Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 01:14 PM EDT

PDB ID	:	4K2S
Title	:	Crystal structure of the mutant P317A of d-mannonate dehydratase from chromohalobacter salexigens complexed with mg and d-gluconate
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.
Deposited on	:	2013-04-09
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

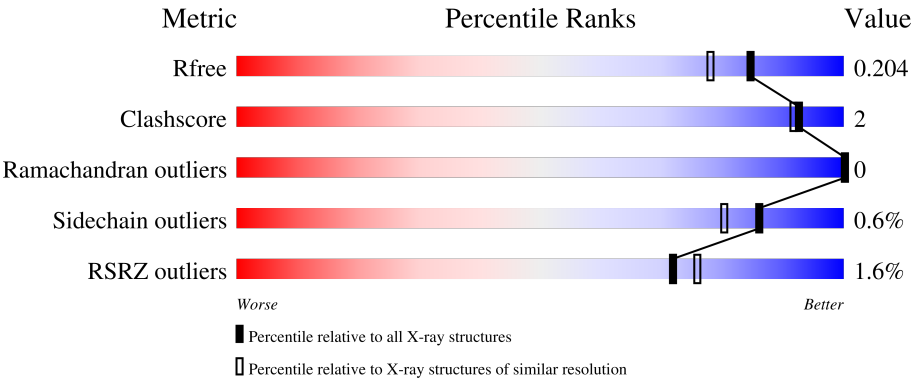
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	405	93%
1	B	405	94%
1	C	405	3% 91% 6%
1	D	405	93%
1	E	405	92%

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Mol	Chain	Length	Quality of chain
1	F	405	93%
1	G	405	2% 91% 6%
1	H	405	2% 94%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28312 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 D-mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	3	0
			3137	1985	563	575	14			
1	B	390	Total	C	N	O	S	0	4	0
			3126	1979	565	568	14			
1	C	393	Total	C	N	O	S	0	2	0
			3122	1977	558	573	14			
1	D	391	Total	C	N	O	S	0	4	0
			3134	1984	562	573	15			
1	E	391	Total	C	N	O	S	0	1	0
			3106	1968	556	568	14			
1	F	390	Total	C	N	O	S	0	5	0
			3132	1984	563	570	15			
1	G	392	Total	C	N	O	S	0	4	0
			3137	1987	562	573	15			
1	H	396	Total	C	N	O	S	0	2	0
			3145	1992	561	578	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q1QT89
A	2	SER	-	expression tag	UNP Q1QT89
A	3	LEU	-	expression tag	UNP Q1QT89
A	317	ALA	PRO	engineered mutation	UNP Q1QT89
B	1	MET	-	initiating methionine	UNP Q1QT89
B	2	SER	-	expression tag	UNP Q1QT89
B	3	LEU	-	expression tag	UNP Q1QT89
B	317	ALA	PRO	engineered mutation	UNP Q1QT89
C	1	MET	-	initiating methionine	UNP Q1QT89
C	2	SER	-	expression tag	UNP Q1QT89
C	3	LEU	-	expression tag	UNP Q1QT89
C	317	ALA	PRO	engineered mutation	UNP Q1QT89
D	1	MET	-	initiating methionine	UNP Q1QT89

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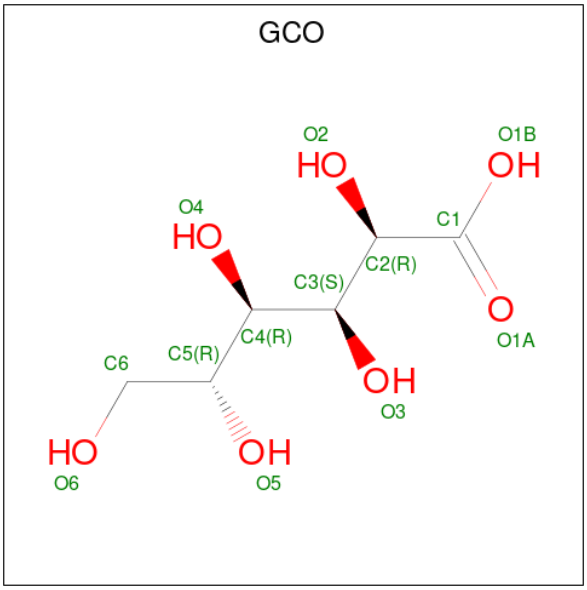
Chain	Residue	Modelled	Actual	Comment	Reference
D	2	SER	-	expression tag	UNP Q1QT89
D	3	LEU	-	expression tag	UNP Q1QT89
D	317	ALA	PRO	engineered mutation	UNP Q1QT89
E	1	MET	-	initiating methionine	UNP Q1QT89
E	2	SER	-	expression tag	UNP Q1QT89
E	3	LEU	-	expression tag	UNP Q1QT89
E	317	ALA	PRO	engineered mutation	UNP Q1QT89
F	1	MET	-	initiating methionine	UNP Q1QT89
F	2	SER	-	expression tag	UNP Q1QT89
F	3	LEU	-	expression tag	UNP Q1QT89
F	317	ALA	PRO	engineered mutation	UNP Q1QT89
G	1	MET	-	initiating methionine	UNP Q1QT89
G	2	SER	-	expression tag	UNP Q1QT89
G	3	LEU	-	expression tag	UNP Q1QT89
G	317	ALA	PRO	engineered mutation	UNP Q1QT89
H	1	MET	-	initiating methionine	UNP Q1QT89
H	2	SER	-	expression tag	UNP Q1QT89
H	3	LEU	-	expression tag	UNP Q1QT89
H	317	ALA	PRO	engineered mutation	UNP Q1QT89

