



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:07 PM EDT

PDB ID : 2NQR  
Title : MoeA D142N  
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Deposited on : 2006-10-31  
Resolution : 2.20 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 : 2.23.2  
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) : 2.23.2

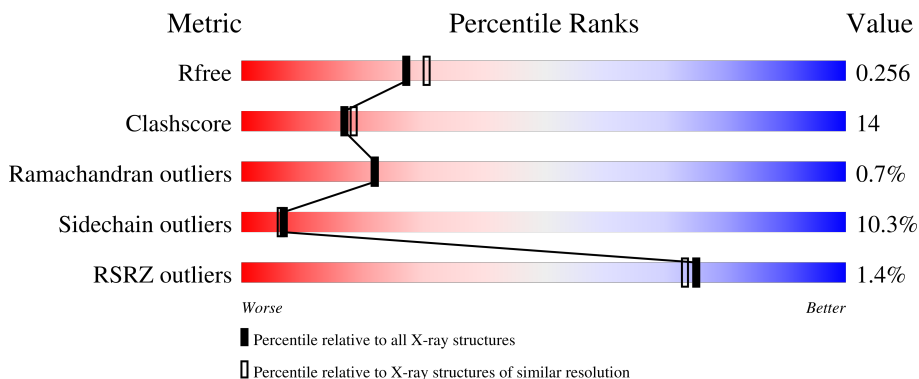
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	411	
1	B	411	

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
2	GOL	A	901	-	-	X	-
2	GOL	A	902	-	-	X	-
2	GOL	A	905	-	X	-	-
2	GOL	A	907	-	-	X	-
2	GOL	A	911	-	-	X	-
2	GOL	A	914	-	-	X	-
2	GOL	B	908	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7031 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 Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3044	1920	533	578	13	0	0	0
1	B	403	3040	1918	532	577	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASN	ASP	engineered mutation	UNP P12281
B	142	ASN	ASP	engineered mutation	UNP P12281

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

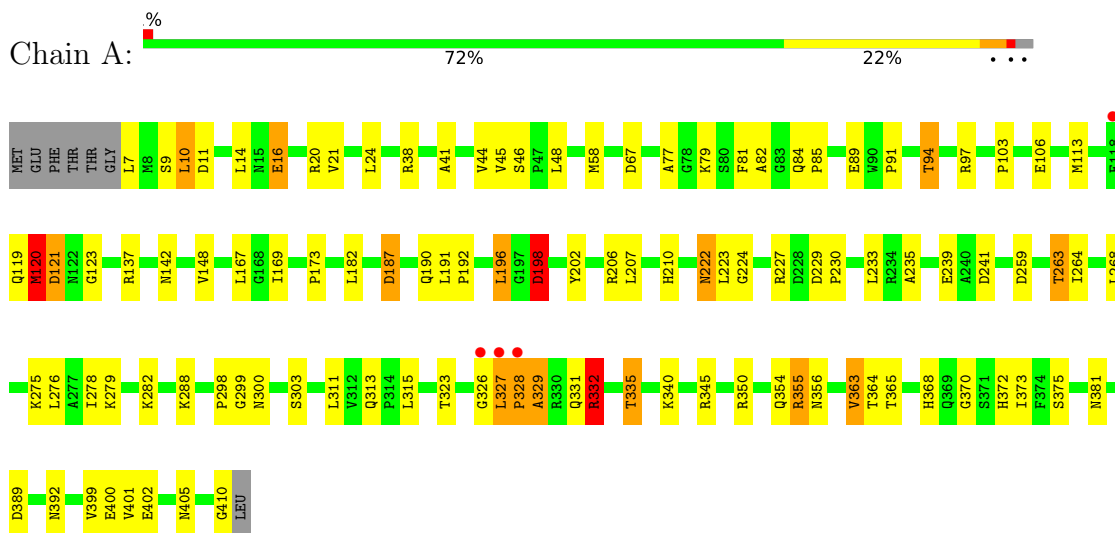
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	438	Total O 438 438	0	0
3	B	401	Total O 401 401	0	0

