



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 AM GMT

PDB ID : 2VXJ  
Title : CRYSTAL STRUCTURE OF PA-IL LECTIN COMPLEXED WITH AGAL13BGAL14GLC AT 1.9 Å RESOLUTION  
Authors : Blanchard, B.; Nurisso, A.; Hollville, E.; Tetaud, C.; Wiels, J.; Pokorna, M.; Wimmerova, M.; Varrot, A.; Imberty, A.  
Deposited on : 2008-07-04  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

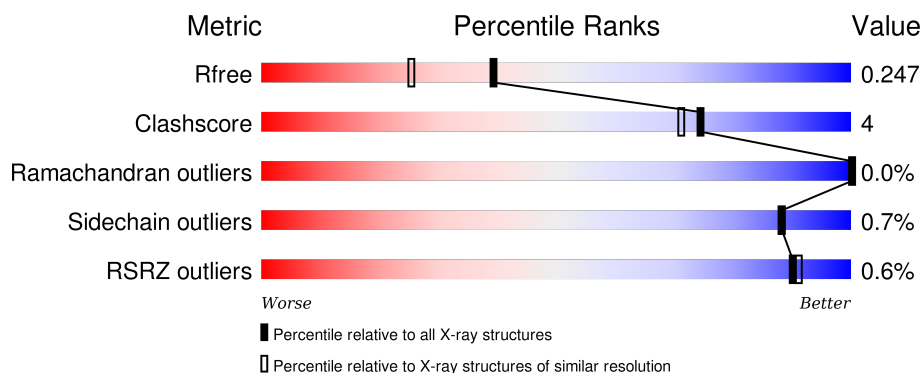
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.






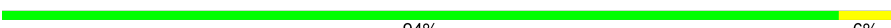









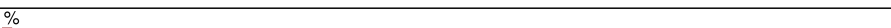





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	121	<div> <div>95%</div> <div>5%</div> </div>
1	B	121	<div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	C	121	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	D	121	<div> <div>91%</div> <div>7%</div> <div>..</div> </div>
1	E	121	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	121	 89% 11%
1	G	121	 87% 12% .
1	H	121	 91% 9%
1	I	121	 94% 6%
1	J	121	 87% 12% .
1	K	121	 91% 9%
1	L	121	 90% 9% .
1	M	121	 93% 7%
1	N	121	 95% . . .
1	O	121	 92% 8%
1	P	121	 88% 11% .
1	Q	121	 92% 8%
1	R	121	 94% 6%
1	S	121	 93% 7%
1	T	121	 92% 8%
1	U	121	 89% 11%
1	V	121	 87% 13%
1	W	121	 90% 10%
1	X	121	 91% 8% .

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
3	BGC	A	203	-	-	-	X
3	GLA	R	201	-	-	-	X
3	BGC	U	203	-	-	-	X
4	EDO	A	1122	-	-	-	X
4	EDO	D	1122	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	E	1122	-	-	-	X
4	EDO	H	1122	-	-	X	X
4	EDO	I	1122	-	-	X	X
4	EDO	L	1122	-	-	-	X
4	EDO	M	1122	-	-	-	X
4	EDO	M	1123	-	-	-	X
4	EDO	O	1122	-	-	-	X
4	EDO	Q	1122	-	-	-	X
4	EDO	S	1122	-	-	-	X
4	EDO	W	1122	-	-	-	X
4	EDO	X	1122	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25600 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 PA-I GALACTOPHILIC LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	B	118	Total	C	N	O	S	0	1	0
			886	558	152	173	3			
1	C	119	Total	C	N	O	S	0	0	0
			886	558	153	172	3			
1	D	120	Total	C	N	O	S	0	1	0
			899	567	155	174	3			
1	E	121	Total	C	N	O	S	0	1	0
			907	572	157	175	3			
1	F	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	G	121	Total	C	N	O	S	0	0	0
			897	564	155	175	3			
1	H	121	Total	C	N	O	S	0	2	0
			914	575	159	177	3			
1	I	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	J	120	Total	C	N	O	S	0	0	0
			894	562	155	174	3			
1	K	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	L	121	Total	C	N	O	S	0	1	0
			908	571	159	175	3			
1	M	121	Total	C	N	O	S	0	1	0
			906	570	157	176	3			
1	N	120	Total	C	N	O	S	0	0	0
			893	563	154	173	3			
1	O	121	Total	C	N	O	S	0	1	0
			907	571	156	177	3			
1	P	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	121	Total	C	N	O	S	0	1	0
			907	571	157	176	3			
1	R	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	S	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	T	121	Total	C	N	O	S	0	2	0
			910	573	156	178	3			
1	U	121	Total	C	N	O	S	0	1	0
			904	569	156	176	3			
1	V	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	W	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	X	121	Total	C	N	O	S	0	1	0
			907	571	156	177	3			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Ca	0	0
			1	1		
2	K	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	W	1	Total	Ca	0	0
			1	1		
2	N	1	Total	Ca	0	0
			1	1		
2	X	1	Total	Ca	0	0
			1	1		
2	S	1	Total	Ca	0	0
			1	1		
2	J	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	V	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	1	Total 1	Ca 1	0	0
2	M	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	I	1	Total 1	Ca 1	0	0
2	U	1	Total 1	Ca 1	0	0
2	L	1	Total 1	Ca 1	0	0
2	G	1	Total 1	Ca 1	0	0
2	Q	1	Total 1	Ca 1	0	0
2	H	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	T	1	Total 1	Ca 1	0	0
2	O	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 1	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	3	Total 34	C 18	O 16	0	0
3	B	3	Total 34	C 18	O 16	0	0
3	D	3	Total 34	C 18	O 16	0	0
3	F	3	Total 34	C 18	O 16	0	0
3	G	3	Total 34	C 18	O 16	0	0
3	H	3	Total 34	C 18	O 16	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	3	Total	C	O	0	0
			34	18	16		
3	J	3	Total	C	O	0	0
			34	18	16		
3	K	3	Total	C	O	0	0
			34	18	16		
3	L	3	Total	C	O	0	0
			34	18	16		
3	M	3	Total	C	O	0	0
			34	18	16		
3	O	3	Total	C	O	0	0
			34	18	16		
3	P	3	Total	C	O	0	0
			34	18	16		
3	Q	3	Total	C	O	0	0
			34	18	16		
3	R	3	Total	C	O	0	0
			34	18	16		
3	S	3	Total	C	O	0	0
			34	18	16		
3	T	3	Total	C	O	0	0
			34	18	16		
3	U	3	Total	C	O	0	0
			34	18	16		
3	V	3	Total	C	O	0	0
			34	18	16		
3	W	3	Total	C	O	0	0
			34	18	16		
3	X	3	Total	C	O	0	0
			34	18	16		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	N	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	C	O	0	0
			4	2	2		
4	U	1	Total	C	O	0	0
			4	2	2		
4	V	1	Total	C	O	0	0
			4	2	2		
4	W	1	Total	C	O	0	0
			4	2	2		
4	W	1	Total	C	O	0	0
			4	2	2		
4	X	1	Total	C	O	0	0
			4	2	2		

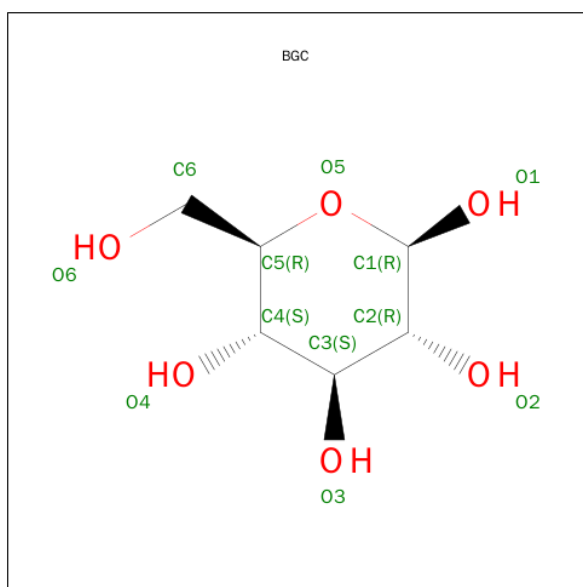
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	3	Total	C	O	0	0
			34	18	16		
5	E	3	Total	C	O	0	0
			34	18	16		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	N	2	Total	C	O	0	0
			22	12	10		

- Molecule 7 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	N	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	143	Total	O	0	0
			143	143		
8	B	119	Total	O	0	0
			119	119		
8	C	115	Total	O	0	0
			115	115		
8	D	124	Total	O	0	0
			124	124		
8	E	129	Total	O	0	0
			129	129		
8	F	113	Total	O	0	0
			113	113		
8	G	125	Total	O	0	0
			125	125		
8	H	139	Total	O	0	0
			139	139		
8	I	137	Total	O	0	0
			137	137		
8	J	122	Total	O	0	0
			122	122		
8	K	137	Total	O	0	0
			137	137		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	134	Total 134	O 134	0	0
8	M	122	Total 122	O 122	0	0
8	N	118	Total 118	O 118	0	0
8	O	107	Total 107	O 107	0	0
8	P	119	Total 119	O 119	0	0
8	Q	136	Total 136	O 136	0	0
8	R	125	Total 125	O 125	0	0
8	S	130	Total 130	O 130	0	0
8	T	138	Total 138	O 138	0	0
8	U	139	Total 139	O 139	0	0
8	V	122	Total 122	O 122	0	0
8	W	125	Total 125	O 125	0	0
8	X	128	Total 128	O 128	0	0