- Molecule 2 is D-gluconic acid (three-letter code: GCO) (formula: $C_6H_{12}O_7$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	2	Total Cl 2 2	0	0

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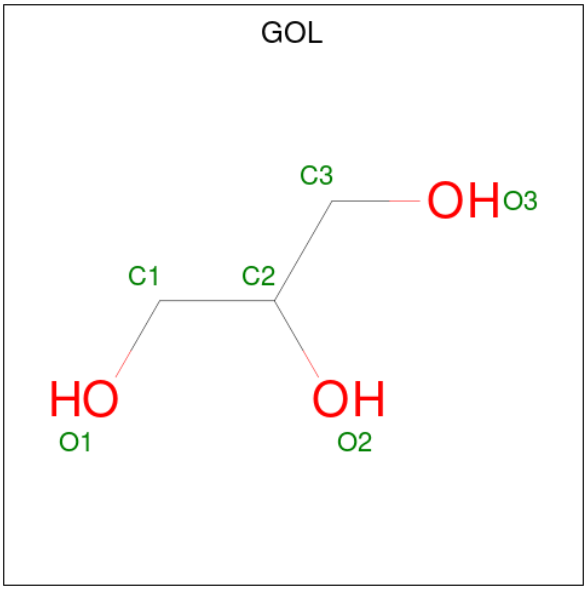
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total Cl 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	393	Total O 394 394	0	1
6	B	417	Total O 419 419	0	2
6	C	368	Total O 370 370	0	2
6	D	378	Total O 378 378	0	0
6	E	402	Total O 403 403	0	1
6	F	400	Total O 402 402	0	2
6	G	392	Total O 395 395	0	3

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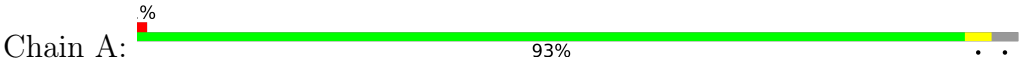
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	383	Total 383	O 383	0	0

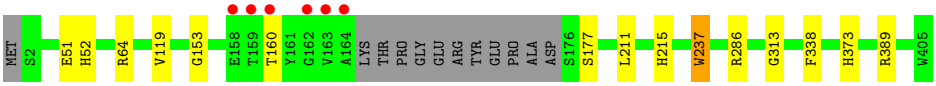
3 Residue-property plots (i)

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: D-mannonate dehydratase

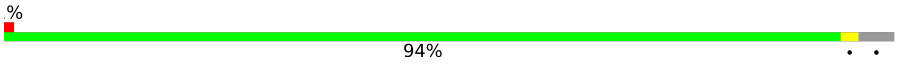
Chain A:

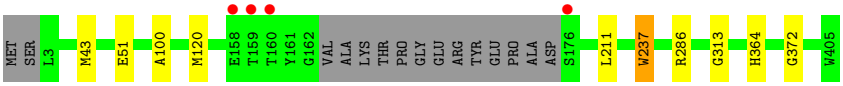




• Molecule 1: D-mannonate dehydratase

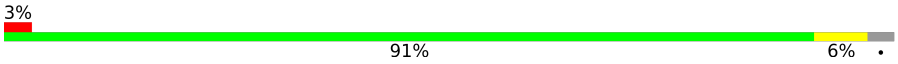
Chain B:

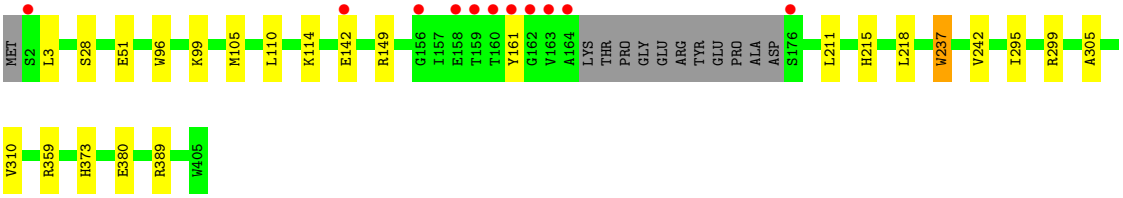




• Molecule 1: D-mannonate dehydratase

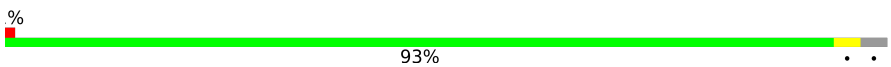
Chain C:

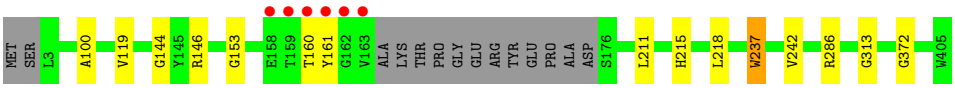




• Molecule 1: D-mannonate dehydratase

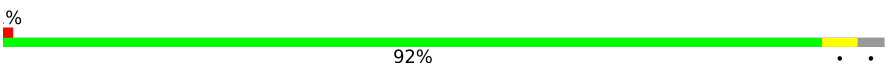
Chain D:

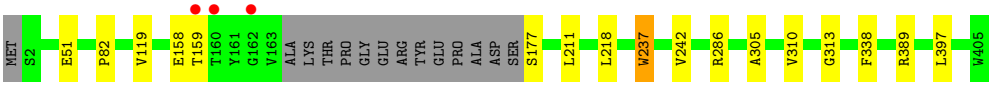




• Molecule 1: D-mannonate dehydratase

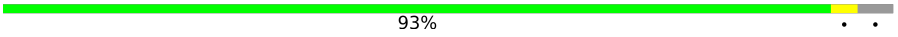
Chain E:

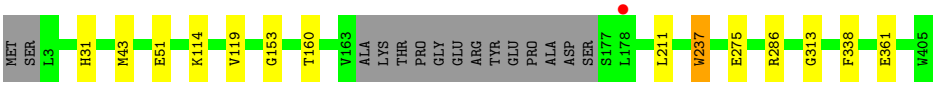




• Molecule 1: D-mannonate dehydratase

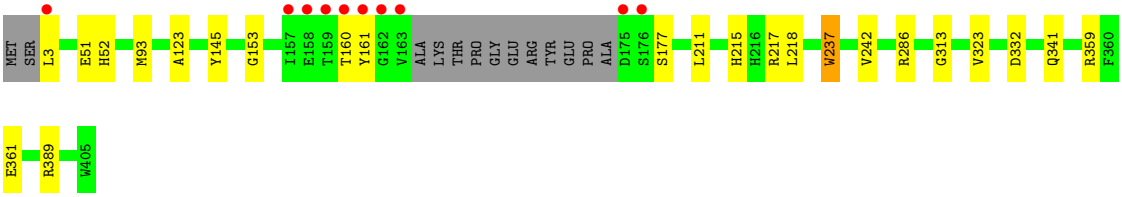
Chain F:





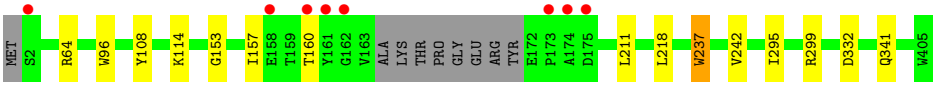
• Molecule 1: D-mannonate dehydratase

Chain G:



• Molecule 1: D-mannonate dehydratase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.33Å 85.79Å 195.64Å 90.00° 110.47° 90.00°	Depositor
Resolution (Å)	44.25 – 1.70 44.25 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.25-1.70) 99.3 (44.25-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.169 , 0.203 0.170 , 0.204	Depositor DCC
R_{free} test set	16774 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28312	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GCO, CL, MG

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	0.35	0/3222	0.53	0/4385
1	B	0.36	0/3217	0.53	0/4376
1	C	0.33	0/3210	0.51	0/4370
1	D	0.34	0/3219	0.52	0/4380
1	E	0.33	0/3191	0.52	0/4344
1	F	0.36	0/3223	0.53	0/4385
1	G	0.35	0/3225	0.55	0/4390
1	H	0.34	0/3234	0.51	0/4405
All	All	0.35	0/25741	0.53	0/35035

