



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:39 pm BST

PDB ID : 5JXX  
Title : Crystal structure of UDP-N-acetylglucosamine O-acyltransferase (LpxA) from *Moraxella catarrhalis* RH4.  
Authors : Pratap, S.; Kesari, P.; Yadav, R.; Narwal, M.; Dev, A.; Kumar, P.  
Deposited on : 2016-05-13  
Resolution : 3.00 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 : 2.11  
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) : 2.11

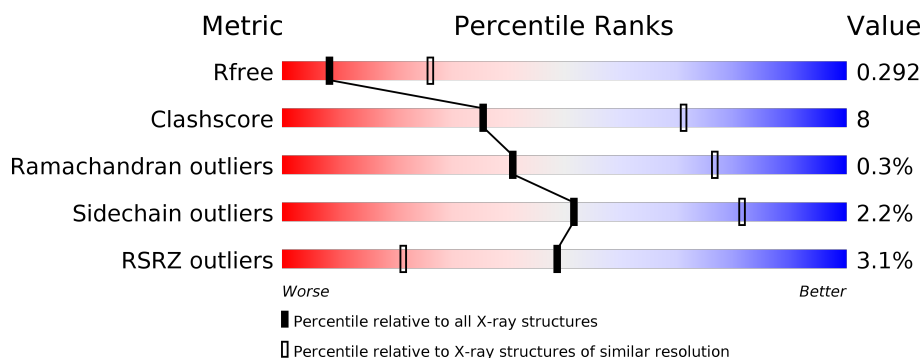
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	257	<div> <div>81%</div> <div>18%</div> <div>•</div> </div>
1	B	257	<div> <div>3%</div> <div>79%</div> <div>20%</div> <div>•</div> </div>
1	C	257	<div> <div>79%</div> <div>21%</div> </div>
1	D	257	<div> <div>76%</div> <div>23%</div> <div>•</div> </div>
1	E	257	<div> <div>6%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>
1	F	257	<div> <div>9%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>

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	B	302	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11891 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 Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase.

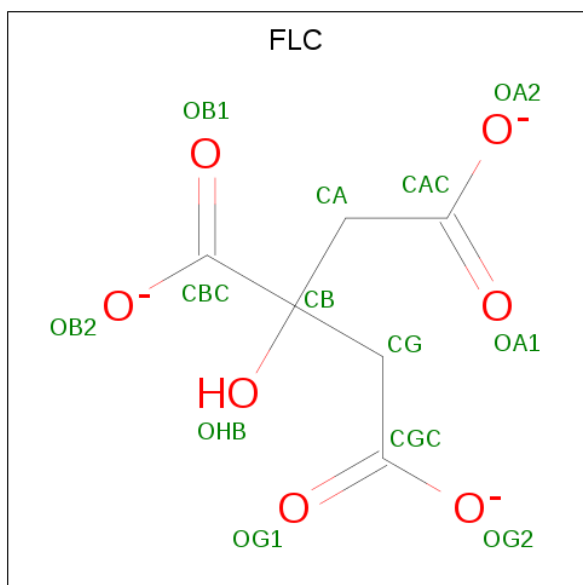
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1964	1221	365	368	10			
1	B	256	Total	C	N	O	S	0	1	0
			1956	1217	361	367	11			
1	C	257	Total	C	N	O	S	0	0	0
			1964	1221	365	368	10			
1	D	257	Total	C	N	O	S	0	0	0
			1964	1221	365	368	10			
1	E	256	Total	C	N	O	S	0	1	0
			1960	1220	363	367	10			
1	F	256	Total	C	N	O	S	0	0	0
			1950	1212	361	367	10			

- 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	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		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $\text{C}_6\text{H}_5\text{O}_7$ ).