### 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 errors 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: PA-I GALACTOPHILIC LECTIN

Chain A: 




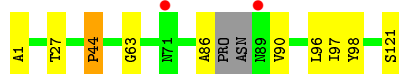
#### • Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain B: 



#### • Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain C: 



#### • Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain D: 




#### • Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain E: 

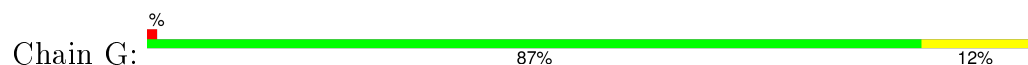


#### • Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain F: 



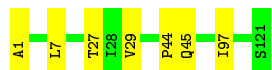
- Molecule 1: PA-I GALACTOPHILIC LECTIN



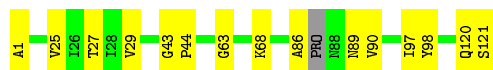
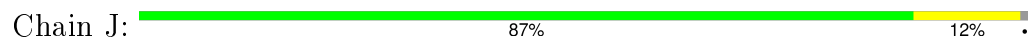
- Molecule 1: PA-I GALACTOPHILIC LECTIN



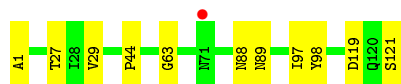
- Molecule 1: PA-I GALACTOPHILIC LECTIN



- Molecule 1: PA-I GALACTOPHILIC LECTIN



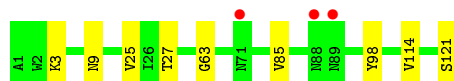
- Molecule 1: PA-I GALACTOPHILIC LECTIN



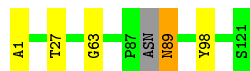
- Molecule 1: PA-I GALACTOPHILIC LECTIN



- Molecule 1: PA-I GALACTOPHILIC LECTIN





## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain N:  95% 

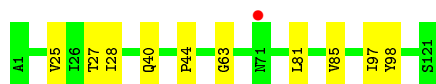
## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain O:  92% 8% 

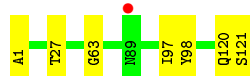
## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain P:  88% 11% 

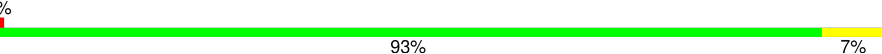
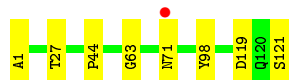

## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain Q:  92% 8% 

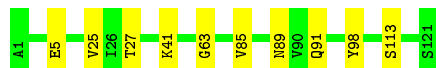
## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain R:  94% 6% 


## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain S:  93% 7% 

## ● Molecule 1: PA-I GALACTOPHILIC LECTIN


Chain T:  92% 8% 

## ● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain U:  89% 11%




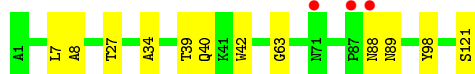
● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain V:  87% 13%




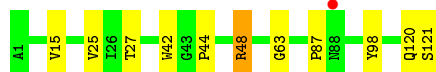
● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain W:  90% 10% 2%



● Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain X:  91% 8% 1%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.18Å 86.52Å 119.08Å 93.93° 98.16° 90.08°	Depositor
Resolution (Å)	55.00 – 1.90 48.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (55.00-1.90) 84.9 (48.96-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.245 0.190 , 0.247	Depositor DCC
$R_{free}$ test set	10734 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.966	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 213320 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.14 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8448e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: BGC, GLA, CA, GLC, EDO, GAL

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	0.80	0/924	0.73	0/1262
1	B	0.76	0/907	0.69	0/1236
1	C	0.75	0/907	0.74	0/1236
1	D	0.73	0/924	0.71	0/1260
1	E	0.78	0/933	0.72	0/1273
1	F	0.79	0/924	0.74	0/1262
1	G	0.78	0/920	0.74	0/1258
1	H	0.76	0/943	0.76	0/1287
1	I	0.81	0/924	0.71	0/1262
1	J	0.75	0/915	0.77	0/1247
1	K	0.75	0/924	0.72	0/1262
1	L	0.77	0/935	0.71	0/1276
1	M	0.74	0/932	0.73	0/1273
1	N	0.77	0/915	0.72	0/1248
1	O	0.77	0/933	0.72	0/1274
1	P	0.76	0/924	0.76	1/1262 (0.1%)
1	Q	0.77	0/933	0.75	0/1274
1	R	0.77	0/924	0.75	0/1262
1	S	0.76	0/924	0.73	0/1262
1	T	0.80	0/939	0.72	0/1282
1	U	0.75	0/930	0.72	0/1270
1	V	0.77	0/924	0.73	0/1262
1	W	0.79	0/924	0.72	0/1262
1	X	0.74	0/933	0.73	1/1274 (0.1%)
All	All	0.77	0/22215	0.73	2/30326 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	24	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	X	48	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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	901	0	861	6	0
1	B	886	0	844	7	0
1	C	886	0	847	9	0
1	D	899	0	862	10	0
1	E	907	0	874	4	0
1	F	901	0	861	8	0
1	G	897	0	850	14	0
1	H	914	0	878	11	0
1	I	901	0	861	7	0
1	J	894	0	853	12	0
1	K	901	0	861	9	0
1	L	908	0	870	10	0
1	M	906	0	867	9	0
1	N	893	0	854	5	0
1	O	907	0	867	9	0
1	P	901	0	861	13	0
1	Q	907	0	869	6	0
1	R	901	0	861	5	0
1	S	901	0	861	8	0
1	T	910	0	872	7	0
1	U	904	0	866	11	0
1	V	901	0	861	13	0
1	W	901	0	861	11	0
1	X	907	0	867	8	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	34	0	28	0	0
3	B	34	0	28	1	0
3	D	34	0	28	0	0
3	F	34	0	28	0	0
3	G	34	0	28	0	0
3	H	34	0	28	0	0
3	I	34	0	28	0	0
3	J	34	0	28	0	0
3	K	34	0	28	0	0
3	L	34	0	28	0	0
3	M	34	0	28	0	0
3	O	34	0	28	3	0
3	P	34	0	28	0	0
3	Q	34	0	29	0	0
3	R	34	0	28	0	0
3	S	34	0	28	0	0
3	T	34	0	28	0	0
3	U	34	0	28	0	0
3	V	34	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	34	0	28	0	0
3	X	34	0	28	0	0
4	A	4	0	6	1	0
4	D	4	0	6	1	0
4	E	4	0	6	1	0
4	H	8	0	12	8	0
4	I	8	0	11	6	0
4	L	4	0	6	1	0
4	M	8	0	12	2	0
4	N	4	0	6	0	0
4	O	4	0	6	1	0
4	Q	8	0	12	1	0
4	S	4	0	6	1	0
4	U	4	0	6	1	0
4	V	4	0	6	2	0
4	W	8	0	12	1	0
4	X	4	0	6	2	0
5	C	34	0	28	0	0
5	E	34	0	28	0	0
6	N	22	0	17	0	0
7	N	12	0	11	0	0
8	A	143	0	0	3	0
8	B	119	0	0	1	0
8	C	115	0	0	0	0
8	D	124	0	0	4	0
8	E	129	0	0	1	0
8	F	113	0	0	0	0
8	G	125	0	0	2	0
8	H	139	0	0	2	0
8	I	137	0	0	0	0
8	J	122	0	0	1	0
8	K	137	0	0	2	0
8	L	134	0	0	1	0
8	M	122	0	0	3	0
8	N	118	0	0	0	0
8	O	107	0	0	2	0
8	P	119	0	0	5	0
8	Q	136	0	0	1	0
8	R	125	0	0	0	0
8	S	130	0	0	2	0
8	T	138	0	0	2	0
8	U	139	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	122	0	0	1	0
8	W	125	0	0	4	0
8	X	128	0	0	2	0
All	All	25600	0	21481	177	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 4.

