



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 08:25 PM EST

PDB ID : 3NZG  
Title : Crystal structure of a putative racemase with Mg ion  
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Deposited on : 2010-07-16  
Resolution : 2.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.16  
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) : 2.16

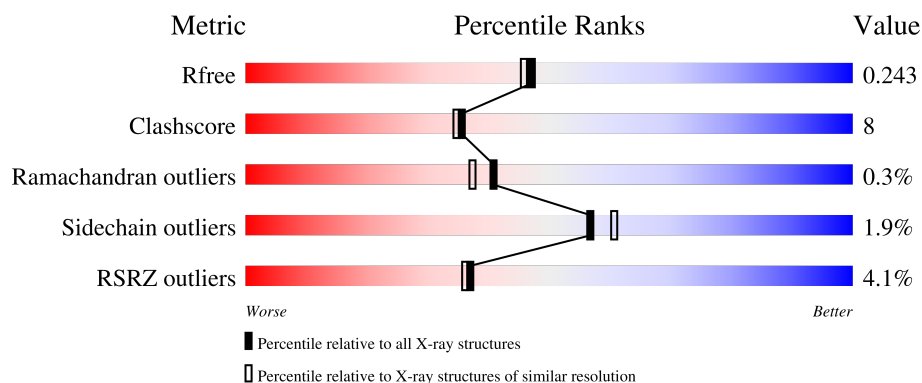
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	394	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	394	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>
1	C	394	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	394	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12214 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 Putative racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	Se	0	0	0
			2945	1886	491	555	4	9			
1	B	377	Total	C	N	O	S	Se	0	0	0
			2945	1886	491	555	4	9			
1	C	377	Total	C	N	O	S	Se	0	0	0
			2945	1886	491	555	4	9			
1	D	380	Total	C	N	O	S	Se	0	0	0
			2963	1898	494	558	4	9			

There are 32 discrepancies between the modelled and reference sequences:

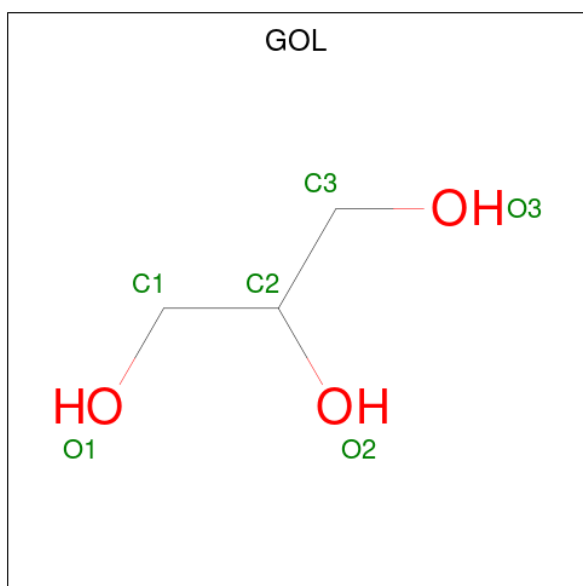
Chain	Residue	Modelled	Actual	Comment	Reference
A	387	GLU	-	expression tag	UNP B6R2Z6
A	388	GLY	-	expression tag	UNP B6R2Z6
A	389	HIS	-	expression tag	UNP B6R2Z6
A	390	HIS	-	expression tag	UNP B6R2Z6
A	391	HIS	-	expression tag	UNP B6R2Z6
A	392	HIS	-	expression tag	UNP B6R2Z6
A	393	HIS	-	expression tag	UNP B6R2Z6
A	394	HIS	-	expression tag	UNP B6R2Z6
B	387	GLU	-	expression tag	UNP B6R2Z6
B	388	GLY	-	expression tag	UNP B6R2Z6
B	389	HIS	-	expression tag	UNP B6R2Z6
B	390	HIS	-	expression tag	UNP B6R2Z6
B	391	HIS	-	expression tag	UNP B6R2Z6
B	392	HIS	-	expression tag	UNP B6R2Z6
B	393	HIS	-	expression tag	UNP B6R2Z6
B	394	HIS	-	expression tag	UNP B6R2Z6
C	387	GLU	-	expression tag	UNP B6R2Z6
C	388	GLY	-	expression tag	UNP B6R2Z6
C	389	HIS	-	expression tag	UNP B6R2Z6
C	390	HIS	-	expression tag	UNP B6R2Z6
C	391	HIS	-	expression tag	UNP B6R2Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP B6R2Z6
C	393	HIS	-	expression tag	UNP B6R2Z6
C	394	HIS	-	expression tag	UNP B6R2Z6
D	387	GLU	-	expression tag	UNP B6R2Z6
D	388	GLY	-	expression tag	UNP B6R2Z6
D	389	HIS	-	expression tag	UNP B6R2Z6
D	390	HIS	-	expression tag	UNP B6R2Z6
D	391	HIS	-	expression tag	UNP B6R2Z6
D	392	HIS	-	expression tag	UNP B6R2Z6
D	393	HIS	-	expression tag	UNP B6R2Z6
D	394	HIS	-	expression tag	UNP B6R2Z6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