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

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

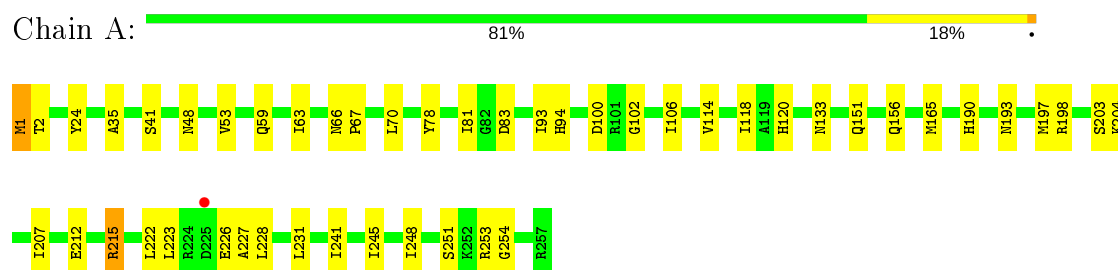
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	7	Total	O	0	0
			7	7		
4	C	7	Total	O	0	0
			7	7		
4	D	7	Total	O	0	0
			7	7		
4	E	5	Total	O	0	0
			5	5		
4	F	5	Total	O	0	0
			5	5		

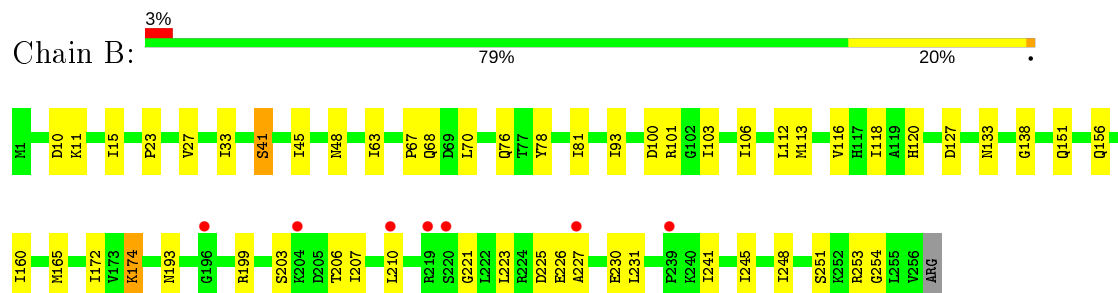
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

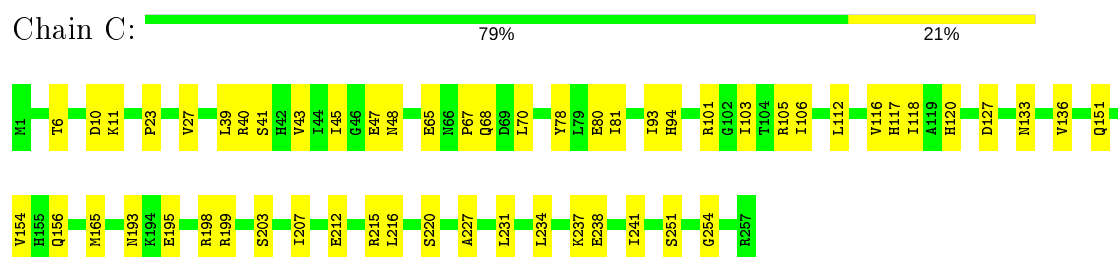
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



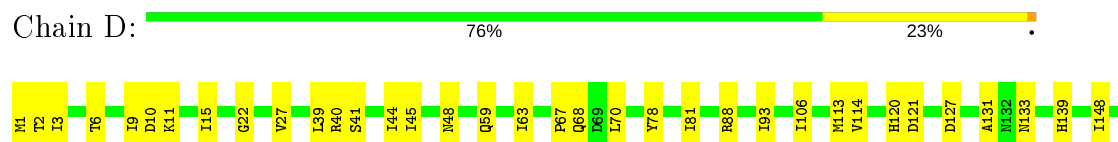
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

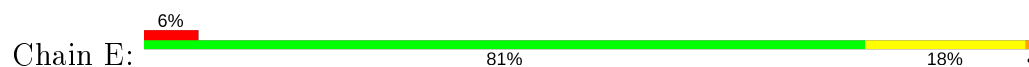


- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

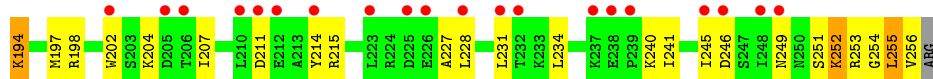
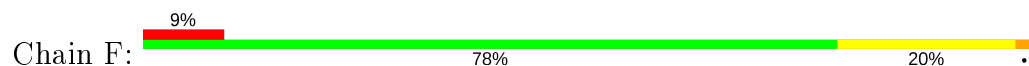




- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.61Å 136.90Å 90.58Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	45.39 – 3.00 45.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	78.3 (45.39-3.00) 78.4 (45.39-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.235 , 0.293 0.237 , 0.292	Depositor DCC
$R_{free}$ test set	1508 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 27.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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

### 5.1 Standard geometry

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

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	0.24	0/1993	0.48	0/2691
1	B	0.24	0/1988	0.46	0/2685
1	C	0.24	0/1993	0.47	0/2691
1	D	0.25	0/1993	0.48	0/2691
1	E	0.24	0/1993	0.46	0/2692
1	F	0.25	0/1979	0.48	0/2673
All	All	0.24	0/11939	0.47	0/16123

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	1964	0	1981	33	0
1	B	1956	0	1973	34	0
1	C	1964	0	1981	34	0
1	D	1964	0	1981	43	0
1	E	1960	0	1975	28	0
1	F	1950	0	1959	37	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	16	0	0
2	C	12	0	16	0	0
2	D	18	0	24	0	0
2	E	12	0	16	0	0
2	F	6	0	8	0	0
3	A	13	0	5	1	0
3	B	13	0	5	2	0
4	A	10	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	11891	0	11948	192	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 8.

All (192) 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:153:GLY:HA3	1:F:151:GLN:HE22	1.48	0.78
1:E:40:ARG:HG3	1:E:41:SER:H	1.54	0.72
1:C:27:VAL:HG22	1:C:45:ILE:HD13	1.72	0.70
1:C:23:PRO:HD2	1:C:41:SER:HB3	1.74	0.69
1:A:66:ASN:O	1:E:88:ARG:NH2	2.26	0.69
1:A:156:GLN:O	1:A:253:ARG:NH1	2.26	0.68
1:B:68:GLN:HE21	1:D:88:ARG:HG3	1.57	0.68
1:D:27:VAL:HG22	1:D:45:ILE:HD13	1.76	0.67
1:D:245:ILE:HA	1:D:248:ILE:HD12	1.77	0.66
1:F:175:ASP:O	1:F:255:LEU:HD13	1.96	0.66
1:A:83:ASP:OD1	1:B:76:GLN:NE2	2.29	0.65
1:F:158:CYS:SG	1:F:253:ARG:NH1	2.70	0.64
1:E:203:SER:O	1:E:206:THR:OG1	2.16	0.64
1:B:245:ILE:HA	1:B:248:ILE:HD12	1.81	0.63
1:F:48:ASN:HB3	1:F:78:TYR:CD2	2.35	0.62
1:D:224:ARG:NH2	1:D:248:ILE:O	2.33	0.61
1:E:245:ILE:HA	1:E:248:ILE:HD12	1.83	0.60
1:F:81:ILE:HG23	1:F:106:ILE:HD11	1.85	0.59
1:B:10:ASP:OD1	1:B:11:LYS:N	2.35	0.59
1:F:175:ASP:O	1:F:255:LEU:CD1	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ILE:HG23	1:B:106:ILE:HD11	1.84	0.58
1:C:10:ASP:OD1	1:C:11:LYS:N	2.36	0.58
1:D:6:THR:O	1:F:24:TYR:OH	2.22	0.57
1:D:203:SER:O	1:D:206:THR:HG22	2.04	0.57
1:A:222:LEU:HB3	1:A:226:GLU:HG3	1.86	0.57
1:C:81:ILE:HG23	1:C:106:ILE:HD11	1.86	0.56
1:B:76:GLN:H	1:B:76:GLN:CD	2.09	0.56
1:A:190:HIS:HA	3:A:302:FLC:HG1	1.87	0.56