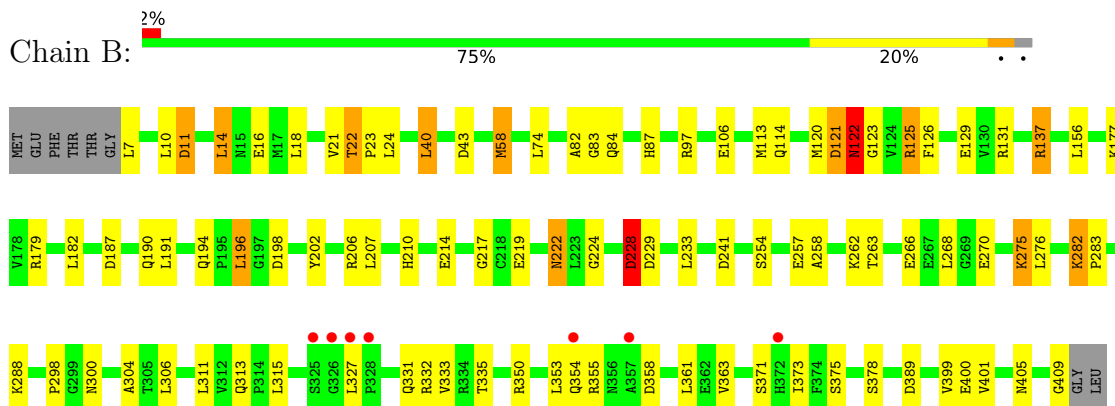
### 3 Residue-property plots [i](#)

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: Molybdopterin biosynthesis protein moeA



- Molecule 1: Molybdopterin biosynthesis protein moeA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.28Å 100.08Å 102.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.20 39.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.64-2.20) 98.8 (39.01-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.162 , 0.253 0.172 , 0.256	Depositor DCC
$R_{free}$ test set	1981 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

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	0.89	0/3103	1.04	12/4217 (0.3%)
1	B	0.95	5/3099 (0.2%)	1.03	12/4212 (0.3%)
All	All	0.92	5/6202 (0.1%)	1.04	24/8429 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLU	CD-OE1	8.27	1.34	1.25
1	B	275	LYS	CD-CE	6.32	1.67	1.51
1	B	214	GLU	CG-CD	5.97	1.60	1.51
1	B	258	ALA	CA-CB	5.08	1.63	1.52
1	B	122	ASN	CB-CG	5.02	1.62	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ASP	CB-CG-OD1	9.43	126.79	118.30
1	A	389	ASP	CB-CG-OD2	9.02	126.41	118.30
1	B	11	ASP	CB-CG-OD2	7.98	125.48	118.30
1	B	275	LYS	CD-CE-NZ	7.82	129.69	111.70
1	B	198	ASP	CB-CG-OD2	7.73	125.26	118.30
1	A	332	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	121	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	259	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	363	VAL	CB-CA-C	-7.31	97.50	111.40
1	A	241	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	198	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	187	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	43	ASP	CB-CG-OD2	6.73	124.36	118.30
1	B	229	ASP	CB-CG-OD2	6.73	124.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	B	358	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	409	GLY	CA-C-O	-6.48	108.94	120.60
1	A	67	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	121	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	241	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	120	MET	CA-CB-CG	5.51	122.66	113.30
1	B	214	GLU	CA-CB-CG	5.48	125.47	113.40
1	A	38	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	335	THR	CB-CA-C	-5.05	97.96	111.60

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	3044	0	3042	88	0
1	B	3040	0	3039	76	0
2	A	78	0	103	43	1
2	B	30	0	40	10	0
3	A	438	0	0	24	3
3	B	401	0	0	18	4
All	All	7031	0	6224	173	5

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 14.