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

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	3137	0	3025	9	0
1	B	3126	0	3027	6	0
1	C	3122	0	3012	15	0
1	D	3134	0	3023	7	0
1	E	3106	0	2998	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3132	0	3030	11	0
1	G	3137	0	3032	16	0
1	H	3145	0	3035	12	0
2	A	13	0	10	0	0
2	B	13	0	10	0	0
2	C	13	0	10	0	0
2	D	13	0	10	1	0
2	E	13	0	10	0	0
2	F	13	0	10	0	0
2	G	13	0	10	0	0
2	H	13	0	10	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	2	0
4	F	2	0	0	1	0
5	C	6	0	8	1	0
6	A	394	0	0	0	0
6	B	419	0	0	0	0
6	C	370	0	0	2	0
6	D	378	0	0	0	0
6	E	403	0	0	0	0
6	F	402	0	0	3	0
6	G	395	0	0	2	0
6	H	383	0	0	3	0
All	All	28312	0	24270	76	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 (76) 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:299:ARG:HD3	1:H:299:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:MET:HG2	5:C:504:GOL:H32	1.82	0.62
1:A:177:SER:HB2	1:A:389:ARG:HG2	1.81	0.61
1:D:153:GLY:HA2	1:D:160:THR:HG21	1.84	0.59
1:E:158:GLU:HG3	1:E:159:THR:HG23	1.86	0.58
1:C:359:ARG:NH2	6:C:759:HOH:O	2.37	0.57
1:G:177:SER:HB2	1:G:389:ARG:HG2	1.88	0.56
1:G:359:ARG:NH2	1:G:361:GLU:OE2	2.39	0.56
1:H:299:ARG:NH1	6:H:770:HOH:O	2.30	0.56
1:A:211:LEU:HD23	1:A:237:TRP:CE2	2.41	0.55
4:F:504:CL:CL	1:G:52:HIS:ND1	2.72	0.55
1:D:161:TYR:HH	2:D:501:GCO:HO3	1.52	0.54
1:C:51:GLU:OE2	1:E:389:ARG:HD3	2.07	0.54
1:H:108:TYR:CE1	1:H:114:LYS:HG3	2.42	0.53
1:C:114:LYS:HE3	1:H:64[B]:ARG:NH2	2.23	0.53
1:A:153:GLY:HA2	1:A:160:THR:HG21	1.92	0.52
1:C:149:ARG:NH1	1:C:161:TYR:OH	2.31	0.52
1:C:380:GLU:HG2	6:C:948:HOH:O	2.08	0.52
1:F:31:HIS:ND1	6:F:998:HOH:O	2.34	0.51
1:D:144:GLY:O	1:D:146:ARG:NH1	2.44	0.51
1:H:153:GLY:HA2	1:H:160:THR:HG21	1.92	0.50
1:H:299:ARG:NE	6:H:979:HOH:O	2.45	0.50
1:G:153:GLY:HA2	1:G:160:THR:HG21	1.94	0.49
1:F:153:GLY:HA2	1:F:160:THR:HG21	1.94	0.49
1:E:211:LEU:HD23	1:E:237:TRP:CE2	2.48	0.49
1:D:218:LEU:O	1:D:242:VAL:HG12	2.14	0.48
1:G:211:LEU:HD23	1:G:237:TRP:CE2	2.48	0.48
1:C:389:ARG:HD3	1:E:51:GLU:OE2	2.14	0.47
1:C:99:LYS:HG2	1:C:110:LEU:HD21	1.95	0.47
1:F:43:MET:CG	1:G:51:GLU:HG2	2.45	0.47
1:F:361:GLU:OE2	6:F:991:HOH:O	2.20	0.47
1:G:218:LEU:O	1:G:242[A]:VAL:HG12	2.14	0.47
1:D:100:ALA:HB3	1:D:372:GLY:HA2	1.97	0.47
1:H:211:LEU:HD23	1:H:237:TRP:CE2	2.50	0.47
1:E:286:ARG:HD2	1:E:313:GLY:O	2.16	0.46
1:D:286:ARG:HD2	1:D:313:GLY:O	2.16	0.46
1:F:43:MET:HG3	1:G:51:GLU:HG2	1.98	0.46
1:F:211:LEU:HD23	1:F:237:TRP:CE2	2.51	0.45
1:B:211:LEU:HD23	1:B:237:TRP:CE2	2.51	0.45
1:G:161:TYR:HB2	1:G:217:ARG:NH2	2.32	0.45