1:D:209:ALA:O	1:D:212:GLU:HG3	2.06	0.55
1:D:81:ILE:HG23	1:D:106:ILE:HD11	1.88	0.55
1:F:255:LEU:HD12	1:F:256:VAL:H	1.70	0.55
1:C:251:SER:OG	1:C:254:GLY:O	2.25	0.55
1:D:215:ARG:HA	1:D:219:ARG:HG3	1.88	0.55
1:F:246:ASP:HA	1:F:249:ASN:ND2	2.22	0.55
1:A:165:MET:HB2	1:A:193:ASN:ND2	2.21	0.55
1:A:81:ILE:HG23	1:A:106:ILE:HD11	1.88	0.55
1:C:227:ALA:O	1:C:231:LEU:HD12	2.07	0.55
1:A:228:LEU:HD21	1:A:245:ILE:HG23	1.89	0.54
1:F:204:LYS:O	1:F:207:ILE:HG13	2.07	0.54
1:D:44:ILE:HG21	1:F:59:GLN:NE2	2.22	0.54
1:B:165:MET:HB2	1:B:193:ASN:ND2	2.23	0.53
1:B:78:TYR:HB2	1:B:103:ILE:HG13	1.89	0.53
1:D:22:GLY:HA3	1:D:40:ARG:O	2.08	0.53
1:A:227:ALA:O	1:A:231:LEU:HD12	2.08	0.53
1:F:27:VAL:HA	1:F:45:ILE:HB	1.91	0.53
1:B:81:ILE:HG12	1:B:106:ILE:HG12	1.91	0.52
1:A:35:ALA:H	1:A:53:VAL:HG12	1.75	0.52
1:D:10:ASP:OD1	1:D:11:LYS:N	2.42	0.52
1:C:165:MET:HB2	1:C:193:ASN:ND2	2.24	0.52
1:D:227:ALA:O	1:D:231:LEU:HD12	2.10	0.52
1:B:203:SER:O	1:B:206:THR:HG22	2.10	0.52
1:D:44:ILE:HG13	1:F:59:GLN:HE21	1.74	0.52
1:F:173:VAL:O	1:F:253:ARG:NH1	2.43	0.52
1:E:58:TYR:HD2	1:E:88:ARG:HD2	1.75	0.52
1:D:216:LEU:HD23	1:D:222:LEU:HD21	1.92	0.52
1:C:48:ASN:HB3	1:C:78:TYR:CD2	2.45	0.51
1:C:212:GLU:HG2	1:C:215:ARG:HH12	1.75	0.51
1:D:121:ASP:HB2	1:D:139:HIS:HD2	1.75	0.51
1:E:81:ILE:HG23	1:E:106:ILE:HD11	1.92	0.51
1:B:226:GLU:O	1:B:230:GLU:HG2	2.11	0.51
1:B:203:SER:O	1:B:207:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:OG	1:A:254:GLY:O	2.28	0.50
1:C:234:LEU:HB3	1:C:241:ILE:HD13	1.91	0.50
1:A:231:LEU:HD23	1:A:241:ILE:HG23	1.94	0.50
1:D:121:ASP:HB2	1:D:139:HIS:CD2	2.46	0.50
1:D:203:SER:O	1:D:207:ILE:HG13	2.11	0.50
1:E:63:ILE:HD12	1:E:93:ILE:HD12	1.94	0.50
1:D:67:PRO:HB3	1:D:120:HIS:HB3	1.94	0.50
1:A:1:MET:SD	1:A:2:THR:HG23	2.51	0.49
1:A:245:ILE:HA	1:A:248:ILE:HD12	1.93	0.49
1:A:48:ASN:HB3	1:A:78:TYR:CD2	2.47	0.49
1:C:40:ARG:O	1:C:41:SER:OG	2.18	0.49
1:B:210:LEU:HD23	1:B:241:ILE:HD13	1.94	0.49
1:C:93:ILE:HG23	1:C:118:ILE:HB	1.94	0.49
1:C:238:GLU:HB3	1:C:241:ILE:HD12	1.95	0.49
1:E:103:ILE:HG21	1:E:105:ARG:HH21	1.78	0.49
1:B:100:ASP:OD1	1:B:101:ARG:NH1	2.45	0.49
1:D:238:GLU:HB3	1:D:241:ILE:HD12	1.94	0.49
1:E:251:SER:OG	1:E:254:GLY:O	2.30	0.49
1:E:78:TYR:HB2	1:E:103:ILE:HG13	1.94	0.49
1:C:231:LEU:HD23	1:C:241:ILE:HG23	1.94	0.48
1:B:23:PRO:O	1:B:41:SER:HA	2.14	0.48
1:B:48:ASN:HB3	1:B:78:TYR:CD2	2.47	0.48
1:F:67:PRO:HB3	1:F:120:HIS:HB3	1.94	0.48
1:A:114:VAL:HG23	1:C:68:GLN:NE2	2.29	0.48
1:A:133:ASN:HB2	1:A:151:GLN:HG2	1.95	0.48
1:D:68:GLN:NE2	1:F:114:VAL:HG23	2.29	0.48
1:B:63:ILE:HD12	1:B:93:ILE:HD12	1.95	0.48
1:D:223:LEU:HB2	1:D:226:GLU:HG2	1.96	0.48