All (173) 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)
2:A:901:GOL:H32	1:B:84:GLN:NE2	1.47	1.26
1:A:187:ASP:OD2	2:A:902:GOL:H2	1.44	1.15
2:B:909:GOL:H32	3:B:987:HOH:O	1.52	1.08
1:B:7:LEU:N	3:B:1050:HOH:O	1.82	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:OD1	2:A:901:GOL:H2	1.54	1.07
1:A:375:SER:HB3	2:A:914:GOL:H12	1.42	1.02
1:B:228:ASP:HB3	3:B:1306:HOH:O	1.60	1.00
2:A:902:GOL:H31	3:A:1007:HOH:O	1.59	1.00
2:A:901:GOL:C3	1:B:84:GLN:NE2	2.23	1.00
1:B:228:ASP:OD2	2:B:908:GOL:H32	1.68	0.94
1:A:44:VAL:HA	2:A:911:GOL:H32	1.49	0.93
2:A:901:GOL:H32	1:B:84:GLN:HE21	1.15	0.91
2:B:909:GOL:C3	3:B:987:HOH:O	2.10	0.91
1:B:363:VAL:HG21	1:B:401:VAL:HG21	1.53	0.90
2:A:902:GOL:C3	3:A:1007:HOH:O	2.17	0.89
1:B:120:MET:HB2	1:B:122:ASN:HD21	1.37	0.89
1:B:120:MET:HB2	1:B:122:ASN:ND2	1.86	0.89
1:A:375:SER:HB3	2:A:914:GOL:C1	2.05	0.87
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.19	0.86
1:A:190:GLN:HE21	1:A:191:LEU:H	1.22	0.85
2:A:901:GOL:H32	1:B:84:GLN:HE22	1.40	0.85
1:B:120:MET:CB	1:B:122:ASN:HD21	1.90	0.84
1:A:300:ASN:HD22	1:A:303:SER:H	1.28	0.81
3:A:1346:HOH:O	1:B:375:SER:HB3	1.81	0.80
1:B:270:GLU:HB3	3:B:1172:HOH:O	1.81	0.79
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.30	0.78
2:A:901:GOL:C3	1:B:84:GLN:HE21	1.91	0.78
1:A:375:SER:CB	2:A:914:GOL:H12	2.14	0.77
1:A:229:ASP:HB3	2:A:918:GOL:H32	1.67	0.76
1:B:378:SER:O	2:B:909:GOL:H2	1.86	0.75
1:B:187:ASP:HB3	3:B:1072:HOH:O	1.89	0.73
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.36	0.72
2:A:901:GOL:H11	3:A:1332:HOH:O	1.88	0.72
1:B:120:MET:CB	1:B:122:ASN:ND2	2.49	0.72
1:A:239:GLU:OE2	2:A:907:GOL:H2	1.89	0.72
1:B:378:SER:O	3:B:987:HOH:O	2.09	0.71
1:B:190:GLN:HE21	1:B:191:LEU:H	1.37	0.71
1:A:79:LYS:HE2	1:A:81:PHE:CE2	2.26	0.70
1:A:263:THR:HG21	3:A:1342:HOH:O	1.91	0.70
1:B:389:ASP:OD2	3:B:1197:HOH:O	2.09	0.70
1:A:187:ASP:OD1	2:A:901:GOL:C2	2.38	0.70
2:A:917:GOL:C1	3:A:1132:HOH:O	2.39	0.70
2:A:917:GOL:H11	3:A:1132:HOH:O	1.91	0.69
1:B:187:ASP:OD2	2:B:908:GOL:H11	1.92	0.69
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HD13	2:A:911:GOL:H31	1.76	0.68
2:A:902:GOL:O2	1:B:82:ALA:O	2.13	0.67
1:A:120:MET:O	1:A:121:ASP:HB2	1.95	0.67
1:A:323:THR:HA	2:A:910:GOL:H32	1.75	0.67
1:A:91:PRO:HD2	1:A:94:THR:HG21	1.77	0.65
1:B:266:GLU:O	3:B:1222:HOH:O	2.12	0.65
1:A:21:VAL:HG21	1:A:315:LEU:HD11	1.79	0.65
1:A:235:ALA:HB1	2:A:907:GOL:H31	1.79	0.65
2:A:901:GOL:C1	3:A:1332:HOH:O	2.41	0.64
2:B:903:GOL:O1	3:B:1132:HOH:O	2.06	0.64
1:B:121:ASP:O	1:B:122:ASN:HB3	1.99	0.62