1:E:397:LEU:HB3	4:E:505:CL:CL	2.54	0.45
1:E:82:PRO:HD2	4:E:504:CL:CL	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:O	1:E:242:VAL:HG12	2.17	0.45
1:B:100:ALA:HB3	1:B:372:GLY:HA2	1.99	0.44
1:C:3:LEU:HD13	1:C:28:SER:HB3	2.00	0.44
1:B:120:MET:HA	1:B:364:HIS:CD2	2.53	0.44
1:C:218:LEU:O	1:C:242:VAL:HG12	2.18	0.44
1:C:305:ALA:HB1	1:C:310:VAL:HB	1.99	0.44
1:A:286:ARG:HD2	1:A:313:GLY:O	2.18	0.43
1:A:64[B]:ARG:NH2	1:F:114:LYS:HD2	2.33	0.43
1:E:177:SER:HB2	1:E:389:ARG:HG2	2.00	0.43
1:A:389:ARG:HD3	1:B:51:GLU:OE2	2.18	0.43
1:E:119:VAL:HG13	1:E:338:PHE:CZ	2.54	0.43
1:C:211:LEU:HD23	1:C:237:TRP:CE2	2.54	0.43
1:F:275:GLU:HG2	6:F:982:HOH:O	2.19	0.42
1:G:93[A]:MET:SD	1:G:323:VAL:HG12	2.60	0.42
1:C:96:TRP:CD1	1:C:295:ILE:HB	2.54	0.42
1:G:51:GLU:HB2	6:G:805:HOH:O	2.18	0.42
1:G:286:ARG:HD2	1:G:313:GLY:O	2.19	0.42
1:H:96:TRP:CD1	1:H:295:ILE:HB	2.54	0.41
1:C:114:LYS:HE3	1:H:64[B]:ARG:CZ	2.51	0.41
1:D:211:LEU:HD23	1:D:237:TRP:CE2	2.55	0.41
1:A:51:GLU:HG3	1:A:52:HIS:CE1	2.56	0.41
1:A:119:VAL:HG13	1:A:338:PHE:CZ	2.56	0.41
1:E:305:ALA:HB1	1:E:310:VAL:HB	2.02	0.41
1:F:286:ARG:HD2	1:F:313:GLY:O	2.20	0.41
1:G:332:ASP:OD2	1:G:341:GLN:NE2	2.45	0.41
1:F:51:GLU:OE2	1:G:389:ARG:HD3	2.21	0.41
1:A:51:GLU:HG2	1:B:43:MET:CG	2.51	0.41
1:H:157:ILE:HG13	6:H:982:HOH:O	2.20	0.41
1:H:332:ASP:OD2	1:H:341:GLN:NE2	2.49	0.41
1:B:286:ARG:HD2	1:B:313:GLY:O	2.21	0.40
1:G:3:LEU:N	6:G:959:HOH:O	2.53	0.40
1:G:123:ALA:HB2	1:G:145:TYR:CE2	2.56	0.40
1:H:218:LEU:O	1:H:242[A]:VAL:HG12	2.21	0.40
1:F:119:VAL:HG13	1:F:338:PHE:CZ	2.56	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	392/405 (97%)	382 (97%)	10 (3%)	0	100	100
1	B	390/405 (96%)	380 (97%)	10 (3%)	0	100	100
1	C	391/405 (96%)	376 (96%)	15 (4%)	0	100	100
1	D	391/405 (96%)	378 (97%)	13 (3%)	0	100	100
1	E	388/405 (96%)	379 (98%)	9 (2%)	0	100	100
1	F	391/405 (96%)	379 (97%)	12 (3%)	0	100	100
1	G	392/405 (97%)	382 (97%)	10 (3%)	0	100	100
1	H	394/405 (97%)	384 (98%)	10 (2%)	0	100	100
All	All	3129/3240 (97%)	3040 (97%)	89 (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	324/331 (98%)	321 (99%)	3 (1%)	78	70
1	B	323/331 (98%)	322 (100%)	1 (0%)	92	89
1	C	323/331 (98%)	319 (99%)	4 (1%)	71	59
1	D	324/331 (98%)	321 (99%)	3 (1%)	78	70
1	E	321/331 (97%)	320 (100%)	1 (0%)	92	89
1	F	324/331 (98%)	323 (100%)	1 (0%)	92	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	325/331 (98%)	323 (99%)	2 (1%)	86 80
1	H	326/331 (98%)	325 (100%)	1 (0%)	92 89
All	All	2590/2648 (98%)	2574 (99%)	16 (1%)	86 80