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

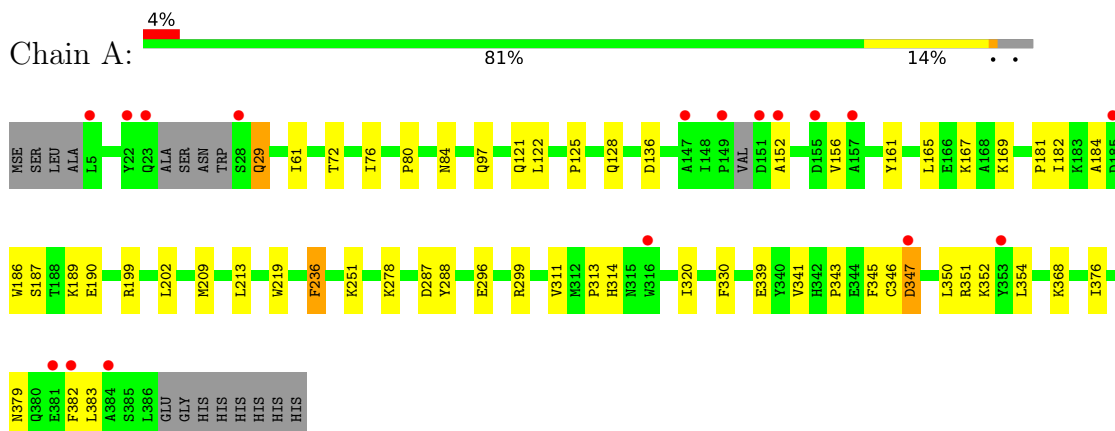
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total 96	O 96	0	0
4	B	91	Total 91	O 91	0	0
4	C	100	Total 100	O 100	0	0
4	D	91	Total 91	O 91	0	0

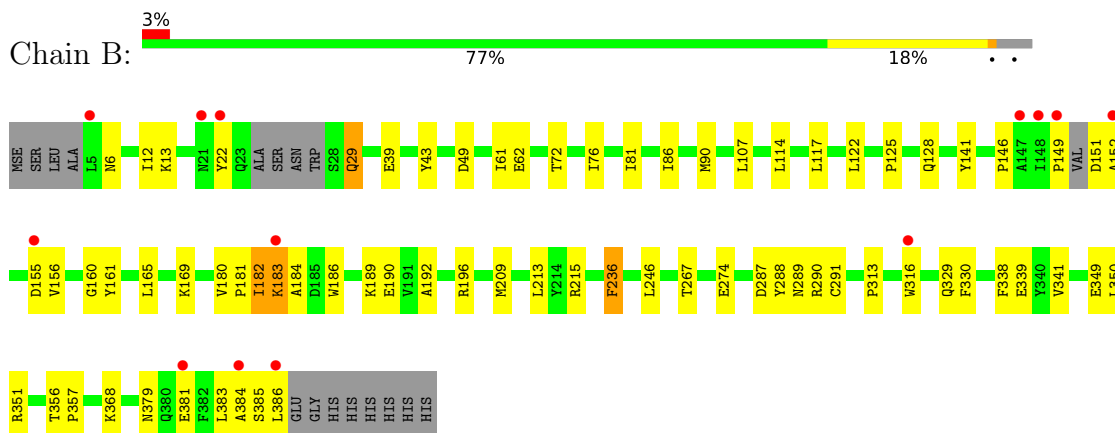
### 3 Residue-property plots [i](#)

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.