All (177) 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:H:44:PRO:HD2	4:H:1122:EDO:H22	1.45	0.98
3:O:202:GAL:H4	8:O:2104:HOH:O	1.78	0.82
1:W:88:ASN:HB2	8:W:2095:HOH:O	1.83	0.78
1:L:5:GLU:HG3	8:L:2005:HOH:O	1.83	0.78
1:G:53:GLN:HG2	1:G:101:VAL:HG21	1.67	0.77
1:U:49:GLU:HG2	8:U:2067:HOH:O	1.84	0.77
1:G:44:PRO:HD2	4:H:1122:EDO:H11	1.64	0.76
1:N:89:ASN:HD22	1:N:89:ASN:N	1.85	0.72
1:X:42:TRP:HB3	4:X:1122:EDO:H12	1.73	0.71
1:H:121:SER:OG	4:H:1123:EDO:H22	1.92	0.70
1:D:71:ASN:ND2	8:D:2078:HOH:O	2.26	0.68
1:P:15:VAL:HG22	8:P:2095:HOH:O	1.92	0.68
1:D:87:PRO:HG2	1:D:90:VAL:HG21	1.75	0.68
1:D:15:VAL:HG23	8:D:2026:HOH:O	1.96	0.66
1:M:121:SER:HA	8:M:2114:HOH:O	1.97	0.64
4:W:1122:EDO:H22	1:X:44:PRO:HD2	1.79	0.64
1:W:7:LEU:HD12	8:W:2011:HOH:O	1.98	0.64
1:I:45:GLN:HG3	4:I:1122:EDO:H11	1.79	0.63
1:S:44:PRO:HD2	4:S:1122:EDO:H11	1.79	0.63
1:J:86:ALA:HB1	1:J:90:VAL:HG22	1.81	0.62
1:I:45:GLN:CG	4:I:1122:EDO:H11	2.31	0.61
1:W:40:GLN:CG	1:W:42:TRP:CH2	2.84	0.61
8:W:2057:HOH:O	4:X:1122:EDO:H22	2.01	0.60
1:W:40:GLN:HG3	1:W:42:TRP:CH2	2.37	0.59
1:B:63:GLY:HA2	1:B:98:TYR:CZ	2.37	0.59
1:O:63:GLY:HA2	1:O:98:TYR:CZ	2.38	0.59
1:L:63:GLY:HA2	1:L:98:TYR:CZ	2.38	0.59
1:S:63:GLY:HA2	1:S:98:TYR:CZ	2.38	0.59
1:G:52:ASP:N	8:G:2063:HOH:O	2.29	0.58
1:C:27:THR:HG21	1:D:27:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:BGC:H1	8:B:2119:HOH:O	2.03	0.57
1:V:1:ALA:N	1:W:121:SER:OXT	2.30	0.57
1:E:1:ALA:N	1:H:121:SER:OXT	2.38	0.57
1:J:89:ASN:ND2	8:J:2100:HOH:O	2.36	0.57
1:M:121:SER:CA	8:M:2114:HOH:O	2.52	0.56
1:G:5:GLU:OE2	1:L:3:LYS:HE2	2.05	0.56
8:A:2106:HOH:O	1:C:121:SER:C	2.42	0.56
1:M:9:ASN:CG	4:M:1123:EDO:H11	2.25	0.56
1:W:27:THR:HG21	1:X:27:THR:HG21	1.88	0.56
1:L:25:VAL:HG22	1:L:85:VAL:CG2	2.36	0.56
1:I:44:PRO:HD2	4:I:1122:EDO:H21	1.88	0.55
1:K:88:ASN:HB2	8:K:2108:HOH:O	2.05	0.55
1:S:71:ASN:HB3	8:S:2085:HOH:O	2.04	0.55
1:W:40:GLN:HG2	1:W:42:TRP:CH2	2.42	0.54
1:R:120:GLN:HG2	1:S:119:ASP:HA	1.90	0.54
1:M:27:THR:HG21	1:N:27:THR:HG21	1.89	0.54
1:J:1:ALA:N	1:K:121:SER:OXT	2.33	0.54
1:W:40:GLN:HG3	1:W:42:TRP:CZ2	2.43	0.54
1:F:63:GLY:HA2	1:F:98:TYR:CZ	2.43	0.53
1:Q:44:PRO:HD2	4:Q:1122:EDO:H12	1.91	0.53
4:I:1122:EDO:H12	1:J:43:GLY:HA3	1.89	0.53
1:H:63:GLY:HA2	1:H:98:TYR:CZ	2.44	0.53
1:K:63:GLY:HA2	1:K:98:TYR:CZ	2.44	0.53
1:D:87:PRO:HG3	8:D:2013:HOH:O	2.07	0.53
1:V:71:ASN:OD1	4:V:1122:EDO:H12	2.09	0.53
1:S:71:ASN:CB	8:S:2085:HOH:O	2.57	0.52
1:Q:27:THR:HG21	1:R:27:THR:HG21	1.90	0.52
1:V:2:TRP:HD1	1:V:17:SER:HG	1.57	0.52
4:V:1122:EDO:H21	8:V:2122:HOH:O	2.08	0.52
1:V:63:GLY:HA2	1:V:98:TYR:CZ	2.45	0.52
1:R:121:SER:OXT	1:S:1:ALA:N	2.37	0.51
1:G:44:PRO:HD2	4:H:1122:EDO:C1	2.38	0.51
1:U:119:ASP:HA	1:X:120:GLN:HG2	1.92	0.51
1:R:63:GLY:HA2	1:R:98:TYR:CZ	2.46	0.51
1:N:89:ASN:N	1:N:89:ASN:ND2	2.57	0.51
1:O:44:PRO:HD2	4:O:1122:EDO:H21	1.93	0.50
1:L:25:VAL:HG22	1:L:85:VAL:HG22	1.91	0.50
1:E:63:GLY:HA2	1:E:98:TYR:CZ	2.46	0.50
1:K:88:ASN:OD1	1:K:89:ASN:ND2	2.45	0.50
1:X:15:VAL:HG22	8:X:2104:HOH:O	2.11	0.50
1:E:27:THR:HG21	1:F:27:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLY:HA2	1:G:98:TYR:CZ	2.46	0.50
1:X:87:PRO:HA	8:X:2097:HOH:O	2.12	0.49
1:U:29:VAL:HG22	1:V:29:VAL:HG22	1.94	0.49
1:W:63:GLY:HA2	1:W:98:TYR:CZ	2.48	0.49
1:H:79:THR:HG22	4:H:1122:EDO:H21	1.95	0.49
1:G:33:TRP:CZ3	1:H:48[A]:ARG:HD2	2.47	0.48
1:G:44:PRO:CD	4:H:1122:EDO:H11	2.38	0.48
1:G:15:VAL:HG12	8:G:2022:HOH:O	2.12	0.48
1:C:86:ALA:HB1	1:C:90:VAL:HG22	1.95	0.48
1:P:115:ASN:ND2	8:P:2110:HOH:O	2.46	0.48
1:M:63:GLY:HA2	1:M:98:TYR:CZ	2.49	0.48
1:N:1:ALA:N	1:O:121:SER:OXT	2.39	0.48
1:I:29:VAL:HG22	1:J:29:VAL:HG22	1.95	0.48
8:D:2079:HOH:O	1:P:68:LYS:NZ	2.47	0.47
4:E:1122:EDO:H22	1:F:44:PRO:HD2	1.96	0.47
1:P:68:LYS:HD2	8:P:2034:HOH:O	2.15	0.47
1:U:33:TRP:CE3	1:V:48:ARG:HD2	2.50	0.47
1:O:33:TRP:CE3	1:P:48:ARG:HD2	2.49	0.47
1:B:5:GLU:HG2	1:B:7:LEU:HD12	1.95	0.47
1:D:86:ALA:HB1	1:D:87:PRO:HD2	1.96	0.47
1:M:121:SER:C	8:M:2114:HOH:O	2.52	0.47
1:F:6:VAL:HG21	1:F:96:LEU:HB3	1.95	0.47
1:P:86:ALA:HB1	1:P:90:VAL:HG22	1.96	0.47
1:C:63:GLY:HA2	1:C:98:TYR:CZ	2.50	0.47
1:D:68:LYS:HE2	8:P:2074:HOH:O	2.15	0.47
1:I:27:THR:HG21	1:J:27:THR:HG21	1.96	0.47
1:R:1:ALA:N	1:S:121:SER:OXT	2.43	0.46
1:J:68:LYS:HG3	1:J:97:ILE:HD11	1.96	0.46
1:W:89:ASN:N	8:W:2095:HOH:O	2.40	0.46
1:T:25:VAL:HG22	1:T:85:VAL:HG22	1.97	0.46
1:G:41:LYS:HD2	8:H:2073:HOH:O	2.15	0.46
1:J:120:GLN:HG2	1:K:119:ASP:HA	1.96	0.46
1:K:44:PRO:HD2	4:L:1122:EDO:H11	1.96	0.46
1:Q:28:ILE:HD12	1:Q:81:LEU:HD12	1.97	0.46
1:P:63:GLY:HA2	1:P:98:TYR:CZ	2.50	0.46
1:U:27:THR:HG21	1:V:27:THR:HG21	1.96	0.46
1:G:55:LEU:CD2	1:G:100:ASP:HA	2.46	0.46
1:J:63:GLY:HA2	1:J:98:TYR:CZ	2.51	0.46
3:O:202:GAL:C4	8:O:2104:HOH:O	2.51	0.45
1:G:15:VAL:HG11	8:K:2108:HOH:O	2.15	0.45
1:O:107:ASN:ND2	3:O:201:GLA:O3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HD12	1:B:74:THR:HG21	1.99	0.45
1:H:15:VAL:HG22	8:H:2119:HOH:O	2.17	0.45
1:F:120:GLN:HG2	1:G:119:ASP:HA	1.99	0.45
1:M:3:LYS:HA	1:M:114:VAL:O	2.16	0.45
1:F:84:TRP:CH2	1:F:86:ALA:HA	2.51	0.45