1:A:187:ASP:CG	2:A:902:GOL:H2	2.19	0.61
1:A:331:GLN:HE22	1:B:331:GLN:HE22	1.48	0.61
1:B:300:ASN:ND2	1:B:371:SER:HB2	2.15	0.60
2:A:901:GOL:C3	1:B:84:GLN:HE22	2.04	0.60
1:A:355:ARG:NH2	1:B:400:GLU:OE2	2.33	0.60
1:A:400:GLU:OE2	1:B:355:ARG:NH2	2.35	0.59
1:A:229:ASP:HB2	1:A:230:PRO:HD2	1.85	0.58
1:A:375:SER:CA	2:A:914:GOL:H12	2.34	0.57
1:A:210:HIS:HD2	1:A:222:ASN:OD1	1.87	0.57
2:A:905:GOL:H32	3:A:943:HOH:O	2.02	0.57
1:B:228:ASP:OD2	2:B:908:GOL:C3	2.48	0.57
1:B:363:VAL:HG21	1:B:401:VAL:CG2	2.31	0.57
2:A:917:GOL:H12	3:A:1132:HOH:O	2.04	0.57
1:A:10:LEU:CD2	1:A:311:LEU:HD21	2.35	0.56
1:B:222:ASN:HD22	1:B:224:GLY:H	1.54	0.56
1:A:227:ARG:HG2	1:A:229:ASP:OD2	2.07	0.55
1:B:332:ARG:HG3	1:B:332:ARG:HH11	1.71	0.55
1:A:381:ASN:HD22	2:A:912:GOL:C1	2.20	0.55
1:A:364:THR:HG22	1:A:365:THR:O	2.07	0.55
1:A:230:PRO:HB3	1:A:264:ILE:HD11	1.90	0.54
1:B:333:VAL:HG13	1:B:361:LEU:O	2.08	0.54
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.73	0.54
1:A:192:PRO:HD2	3:A:976:HOH:O	2.07	0.53
1:A:190:GLN:HE21	1:A:191:LEU:N	2.00	0.53
1:A:206:ARG:HD2	1:A:222:ASN:HD21	1.73	0.53
1:A:222:ASN:HD22	1:A:224:GLY:H	1.55	0.53
1:B:353:LEU:HD13	1:B:363:VAL:HG22	1.90	0.53
1:B:300:ASN:HB2	3:B:1100:HOH:O	2.09	0.53
1:B:206:ARG:HH11	1:B:222:ASN:ND2	2.00	0.52
1:B:21:VAL:HG21	1:B:315:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:N	3:A:1039:HOH:O	2.42	0.52
1:B:58:MET:SD	1:B:113:MET:HE2	2.50	0.51
1:A:7:LEU:N	3:A:1079:HOH:O	2.44	0.50
1:A:77:ALA:HB2	1:A:94:THR:CG2	2.42	0.50
1:B:254:SER:HA	1:B:257:GLU:OE1	2.12	0.50
1:B:7:LEU:HD23	3:B:995:HOH:O	2.11	0.49
1:A:223:LEU:HD12	1:A:223:LEU:N	2.28	0.49
1:A:16:GLU:O	1:A:20:ARG:HG2	2.11	0.49
1:A:196:LEU:HD13	1:A:202:TYR:CZ	2.48	0.49
1:B:196:LEU:HD13	1:B:202:TYR:CZ	2.48	0.49
1:A:381:ASN:HD22	2:A:912:GOL:H11	1.78	0.49
1:A:235:ALA:O	2:A:907:GOL:H32	2.12	0.48
1:A:279:LYS:HD2	1:A:345:ARG:NH2	2.28	0.48
1:A:328:PRO:O	1:A:329:ALA:HB3	2.13	0.48
1:B:262:LYS:HE2	3:B:1301:HOH:O	2.12	0.48
1:A:375:SER:HB3	2:A:914:GOL:H11	1.94	0.48
1:A:142:ASN:CG	1:B:373:ILE:HG22	2.34	0.48
1:A:239:GLU:OE2	2:A:907:GOL:C1	2.62	0.48
1:A:368:HIS:CD2	1:A:370:GLY:H	2.32	0.48
1:A:85:PRO:HG3	1:A:103:PRO:HG2	1.95	0.47
1:A:77:ALA:HB2	1:A:94:THR:HG23	1.97	0.47
1:A:206:ARG:HH11	1:A:222:ASN:ND2	2.08	0.47
1:B:282:LYS:HB3	1:B:283:PRO:HD3	1.97	0.47
1:A:402:GLU:HG2	3:A:1126:HOH:O	2.14	0.47
1:B:298:PRO:O	1:B:304:ALA:HB2	2.14	0.47
1:A:46:SER:OG	1:A:167:LEU:HD22	2.15	0.47
1:B:74:LEU:HD12	1:B:126:PHE:CE1	2.49	0.47
1:B:306:LEU:C	1:B:306:LEU:HD13	2.35	0.47