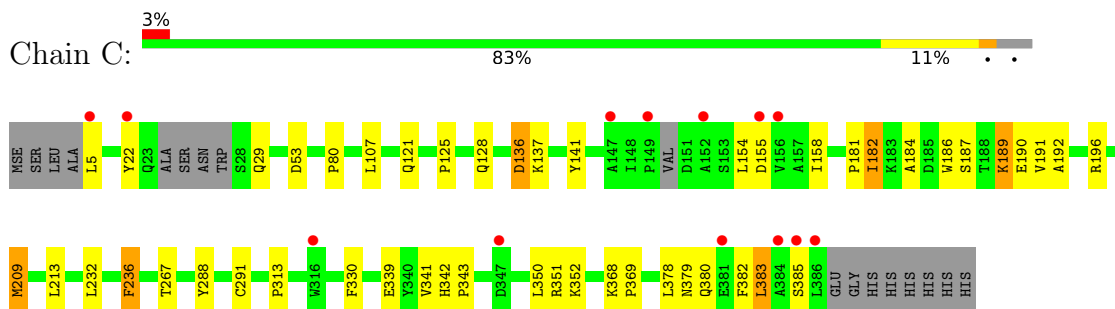
#### • Molecule 1: Putative racemase



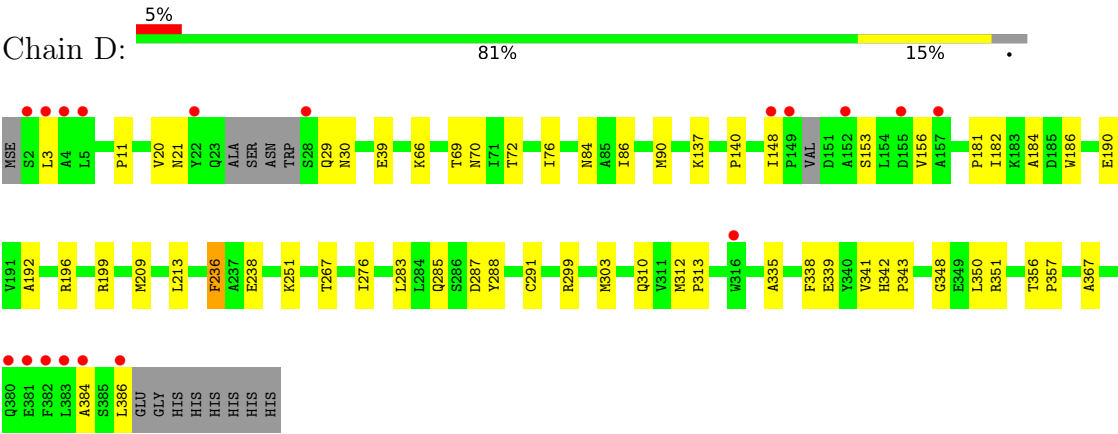
#### • Molecule 1: Putative racemase



#### • Molecule 1: Putative racemase



● Molecule 1: Putative racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.14Å 165.41Å 165.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.28 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.00) 96.9 (49.28-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.86 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.244 0.221 , 0.243	Depositor DCC
$R_{free}$ test set	4808 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, 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	0.32	0/3004	0.58	0/4073
1	B	0.34	0/3004	0.60	1/4073 (0.0%)
1	C	0.33	0/3004	0.59	0/4073
1	D	0.33	0/3022	0.60	0/4098
All	All	0.33	0/12034	0.59	1/16317 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	TYR	N-CA-C	-5.01	97.46	111.00

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	2945	0	2882	43	0
1	B	2945	0	2882	57	0
1	C	2945	0	2882	42	0
1	D	2963	0	2900	50	0
2	A	6	0	6	1	0
2	B	6	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	14	1	0
2	D	6	0	6	1	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	96	0	0	2	0
4	B	91	0	0	1	1
4	C	100	0	0	0	0
4	D	91	0	0	0	1
All	All	12214	0	11578	190	1

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 8.

