



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:42 AM BST

PDB ID : 3UJQ  
Title : Galactose-specific lectin from Dolichos lablab in complex with galactose  
Authors : Shetty, K.N.; Latha, V.L.; Rao, R.N.; Nadimpalli, S.K.; Suguna, K.  
Deposited on : 2011-11-08  
Resolution : 2.06 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

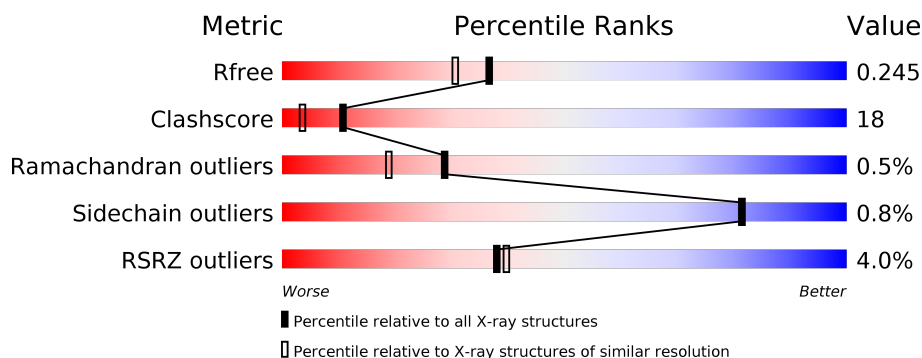
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	281	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>
1	B	281	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>10%</div> </div> </div>
1	C	281	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>11%</div> </div> </div>
1	D	281	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

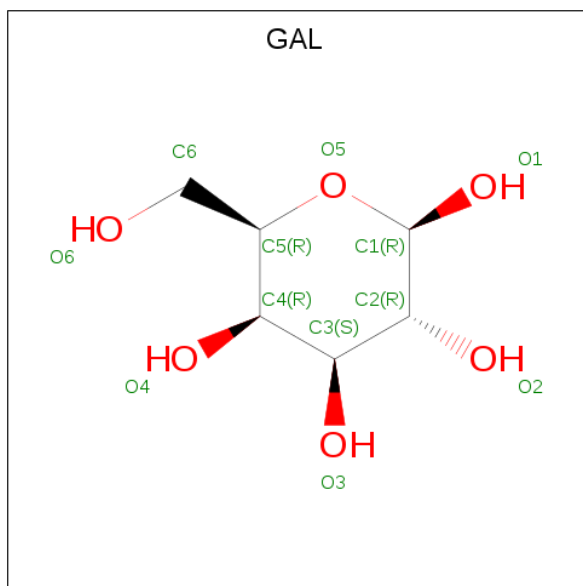
There are 7 unique types of molecules in this entry. The entry contains 7922 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Legume lectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	0	0	0
			1926	1224	316	386			
1	B	253	Total	C	N	O	0	0	0
			1930	1227	317	386			
1	C	250	Total	C	N	O	0	0	0
			1904	1213	314	377			
1	D	250	Total	C	N	O	0	0	0
			1904	1213	314	377			

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

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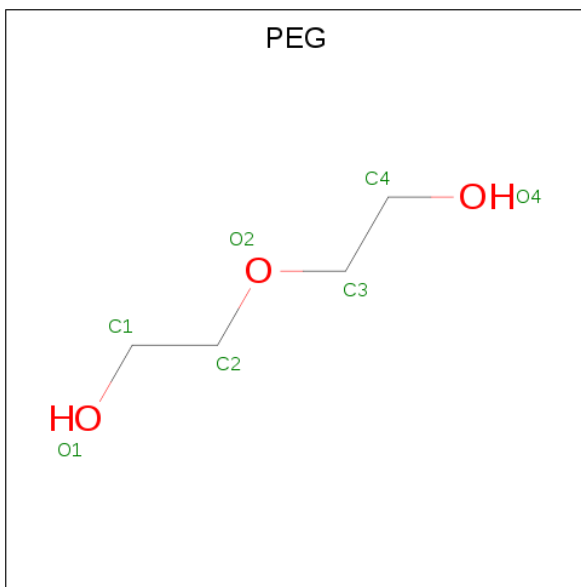
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