1:A:368:HIS:CD2	1:A:372:HIS:HE1	2.33	0.46
1:B:120:MET:HB3	1:B:122:ASN:HD21	1.73	0.46
2:A:902:GOL:H12	2:A:906:GOL:H12	1.97	0.46
1:A:328:PRO:CG	1:A:329:ALA:H	2.28	0.46
1:B:121:ASP:O	1:B:122:ASN:CB	2.63	0.46
1:A:45:VAL:H	2:A:911:GOL:H2	1.81	0.46
1:A:7:LEU:HD12	3:A:1336:HOH:O	2.15	0.46
1:A:278:ILE:O	1:A:345:ARG:HD2	2.16	0.45
1:A:148:VAL:HG23	1:A:148:VAL:O	2.16	0.45
1:B:120:MET:HB3	1:B:122:ASN:ND2	2.29	0.45
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.09	0.45
1:B:300:ASN:ND2	1:B:371:SER:CB	2.80	0.45
1:A:327:LEU:C	1:A:327:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:HE2	3:A:1189:HOH:O	2.16	0.44
1:B:137:ARG:NH1	3:B:1206:HOH:O	2.51	0.44
1:A:410:GLY:O	3:A:1275:HOH:O	2.21	0.44
1:A:239:GLU:OE2	2:A:907:GOL:C2	2.64	0.44
1:B:177:LYS:HD3	1:B:217:GLY:O	2.18	0.44
1:B:206:ARG:NH1	1:B:222:ASN:HD21	1.99	0.44
1:B:210:HIS:HD2	1:B:222:ASN:OD1	2.00	0.44
1:B:40:LEU:HD13	1:B:156:LEU:HD11	2.00	0.44
1:A:82:ALA:HB3	2:B:908:GOL:O2	2.18	0.43
1:A:198:ASP:O	3:A:1208:HOH:O	2.21	0.43
1:A:340:LYS:HA	1:A:392:ASN:OD1	2.18	0.43
1:A:298:PRO:HG3	3:A:1076:HOH:O	2.18	0.43
1:A:120:MET:HB2	1:A:123:GLY:O	2.19	0.43
1:B:353:LEU:CD1	1:B:363:VAL:HG22	2.48	0.43
1:A:326:GLY:CA	3:A:965:HOH:O	2.66	0.43
1:B:22:THR:HA	1:B:23:PRO:HD3	1.92	0.43
1:B:14:LEU:HD22	1:B:18:LEU:HG	2.01	0.43
1:B:122:ASN:HD22	1:B:123:GLY:N	2.17	0.43
1:A:328:PRO:CD	1:A:329:ALA:H	2.32	0.43
1:B:125:ARG:HG3	3:B:1007:HOH:O	2.19	0.42
1:A:356:ASN:C	1:A:356:ASN:OD1	2.57	0.42
1:B:257:GLU:H	1:B:257:GLU:CD	2.22	0.42
1:A:82:ALA:C	2:B:908:GOL:O2	2.52	0.42
1:A:120:MET:O	1:A:121:ASP:CB	2.64	0.42
1:A:45:VAL:HG22	1:A:148:VAL:HG12	2.00	0.42
1:A:223:LEU:N	1:A:223:LEU:CD1	2.83	0.41
1:A:313:GLN:HE22	1:A:405:ASN:ND2	2.09	0.41
1:B:14:LEU:HG	1:B:311:LEU:HD23	2.02	0.41
1:B:187:ASP:CG	2:B:908:GOL:H11	2.40	0.41
1:B:363:VAL:CG2	1:B:401:VAL:HG21	2.38	0.41
1:A:41:ALA:HB3	1:A:173:PRO:HB2	2.01	0.41
1:B:74:LEU:HD12	1:B:126:PHE:HE1	1.86	0.41
1:B:129:GLU:CG	3:B:1201:HOH:O	2.68	0.41
1:A:192:PRO:CD	3:A:976:HOH:O	2.67	0.41
3:A:1167:HOH:O	1:B:87:HIS:HD2	2.04	0.41
1:A:187:ASP:OD1	2:A:901:GOL:C3	2.68	0.41
1:B:125:ARG:CG	3:B:1007:HOH:O	2.69	0.41
1:B:179:ARG:NH2	1:B:219:GLU:OE1	2.54	0.41
2:A:901:GOL:O1	1:B:83:GLY:O	2.37	0.41
2:A:906:GOL:O1	3:A:1200:HOH:O	2.06	0.41
1:A:381:ASN:ND2	2:A:912:GOL:H11	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:O	2:A:904:GOL:H31	2.21	0.40
1:B:129:GLU:HG2	3:B:1201:HOH:O	2.21	0.40
1:A:137:ARG:HD2	3:A:1095:HOH:O	2.21	0.40
1:A:229:ASP:CB	2:A:918:GOL:H32	2.45	0.40
1:A:300:ASN:ND2	1:A:303:SER:H	2.06	0.40