1:V:25:VAL:HG22	1:V:85:VAL:HG22	1.99	0.45
1:I:7:LEU:HD23	4:I:1123:EDO:H11	1.98	0.45
1:W:8:ALA:HB2	1:W:34:ALA:HB1	1.99	0.45
8:A:2106:HOH:O	1:C:121:SER:CA	2.65	0.44
1:E:119:ASP:HA	1:H:120:GLN:HG2	2.00	0.44
1:M:25:VAL:HG22	1:M:85:VAL:HG22	1.99	0.44
1:M:9:ASN:ND2	4:M:1123:EDO:H11	2.32	0.44
1:L:48[B]:ARG:HH11	1:L:48[B]:ARG:HB2	1.82	0.44
1:H:44:PRO:CD	4:H:1122:EDO:H22	2.32	0.44
1:D:63:GLY:HA2	1:D:98:TYR:CZ	2.52	0.44
1:A:40:GLN:NE2	8:A:2055:HOH:O	2.41	0.44
1:V:1:ALA:HB1	1:V:116:ILE:O	2.18	0.44
1:X:25:VAL:HG23	1:X:121:SER:HB3	1.99	0.44
1:Q:25:VAL:HG22	1:Q:85:VAL:HG22	2.00	0.44
1:K:29:VAL:HG22	1:L:29:VAL:HG22	2.00	0.44
1:F:25:VAL:HG22	1:F:85:VAL:HG22	1.99	0.44
1:O:29:VAL:HG22	1:P:29:VAL:HG22	2.00	0.44
1:V:2:TRP:CZ2	1:V:4:GLY:HA3	2.53	0.44
1:O:27:THR:HG21	1:P:27:THR:HG21	1.99	0.44
1:C:86:ALA:HB1	1:C:90:VAL:CG2	2.47	0.43
1:U:69:ILE:HG12	1:U:94:ILE:HG12	2.00	0.43
1:X:63:GLY:HA2	1:X:98:TYR:CZ	2.53	0.43
1:L:8:ALA:HB2	1:L:34:ALA:HB1	2.00	0.43
1:J:121:SER:OXT	1:K:1:ALA:N	2.36	0.43
1:C:44:PRO:HD2	4:D:1122:EDO:H22	1.99	0.43
1:U:33:TRP:CZ3	1:V:48:ARG:HD2	2.53	0.43
1:T:5[A]:GLU:OE2	1:T:113[A]:SER:HB2	2.19	0.43
1:G:43:GLY:HA3	4:H:1122:EDO:H11	1.99	0.43
1:Q:63:GLY:HA2	1:Q:98:TYR:CZ	2.54	0.43
1:S:27:THR:HG21	1:T:27:THR:HG21	2.01	0.43
1:P:24:ASP:OD2	1:P:118:LYS:NZ	2.45	0.43
1:U:45:GLN:HG3	4:U:1122:EDO:H12	1.99	0.43
1:A:33:TRP:CZ3	1:B:48:ARG:HD2	2.54	0.43
1:B:121:SER:OXT	1:C:1:ALA:N	2.45	0.43
1:P:5:GLU:OE1	8:P:2004:HOH:O	2.22	0.43
1:V:69:ILE:HB	1:V:90:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:28:ILE:HG12	1:U:116:ILE:HG12	2.02	0.42
1:I:1:ALA:N	1:L:121:SER:OXT	2.40	0.42
1:J:25:VAL:HG23	1:J:121:SER:HB3	2.01	0.42
1:A:28:ILE:O	1:A:80:GLY:HA3	2.20	0.42
4:I:1122:EDO:H22	1:J:44:PRO:HD2	2.01	0.42
1:T:91:GLN:HG3	8:T:2041:HOH:O	2.18	0.42
1:Q:40[A]:GLN:NE2	8:Q:2057:HOH:O	2.25	0.42
1:A:44:PRO:HD2	4:A:1122:EDO:H21	2.02	0.42
1:O:33:TRP:CZ3	1:P:48:ARG:HD2	2.55	0.42
1:U:104:THR:HG22	8:U:2115:HOH:O	2.20	0.42
1:C:96:LEU:C	1:C:97:ILE:HG13	2.39	0.42
1:K:27:THR:HG21	1:L:27:THR:HG21	2.02	0.41
1:A:119:ASP:HA	1:D:120[B]:GLN:HG2	2.01	0.41
1:N:63:GLY:HA2	1:N:98:TYR:CZ	2.55	0.41
1:A:33:TRP:CE3	1:B:48:ARG:HD2	2.56	0.41
1:B:28:ILE:O	1:B:80:GLY:HA3	2.21	0.41
1:D:71:ASN:OD1	1:P:97:ILE:HD13	2.21	0.41
1:H:25:VAL:HG22	1:H:85:VAL:HG22	2.02	0.41
1:T:41:LYS:NZ	8:T:2060:HOH:O	2.40	0.41
1:H:102:PRO:HG2	1:T:89:ASN:O	2.21	0.41
1:U:48:ARG:HD2	1:V:33:TRP:CE3	2.55	0.41
8:E:2070:HOH:O	1:F:40:GLN:HG3	2.19	0.41
1:O:11:GLU:OE2	1:O:102:PRO:HA	2.21	0.41
1:T:63:GLY:HA2	1:T:98:TYR: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	119/121 (98%)	115 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	115/121 (95%)	112 (97%)	3 (3%)	0	100	100
1	C	115/121 (95%)	111 (96%)	4 (4%)	0	100	100
1	D	117/121 (97%)	114 (97%)	3 (3%)	0	100	100
1	E	120/121 (99%)	115 (96%)	5 (4%)	0	100	100
1	F	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
1	G	119/121 (98%)	114 (96%)	4 (3%)	1 (1%)	24	11
1	H	121/121 (100%)	118 (98%)	3 (2%)	0	100	100
1	I	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
1	J	116/121 (96%)	112 (97%)	4 (3%)	0	100	100
1	K	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
1	L	120/121 (99%)	117 (98%)	3 (2%)	0	100	100
1	M	120/121 (99%)	115 (96%)	5 (4%)	0	100	100
1	N	116/121 (96%)	113 (97%)	3 (3%)	0	100	100
1	O	120/121 (99%)	117 (98%)	3 (2%)	0	100	100
1	P	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
1	Q	120/121 (99%)	117 (98%)	3 (2%)	0	100	100
1	R	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
1	S	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	T	121/121 (100%)	118 (98%)	3 (2%)	0	100	100
1	U	120/121 (99%)	118 (98%)	2 (2%)	0	100	100
1	V	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	W	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
1	X	120/121 (99%)	117 (98%)	3 (2%)	0	100	100
All	All	2851/2904 (98%)	2761 (97%)	89 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	54	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	94/94 (100%)	94 (100%)	0	100	100
1	B	92/94 (98%)	92 (100%)	0	100	100
1	C	92/94 (98%)	91 (99%)	1 (1%)	80	79
1	D	94/94 (100%)	93 (99%)	1 (1%)	80	79
1	E	95/94 (101%)	94 (99%)	1 (1%)	80	79
1	F	94/94 (100%)	93 (99%)	1 (1%)	80	79
1	G	93/94 (99%)	91 (98%)	2 (2%)	60	53
1	H	96/94 (102%)	96 (100%)	0	100	100
1	I	94/94 (100%)	93 (99%)	1 (1%)	80	79
1	J	93/94 (99%)	93 (100%)	0	100	100
1	K	94/94 (100%)	93 (99%)	1 (1%)	80	79
1	L	95/94 (101%)	93 (98%)	2 (2%)	61	55
1	M	95/94 (101%)	95 (100%)	0	100	100
1	N	93/94 (99%)	92 (99%)	1 (1%)	80	79
1	O	95/94 (101%)	95 (100%)	0	100	100
1	P	94/94 (100%)	94 (100%)	0	100	100
1	Q	95/94 (101%)	94 (99%)	1 (1%)	80	79
1	R	94/94 (100%)	93 (99%)	1 (1%)	80	79
1	S	94/94 (100%)	94 (100%)	0	100	100
1	T	96/94 (102%)	96 (100%)	0	100	100
1	U	95/94 (101%)	94 (99%)	1 (1%)	80	79
1	V	94/94 (100%)	94 (100%)	0	100	100
1	W	94/94 (100%)	93 (99%)	1 (1%)	80	79
1	X	95/94 (101%)	94 (99%)	1 (1%)	80	79
All	All	2260/2256 (100%)	2244 (99%)	16 (1%)	88	88