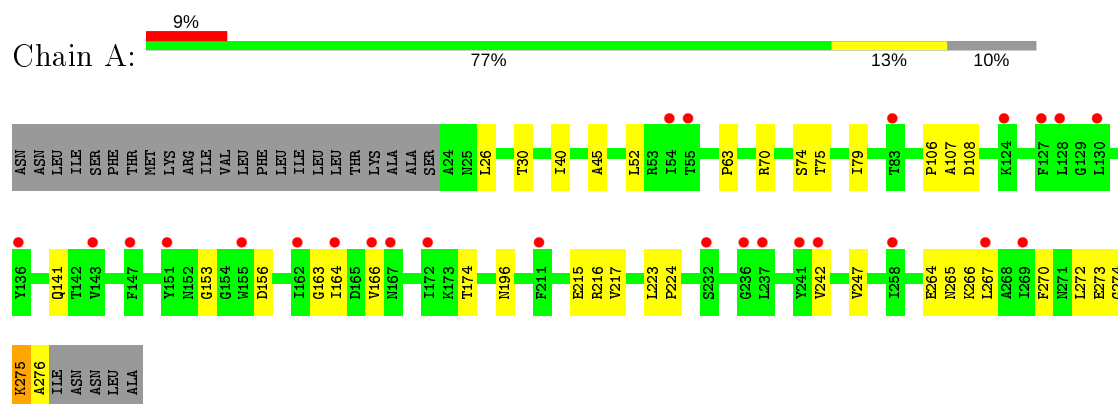
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	43	Total 43	O 43	0	0
7	B	40	Total 40	O 40	0	0
7	C	42	Total 42	O 42	0	0
7	D	36	Total 36	O 36	0	0

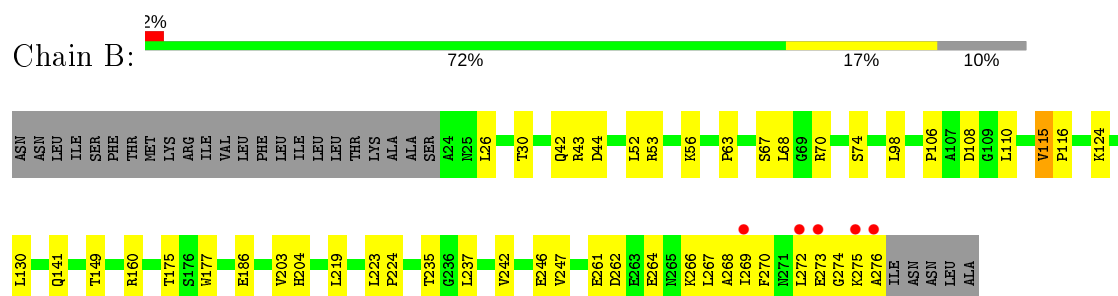
### 3 Residue-property plots

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.