All (5) 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)
2:A:911:GOL:O2	3:A:1261:HOH:O[4_465]	1.78	0.42
3:B:981:HOH:O	3:B:1316:HOH:O[1_545]	1.93	0.27
3:B:943:HOH:O	3:B:1243:HOH:O[3_645]	2.06	0.14
3:A:1073:HOH:O	3:B:1269:HOH:O[3_545]	2.16	0.04
3:A:1029:HOH:O	3:B:1027:HOH:O[3_545]	2.18	0.02

## 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	402/411 (98%)	390 (97%)	8 (2%)	4 (1%)	15	14
1	B	401/411 (98%)	387 (96%)	12 (3%)	2 (0%)	29	31
All	All	803/822 (98%)	777 (97%)	20 (2%)	6 (1%)	22	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	282	LYS
1	A	328	PRO
1	B	122	ASN

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Mol	Chain	Res	Type
1	B	282	LYS
1	A	329	ALA

### 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	325/331 (98%)	290 (89%)	35 (11%)	6	6
1	B	325/331 (98%)	293 (90%)	32 (10%)	8	7
All	All	650/662 (98%)	583 (90%)	67 (10%)	7	6

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	LEU
1	A	11	ASP
1	A	14	LEU
1	A	16	GLU
1	A	24	LEU
1	A	48	LEU
1	A	58	MET
1	A	84	GLN
1	A	89	GLU
1	A	94	THR
1	A	97	ARG
1	A	106	GLU
1	A	113	MET
1	A	119	GLN
1	A	120	MET
1	A	182	LEU
1	A	196	LEU
1	A	207	LEU
1	A	222	ASN
1	A	233	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	263	THR
1	A	268	LEU
1	A	276	LEU
1	A	288	LYS
1	A	327	LEU
1	A	332	ARG
1	A	335	THR
1	A	350	ARG
1	A	354	GLN
1	A	355	ARG
1	A	363	VAL
1	A	373	ILE
1	A	399	VAL
1	A	401	VAL
1	B	10	LEU
1	B	11	ASP
1	B	14	LEU
1	B	16	GLU
1	B	22	THR
1	B	24	LEU
1	B	40	LEU
1	B	58	MET
1	B	97	ARG
1	B	106	GLU
1	B	114	GLN
1	B	122	ASN
1	B	125	ARG
1	B	131	ARG
1	B	137	ARG
1	B	182	LEU
1	B	194	GLN
1	B	196	LEU
1	B	207	LEU
1	B	222	ASN
1	B	228	ASP
1	B	233	LEU
1	B	263	THR
1	B	268	LEU
1	B	275	LYS
1	B	276	LEU
1	B	288	LYS
1	B	327	LEU

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Mol	Chain	Res	Type
1	B	335	THR
1	B	350	ARG
1	B	354	GLN
1	B	399	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	84	GLN
1	A	190	GLN
1	A	210	HIS
1	A	222	ASN
1	A	300	ASN
1	A	313	GLN
1	A	368	HIS
1	B	15	ASN
1	B	34	GLN
1	B	84	GLN
1	B	122	ASN
1	B	135	ASN
1	B	190	GLN
1	B	210	HIS
1	B	222	ASN
1	B	243	GLN
1	B	300	ASN
1	B	313	GLN
1	B	331	GLN
1	B	368	HIS