1:D:48:ASN:HB3	1:D:78:TYR:CD2	2.48	0.48
1:C:81:ILE:HG12	1:C:106:ILE:HG12	1.96	0.47
1:A:67:PRO:HB3	1:A:120:HIS:HB3	1.95	0.47
1:B:223:LEU:HD23	1:B:225:ASP:H	1.79	0.47
1:A:81:ILE:HG12	1:A:106:ILE:HG12	1.96	0.47
1:F:35:ALA:O	1:F:53:VAL:HG23	2.14	0.47
1:F:227:ALA:O	1:F:231:LEU:HD12	2.15	0.47
1:B:227:ALA:O	1:B:231:LEU:HD12	2.15	0.47
1:D:9:ILE:HG23	1:D:27:VAL:HB	1.97	0.47
1:A:197:MET:SD	1:A:207:ILE:HG23	2.55	0.47
1:E:67:PRO:HB3	1:E:120:HIS:HB3	1.97	0.47
1:A:63:ILE:HD12	1:A:93:ILE:HD12	1.97	0.46
1:A:114:VAL:HG23	1:C:68:GLN:HE22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:LEU:HD11	1:F:245:ILE:HG23	1.96	0.46
1:F:194:LYS:O	1:F:198:ARG:CB	2.64	0.46
1:F:234:LEU:HB3	1:F:241:ILE:HD13	1.98	0.46
1:C:151:GLN:NE2	1:E:133:ASN:O	2.47	0.46
1:D:63:ILE:HD12	1:D:93:ILE:HD12	1.97	0.46
1:B:251:SER:OG	1:B:254:GLY:O	2.34	0.46
1:F:67:PRO:HG3	1:F:95:ARG:O	2.16	0.46
1:E:48:ASN:HB3	1:E:78:TYR:CD2	2.51	0.45
1:A:223:LEU:HD23	1:A:226:GLU:HG2	1.97	0.45
1:B:174:LYS:HD3	1:B:253:ARG:O	2.17	0.45
1:F:150:GLY:O	1:F:151:GLN:HG2	2.16	0.45
1:C:195:GLU:O	1:C:198:ARG:HG2	2.16	0.45
1:D:39:LEU:CD2	1:D:45:ILE:HD11	2.45	0.45
1:D:9:ILE:HG21	1:D:15:ILE:HD11	1.98	0.45
1:F:192:LEU:HD13	1:F:214:TYR:HB2	1.97	0.45
1:E:112:LEU:HG	1:E:116:VAL:HG11	1.97	0.45
1:E:27:VAL:HA	1:E:45:ILE:HB	1.98	0.45
1:A:41:SER:O	1:A:59:GLN:HA	2.17	0.45
1:B:112:LEU:HG	1:B:116:VAL:HG11	1.98	0.45
1:A:35:ALA:N	1:A:53:VAL:HG12	2.31	0.44
1:D:81:ILE:HG12	1:D:106:ILE:HG12	1.97	0.44
1:B:27:VAL:HA	1:B:45:ILE:HB	1.99	0.44
1:F:252:LYS:HB3	1:F:252:LYS:HE3	1.77	0.44
1:C:112:LEU:HG	1:C:116:VAL:HG11	1.99	0.44
1:C:39:LEU:HB3	1:C:43:VAL:HG21	1.99	0.44
1:B:156:GLN:OE1	3:B:303:FLC:HG1	2.17	0.44
1:D:197:MET:SD	1:D:207:ILE:HG23	2.58	0.44
1:D:44:ILE:HG21	1:F:59:GLN:HE21	1.83	0.44
1:B:138:GLY:H	3:B:303:FLC:HOB	1.62	0.44
1:C:47:GLU:HG2	1:C:48:ASN:CG	2.38	0.44
1:D:113:MET:SD	1:D:131:ALA:HA	2.58	0.44
1:E:133:ASN:HB2	1:E:151:GLN:HG2	2.00	0.44
1:D:41:SER:O	1:D:59:GLN:HA	2.18	0.44
1:E:100:ASP:C	1:E:102:GLY:H	2.20	0.44
1:C:78:TYR:HB2	1:C:103:ILE:HG13	2.00	0.43
1:C:80:GLU:HB2	1:C:105:ARG:HD2	2.00	0.43
1:F:63:ILE:HD12	1:F:93:ILE:HD12	1.99	0.43
1:A:94:HIS:HE1	1:E:89:GLU:OE2	2.02	0.43
1:B:68:GLN:HE22	1:D:114:VAL:HG23	1.84	0.43
1:F:112:LEU:HG	1:F:116:VAL:HG11	1.99	0.43
1:C:216:LEU:O	1:C:220:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:HIS:HD2	1:E:253:ARG:NH2	2.17	0.43
1:E:203:SER:O	1:E:207:ILE:HG12	2.19	0.43
1:F:252:LYS:HE3	1:F:253:ARG:HG2	2.00	0.43
1:C:203:SER:O	1:C:207:ILE:HG13	2.18	0.43
1:A:203:SER:O	1:A:207:ILE:HG13	2.19	0.43
1:B:67:PRO:HB3	1:B:120:HIS:HB3	2.00	0.43
1:A:24:TYR:OH	1:C:6:THR:O	2.35	0.43