All (190) 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:D:283:LEU:HD11	1:D:312:MSE:HE2	1.26	1.12
1:A:189:LYS:HA	1:A:189:LYS:HE2	1.38	1.03
1:D:283:LEU:CD1	1:D:312:MSE:HE2	1.99	0.93
1:B:189:LYS:HE2	1:B:189:LYS:HA	1.52	0.92
1:D:236:PHE:CE2	1:D:312:MSE:HE1	2.04	0.92
1:B:341:VAL:HG13	1:B:351:ARG:HE	1.35	0.91
1:D:236:PHE:HE2	1:D:312:MSE:HE1	1.36	0.90
1:D:341:VAL:HG23	1:D:351:ARG:HE	1.38	0.87
1:C:189:LYS:HA	1:C:189:LYS:HE2	1.57	0.83
1:B:22:TYR:HB3	1:B:350:LEU:HD11	1.65	0.79
1:A:29:GLN:HE22	1:A:350:LEU:H	1.30	0.78
1:C:341:VAL:HG13	1:C:351:ARG:HE	1.50	0.76
1:B:385:SER:O	1:B:386:LEU:HB2	1.85	0.75
1:B:29:GLN:HB2	1:B:350:LEU:HD13	1.68	0.75
1:D:181:PRO:HG2	1:D:184:ALA:HB2	1.71	0.73
1:B:81:ILE:HD13	1:B:122:LEU:HD11	1.71	0.73
1:A:341:VAL:HG13	1:A:351:ARG:HE	1.53	0.72
1:D:11:PRO:HD2	1:D:39:GLU:HG3	1.72	0.72
1:A:343:PRO:HB3	1:A:352:LYS:HG2	1.72	0.72
1:A:181:PRO:HB2	1:A:184:ALA:HB2	1.72	0.70
1:C:125:PRO:HG2	1:C:128:GLN:HG3	1.74	0.69
1:B:181:PRO:HB2	1:B:184:ALA:HB2	1.73	0.69
1:A:169:LYS:HD3	1:A:202:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:HG2	1:A:128:GLN:HG3	1.73	0.68
1:D:236:PHE:HE2	1:D:312:MSE:CE	2.06	0.68
1:A:287:ASP:OD2	1:A:314:HIS:HD2	1.77	0.67
1:C:181:PRO:HB2	1:C:184:ALA:HB2	1.77	0.66
1:B:151:ASP:N	1:B:183:LYS:HB2	2.12	0.64
1:B:149:PRO:HD2	1:B:152:ALA:HB2	1.79	0.64
1:B:22:TYR:CB	1:B:350:LEU:HD11	2.28	0.63
1:B:246:LEU:CD2	1:B:274:GLU:HG2	2.29	0.63
1:D:236:PHE:CE2	1:D:312:MSE:CE	2.81	0.60
1:A:330:PHE:CE1	1:A:368:LYS:HG2	2.37	0.60
1:C:379:ASN:ND2	1:C:382:PHE:HB2	2.18	0.59
1:A:379:ASN:ND2	1:A:382:PHE:HB2	2.18	0.58
1:D:384:ALA:C	1:D:386:LEU:H	2.07	0.58
1:D:21:ASN:OD1	1:D:30:ASN:HB3	2.03	0.57
1:C:29:GLN:HE21	1:C:350:LEU:HB2	1.68	0.57
1:D:29:GLN:HE22	1:D:350:LEU:H	1.51	0.57
1:B:29:GLN:HE21	1:B:350:LEU:HD13	1.71	0.56
1:A:29:GLN:NE2	1:A:350:LEU:H	2.01	0.55
1:C:29:GLN:HE22	1:C:350:LEU:H	1.54	0.55
1:C:330:PHE:CE1	1:C:368:LYS:HG2	2.40	0.55
1:D:84:ASN:ND2	1:D:299:ARG:HH12	2.03	0.55
1:A:288:TYR:OH	1:A:313:PRO:HG2	2.07	0.55
1:B:330:PHE:CE1	1:B:368:LYS:HG2	2.40	0.55
1:A:187:SER:OG	1:A:190:GLU:HG3	2.07	0.55
1:B:341:VAL:HG13	1:B:351:ARG:NE	2.15	0.55
1:A:72:THR:O	1:A:76:ILE:HG12	2.08	0.54
1:B:385:SER:O	1:B:386:LEU:CB	2.56	0.54
1:D:84:ASN:HD21	1:D:299:ARG:NH1	2.06	0.54
1:C:288:TYR:CE2	1:C:313:PRO:HB2	2.42	0.54
1:D:339:GLU:OE2	2:D:601:GOL:O3	2.26	0.54
1:C:187:SER:OG	1:C:190:GLU:HG3	2.08	0.54
1:D:84:ASN:HD21	1:D:299:ARG:HH12	1.55	0.54
1:B:180:VAL:O	1:B:213:LEU:HD12	2.08	0.54
1:C:186:TRP:HA	1:C:190:GLU:OE1	2.08	0.54
1:B:22:TYR:OH	1:B:349:GLU:HG2	2.08	0.54
1:B:29:GLN:NE2	1:B:350:LEU:HD13	2.23	0.54
1:A:339:GLU:OE2	2:A:601:GOL:O3	2.27	0.53
1:B:149:PRO:HB2	1:B:152:ALA:HB2	1.90	0.53
1:D:283:LEU:HD11	1:D:312:MSE:CE	2.19	0.53
1:B:165:LEU:O	1:B:169:LYS:HG3	2.08	0.53