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

Mol	Chain	Res	Type
1	C	44	PRO

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Mol	Chain	Res	Type
1	D	71	ASN
1	E	71	ASN
1	F	7	LEU
1	G	53	GLN
1	G	59	ASP
1	I	97	ILE
1	K	97	ILE
1	L	48[A]	ARG
1	L	48[B]	ARG
1	N	89	ASN
1	Q	97	ILE
1	R	97	ILE
1	U	97	ILE
1	W	39	THR
1	X	48	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	D	71	ASN
1	K	89	ASN
1	W	91	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](#)

71 carbohydrates 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$
3	GLA	A	201	3,2	11,11,12	0.91	0	14,15,17	1.35	1 (7%)
3	GAL	A	202	3	11,11,12	0.90	1 (9%)	14,15,17	1.30	2 (14%)
3	BGC	A	203	3	12,12,12	0.89	1 (8%)	17,17,17	0.91	0
3	GLA	B	201	3,2	11,11,12	0.82	0	14,15,17	1.38	2 (14%)
3	GAL	B	202	3	11,11,12	1.00	1 (9%)	14,15,17	0.83	1 (7%)
3	BGC	B	203	3	12,12,12	0.48	0	17,17,17	1.24	3 (17%)
5	GLA	C	201	2,5	11,11,12	0.54	0	14,15,17	1.36	2 (14%)
5	GAL	C	202	5	11,11,12	0.80	0	14,15,17	1.61	4 (28%)
5	GLC	C	203	5	12,12,12	0.50	0	17,17,17	1.01	0
3	GLA	D	201	3,2	11,11,12	0.58	0	14,15,17	1.11	1 (7%)
3	GAL	D	202	3	11,11,12	0.76	0	14,15,17	1.01	0
3	BGC	D	203	3	12,12,12	0.45	0	17,17,17	1.17	2 (11%)
5	GLA	E	201	2,5	11,11,12	0.76	0	14,15,17	1.48	3 (21%)
5	GAL	E	202	5	11,11,12	0.89	0	14,15,17	1.33	1 (7%)
5	GLC	E	203	5	12,12,12	0.55	0	17,17,17	2.12	5 (29%)
3	GLA	F	201	3,2	11,11,12	0.69	0	14,15,17	1.44	1 (7%)
3	GAL	F	202	3	11,11,12	0.99	1 (9%)	14,15,17	1.09	1 (7%)
3	BGC	F	203	3	12,12,12	0.56	0	17,17,17	0.88	1 (5%)
3	GLA	G	201	3,2	11,11,12	1.27	2 (18%)	14,15,17	2.11	3 (21%)
3	GAL	G	202	3	11,11,12	0.74	0	14,15,17	1.14	1 (7%)
3	BGC	G	203	3	12,12,12	0.68	0	17,17,17	1.22	1 (5%)
3	GLA	H	201	3,2	11,11,12	0.54	0	14,15,17	1.40	2 (14%)
3	GAL	H	202	3	11,11,12	0.63	0	14,15,17	0.82	1 (7%)
3	BGC	H	203	3	12,12,12	0.42	0	17,17,17	1.44	2 (11%)
3	GLA	I	201	3,2	11,11,12	0.85	0	14,15,17	1.71	4 (28%)
3	GAL	I	202	3	11,11,12	0.69	0	14,15,17	1.38	5 (35%)
3	BGC	I	203	3	12,12,12	0.67	0	17,17,17	0.93	1 (5%)
3	GLA	J	201	3,2	11,11,12	0.56	0	14,15,17	1.29	1 (7%)
3	GAL	J	202	3	11,11,12	0.96	1 (9%)	14,15,17	1.07	1 (7%)
3	BGC	J	203	3	12,12,12	0.64	0	17,17,17	1.29	2 (11%)
3	GLA	K	201	3,2	11,11,12	0.54	0	14,15,17	1.53	4 (28%)
3	GAL	K	202	3	11,11,12	0.55	0	14,15,17	1.17	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	K	203	3	12,12,12	0.69	0	17,17,17	1.31	3 (17%)
3	GLA	L	201	3,2	11,11,12	0.41	0	14,15,17	1.33	2 (14%)
3	GAL	L	202	3	11,11,12	1.01	1 (9%)	14,15,17	1.12	0
3	BGC	L	203	3	12,12,12	0.57	0	17,17,17	1.56	4 (23%)
3	GLA	M	201	3,2	11,11,12	0.75	0	14,15,17	1.33	2 (14%)
3	GAL	M	202	3	11,11,12	1.20	1 (9%)	14,15,17	1.06	1 (7%)
3	BGC	M	203	3	12,12,12	0.60	0	17,17,17	1.61	4 (23%)
6	GLA	N	201	2,6	11,11,12	0.59	0	14,15,17	1.68	4 (28%)
6	GAL	N	202	7,6	11,11,12	0.69	0	14,15,17	1.61	3 (21%)
3	GLA	O	201	3,2	11,11,12	0.84	0	14,15,17	1.37	2 (14%)
3	GAL	O	202	3	11,11,12	0.80	0	14,15,17	0.98	0
3	BGC	O	203	3	12,12,12	0.52	0	17,17,17	1.09	2 (11%)
3	GLA	P	201	3,2	11,11,12	0.53	0	14,15,17	1.31	1 (7%)
3	GAL	P	202	3	11,11,12	0.66	0	14,15,17	0.70	0
3	BGC	P	203	3	12,12,12	0.57	0	17,17,17	1.06	2 (11%)
3	GLA	Q	201	3,2	11,11,12	0.75	0	14,15,17	1.85	5 (35%)
3	GAL	Q	202	3	11,11,12	0.81	0	14,15,17	1.07	1 (7%)
3	BGC	Q	203	3	12,12,12	0.59	0	17,17,17	0.95	0
3	GLA	R	201	3,2	11,11,12	0.61	0	14,15,17	0.94	0
3	GAL	R	202	3	11,11,12	0.87	0	14,15,17	0.76	0
3	BGC	R	203	3	12,12,12	0.53	0	17,17,17	1.11	0
3	GLA	S	201	3,2	11,11,12	0.57	0	14,15,17	1.73	4 (28%)
3	GAL	S	202	3	11,11,12	0.69	0	14,15,17	0.70	0
3	BGC	S	203	3	12,12,12	0.55	0	17,17,17	1.70	3 (17%)
3	GLA	T	201	3,2	11,11,12	0.43	0	14,15,17	1.54	3 (21%)
3	GAL	T	202	3	11,11,12	0.60	0	14,15,17	1.01	0
3	BGC	T	203	3	12,12,12	0.66	0	17,17,17	1.29	1 (5%)
3	GLA	U	201	3,2	11,11,12	0.62	0	14,15,17	1.50	2 (14%)
3	GAL	U	202	3	11,11,12	0.58	0	14,15,17	0.95	0
3	BGC	U	203	3	12,12,12	0.61	0	17,17,17	2.46	6 (35%)
3	GLA	V	201	3,2	11,11,12	0.62	0	14,15,17	1.19	1 (7%)
3	GAL	V	202	3	11,11,12	0.89	1 (9%)	14,15,17	1.17	2 (14%)
3	BGC	V	203	3	12,12,12	0.69	0	17,17,17	0.96	0
3	GLA	W	201	3,2	11,11,12	0.56	0	14,15,17	1.42	2 (14%)
3	GAL	W	202	3	11,11,12	0.58	0	14,15,17	0.98	0
3	BGC	W	203	3	12,12,12	0.63	0	17,17,17	1.29	2 (11%)
3	GLA	X	201	3,2	11,11,12	0.73	0	14,15,17	1.37	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GAL	X	202	3	11,11,12	0.90	1 (9%)	14,15,17	0.80	0
3	BGC	X	203	3	12,12,12	0.66	0	17,17,17	0.96	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
3	GLA	A	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	A	202	3	-	0/2/19/22	0/1/1/1
3	BGC	A	203	3	-	0/2/22/22	0/1/1/1
3	GLA	B	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	B	202	3	-	0/2/19/22	0/1/1/1
3	BGC	B	203	3	-	0/2/22/22	0/1/1/1
5	GLA	C	201	2,5	-	0/2/19/22	0/1/1/1
5	GAL	C	202	5	-	0/2/19/22	0/1/1/1
5	GLC	C	203	5	-	0/2/22/22	0/1/1/1
3	GLA	D	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	D	202	3	-	0/2/19/22	0/1/1/1
3	BGC	D	203	3	-	0/2/22/22	0/1/1/1
5	GLA	E	201	2,5	-	0/2/19/22	0/1/1/1
5	GAL	E	202	5	-	0/2/19/22	0/1/1/1
5	GLC	E	203	5	-	0/2/22/22	0/1/1/1
3	GLA	F	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	F	202	3	-	0/2/19/22	0/1/1/1
3	BGC	F	203	3	-	0/2/22/22	0/1/1/1
3	GLA	G	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	G	202	3	-	0/2/19/22	0/1/1/1
3	BGC	G	203	3	-	0/2/22/22	0/1/1/1
3	GLA	H	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	H	202	3	-	0/2/19/22	0/1/1/1
3	BGC	H	203	3	-	0/2/22/22	0/1/1/1
3	GLA	I	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	I	202	3	-	0/2/19/22	0/1/1/1
3	BGC	I	203	3	-	0/2/22/22	0/1/1/1
3	GLA	J	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	J	202	3	-	0/2/19/22	0/1/1/1
3	BGC	J	203	3	-	0/2/22/22	0/1/1/1
3	GLA	K	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	K	202	3	-	0/2/19/22	0/1/1/1
3	BGC	K	203	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLA	L	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	L	202	3	-	0/2/19/22	0/1/1/1
3	BGC	L	203	3	-	0/2/22/22	0/1/1/1
3	GLA	M	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	M	202	3	-	0/2/19/22	0/1/1/1
3	BGC	M	203	3	-	0/2/22/22	0/1/1/1
6	GLA	N	201	2,6	-	0/2/19/22	0/1/1/1
6	GAL	N	202	7,6	-	0/2/19/22	0/1/1/1
3	GLA	O	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	O	202	3	-	0/2/19/22	0/1/1/1
3	BGC	O	203	3	-	0/2/22/22	0/1/1/1
3	GLA	P	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	P	202	3	-	0/2/19/22	0/1/1/1
3	BGC	P	203	3	-	0/2/22/22	0/1/1/1
3	GLA	Q	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	Q	202	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	203	3	-	0/2/22/22	0/1/1/1
3	GLA	R	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	R	202	3	-	0/2/19/22	0/1/1/1
3	BGC	R	203	3	-	0/2/22/22	0/1/1/1
3	GLA	S	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	S	202	3	-	0/2/19/22	0/1/1/1
3	BGC	S	203	3	-	0/2/22/22	0/1/1/1
3	GLA	T	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	T	202	3	-	0/2/19/22	0/1/1/1
3	BGC	T	203	3	-	0/2/22/22	0/1/1/1
3	GLA	U	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	U	202	3	-	0/2/19/22	0/1/1/1
3	BGC	U	203	3	-	0/2/22/22	0/1/1/1
3	GLA	V	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	V	202	3	-	0/2/19/22	0/1/1/1
3	BGC	V	203	3	-	0/2/22/22	0/1/1/1
3	GLA	W	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	W	202	3	-	0/2/19/22	0/1/1/1
3	BGC	W	203	3	-	0/2/22/22	0/1/1/1
3	GLA	X	201	3,2	-	0/2/19/22	0/1/1/1
3	GAL	X	202	3	-	0/2/19/22	0/1/1/1
3	BGC	X	203	3	-	0/2/22/22	0/1/1/1