1:E:234:LEU:HB3	1:E:241:ILE:HD13	2.01	0.43
1:A:100:ASP:C	1:A:102:GLY:H	2.21	0.43
1:A:198:ARG:HE	1:A:198:ARG:HB2	1.52	0.42
1:C:65:GLU:HB3	1:C:94:HIS:HD2	1.83	0.42
1:C:133:ASN:HB2	1:C:151:GLN:HG2	1.99	0.42
1:B:160:ILE:HD11	1:B:172:ILE:HG21	2.00	0.42
1:D:113:MET:HB3	1:D:113:MET:HE2	1.64	0.42
1:E:216:LEU:O	1:E:220:SER:OG	2.38	0.42
1:E:79:LEU:HD12	1:E:104:THR:O	2.20	0.42
1:A:212:GLU:OE2	1:A:215:ARG:NH1	2.53	0.42
1:C:117:HIS:O	1:C:136:VAL:HG12	2.20	0.42
1:C:237:LYS:N	1:C:237:LYS:HD2	2.34	0.42
1:D:216:LEU:HD11	1:D:230:GLU:HB3	2.02	0.42
1:F:81:ILE:HG12	1:F:106:ILE:HG12	2.02	0.42
1:A:253:ARG:HB3	1:A:253:ARG:HE	1.68	0.42
1:A:93:ILE:HG23	1:A:118:ILE:HB	2.02	0.42
1:D:234:LEU:HB3	1:D:241:ILE:HD13	2.02	0.42
1:B:93:ILE:HG23	1:B:118:ILE:HB	2.02	0.42
1:C:67:PRO:HB3	1:C:120:HIS:HB3	2.01	0.42
1:D:148:ILE:HA	1:D:166:VAL:HB	2.02	0.42
1:D:1:MET:C	1:D:3:ILE:H	2.23	0.42
1:C:195:GLU:O	1:C:199:ARG:HG2	2.20	0.41
1:F:179:TYR:OH	1:F:240:LYS:HG3	2.20	0.41
1:B:68:GLN:NE2	1:D:114:VAL:HG23	2.34	0.41
1:B:113:MET:SD	1:F:68:GLN:NE2	2.93	0.41
1:D:231:LEU:HD23	1:D:241:ILE:HG23	2.01	0.41
1:E:10:ASP:OD2	1:E:12:SER:OG	2.30	0.41
1:F:211:ASP:OD2	1:F:215:ARG:NH2	2.53	0.41
1:E:193:ASN:O	1:E:197:MET:HG2	2.21	0.41
1:F:251:SER:OG	1:F:254:GLY:O	2.38	0.41
1:D:204:LYS:HD3	1:D:204:LYS:H	1.84	0.41
1:F:49:THR:HG23	1:F:79:LEU:HD23	2.03	0.41
1:B:15:ILE:HD12	1:B:33:ILE:HD12	2.03	0.41
1:F:65:GLU:HB3	1:F:94:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HD23	1:B:241:ILE:HG23	2.03	0.41
1:E:88:ARG:NH1	1:E:89:GLU:OE1	2.54	0.41
1:C:136:VAL:HG23	1:C:154:VAL:HB	2.03	0.41
1:D:133:ASN:HB2	1:D:151:GLN:HG2	2.02	0.40
1:F:197:MET:HB2	1:F:202:TRP:CD2	2.56	0.40
1:B:133:ASN:HB2	1:B:151:GLN:HG2	2.04	0.40
1:E:100:ASP:O	1:E:102:GLY:N	2.55	0.40
1:E:82:GLY:HA3	1:E:108:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
1	B	255/257 (99%)	244 (96%)	9 (4%)	2 (1%)	19	57
1	C	255/257 (99%)	246 (96%)	8 (3%)	1 (0%)	34	72
1	D	255/257 (99%)	245 (96%)	8 (3%)	2 (1%)	19	57
1	E	255/257 (99%)	242 (95%)	13 (5%)	0	100	100
1	F	254/257 (99%)	240 (94%)	14 (6%)	0	100	100
All	All	1529/1542 (99%)	1463 (96%)	61 (4%)	5 (0%)	41	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	221	GLY
1	B	41	SER
1	C	101	ARG
1	D	2	THR
1	B	221	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	210/210 (100%)	206 (98%)	4 (2%)	57	84
1	B	210/210 (100%)	206 (98%)	4 (2%)	57	84
1	C	210/210 (100%)	207 (99%)	3 (1%)	67	88
1	D	210/210 (100%)	206 (98%)	4 (2%)	57	84
1	E	210/210 (100%)	202 (96%)	8 (4%)	33	69
1	F	208/210 (99%)	202 (97%)	6 (3%)	42	76
All	All	1258/1260 (100%)	1229 (98%)	29 (2%)	52	80