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	237	TRP
1	A	373	HIS
1	B	237	TRP
1	C	142	GLU
1	C	215	HIS
1	C	237	TRP
1	C	373	HIS
1	D	119	VAL
1	D	215	HIS
1	D	237	TRP
1	E	237	TRP
1	F	237	TRP
1	G	215	HIS
1	G	237	TRP
1	H	237	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 19 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	GCO	B	501	3	12,12,12	1.50	2 (16%)	16,16,16	1.36	4 (25%)
5	GOL	C	504	-	5,5,5	0.33	0	5,5,5	0.33	0
2	GCO	D	501	3	12,12,12	1.42	1 (8%)	16,16,16	1.53	4 (25%)
2	GCO	C	501	3	12,12,12	1.46	2 (16%)	16,16,16	1.43	3 (18%)
2	GCO	F	501	3	12,12,12	1.44	1 (8%)	16,16,16	1.47	4 (25%)
2	GCO	H	501	3	12,12,12	1.55	1 (8%)	16,16,16	1.41	4 (25%)
2	GCO	A	501	3	12,12,12	1.48	1 (8%)	16,16,16	1.54	4 (25%)
2	GCO	G	501	3	12,12,12	1.59	3 (25%)	16,16,16	1.28	4 (25%)
2	GCO	E	501	3	12,12,12	1.46	1 (8%)	16,16,16	1.50	4 (25%)

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
2	GCO	B	501	3	-	8/18/18/18	-
5	GOL	C	504	-	-	3/4/4/4	-
2	GCO	D	501	3	-	7/18/18/18	-
2	GCO	C	501	3	-	6/18/18/18	-
2	GCO	F	501	3	-	8/18/18/18	-
2	GCO	H	501	3	-	8/18/18/18	-
2	GCO	A	501	3	-	8/18/18/18	-
2	GCO	G	501	3	-	8/18/18/18	-
2	GCO	E	501	3	-	8/18/18/18	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	GCO	O5-C5	-2.74	1.37	1.43
2	G	501	GCO	O5-C5	-2.58	1.37	1.43
2	E	501	GCO	O5-C5	-2.49	1.38	1.43
2	A	501	GCO	O5-C5	-2.43	1.38	1.43
2	F	501	GCO	C2-C1	-2.34	1.49	1.52
2	C	501	GCO	C2-C1	-2.32	1.49	1.52
2	B	501	GCO	O5-C5	-2.25	1.38	1.43
2	C	501	GCO	O5-C5	-2.23	1.38	1.43
2	G	501	GCO	C2-C1	-2.18	1.49	1.52
2	D	501	GCO	O5-C5	-2.06	1.39	1.43
2	B	501	GCO	C2-C1	-2.03	1.49	1.52
2	G	501	GCO	O4-C4	-2.03	1.38	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	GCO	C3-C2-C1	3.70	113.97	109.32
2	D	501	GCO	C3-C2-C1	3.60	113.85	109.32
2	A	501	GCO	C3-C2-C1	3.57	113.81	109.32
2	C	501	GCO	O6-C6-C5	3.47	118.63	111.07
2	H	501	GCO	C3-C2-C1	3.31	113.48	109.32
2	B	501	GCO	C3-C2-C1	2.97	113.05	109.32
2	A	501	GCO	C4-C3-C2	-2.91	108.44	113.60
2	G	501	GCO	C3-C2-C1	2.87	112.93	109.32
2	F	501	GCO	O6-C6-C5	2.80	117.18	111.07
2	F	501	GCO	C4-C3-C2	-2.77	108.69	113.60
2	F	501	GCO	C3-C2-C1	2.63	112.63	109.32
2	D	501	GCO	O1B-C1-C2	2.59	120.27	113.27
2	C	501	GCO	C3-C2-C1	2.59	112.57	109.32
2	B	501	GCO	C4-C3-C2	-2.46	109.23	113.60
2	E	501	GCO	O1B-C1-C2	2.43	119.84	113.27
2	E	501	GCO	O6-C6-C5	2.41	116.33	111.07
2	D	501	GCO	O6-C6-C5	2.40	116.31	111.07
2	A	501	GCO	O1B-C1-C2	2.36	119.65	113.27
2	C	501	GCO	O1B-C1-C2	2.31	119.52	113.27
2	G	501	GCO	C4-C3-C2	-2.30	109.52	113.60
2	H	501	GCO	C4-C3-C2	-2.26	109.60	113.60
2	F	501	GCO	O1B-C1-C2	2.26	119.37	113.27
2	B	501	GCO	O1B-C1-C2	2.26	119.37	113.27
2	E	501	GCO	C4-C3-C2	-2.24	109.63	113.60
2	G	501	GCO	O6-C6-C5	2.22	115.90	111.07
2	H	501	GCO	O1B-C1-C2	2.19	119.18	113.27
2	B	501	GCO	O6-C6-C5	2.14	115.74	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	GCO	C4-C3-C2	-2.14	109.81	113.60
2	G	501	GCO	O1B-C1-C2	2.09	118.93	113.27
2	A	501	GCO	O6-C6-C5	2.04	115.53	111.07
2	H	501	GCO	O6-C6-C5	2.04	115.52	111.07