All (11) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	202	GAL	O5-C1	-3.20	1.38	1.43
3	J	202	GAL	O5-C1	-2.49	1.39	1.43
3	L	202	GAL	O5-C1	-2.44	1.39	1.43
3	B	202	GAL	O5-C1	-2.43	1.39	1.43
3	V	202	GAL	O5-C1	-2.35	1.39	1.43
3	F	202	GAL	O5-C1	-2.33	1.39	1.43
3	A	202	GAL	O5-C1	-2.17	1.40	1.43
3	G	201	GLA	O5-C1	-2.06	1.40	1.43
3	X	202	GAL	O5-C1	-2.05	1.40	1.43
3	A	203	BGC	O4-C4	-2.00	1.38	1.43
3	G	201	GLA	O4-C4	3.27	1.50	1.43

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	202	GAL	C1-O5-C5	-4.04	107.12	112.25
3	M	203	BGC	C1-C2-C3	-3.58	105.10	110.43
3	U	203	BGC	O1-C1-O5	-3.27	101.30	110.25
3	H	203	BGC	O4-C4-C3	-3.27	102.99	110.34
3	M	203	BGC	O5-C1-C2	-3.24	104.62	109.80
6	N	201	GLA	O4-C4-C3	-3.00	103.59	110.34
3	J	203	BGC	O6-C6-C5	-2.96	101.54	111.33
3	W	203	BGC	C1-C2-C3	-2.90	106.12	110.43
5	E	203	GLC	O2-C2-C3	-2.81	104.01	110.34
3	G	203	BGC	O4-C4-C3	-2.80	104.04	110.34
3	B	203	BGC	C1-C2-C3	-2.76	106.32	110.43
3	Q	201	GLA	O5-C1-C2	-2.70	106.47	110.86
3	K	203	BGC	C1-C2-C3	-2.67	106.46	110.43
3	S	203	BGC	C1-C2-C3	-2.66	106.48	110.43
3	S	203	BGC	O4-C4-C3	-2.64	104.39	110.34
3	X	201	GLA	O2-C2-C3	-2.64	104.81	110.12
3	T	201	GLA	C2-C3-C4	-2.64	106.56	111.04
3	O	201	GLA	O5-C1-C2	-2.60	106.63	110.86
3	W	203	BGC	O5-C1-C2	-2.59	105.67	109.80
3	K	201	GLA	C1-C2-C3	-2.55	106.52	109.54
3	B	201	GLA	O5-C1-C2	-2.55	106.73	110.86
3	O	201	GLA	O4-C4-C3	-2.46	104.80	110.34
3	L	203	BGC	O6-C6-C5	-2.46	103.21	111.33
3	D	203	BGC	O2-C2-C3	-2.45	104.83	110.34
5	C	201	GLA	O3-C3-C2	-2.44	105.60	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	203	BGC	C1-O5-C5	-2.43	108.98	113.47
3	L	203	BGC	C1-C2-C3	-2.42	106.82	110.43
5	E	203	GLC	O3-C3-C2	-2.41	104.91	110.34
3	M	202	GAL	C3-C4-C5	-2.39	106.03	110.20
6	N	201	GLA	O3-C3-C2	-2.37	105.72	110.00
3	W	201	GLA	O3-C3-C2	-2.37	105.72	110.00
5	C	202	GAL	C3-C4-C5	-2.36	106.08	110.20
3	I	201	GLA	O3-C3-C2	-2.35	105.76	110.00
3	T	203	BGC	C1-O5-C5	-2.34	109.14	113.47
3	J	203	BGC	C1-C2-C3	-2.33	106.96	110.43
3	I	202	GAL	O6-C6-C5	-2.30	103.73	111.33
3	B	203	BGC	O4-C4-C3	-2.28	105.20	110.34
3	Q	202	GAL	C3-C4-C5	-2.28	106.23	110.20
5	C	202	GAL	C1-O5-C5	-2.23	109.41	112.25
3	U	203	BGC	O4-C4-C3	-2.18	105.42	110.34
3	O	203	BGC	O4-C4-C3	-2.17	105.44	110.34
3	I	202	GAL	O3-C3-C4	-2.14	105.51	110.34
3	S	201	GLA	O3-C3-C2	-2.14	106.13	110.00
3	H	202	GAL	C1-O5-C5	-2.14	109.53	112.25
3	F	202	GAL	C2-C3-C4	-2.11	107.45	111.04
6	N	202	GAL	O2-C2-C1	-2.10	104.99	109.21
3	G	201	GLA	C3-C4-C5	-2.09	106.56	110.20
3	Q	201	GLA	C3-C4-C5	-2.07	106.59	110.20
3	K	203	BGC	C1-O5-C5	-2.04	109.70	113.47
3	I	202	GAL	C3-C4-C5	-2.02	106.67	110.20
3	S	201	GLA	O4-C4-C3	-2.01	105.81	110.34
3	M	203	BGC	O1-C1-C2	2.00	114.57	109.21
3	M	201	GLA	O2-C2-C1	2.02	113.26	109.21
3	L	203	BGC	O2-C2-C1	2.06	114.35	109.82
3	I	203	BGC	C1-O5-C5	2.06	117.28	113.47
3	D	203	BGC	O5-C1-C2	2.07	113.10	109.80
3	P	203	BGC	C1-C2-C3	2.08	113.52	110.43
3	B	203	BGC	C3-C4-C5	2.09	113.84	110.20
3	T	201	GLA	O3-C3-C4	2.12	115.12	110.34
3	I	201	GLA	O2-C2-C1	2.13	113.47	109.21
3	P	203	BGC	C3-C4-C5	2.13	113.91	110.20
3	K	201	GLA	O4-C4-C5	2.13	114.89	109.24
3	A	202	GAL	O5-C5-C6	2.15	112.01	107.35
5	E	201	GLA	O4-C4-C5	2.18	115.03	109.24
5	C	202	GAL	O5-C5-C6	2.19	112.08	107.35
3	K	203	BGC	O3-C3-C4	2.19	115.27	110.34
3	B	202	GAL	C1-C2-C3	2.22	112.17	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	202	GAL	O5-C5-C6	2.22	112.15	107.35
3	I	202	GAL	O5-C5-C6	2.23	112.18	107.35
3	U	201	GLA	C1-C2-C3	2.23	112.18	109.54
3	H	201	GLA	O4-C4-C5	2.36	115.50	109.24
3	X	201	GLA	C1-O5-C5	2.37	115.26	112.25
3	O	203	BGC	O5-C5-C6	2.39	112.41	106.36
3	V	201	GLA	C1-O5-C5	2.42	115.32	112.25
3	I	202	GAL	O5-C1-C2	2.44	114.81	110.86
6	N	201	GLA	O4-C4-C5	2.48	115.81	109.24
3	D	201	GLA	O5-C5-C6	2.50	112.77	107.35
3	V	202	GAL	C1-C2-C3	2.51	112.51	109.54
3	W	201	GLA	C1-O5-C5	2.54	115.47	112.25
3	Q	201	GLA	O4-C4-C5	2.55	115.99	109.24
3	K	202	GAL	O5-C5-C6	2.55	112.87	107.35
3	H	201	GLA	O2-C2-C1	2.59	114.40	109.21
6	N	202	GAL	O2-C2-C3	2.60	115.34	110.12
3	M	201	GLA	C1-O5-C5	2.65	115.62	112.25
3	L	201	GLA	C1-O5-C5	2.67	115.64	112.25
3	L	201	GLA	O4-C4-C5	2.68	116.33	109.24
3	F	203	BGC	C3-C4-C5	2.72	114.93	110.20
3	X	201	GLA	O5-C5-C6	2.73	113.27	107.35
5	E	201	GLA	C1-O5-C5	2.74	115.72	112.25
3	H	203	BGC	O5-C1-C2	2.74	114.17	109.80
3	K	201	GLA	O5-C5-C6	2.79	113.39	107.35
3	K	201	GLA	O2-C2-C1	2.80	114.82	109.21
3	J	202	GAL	C1-C2-C3	2.85	112.91	109.54
5	C	202	GAL	C1-C2-C3	2.86	112.93	109.54
3	G	202	GAL	C1-C2-C3	2.87	112.94	109.54
3	T	201	GLA	O2-C2-C1	2.88	114.99	109.21
3	A	201	GLA	C1-O5-C5	2.94	115.98	112.25
6	N	201	GLA	C1-O5-C5	3.01	116.06	112.25
3	B	201	GLA	C1-O5-C5	3.03	116.09	112.25
3	Q	201	GLA	C1-C2-C3	3.11	113.22	109.54
3	I	201	GLA	O4-C4-C5	3.11	117.48	109.24
5	E	201	GLA	O2-C2-C1	3.11	115.45	109.21
5	C	201	GLA	O4-C4-C5	3.16	117.62	109.24
3	A	202	GAL	C1-C2-C3	3.28	113.42	109.54
3	L	203	BGC	C3-C4-C5	3.29	115.93	110.20
3	S	201	GLA	C1-O5-C5	3.30	116.43	112.25
3	I	201	GLA	C1-O5-C5	3.35	116.50	112.25
3	J	201	GLA	C1-O5-C5	3.35	116.50	112.25
3	U	203	BGC	C3-C4-C5	3.36	116.05	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	203	GLC	O2-C2-C1	3.55	117.63	109.82
3	Q	201	GLA	C1-O5-C5	3.60	116.82	112.25
3	F	201	GLA	C1-O5-C5	3.72	116.97	112.25
5	E	203	GLC	C1-O5-C5	3.75	120.41	113.47
3	S	201	GLA	O4-C4-C5	3.75	119.18	109.24
3	U	203	BGC	O5-C5-C4	3.76	116.74	109.68
3	P	201	GLA	C1-O5-C5	3.76	117.03	112.25
5	E	202	GAL	C1-C2-C3	3.81	114.05	109.54
3	U	201	GLA	C1-O5-C5	3.88	117.17	112.25
3	S	203	BGC	C3-C4-C5	4.01	117.19	110.20
5	E	203	GLC	O5-C1-C2	4.15	116.42	109.80
3	G	201	GLA	O4-C4-C5	4.85	122.08	109.24
3	G	201	GLA	C1-C2-C3	4.85	115.28	109.54
3	U	203	BGC	O5-C1-C2	4.99	117.76	109.80
3	U	203	BGC	C1-O5-C5	5.55	123.73	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	BGC	1	0
3	O	201	GLA	1	0
3	O	202	GAL	2	0