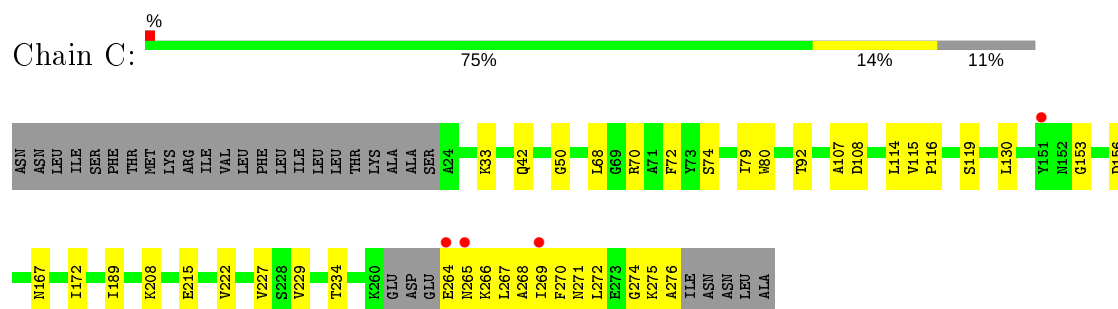
#### • Molecule 1: Legume lectin



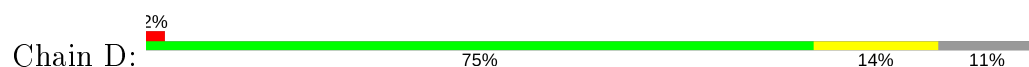
#### • Molecule 1: Legume lectin

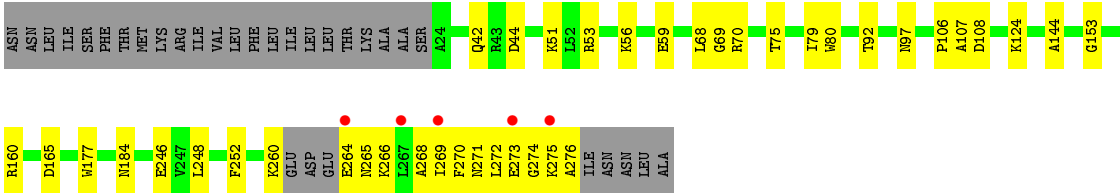


#### • Molecule 1: Legume lectin



#### • Molecule 1: Legume lectin







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.99 Å 89.99 Å 125.08 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.34 – 2.06 41.69 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.34-2.06) 99.6 (41.69-2.06)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.06 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.197 , 0.246 0.197 , 0.245	Depositor DCC
$R_{free}$ test set	3509 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 9.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.468 for h,-h-k,-l 0.468 for -k,-h,-l	Xtriage
Reported twinning fraction	0.251 for H, K, L 0.249 for -H, H+K, -L 0.249 for -h,-k,l 0.252 for -H-K, K, -L	Depositor
Outliers	0 of 69386 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: PEG, GAL, CA, MN, EDO

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	0.33	0/1969	0.44	0/2683
1	B	0.33	0/1973	0.47	0/2687
1	C	0.32	0/1946	0.47	0/2649
1	D	0.32	0/1946	0.48	0/2649
All	All	0.33	0/7834	0.47	0/10668

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 [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	1926	0	1852	135	0
1	B	1930	0	1868	82	0
1	C	1904	0	1851	160	0
1	D	1904	0	1849	77	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	12	0	0
3	D	8	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	14	0	20	0	0
6	D	7	0	10	0	0
7	A	43	0	0	0	0
7	B	40	0	0	0	0
7	C	42	0	0	0	0
7	D	36	0	0	0	0
All	All	7922	0	7528	280	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 18.