1:B:339:GLU:OE2	2:B:601:GOL:O3	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ASN:HD22	1:C:382:PHE:HB2	1.73	0.53
1:D:186:TRP:HB3	1:D:190:GLU:HB2	1.92	0.52
1:D:236:PHE:CD2	1:D:312:MSE:HE1	2.41	0.52
1:C:22:TYR:HB2	1:C:350:LEU:HD13	1.91	0.52
1:A:311:VAL:HG12	1:A:313:PRO:HD3	1.91	0.52
1:B:246:LEU:HD23	1:B:274:GLU:HG2	1.93	0.51
1:A:186:TRP:HB3	1:A:190:GLU:HB2	1.93	0.51
1:B:22:TYR:CZ	1:B:349:GLU:HG2	2.45	0.51
1:D:236:PHE:C	1:D:236:PHE:CD1	2.84	0.51
1:D:69:THR:HG22	1:D:70:ASN:N	2.26	0.51
1:D:29:GLN:NE2	1:D:350:LEU:H	2.09	0.50
1:B:13:LYS:HE3	1:B:39:GLU:HA	1.93	0.50
1:D:181:PRO:HG2	1:D:184:ALA:CB	2.40	0.50
1:D:288:TYR:CE2	1:D:313:PRO:HB2	2.46	0.50
1:D:11:PRO:O	1:D:39:GLU:HG2	2.12	0.50
1:A:189:LYS:HA	1:A:189:LYS:CE	2.24	0.49
1:B:86:ILE:HG22	1:B:90:MSE:HE2	1.93	0.49
4:A:426:HOH:O	1:D:251:LYS:HE2	2.13	0.49
1:B:182:ILE:HG21	1:D:66:LYS:HD2	1.94	0.49
1:C:186:TRP:HB3	1:C:190:GLU:HB2	1.94	0.49
1:A:29:GLN:HE21	1:A:350:LEU:HB2	1.77	0.48
1:B:383:LEU:HD23	1:B:383:LEU:O	2.13	0.48
1:A:341:VAL:O	1:A:341:VAL:HG13	2.14	0.48
1:B:12:ILE:HD11	1:B:114:LEU:HD21	1.95	0.48
1:A:189:LYS:CA	1:A:189:LYS:HE2	2.26	0.47
1:B:288:TYR:CE2	1:B:313:PRO:HB2	2.49	0.47
1:C:236:PHE:C	1:C:236:PHE:CD1	2.88	0.47
1:D:342:HIS:ND1	1:D:343:PRO:HD2	2.30	0.47
1:B:146:PRO:HB3	1:B:160:GLY:O	2.15	0.47
1:A:182:ILE:HG13	1:A:213:LEU:HD13	1.95	0.47
1:C:187:SER:O	1:C:191:VAL:HG23	2.15	0.47
1:A:219:TRP:CE2	1:A:251:LYS:HD3	2.50	0.47
1:C:29:GLN:NE2	1:C:350:LEU:H	2.13	0.47
1:A:84:ASN:HD21	1:A:299:ARG:NH1	2.13	0.47
1:B:356:THR:OG1	1:B:357:PRO:HA	2.15	0.46
1:B:61:ILE:C	1:B:61:ILE:HD12	2.35	0.46
1:C:379:ASN:HD22	1:C:382:PHE:CB	2.28	0.46
1:D:20:VAL:O	1:D:30:ASN:HA	2.15	0.46
1:C:380:GLN:HE21	1:C:380:GLN:HA	1.80	0.46
1:A:29:GLN:NE2	1:A:350:LEU:HB2	2.31	0.46
1:D:153:SER:OG	1:D:156:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLU:O	1:B:384:ALA:HB3	2.16	0.46
1:B:125:PRO:HG2	1:B:128:GLN:HG3	1.97	0.46
1:B:72:THR:O	1:B:76:ILE:HG12	2.15	0.46
1:A:278:LYS:HB2	1:A:278:LYS:NZ	2.31	0.45
1:D:209:MSE:HG2	1:D:236:PHE:CE2	2.51	0.45
1:A:80:PRO:HG2	1:A:121:GLN:OE1	2.17	0.45
1:D:182:ILE:HG13	1:D:213:LEU:HD13	1.98	0.45
1:B:186:TRP:HB3	1:B:190:GLU:HB2	1.98	0.45
1:C:288:TYR:CZ	1:C:313:PRO:HB2	2.51	0.45
1:C:343:PRO:O	1:C:352:LYS:HE2	2.17	0.45
1:D:236:PHE:C	1:D:236:PHE:HD1	2.19	0.45
1:D:288:TYR:CZ	1:D:313:PRO:HB2	2.52	0.45
1:A:122:LEU:O	1:B:6:ASN:HB2	2.17	0.45
1:B:287:ASP:HB3	1:B:290:ARG:HB2	1.98	0.45
1:A:236:PHE:C	1:A:236:PHE:CD1	2.91	0.45
1:B:149:PRO:CD	1:B:152:ALA:HB2	2.44	0.45
1:B:316:TRP:HE3	2:B:601:GOL:H32	1.82	0.45
1:C:380:GLN:NE2	1:C:380:GLN:HA	2.32	0.45
1:A:288:TYR:CZ	1:A:313:PRO:HG2	2.51	0.45
1:B:316:TRP:CE3	2:B:601:GOL:H32	2.52	0.44
1:C:154:LEU:O	1:C:158:ILE:HG13	2.17	0.44
1:D:276:ILE:HD12	1:D:303:MSE:HE3	1.99	0.44
1:D:137:LYS:HD2	1:D:367:ALA:HA	1.98	0.44