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 24 are monoatomic - leaving 21 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	$\# Z  > 2$
4	EDO	A	1122	-	3,3,3	0.38	0	2,2,2	0.35	0
4	EDO	D	1122	-	3,3,3	0.14	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	E	1122	-	3,3,3	0.24	0	2,2,2	0.27	0
4	EDO	H	1122	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	H	1123	-	3,3,3	0.54	0	2,2,2	0.25	0
4	EDO	I	1122	-	3,3,3	0.67	0	2,2,2	0.95	0
4	EDO	I	1123	-	3,3,3	0.61	0	2,2,2	0.39	0
4	EDO	L	1122	-	3,3,3	0.31	0	2,2,2	0.06	0
4	EDO	M	1122	-	3,3,3	0.15	0	2,2,2	0.71	0
4	EDO	M	1123	-	3,3,3	0.45	0	2,2,2	0.96	0
4	EDO	N	1122	-	3,3,3	0.56	0	2,2,2	0.44	0
7	BGC	N	203	6	12,12,12	0.60	0	17,17,17	1.37	2 (11%)
4	EDO	O	1122	-	3,3,3	0.42	0	2,2,2	0.44	0
4	EDO	Q	1122	-	3,3,3	0.54	0	2,2,2	0.33	0
4	EDO	Q	1123	-	3,3,3	0.46	0	2,2,2	0.47	0
4	EDO	S	1122	-	3,3,3	0.22	0	2,2,2	0.50	0
4	EDO	U	1122	-	3,3,3	0.18	0	2,2,2	0.24	0
4	EDO	V	1122	-	3,3,3	0.39	0	2,2,2	0.56	0
4	EDO	W	1122	-	3,3,3	0.35	0	2,2,2	0.33	0
4	EDO	W	1123	-	3,3,3	0.58	0	2,2,2	0.21	0
4	EDO	X	1122	-	3,3,3	0.46	0	2,2,2	0.75	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
4	EDO	A	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	H	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	H	1123	-	-	0/1/1/1	0/0/0/0
4	EDO	I	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	I	1123	-	-	0/1/1/1	0/0/0/0
4	EDO	L	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	M	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	M	1123	-	-	0/1/1/1	0/0/0/0
4	EDO	N	1122	-	-	0/1/1/1	0/0/0/0
7	BGC	N	203	6	-	0/2/22/22	0/1/1/1
4	EDO	O	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	Q	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	Q	1123	-	-	0/1/1/1	0/0/0/0
4	EDO	S	1122	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	U	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	V	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	W	1122	-	-	0/1/1/1	0/0/0/0
4	EDO	W	1123	-	-	0/1/1/1	0/0/0/0
4	EDO	X	1122	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	203	BGC	O4-C4-C3	-2.94	103.72	110.34
7	N	203	BGC	C3-C4-C5	2.25	114.13	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1122	EDO	1	0
4	D	1122	EDO	1	0
4	E	1122	EDO	1	0
4	H	1122	EDO	7	0
4	H	1123	EDO	1	0
4	I	1122	EDO	5	0
4	I	1123	EDO	1	0
4	L	1122	EDO	1	0
4	M	1123	EDO	2	0
4	O	1122	EDO	1	0
4	Q	1122	EDO	1	0
4	S	1122	EDO	1	0
4	U	1122	EDO	1	0
4	V	1122	EDO	2	0
4	W	1122	EDO	1	0
4	X	1122	EDO	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	121/121 (100%)	-0.51	0 100 100	7, 11, 19, 25	0
1	B	118/121 (97%)	-0.46	0 100 100	7, 11, 18, 21	0
1	C	119/121 (98%)	-0.29	2 (1%) 73 76	9, 14, 23, 25	2 (1%)
1	D	120/121 (99%)	-0.43	0 100 100	9, 12, 20, 27	0
1	E	121/121 (100%)	-0.35	2 (1%) 73 76	8, 13, 21, 30	0
1	F	121/121 (100%)	-0.40	0 100 100	7, 12, 18, 29	0
1	G	121/121 (100%)	-0.18	1 (0%) 87 88	7, 14, 24, 27	0
1	H	121/121 (100%)	-0.47	0 100 100	5, 10, 17, 24	0
1	I	121/121 (100%)	-0.44	0 100 100	6, 10, 18, 23	0
1	J	120/121 (99%)	-0.40	0 100 100	6, 10, 18, 24	1 (0%)
1	K	121/121 (100%)	-0.50	1 (0%) 87 88	7, 11, 17, 23	1 (0%)
1	L	121/121 (100%)	-0.44	0 100 100	7, 11, 18, 21	0
1	M	121/121 (100%)	-0.30	3 (2%) 61 64	8, 13, 21, 29	0
1	N	120/121 (99%)	-0.43	0 100 100	7, 12, 19, 24	0
1	O	121/121 (100%)	-0.23	0 100 100	7, 14, 22, 26	0
1	P	121/121 (100%)	-0.45	0 100 100	6, 10, 18, 24	0
1	Q	121/121 (100%)	-0.45	1 (0%) 87 88	6, 11, 17, 27	0
1	R	121/121 (100%)	-0.33	1 (0%) 87 88	7, 11, 18, 19	1 (0%)
1	S	121/121 (100%)	-0.50	1 (0%) 87 88	6, 11, 18, 26	0
1	T	121/121 (100%)	-0.44	0 100 100	7, 11, 19, 23	0
1	U	121/121 (100%)	-0.51	0 100 100	7, 11, 18, 27	1 (0%)
1	V	121/121 (100%)	-0.51	0 100 100	6, 11, 18, 24	0
1	W	121/121 (100%)	-0.31	3 (2%) 61 64	8, 14, 23, 33	0
1	X	121/121 (100%)	-0.47	1 (0%) 87 88	8, 12, 19, 23	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2896/2904 (99%)	-0.41	16 (0%) 90 91	5, 12, 20, 33	7 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	89	ASN	15.6
1	C	71	ASN	3.3
1	X	88	ASN	3.2
1	W	88	ASN	3.2
1	M	71	ASN	3.1
1	W	71	ASN	2.5
1	Q	71	ASN	2.3
1	E	71	ASN	2.2
1	E	89	ASN	2.2
1	M	89	ASN	2.2
1	K	71	ASN	2.2
1	C	89	ASN	2.1
1	G	71	ASN	2.1
1	S	71	ASN	2.1
1	M	88[A]	ASN	2.1
1	W	87	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	A	203	12/12	0.88	0.16	23.24	11,19,23,28	0
3	BGC	U	203	12/12	0.87	0.15	6.08	17,24,31,32	0
3	GLA	R	201	11/12	0.95	0.11	2.45	15,17,18,19	0
3	GLA	H	201	11/12	0.98	0.09	1.92	10,14,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLA	S	201	11/12	0.94	0.10	1.57	12,17,18,20	0
3	GLA	J	201	11/12	0.97	0.08	1.28	10,12,14,14	0
3	GLA	D	201	11/12	0.94	0.12	1.13	13,15,18,18	0
6	GLA	N	201	11/12	0.93	0.12	1.08	14,16,19,19	0
3	GLA	M	201	11/12	0.95	0.10	1.01	11,14,16,17	0
3	GLA	L	201	11/12	0.96	0.12	0.97	11,15,19,19	0
3	GLA	T	201	11/12	0.95	0.12	0.96	12,15,18,19	0
5	GLA	C	201	11/12	0.91	0.12	0.64	17,18,20,22	0
5	GLA	E	201	11/12	0.92	0.09	0.57	12,14,16,19	0
3	GLA	I	201	11/12	0.95	0.09	0.45	9,11,12,14	0
3	GLA	P	201	11/12	0.97	0.08	0.43	9,12,14,15	0
3	GLA	X	201	11/12	0.97	0.09	0.31	11,13,15,15	0
3	BGC	Q	203	12/12	0.93	0.10	0.27	15,22,27,29	0
3	GLA	O	201	11/12	0.92	0.12	0.14	18,22,24,25	0
3	GLA	K	201	11/12	0.95	0.08	0.10	12,14,16,17	0
3	GLA	G	201	11/12	0.89	0.12	0.09	6,14,18,18	0
3	GLA	B	201	11/12	0.95	0.09	0.00	16,18,19,20	0
3	GLA	F	201	11/12	0.96	0.09	-0.11	11,15,18,19	0
3	GLA	V	201	11/12	0.96	0.08	-0.23	13,16,17,18	0
3	GLA	W	201	11/12	0.95	0.09	-0.36	15,16,18,18	0
3	GLA	A	201	11/12	0.98	0.07	-0.41	7,9,11,13	0
3	GLA	Q	201	11/12	0.98	0.07	-0.41	7,11,13,13	0
3	GLA	U	201	11/12	0.98	0.07	-0.52	9,11,12,14	0
5	GLC	C	203	12/12	0.88	0.18	-	24,29,36,37	0
3	GAL	B	202	11/12	0.92	0.18	-	21,24,29,30	0
3	BGC	B	203	12/12	0.82	0.21	-	24,31,34,34	0
3	GAL	V	202	11/12	0.91	0.18	-	18,23,26,28	0
3	GAL	H	202	11/12	0.94	0.18	-	17,19,26,26	0
3	BGC	R	203	12/12	0.85	0.21	-	23,30,34,37	0
5	GLC	E	203	12/12	0.90	0.16	-	14,23,26,27	0
3	BGC	J	203	12/12	0.84	0.20	-	23,30,35,38	0
3	GAL	P	202	11/12	0.93	0.15	-	15,20,25,26	0
3	BGC	L	203	12/12	0.72	0.26	-	30,35,39,41	0
3	GAL	O	202	11/12	0.93	0.15	-	25,27,28,28	0
3	BGC	K	203	12/12	0.91	0.16	-	21,26,29,31	0
3	GAL	G	202	11/12	0.90	0.16	-	19,24,27,30	0
3	GAL	L	202	11/12	0.91	0.21	-	19,25,30,32	0
3	GAL	J	202	11/12	0.95	0.15	-	15,22,26,28	0
5	GAL	C	202	11/12	0.85	0.17	-	19,24,33,37	0
3	BGC	I	203	12/12	0.90	0.16	-	15,22,28,31	0
3	BGC	S	203	12/12	0.84	0.20	-	25,30,36,37	0
3	BGC	X	203	12/12	0.84	0.28	-	26,34,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BGC	P	203	12/12	0.84	0.25	-	23,30,32,33	0
3	GAL	A	202	11/12	0.94	0.11	-	10,14,23,28	0
3	GAL	D	202	11/12	0.93	0.16	-	19,23,26,28	0
3	GAL	T	202	11/12	0.94	0.20	-	22,24,31,34	0
3	GAL	U	202	11/12	0.94	0.09	-	14,16,22,22	0
3	BGC	H	203	12/12	0.91	0.19	-	20,25,31,32	0
3	BGC	O	203	12/12	0.82	0.18	-	25,30,36,37	0
3	BGC	V	203	12/12	0.91	0.19	-	26,35,38,38	0
3	GAL	I	202	11/12	0.94	0.10	-	15,17,20,23	0
3	GAL	R	202	11/12	0.90	0.18	-	17,20,27,29	0
5	GAL	E	202	11/12	0.95	0.12	-	15,16,21,23	0
3	BGC	T	203	12/12	0.83	0.25	-	28,35,40,40	0
3	GAL	W	202	11/12	0.91	0.17	-	21,22,25,27	0
6	GAL	N	202	11/12	0.90	0.20	-	21,23,29,29	0
3	GAL	M	202	11/12	0.96	0.09	-	11,14,18,21	0
3	GAL	S	202	11/12	0.92	0.14	-	14,17,20,21	0
3	GAL	Q	202	11/12	0.96	0.07	-	13,16,20,22	0
3	BGC	F	203	12/12	0.83	0.28	-	26,31,34,36	0
3	BGC	D	203	12/12	0.88	0.24	-	19,25,28,32	0
3	GAL	F	202	11/12	0.93	0.17	-	19,22,26,28	0
3	GAL	K	202	11/12	0.94	0.11	-	16,20,22,23	0
3	GAL	X	202	11/12	0.90	0.17	-	18,21,27,32	0
3	BGC	G	203	12/12	0.83	0.17	-	22,25,29,30	0
3	BGC	W	203	12/12	0.88	0.20	-	21,25,31,34	0
3	BGC	M	203	12/12	0.92	0.14	-	16,21,28,33	0