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GCO	C2-C3-C4-C5
2	A	501	GCO	C2-C3-C4-O4
2	A	501	GCO	O3-C3-C4-C5
2	B	501	GCO	C2-C3-C4-C5
2	B	501	GCO	C2-C3-C4-O4
2	B	501	GCO	O3-C3-C4-C5
2	B	501	GCO	O3-C3-C4-O4
2	C	501	GCO	C2-C3-C4-C5
2	C	501	GCO	C2-C3-C4-O4
2	C	501	GCO	O3-C3-C4-C5
2	D	501	GCO	C2-C3-C4-C5
2	D	501	GCO	C2-C3-C4-O4
2	D	501	GCO	O3-C3-C4-C5
2	E	501	GCO	C2-C3-C4-C5
2	E	501	GCO	C2-C3-C4-O4
2	E	501	GCO	O3-C3-C4-C5
2	F	501	GCO	C2-C3-C4-C5
2	F	501	GCO	C2-C3-C4-O4
2	F	501	GCO	O3-C3-C4-C5
2	G	501	GCO	C2-C3-C4-C5
2	G	501	GCO	C2-C3-C4-O4
2	G	501	GCO	O3-C3-C4-C5
2	H	501	GCO	C2-C3-C4-C5
2	H	501	GCO	C2-C3-C4-O4
2	H	501	GCO	O3-C3-C4-C5
2	H	501	GCO	O1B-C1-C2-C3
2	A	501	GCO	O3-C3-C4-O4
2	C	501	GCO	O3-C3-C4-O4
2	D	501	GCO	O3-C3-C4-O4
2	E	501	GCO	O3-C3-C4-O4
2	F	501	GCO	O3-C3-C4-O4
2	G	501	GCO	O3-C3-C4-O4
2	H	501	GCO	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	H	501	GCO	O1A-C1-C2-C3
2	A	501	GCO	O1B-C1-C2-C3
2	E	501	GCO	O1B-C1-C2-C3
2	F	501	GCO	O1B-C1-C2-C3
2	G	501	GCO	O1B-C1-C2-C3
5	C	504	GOL	O1-C1-C2-C3
5	C	504	GOL	C1-C2-C3-O3
5	C	504	GOL	O2-C2-C3-O3
2	B	501	GCO	O1A-C1-C2-C3
2	D	501	GCO	O1A-C1-C2-C3
2	F	501	GCO	O1A-C1-C2-C3
2	H	501	GCO	O1A-C1-C2-O2
2	A	501	GCO	O1A-C1-C2-C3
2	B	501	GCO	O1B-C1-C2-C3
2	D	501	GCO	O1B-C1-C2-C3
2	E	501	GCO	O1A-C1-C2-C3
2	G	501	GCO	O1A-C1-C2-C3
2	C	501	GCO	O1A-C1-C2-C3
2	H	501	GCO	O1B-C1-C2-O2
2	C	501	GCO	O1B-C1-C2-C3
2	A	501	GCO	O1A-C1-C2-O2
2	A	501	GCO	O1B-C1-C2-O2
2	E	501	GCO	O1B-C1-C2-O2
2	F	501	GCO	O1B-C1-C2-O2
2	E	501	GCO	O1A-C1-C2-O2
2	F	501	GCO	O1A-C1-C2-O2
2	B	501	GCO	O1A-C1-C2-O2
2	G	501	GCO	O1A-C1-C2-O2
2	G	501	GCO	O1B-C1-C2-O2
2	D	501	GCO	O1A-C1-C2-O2
2	B	501	GCO	O1B-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	GOL	1	0
2	D	501	GCO	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, 95^{th} 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	393/405 (97%)	-0.59	6 (1%)	73 77	8, 13, 29, 53	0
1	B	390/405 (96%)	-0.55	4 (1%)	82 85	8, 12, 27, 54	0
1	C	393/405 (97%)	-0.36	11 (2%)	53 57	11, 17, 34, 55	0
1	D	391/405 (96%)	-0.42	6 (1%)	73 77	10, 16, 31, 60	0
1	E	391/405 (96%)	-0.52	3 (0%)	86 88	9, 15, 30, 53	0
1	F	390/405 (96%)	-0.50	1 (0%)	94 94	8, 13, 27, 46	0
1	G	392/405 (96%)	-0.52	10 (2%)	56 60	8, 13, 29, 65	0
1	H	396/405 (97%)	-0.50	8 (2%)	65 69	9, 15, 31, 52	0