### 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](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	916	-	5,5,5	0.50	0	5,5,5	0.32	0
2	GOL	A	905	-	5,5,5	1.06	0	5,5,5	2.03	2 (40%)
2	GOL	A	917	-	5,5,5	0.51	0	5,5,5	0.58	0
2	GOL	A	904	-	5,5,5	0.58	0	5,5,5	0.99	0
2	GOL	A	906	-	5,5,5	0.48	0	5,5,5	0.77	0
2	GOL	A	907	-	5,5,5	0.79	0	5,5,5	1.77	2 (40%)
2	GOL	A	911	-	5,5,5	0.60	0	5,5,5	1.41	1 (20%)
2	GOL	A	918	-	5,5,5	0.55	0	5,5,5	0.78	0
2	GOL	B	903	-	5,5,5	0.54	0	5,5,5	0.55	0
2	GOL	A	910	-	5,5,5	0.38	0	5,5,5	0.43	0
2	GOL	A	912	-	5,5,5	0.37	0	5,5,5	0.21	0
2	GOL	B	908	1	5,5,5	0.65	0	5,5,5	1.02	0
2	GOL	A	902	-	5,5,5	2.04	1 (20%)	5,5,5	0.98	0
2	GOL	B	909	-	5,5,5	0.73	0	5,5,5	0.40	0
2	GOL	B	913	-	5,5,5	0.71	0	5,5,5	1.39	1 (20%)
2	GOL	A	915	-	5,5,5	0.40	0	5,5,5	0.19	0
2	GOL	A	901	-	5,5,5	1.72	1 (20%)	5,5,5	0.92	0
2	GOL	A	914	-	5,5,5	0.45	0	5,5,5	1.46	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	916	-	-	2/4/4/4	-
2	GOL	A	905	-	-	4/4/4/4	-
2	GOL	A	917	-	-	4/4/4/4	-
2	GOL	A	904	-	-	2/4/4/4	-
2	GOL	A	906	-	-	2/4/4/4	-
2	GOL	A	907	-	-	0/4/4/4	-
2	GOL	A	911	-	-	1/4/4/4	-
2	GOL	A	918	-	-	2/4/4/4	-
2	GOL	B	903	-	-	4/4/4/4	-
2	GOL	A	910	-	-	4/4/4/4	-
2	GOL	A	912	-	-	2/4/4/4	-
2	GOL	B	908	1	-	2/4/4/4	-
2	GOL	A	902	-	-	2/4/4/4	-
2	GOL	B	909	-	-	4/4/4/4	-
2	GOL	B	913	-	-	2/4/4/4	-
2	GOL	A	915	-	-	4/4/4/4	-
2	GOL	A	901	-	-	2/4/4/4	-
2	GOL	A	914	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	GOL	O2-C2	-4.42	1.30	1.43
2	A	901	GOL	C3-C2	-3.55	1.37	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	905	GOL	O3-C3-C2	3.66	127.73	110.20
2	A	907	GOL	O1-C1-C2	2.88	124.02	110.20
2	A	914	GOL	O1-C1-C2	2.77	123.47	110.20
2	A	911	GOL	O3-C3-C2	2.55	122.41	110.20
2	A	905	GOL	O2-C2-C3	2.37	119.55	109.12
2	B	913	GOL	O2-C2-C1	-2.08	99.95	109.12
2	A	907	GOL	O2-C2-C1	2.06	118.18	109.12