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	E	1122	4/4	0.91	0.14	7.74	9,11,16,16	0
4	EDO	H	1122	4/4	0.91	0.14	6.49	8,13,14,17	0
4	EDO	X	1122	4/4	0.92	0.18	5.63	16,16,17,19	0
4	EDO	S	1122	4/4	0.94	0.12	5.57	7,8,12,15	0
4	EDO	M	1122	4/4	0.94	0.13	5.12	9,10,14,16	0
4	EDO	I	1122	4/4	0.97	0.13	4.57	12,13,14,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	Q	1122	4/4	0.95	0.12	4.20	10,11,13,15	0
4	EDO	D	1122	4/4	0.94	0.11	4.05	13,14,17,20	0
4	EDO	O	1122	4/4	0.92	0.13	3.74	12,13,16,17	0
4	EDO	M	1123	4/4	0.96	0.12	3.50	14,15,17,19	0
4	EDO	W	1122	4/4	0.95	0.11	3.49	12,13,14,15	0
4	EDO	A	1122	4/4	0.95	0.10	3.43	11,13,15,19	0
4	EDO	L	1122	4/4	0.95	0.11	2.91	17,17,18,21	0
4	EDO	I	1123	4/4	0.97	0.09	1.96	10,11,13,13	0
4	EDO	U	1122	4/4	0.96	0.10	1.96	11,12,12,18	0
4	EDO	V	1122	4/4	0.94	0.12	1.53	16,17,17,18	0
4	EDO	H	1123	4/4	0.95	0.10	0.91	15,21,22,22	0
4	EDO	W	1123	4/4	0.95	0.09	0.39	20,23,24,26	0
4	EDO	N	1122	4/4	0.97	0.09	0.13	17,18,18,19	0
2	CA	Q	200	1/1	1.00	0.08	0.11	10,10,10,10	0
4	EDO	Q	1123	4/4	0.96	0.07	-0.24	16,16,16,17	0
2	CA	I	200	1/1	1.00	0.07	-0.76	10,10,10,10	0
2	CA	M	200	1/1	0.99	0.05	-1.35	11,11,11,11	0
2	CA	E	200	1/1	0.99	0.05	-2.37	12,12,12,12	0
2	CA	N	200	1/1	0.99	0.04	-2.61	15,15,15,15	0
2	CA	X	200	1/1	1.00	0.04	-2.72	12,12,12,12	0
2	CA	P	200	1/1	1.00	0.04	-2.77	10,10,10,10	0
2	CA	F	200	1/1	0.99	0.02	-2.91	10,10,10,10	0
2	CA	O	200	1/1	0.96	0.06	-2.94	19,19,19,19	0
2	CA	K	200	1/1	0.99	0.04	-2.99	12,12,12,12	0
2	CA	S	200	1/1	1.00	0.04	-3.03	11,11,11,11	0
2	CA	D	200	1/1	1.00	0.02	-3.06	13,13,13,13	0
2	CA	W	200	1/1	0.99	0.04	-3.21	14,14,14,14	0
2	CA	U	200	1/1	0.99	0.04	-3.38	14,14,14,14	0
2	CA	G	200	1/1	0.99	0.06	-3.51	16,16,16,16	0
2	CA	R	200	1/1	1.00	0.03	-3.53	13,13,13,13	0
2	CA	L	200	1/1	0.99	0.03	-3.69	14,14,14,14	0
2	CA	B	200	1/1	0.99	0.03	-3.93	13,13,13,13	0
2	CA	H	200	1/1	1.00	0.03	-4.31	8,8,8,8	0
2	CA	T	200	1/1	1.00	0.03	-4.92	14,14,14,14	0
2	CA	V	200	1/1	1.00	0.03	-5.03	12,12,12,12	0
2	CA	J	200	1/1	0.99	0.04	-5.28	11,11,11,11	0
2	CA	A	200	1/1	1.00	0.03	-5.30	10,10,10,10	0
2	CA	C	200	1/1	0.97	0.05	-6.13	16,16,16,16	0
7	BGC	N	203	12/12	0.81	0.25	-	30,35,39,41	0

## 6.5 Other polymers

There are no such residues in this entry.