1:A:61:ILE:HD13	1:A:97:GLN:NE2	2.33	0.44
1:A:379:ASN:ND2	1:A:382:PHE:CB	2.81	0.44
1:D:72:THR:O	1:D:76:ILE:HG12	2.17	0.44
1:B:192:ALA:O	1:B:196:ARG:HG3	2.18	0.44
1:C:339:GLU:OE2	2:C:601:GOL:O3	2.35	0.44
1:D:310:GLN:HB3	1:D:335:ALA:HB2	1.99	0.44
1:B:189:LYS:CE	1:B:189:LYS:HA	2.34	0.44
1:C:141:TYR:CD2	1:C:209:MSE:HE2	2.53	0.44
1:D:341:VAL:HG23	1:D:341:VAL:O	2.18	0.44
1:B:196:ARG:NH1	1:B:196:ARG:HG2	2.32	0.43
1:B:379:ASN:OD1	1:B:381:GLU:HB2	2.18	0.43
1:C:192:ALA:O	1:C:196:ARG:HG3	2.18	0.43
1:C:379:ASN:ND2	1:C:382:PHE:CB	2.81	0.43
1:B:196:ARG:HG2	1:B:196:ARG:HH11	1.82	0.43
1:B:182:ILE:HG13	1:B:213:LEU:HD13	1.99	0.43
1:C:236:PHE:HD1	1:C:236:PHE:C	2.22	0.43
1:D:192:ALA:O	1:D:196:ARG:HG3	2.18	0.43
1:B:149:PRO:HD2	1:B:156:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:HG2	1:D:196:ARG:NH1	2.33	0.43
1:D:140:PRO:HB3	1:D:338:PHE:CZ	2.54	0.43
1:D:148:ILE:O	1:D:148:ILE:HG13	2.18	0.43
1:C:136:ASP:O	1:C:137:LYS:HG2	2.18	0.43
1:B:288:TYR:CZ	1:B:313:PRO:HB2	2.54	0.43
1:C:341:VAL:HG13	1:C:341:VAL:O	2.17	0.43
1:C:343:PRO:HB3	1:C:352:LYS:HG2	2.00	0.43
1:D:356:THR:OG1	1:D:357:PRO:HA	2.19	0.42
1:A:346:CYS:SG	1:A:347:ASP:N	2.92	0.42
1:B:49:ASP:HB2	1:B:289:ASN:OD1	2.20	0.42
1:D:287:ASP:OD1	1:D:288:TYR:N	2.52	0.42
1:D:267:THR:HA	1:D:291:CYS:HA	2.01	0.42
1:A:152:ALA:HB1	1:A:156:VAL:HB	2.00	0.42
1:A:320:ILE:HG12	1:A:376:ILE:HD12	2.00	0.42
1:A:161:TYR:O	1:A:165:LEU:HG	2.20	0.42
1:C:342:HIS:HA	1:C:343:PRO:HD3	1.90	0.42
1:C:267:THR:HA	1:C:291:CYS:HA	2.02	0.42
1:C:378:LEU:HD13	1:C:383:LEU:HD11	2.01	0.42
1:C:80:PRO:HG2	1:C:121:GLN:OE1	2.19	0.42
1:A:84:ASN:ND2	4:A:436:HOH:O	2.52	0.42
1:D:86:ILE:HG22	1:D:90:MSE:HE2	2.01	0.42
1:A:236:PHE:HD1	1:A:236:PHE:C	2.23	0.41
1:B:215:ARG:HD2	4:B:443:HOH:O	2.20	0.41
1:A:186:TRP:HA	1:A:190:GLU:OE1	2.19	0.41
1:D:238:GLU:HG3	1:D:285:GLN:OE1	2.20	0.41
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.91	0.41
1:C:182:ILE:CG1	1:C:213:LEU:HD13	2.51	0.41
1:A:320:ILE:HA	1:A:376:ILE:HD13	2.03	0.41
1:B:107:LEU:O	1:B:107:LEU:HD23	2.21	0.41
1:D:196:ARG:HG2	1:D:196:ARG:HH11	1.86	0.41
1:B:350:LEU:H	1:B:350:LEU:HD12	1.85	0.41
1:C:107:LEU:HD23	1:C:107:LEU:C	2.41	0.41
1:A:296:GLU:HA	1:A:296:GLU:OE1	2.21	0.41
1:B:209:MSE:HB3	1:B:236:PHE:CE1	2.56	0.41
1:B:267:THR:HA	1:B:291:CYS:HA	2.03	0.41
1:D:384:ALA:C	1:D:386:LEU:N	2.73	0.41
1:B:329:GLN:HG2	1:B:338:PHE:CD2	2.56	0.41
1:A:167:LYS:HG2	1:A:345:PHE:CE1	2.56	0.40
1:C:182:ILE:HG13	1:C:213:LEU:HD13	2.03	0.40
1:C:53:ASP:OD1	1:C:53:ASP:N	2.53	0.40
1:C:196:ARG:HG2	1:C:232:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LYS:HA	1:C:369:PRO:HD3	1.95	0.40
1:C:341:VAL:HG13	1:C:351:ARG:NE	2.25	0.40
1:B:43:TYR:HA	1:B:117:LEU:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:486:HOH:O	4:D:468:HOH:O[3_455]	2.12	0.08