All (280) 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:A:267:LEU:HB3	1:C:275:LYS:CG	1.28	1.61
1:A:265:ASN:ND2	1:C:272:LEU:CB	1.69	1.51
1:A:272:LEU:HB3	1:C:265:ASN:CG	1.21	1.49
1:A:272:LEU:HD13	1:C:265:ASN:ND2	1.32	1.44
1:C:266:LYS:HE2	1:C:269:ILE:CB	1.48	1.44
1:A:265:ASN:ND2	1:C:272:LEU:CG	1.83	1.40
1:A:265:ASN:ND2	1:C:272:LEU:HB3	1.18	1.37
1:A:272:LEU:HB3	1:C:265:ASN:OD1	1.21	1.36
1:A:276:ALA:N	1:C:265:ASN:O	1.56	1.35
1:A:276:ALA:CB	1:C:265:ASN:HB3	1.57	1.34
1:C:266:LYS:CE	1:C:269:ILE:CB	2.05	1.32
1:C:272:LEU:HA	1:C:276:ALA:N	1.41	1.32
1:A:272:LEU:CD1	1:C:265:ASN:ND2	1.95	1.29
1:B:275:LYS:O	1:D:264:GLU:HB2	1.17	1.28
1:A:275:LYS:O	1:C:264:GLU:CB	1.81	1.27
1:A:275:LYS:O	1:C:264:GLU:HB3	1.09	1.26
1:A:267:LEU:CB	1:C:275:LYS:HG3	1.66	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:CG	1:C:272:LEU:HB3	1.56	1.25
1:A:267:LEU:CB	1:C:275:LYS:CG	2.14	1.25
1:A:270:PHE:O	1:C:266:LYS:CG	1.86	1.24
1:A:276:ALA:CB	1:C:265:ASN:CB	2.16	1.22
1:A:272:LEU:CB	1:C:265:ASN:CG	2.07	1.22
1:A:272:LEU:CD1	1:C:265:ASN:HD21	1.50	1.22
1:B:270:PHE:N	1:D:270:PHE:CB	1.70	1.21
1:B:270:PHE:N	1:D:270:PHE:HB2	1.25	1.20
1:A:265:ASN:ND2	1:C:276:ALA:CB	1.98	1.20
1:B:266:LYS:O	1:D:272:LEU:N	1.75	1.19
1:A:265:ASN:ND2	1:C:272:LEU:CD2	2.05	1.18
1:B:266:LYS:HE3	1:B:269:ILE:CB	1.73	1.18
1:A:265:ASN:HD22	1:C:272:LEU:CD2	1.59	1.16
1:A:270:PHE:O	1:C:266:LYS:HG2	1.02	1.15
1:B:275:LYS:O	1:D:264:GLU:CB	1.93	1.15
1:A:273:GLU:OE1	1:C:269:ILE:CB	1.95	1.15
1:A:272:LEU:CG	1:C:265:ASN:ND2	2.09	1.15
1:A:276:ALA:HB3	1:C:265:ASN:CB	1.73	1.14
1:C:275:LYS:HA	1:C:275:LYS:HE2	1.17	1.12
1:A:267:LEU:CB	1:C:275:LYS:CB	2.26	1.12
1:A:276:ALA:CB	1:C:265:ASN:CA	2.28	1.12
1:A:275:LYS:HA	1:A:275:LYS:HE2	1.15	1.11
1:A:265:ASN:CG	1:C:272:LEU:CB	2.13	1.10
1:B:270:PHE:O	1:D:266:LYS:HG2	1.36	1.09
1:B:266:LYS:HG2	1:D:270:PHE:O	1.34	1.08
1:A:265:ASN:ND2	1:C:272:LEU:CD1	2.18	1.07
1:A:265:ASN:HD22	1:C:276:ALA:HB1	1.04	1.07
1:A:276:ALA:CA	1:C:265:ASN:O	2.03	1.07
1:B:272:LEU:O	1:B:276:ALA:O	1.74	1.06
1:C:272:LEU:HA	1:C:276:ALA:CA	1.72	1.06
1:B:266:LYS:C	1:D:272:LEU:N	1.81	1.06
1:B:270:PHE:O	1:D:266:LYS:CG	1.94	1.06
1:A:272:LEU:HD22	1:C:265:ASN:ND2	1.68	1.06
1:A:276:ALA:HB1	1:C:265:ASN:CB	1.85	1.06
1:A:276:ALA:HB3	1:C:265:ASN:HB3	1.16	1.05
1:A:265:ASN:ND2	1:C:272:LEU:HD22	1.63	1.05