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	70	LEU
1	A	204	LYS
1	A	215	ARG
1	B	70	LEU
1	B	127	ASP
1	B	174	LYS
1	B	199	ARG
1	C	70	LEU
1	C	127	ASP
1	C	156	GLN
1	D	70	LEU
1	D	127	ASP
1	D	204	LYS
1	D	212	GLU
1	E	70	LEU
1	E	159	ARG
1	E	190[A]	HIS
1	E	190[B]	HIS
1	E	193	ASN
1	E	199	ARG
1	E	200	LYS

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Mol	Chain	Res	Type
1	E	253	ARG
1	F	59	GLN
1	F	70	LEU
1	F	159	ARG
1	F	194	LYS
1	F	252	LYS
1	F	255	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	B	68	GLN
1	C	68	GLN
1	D	42	HIS
1	D	68	GLN
1	D	94	HIS
1	D	133	ASN
1	D	151	GLN
1	F	151	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	D	302	-	5,5,5	0.36	0	5,5,5	0.30	0
2	GOL	B	302	-	5,5,5	0.36	0	5,5,5	0.23	0
2	GOL	D	301	-	5,5,5	0.37	0	5,5,5	0.35	0
2	GOL	F	301	-	5,5,5	0.36	0	5,5,5	0.26	0
2	GOL	E	301	-	5,5,5	0.38	0	5,5,5	0.21	0
2	GOL	B	301	-	5,5,5	0.36	0	5,5,5	0.25	0
2	GOL	A	301	-	5,5,5	0.37	0	5,5,5	0.29	0
2	GOL	C	301	-	5,5,5	0.38	0	5,5,5	0.31	0
2	GOL	E	302	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	C	302	-	5,5,5	0.36	0	5,5,5	0.29	0
3	FLC	A	302	-	3,12,12	1.38	0	3,17,17	2.81	2 (66%)
2	GOL	D	303	-	5,5,5	0.36	0	5,5,5	0.31	0
3	FLC	B	303	-	3,12,12	1.37	0	3,17,17	2.81	2 (66%)