## 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	371/394 (94%)	354 (95%)	17 (5%)	0	100	100
1	B	371/394 (94%)	352 (95%)	18 (5%)	1 (0%)	41	37
1	C	371/394 (94%)	350 (94%)	20 (5%)	1 (0%)	41	37
1	D	374/394 (95%)	355 (95%)	17 (4%)	2 (0%)	29	23
All	All	1487/1576 (94%)	1411 (95%)	72 (5%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	LEU
1	B	182	ILE
1	C	182	ILE
1	D	348	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/313 (97%)	298 (98%)	7 (2%)	50	53
1	B	305/313 (97%)	299 (98%)	6 (2%)	55	58
1	C	305/313 (97%)	297 (97%)	8 (3%)	46	48
1	D	306/313 (98%)	304 (99%)	2 (1%)	84	88
All	All	1221/1252 (98%)	1198 (98%)	23 (2%)	57	61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	136	ASP
1	A	199	ARG
1	A	209	MSE
1	A	236	PHE
1	A	347	ASP
1	A	383	LEU
1	B	29	GLN
1	B	62	GLU
1	B	155	ASP
1	B	161	TYR
1	B	183	LYS
1	B	236	PHE
1	C	5	LEU
1	C	136	ASP
1	C	155	ASP
1	C	189	LYS
1	C	209	MSE
1	C	236	PHE
1	C	383	LEU
1	C	385	SER
1	D	199	ARG
1	D	236	PHE