1:A:265:ASN:HD22	1:C:272:LEU:HD22	1.08	1.04
1:A:276:ALA:O	1:C:265:ASN:C	1.80	1.04
1:A:272:LEU:CD2	1:C:265:ASN:ND2	2.21	1.03
1:B:266:LYS:CG	1:D:270:PHE:O	1.98	1.03
1:B:266:LYS:HB3	1:D:273:GLU:N	1.61	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LYS:HE2	1:C:269:ILE:CA	1.90	1.01
1:A:275:LYS:CA	1:A:275:LYS:HE2	1.91	1.00
1:A:276:ALA:HB3	1:C:265:ASN:CA	1.88	0.98
1:C:275:LYS:CA	1:C:275:LYS:HE2	1.93	0.98
1:A:267:LEU:HB2	1:C:275:LYS:CB	1.93	0.98
1:A:265:ASN:ND2	1:C:276:ALA:HB3	1.76	0.97
1:A:272:LEU:HB3	1:C:265:ASN:ND2	1.80	0.97
1:A:272:LEU:HD22	1:C:265:ASN:HD22	1.20	0.96
1:A:276:ALA:HB3	1:C:265:ASN:C	1.85	0.95
1:C:272:LEU:HA	1:C:276:ALA:H	1.26	0.95
1:C:266:LYS:HE2	1:C:269:ILE:N	1.82	0.95
1:A:265:ASN:ND2	1:C:272:LEU:HD13	1.79	0.94
1:C:266:LYS:NZ	1:C:269:ILE:CB	2.30	0.94
1:B:266:LYS:HD3	1:D:273:GLU:HB2	1.47	0.93
1:A:265:ASN:CG	1:C:272:LEU:CA	2.33	0.93
1:A:275:LYS:O	1:C:264:GLU:OE1	1.87	0.92
1:A:274:GLY:N	1:C:266:LYS:HA	1.82	0.92
1:A:272:LEU:CB	1:C:265:ASN:OD1	2.13	0.91
1:A:272:LEU:CB	1:C:265:ASN:ND2	2.32	0.90
1:C:272:LEU:CA	1:C:276:ALA:N	2.33	0.90
1:A:276:ALA:HB1	1:C:265:ASN:HB3	1.46	0.90
1:A:272:LEU:CD2	1:C:265:ASN:HD22	1.85	0.89
1:B:275:LYS:C	1:D:264:GLU:HB2	1.83	0.88
1:D:271:ASN:C	1:D:276:ALA:HB3	1.91	0.88
1:A:267:LEU:HB3	1:C:275:LYS:HG2	1.54	0.87
1:A:275:LYS:C	1:C:264:GLU:HB3	1.95	0.87
1:A:272:LEU:HD22	1:C:265:ASN:CB	2.07	0.85
1:A:265:ASN:OD1	1:C:272:LEU:HB3	1.77	0.84
1:B:269:ILE:C	1:D:270:PHE:HB2	1.98	0.83
1:A:267:LEU:HD12	1:A:267:LEU:O	1.79	0.83
1:A:272:LEU:HD22	1:C:265:ASN:HB3	1.59	0.83
1:B:273:GLU:HB2	1:D:266:LYS:HB3	1.59	0.82
1:B:273:GLU:N	1:D:266:LYS:HB3	1.94	0.81
1:A:272:LEU:HD13	1:C:265:ASN:HD21	0.68	0.81
1:A:270:PHE:O	1:C:267:LEU:N	2.13	0.81
1:B:266:LYS:CE	1:B:269:ILE:CB	2.57	0.80
1:B:266:LYS:CA	1:D:271:ASN:C	2.29	0.80
1:A:275:LYS:CE	1:A:275:LYS:HA	2.03	0.79
1:B:275:LYS:H	1:D:266:LYS:HA	1.47	0.79
1:A:264:GLU:HG3	1:C:275:LYS:O	1.84	0.77
1:D:266:LYS:HE3	1:D:269:ILE:CB	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLY:N	1:C:266:LYS:CA	2.47	0.77
1:A:272:LEU:CD2	1:C:265:ASN:HB3	2.15	0.77
1:A:267:LEU:HB3	1:C:275:LYS:HG3	0.79	0.77
1:B:266:LYS:HB3	1:D:273:GLU:HB2	1.66	0.76
1:A:276:ALA:CB	1:C:265:ASN:O	2.33	0.76
1:A:276:ALA:CB	1:C:265:ASN:C	2.53	0.75
1:A:270:PHE:CD1	1:C:266:LYS:HE2	2.22	0.74
1:C:275:LYS:CE	1:C:275:LYS:HA	2.02	0.73