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	D	302	-	-	2/4/4/4	-
2	GOL	B	302	-	-	2/4/4/4	-
2	GOL	D	301	-	-	0/4/4/4	-
2	GOL	F	301	-	-	0/4/4/4	-
2	GOL	E	301	-	-	1/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	E	302	-	-	2/4/4/4	-
2	GOL	C	302	-	-	1/4/4/4	-
3	FLC	A	302	-	-	1/6/16/16	-
2	GOL	D	303	-	-	2/4/4/4	-
3	FLC	B	303	-	-	1/6/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	FLC	CB-CA-CAC	-3.47	109.43	114.98
3	B	303	FLC	CB-CA-CAC	-3.45	109.46	114.98
3	B	303	FLC	CB-CG-CGC	-3.44	109.48	114.98
3	A	302	FLC	CB-CG-CGC	-3.42	109.50	114.98

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	302	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-C3
2	E	302	GOL	O1-C1-C2-C3
2	D	302	GOL	C1-C2-C3-O3
2	A	301	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-C3
2	C	302	GOL	O1-C1-C2-C3
2	D	303	GOL	O1-C1-C2-C3
2	B	302	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-O2
2	E	302	GOL	O1-C1-C2-O2
2	D	302	GOL	O2-C2-C3-O3
2	C	301	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-O2
2	D	303	GOL	O1-C1-C2-O2
3	B	303	FLC	OHB-CB-CG-CGC
3	A	302	FLC	OHB-CB-CG-CGC
2	E	301	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	FLC	1	0
3	B	303	FLC	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	257/257 (100%)	-0.26	1 (0%) 92 79	21, 41, 70, 90	0
1	B	256/257 (99%)	-0.10	7 (2%) 54 26	21, 39, 92, 105	0
1	C	257/257 (100%)	-0.22	0 100 100	24, 40, 65, 79	0
1	D	257/257 (100%)	-0.34	1 (0%) 92 79	21, 40, 69, 90	0
1	E	256/257 (99%)	-0.01	15 (5%) 22 7	27, 49, 97, 112	0
1	F	256/257 (99%)	0.18	23 (8%) 9 3	31, 55, 107, 121	0
All	All	1539/1542 (99%)	-0.12	47 (3%) 49 21	21, 44, 91, 121	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	214	TYR	4.4
1	E	206	THR	4.0
1	F	249	ASN	3.8
1	E	210	LEU	3.6
1	F	211	ASP	3.3
1	F	212	GLU	3.2
1	E	203	SER	3.0
1	F	192	LEU	3.0
1	E	207	ILE	2.9
1	E	216	LEU	2.8
1	F	179	TYR	2.8
1	F	205	ASP	2.7
1	F	225	ASP	2.6
1	F	237	LYS	2.6
1	B	220	SER	2.6
1	F	245	ILE	2.5
1	B	210	LEU	2.5
1	F	226	GLU	2.5
1	B	196	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	2.5
1	F	248	ILE	2.5
1	E	232	THR	2.4
1	E	201	GLY	2.4
1	F	239	PRO	2.4
1	F	228	LEU	2.3
1	F	232	THR	2.3
1	E	211	ASP	2.2
1	F	246	ASP	2.2
1	B	239	PRO	2.2
1	F	191	GLY	2.2
1	D	236	GLU	2.2
1	B	204	LYS	2.1
1	F	202	TRP	2.1
1	E	212	GLU	2.1
1	E	233	LYS	2.1
1	F	210	LEU	2.1
1	E	179	TYR	2.1
1	B	219	ARG	2.1
1	E	241	ILE	2.1
1	F	223	LEU	2.1
1	E	208	LYS	2.1
1	E	199	ARG	2.0
1	F	206	THR	2.0
1	E	195	GLU	2.0
1	F	238	GLU	2.0
1	A	225	ASP	2.0
1	F	231	LEU	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 carbohydrates 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	B	302	6/6	0.68	0.56	57,72,79,80	0
2	GOL	B	301	6/6	0.83	0.21	58,64,66,73	0
2	GOL	E	302	6/6	0.83	0.26	47,51,71,76	0
2	GOL	D	302	6/6	0.86	0.13	37,54,66,71	0
3	FLC	B	303	13/13	0.90	0.23	23,46,66,69	0
2	GOL	C	302	6/6	0.92	0.20	31,43,44,58	0
2	GOL	D	301	6/6	0.92	0.34	26,32,38,39	0
2	GOL	F	301	6/6	0.94	0.24	31,33,38,45	0
3	FLC	A	302	13/13	0.94	0.14	48,54,64,76	0
2	GOL	D	303	6/6	0.94	0.19	42,45,51,51	0
2	GOL	E	301	6/6	0.94	0.38	18,33,38,39	0
2	GOL	A	301	6/6	0.95	0.28	29,33,37,46	0
2	GOL	C	301	6/6	0.96	0.23	24,28,29,30	0

## 6.5 Other polymers

There are no such residues in this entry.