197	VAL	2.0
1	B	358	HIS	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
5	GOL	C	395	6/6	0.79	0.14	25,40,42,45	0
4	D54	C	401	12/12	0.83	0.14	23,33,40,47	0
4	D54	D	401	12/12	0.84	0.13	25,32,42,42	0
4	D54	B	401	12/12	0.87	0.11	26,33,38,43	0
3	DGU	A	401	13/13	0.89	0.10	20,29,38,44	0
2	MG	A	393	1/1	0.94	0.07	26,26,26,26	0
2	MG	B	394	1/1	0.95	0.10	26,26,26,26	0
2	MG	B	393	1/1	0.96	0.12	29,29,29,29	0
2	MG	C	393	1/1	0.98	0.06	22,22,22,22	0
2	MG	C	394	1/1	0.98	0.10	27,27,27,27	0
2	MG	D	394	1/1	0.98	0.05	25,25,25,25	0
2	MG	A	394	1/1	0.98	0.06	23,23,23,23	0
2	MG	D	393	1/1	0.99	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.