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	84	ASN
1	A	308	ASN
1	A	314	HIS
1	A	379	ASN
1	B	29	GLN
1	B	84	ASN
1	B	242	GLN
1	B	308	ASN
1	C	29	GLN
1	C	84	ASN
1	C	242	GLN
1	C	379	ASN
1	C	380	GLN
1	D	29	GLN
1	D	84	ASN
1	D	242	GLN
1	D	379	ASN

### 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 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	$\# Z  > 2$
2	GOL	C	602	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	C	601	3	5,5,5	0.36	0	5,5,5	0.64	0
2	GOL	A	601	3	5,5,5	0.35	0	5,5,5	0.68	0
2	GOL	D	601	3	5,5,5	0.33	0	5,5,5	0.53	0
2	GOL	B	601	3	5,5,5	0.35	0	5,5,5	0.53	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
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	C	601	3	-	4/4/4/4	-
2	GOL	A	601	3	-	3/4/4/4	-
2	GOL	D	601	3	-	3/4/4/4	-
2	GOL	B	601	3	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	GOL	1	0
2	A	601	GOL	1	0
2	D	601	GOL	1	0
2	B	601	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	368/394 (93%)	0.09	17 (4%) 32 31	9, 25, 41, 46	0
1	B	368/394 (93%)	0.04	13 (3%) 44 43	9, 25, 40, 47	0
1	C	368/394 (93%)	0.05	13 (3%) 44 43	8, 23, 40, 46	0
1	D	371/394 (94%)	0.13	18 (4%) 29 28	10, 24, 41, 48	0
All	All	1475/1576 (93%)	0.08	61 (4%) 37 36	8, 24, 40, 48	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	8.8
1	D	2	SER	7.4
1	D	149	PRO	7.2
1	D	4	ALA	6.2
1	B	384	ALA	5.9
1	C	386	LEU	5.5
1	C	384	ALA	4.9
1	A	384	ALA	4.8
1	D	152	ALA	4.6
1	A	5	LEU	4.5
1	A	347	ASP	3.9
1	D	383	LEU	3.8
1	D	386	LEU	3.7
1	D	384	ALA	3.6
1	C	147	ALA	3.5
1	A	147	ALA	3.5
1	C	152	ALA	3.4
1	B	149	PRO	3.4
1	B	22	TYR	3.4
1	D	22	TYR	3.4
1	B	381	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	149	PRO	3.2
1	B	5	LEU	3.2
1	C	156	VAL	3.2
1	D	28	SER	3.2
1	D	5	LEU	3.1
1	A	382	PHE	3.1
1	C	385	SER	3.1
1	D	316	TRP	2.9
1	B	155	ASP	2.8
1	A	353	TYR	2.8
1	C	347	ASP	2.8
1	D	380	GLN	2.8
1	C	155	ASP	2.7
1	A	157	ALA	2.7
1	C	22	TYR	2.7
1	B	316	TRP	2.6
1	C	5	LEU	2.6
1	A	28	SER	2.6
1	A	22	TYR	2.5
1	D	381	GLU	2.5
1	D	382	PHE	2.5
1	A	316	TRP	2.5
1	C	316	TRP	2.5
1	C	149	PRO	2.5
1	B	183	LYS	2.5
1	B	148	ILE	2.4
1	A	23	GLN	2.4
1	A	381	GLU	2.3
1	A	185	ASP	2.3
1	B	386	LEU	2.3
1	B	152	ALA	2.2
1	A	152	ALA	2.2
1	B	147	ALA	2.2
1	C	381	GLU	2.1
1	B	21	ASN	2.1
1	A	151	ASP	2.1
1	D	155	ASP	2.1
1	A	155	ASP	2.1
1	D	148	ILE	2.1
1	D	157	ALA	2.1

## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	601	6/6	0.77	0.23	32,35,36,37	0
2	GOL	C	602	6/6	0.79	0.16	32,35,36,37	0
2	GOL	C	601	6/6	0.81	0.23	31,35,36,37	0
2	GOL	B	601	6/6	0.81	0.24	37,39,40,41	0
3	MG	B	506	1/1	0.86	0.14	35,35,35,35	0
3	MG	C	508	1/1	0.86	0.08	29,29,29,29	0
2	GOL	D	601	6/6	0.90	0.19	31,34,35,35	0
3	MG	A	507	1/1	0.94	0.20	27,27,27,27	0
3	MG	D	505	1/1	0.97	0.13	29,29,29,29	0
3	MG	D	502	1/1	0.98	0.07	17,17,17,17	0
3	MG	B	501	1/1	0.99	0.06	17,17,17,17	0
3	MG	A	504	1/1	0.99	0.05	15,15,15,15	0
3	MG	B	503	1/1	1.00	0.04	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.