All	All	3136/3240 (96%)	-0.49	49 (1%)	72 76	8, 15, 30, 65	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	SER	4.8
1	G	160	THR	4.1
1	D	160	THR	3.9
1	C	163	VAL	3.8
1	E	160	THR	3.7
1	G	163	VAL	3.7
1	C	160	THR	3.6
1	D	161	TYR	3.5
1	C	164	ALA	3.5
1	C	2	SER	3.5
1	G	3	LEU	3.4
1	H	174	ALA	3.3
1	D	163	VAL	3.2
1	G	157	ILE	3.2
1	E	159	THR	3.1
1	C	161	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	164	ALA	3.0
1	D	158	GLU	3.0
1	B	160	THR	2.9
1	G	161	TYR	2.9
1	G	159	THR	2.8
1	C	159	THR	2.8
1	H	175	ASP	2.8
1	G	162	GLY	2.7
1	C	142	GLU	2.6
1	H	160	THR	2.6
1	H	173	PRO	2.6
1	G	176	SER	2.6
1	B	159	THR	2.5
1	B	158	GLU	2.5
1	C	158	GLU	2.5
1	D	159	THR	2.5
1	H	161	TYR	2.4
1	A	160	THR	2.4
1	E	162	GLY	2.3
1	B	176	SER	2.3
1	G	158	GLU	2.3
1	H	2	SER	2.3
1	G	175	ASP	2.3
1	A	158	GLU	2.2
1	D	162	GLY	2.2
1	F	178	LEU	2.2
1	A	159	THR	2.2
1	A	163	VAL	2.1
1	H	158	GLU	2.0
1	A	162	GLY	2.0
1	C	156	GLY	2.0
1	C	162	GLY	2.0
1	H	162	GLY	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 monosaccharides 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, 95^{th} 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	504	6/6	0.83	0.19	29,32,35,35	0
4	CL	E	505	1/1	0.89	0.11	45,45,45,45	0
4	CL	F	503	1/1	0.91	0.07	19,19,19,19	0
4	CL	D	504	1/1	0.91	0.09	20,20,20,20	0
4	CL	F	504	1/1	0.92	0.10	45,45,45,45	0
2	GCO	E	501	13/13	0.94	0.07	11,16,19,22	0
2	GCO	C	501	13/13	0.95	0.06	12,16,20,21	0
2	GCO	D	501	13/13	0.95	0.07	11,14,21,21	0
2	GCO	A	501	13/13	0.95	0.06	11,14,18,21	0
2	GCO	H	501	13/13	0.95	0.07	10,15,19,21	0
4	CL	A	503	1/1	0.95	0.08	18,18,18,18	0
2	GCO	B	501	13/13	0.96	0.06	9,12,16,20	0
4	CL	E	504	1/1	0.96	0.10	24,24,24,24	0
2	GCO	F	501	13/13	0.96	0.06	9,13,15,15	0
3	MG	D	503	1/1	0.97	0.09	15,15,15,15	1
3	MG	G	503	1/1	0.97	0.04	4,4,4,4	1
2	GCO	G	501	13/13	0.97	0.06	11,13,19,21	0
3	MG	C	503	1/1	0.98	0.09	5,5,5,5	1
3	MG	C	502	1/1	0.98	0.03	12,12,12,12	0
3	MG	D	502	1/1	0.99	0.03	11,11,11,11	0
3	MG	B	503	1/1	0.99	0.03	5,5,5,5	1
3	MG	E	502	1/1	0.99	0.02	12,12,12,12	0
3	MG	G	502	1/1	0.99	0.05	11,11,11,11	0
3	MG	A	502	1/1	0.99	0.03	9,9,9,9	0
3	MG	B	502	1/1	0.99	0.05	9,9,9,9	0
3	MG	F	502	1/1	1.00	0.01	9,9,9,9	0
3	MG	H	502	1/1	1.00	0.05	9,9,9,9	0
3	MG	E	503	1/1	1.00	0.05	9,9,9,9	1

6.5 Other polymers (i)

There are no such residues in this entry.