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-C3
2	A	902	GOL	C1-C2-C3-O3
2	A	902	GOL	O2-C2-C3-O3
2	A	904	GOL	C1-C2-C3-O3
2	A	905	GOL	C1-C2-C3-O3
2	A	905	GOL	O2-C2-C3-O3
2	A	910	GOL	C1-C2-C3-O3
2	A	910	GOL	O2-C2-C3-O3
2	A	911	GOL	O1-C1-C2-C3
2	A	914	GOL	O1-C1-C2-O2
2	A	918	GOL	O1-C1-C2-C3
2	B	903	GOL	O1-C1-C2-O2
2	B	903	GOL	O1-C1-C2-C3
2	B	903	GOL	C1-C2-C3-O3
2	B	908	GOL	O1-C1-C2-C3
2	B	909	GOL	C1-C2-C3-O3
2	B	916	GOL	C1-C2-C3-O3
2	A	915	GOL	O1-C1-C2-O2
2	A	917	GOL	O1-C1-C2-O2
2	B	909	GOL	O1-C1-C2-O2
2	B	909	GOL	O2-C2-C3-O3
2	A	905	GOL	O1-C1-C2-C3
2	A	910	GOL	O1-C1-C2-C3
2	A	912	GOL	O1-C1-C2-C3
2	A	914	GOL	O1-C1-C2-C3
2	A	915	GOL	O1-C1-C2-C3
2	A	915	GOL	C1-C2-C3-O3
2	A	917	GOL	O1-C1-C2-C3
2	A	917	GOL	C1-C2-C3-O3
2	B	909	GOL	O1-C1-C2-C3
2	B	913	GOL	O1-C1-C2-C3
2	A	901	GOL	O1-C1-C2-O2
2	A	905	GOL	O1-C1-C2-O2
2	A	910	GOL	O1-C1-C2-O2
2	A	912	GOL	O1-C1-C2-O2
2	A	915	GOL	O2-C2-C3-O3
2	B	908	GOL	O1-C1-C2-O2
2	B	916	GOL	O2-C2-C3-O3
2	A	904	GOL	O2-C2-C3-O3
2	A	906	GOL	C1-C2-C3-O3
2	B	913	GOL	O1-C1-C2-O2
2	A	917	GOL	O2-C2-C3-O3
2	A	918	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	903	GOL	O2-C2-C3-O3
2	A	914	GOL	O2-C2-C3-O3
2	A	906	GOL	O2-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	905	GOL	1	0
2	A	917	GOL	3	0
2	A	904	GOL	1	0
2	A	906	GOL	2	0
2	A	907	GOL	5	0
2	A	911	GOL	3	1
2	A	918	GOL	2	0
2	B	903	GOL	1	0
2	A	910	GOL	1	0
2	A	912	GOL	3	0
2	B	908	GOL	6	0
2	A	902	GOL	6	0
2	B	909	GOL	3	0
2	A	901	GOL	12	0
2	A	914	GOL	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	404/411 (98%)	-0.58	4 (0%) 82 81	11, 20, 35, 57	0
1	B	403/411 (98%)	-0.52	7 (1%) 70 68	9, 20, 38, 63	0
All	All	807/822 (98%)	-0.55	11 (1%) 75 73	9, 20, 36, 63	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	LEU	7.3
1	A	327	LEU	4.8
1	B	326	GLY	4.3
1	B	357	ALA	3.5
1	A	328	PRO	3.4
1	B	328	PRO	3.4
1	B	325	SER	3.0
1	A	326	GLY	2.8
1	A	118	GLU	2.2
1	B	372	HIS	2.2
1	B	354	GLN	2.2

### 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(Å <sup>2</sup> )	Q<0.9
2	GOL	A	907	6/6	0.78	0.18	26,30,32,35	0
2	GOL	B	916	6/6	0.78	0.24	55,56,57,58	0
2	GOL	A	911	6/6	0.81	0.15	37,41,43,46	0
2	GOL	A	914	6/6	0.82	0.30	36,41,43,47	0
2	GOL	A	905	6/6	0.82	0.17	24,28,31,33	0
2	GOL	A	915	6/6	0.83	0.34	49,49,51,51	0
2	GOL	B	909	6/6	0.84	0.13	46,47,48,49	0
2	GOL	A	901	6/6	0.84	0.20	7,19,23,24	0
2	GOL	A	917	6/6	0.85	0.27	40,48,50,52	0
2	GOL	B	908	6/6	0.86	0.30	39,40,40,44	0
2	GOL	B	913	6/6	0.87	0.18	21,33,36,39	0
2	GOL	A	912	6/6	0.88	0.13	43,45,46,48	0
2	GOL	A	910	6/6	0.88	0.28	44,45,45,47	0
2	GOL	A	918	6/6	0.89	0.16	31,38,41,42	0
2	GOL	A	906	6/6	0.90	0.13	38,43,44,46	0
2	GOL	A	902	6/6	0.91	0.16	14,16,25,25	0
2	GOL	A	904	6/6	0.91	0.14	15,25,27,34	0
2	GOL	B	903	6/6	0.95	0.18	30,36,37,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.