1:A:274:GLY:H	1:C:266:LYS:HA	1.53	0.73
1:A:275:LYS:CE	1:A:275:LYS:CA	2.65	0.73
1:B:266:LYS:HA	1:D:275:LYS:N	2.04	0.73
1:A:272:LEU:HD22	1:C:265:ASN:CG	2.08	0.73
1:B:275:LYS:C	1:D:264:GLU:CB	2.44	0.73
1:A:270:PHE:C	1:C:266:LYS:HG2	2.06	0.72
1:A:267:LEU:CB	1:C:275:LYS:HB2	1.90	0.72
1:C:266:LYS:HE2	1:C:269:ILE:H	1.53	0.72
1:A:276:ALA:CA	1:C:265:ASN:C	2.57	0.71
1:C:274:GLY:O	1:C:275:LYS:HE2	1.89	0.71
1:A:270:PHE:HD1	1:C:266:LYS:HE2	1.53	0.70
1:C:271:ASN:O	1:C:276:ALA:N	2.20	0.69
1:C:266:LYS:CD	1:C:269:ILE:CB	2.70	0.69
1:B:270:PHE:CA	1:D:269:ILE:N	2.49	0.69
1:C:275:LYS:CE	1:C:275:LYS:CA	2.67	0.68
1:C:272:LEU:CA	1:C:276:ALA:CA	2.60	0.68
1:B:264:GLU:HB3	1:D:275:LYS:O	1.94	0.68
1:B:273:GLU:N	1:D:266:LYS:CB	2.43	0.68
1:A:265:ASN:CG	1:C:272:LEU:HA	2.08	0.68
1:A:276:ALA:HB3	1:C:265:ASN:O	1.92	0.68
1:B:273:GLU:CB	1:D:266:LYS:HB3	2.12	0.67
1:C:272:LEU:HA	1:C:276:ALA:C	2.13	0.67
1:B:53:ARG:HG2	1:B:246:GLU:HG2	1.75	0.67
1:C:272:LEU:CA	1:C:276:ALA:H	1.97	0.67
1:A:276:ALA:CB	1:C:265:ASN:N	2.20	0.67
1:A:276:ALA:HB1	1:C:265:ASN:N	2.10	0.67
1:B:115:VAL:HG22	1:B:116:PRO:HD2	1.75	0.66
1:D:272:LEU:CD2	1:D:276:ALA:HB1	1.94	0.66
1:B:273:GLU:H	1:D:266:LYS:HB3	1.60	0.66
1:A:270:PHE:CD1	1:C:266:LYS:CE	2.79	0.66
1:B:266:LYS:HA	1:D:274:GLY:C	2.15	0.66
1:B:44:ASP:HB3	1:B:56:LYS:HG3	1.77	0.65
1:B:269:ILE:N	1:D:270:PHE:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:O	1:C:268:ALA:N	2.17	0.65
1:B:266:LYS:CD	1:D:273:GLU:HB2	2.26	0.64
1:D:272:LEU:HD23	1:D:276:ALA:HB1	1.00	0.64
1:A:267:LEU:HB2	1:C:275:LYS:HB3	1.80	0.63
1:A:265:ASN:HD22	1:C:272:LEU:CD1	1.94	0.63
1:A:265:ASN:CG	1:C:272:LEU:HD22	2.07	0.63
1:A:265:ASN:HD22	1:C:272:LEU:HD13	1.57	0.62
1:B:275:LYS:O	1:D:264:GLU:OE1	2.16	0.62
1:C:274:GLY:O	1:C:275:LYS:CE	2.47	0.62
1:A:275:LYS:O	1:C:264:GLU:HB2	1.95	0.62
1:A:272:LEU:CD2	1:C:265:ASN:CG	2.68	0.62
1:B:266:LYS:HB3	1:D:273:GLU:CB	2.01	0.62
1:A:270:PHE:O	1:C:266:LYS:C	2.39	0.61
1:A:272:LEU:HA	1:A:276:ALA:HB3	1.81	0.61
1:B:270:PHE:HA	1:D:269:ILE:N	2.15	0.61
1:B:269:ILE:N	1:D:270:PHE:CA	2.56	0.61
1:A:267:LEU:HB2	1:C:275:LYS:HB2	1.62	0.61
1:D:272:LEU:HD23	1:D:276:ALA:CB	1.81	0.61
1:A:276:ALA:CA	1:C:264:GLU:HB3	2.30	0.60
1:B:275:LYS:N	1:D:266:LYS:HA	2.16	0.60
1:C:271:ASN:C	1:C:276:ALA:H	2.04	0.60
1:C:272:LEU:O	1:C:276:ALA:O	2.09	0.60
1:C:74:SER:HB2	1:D:75:THR:HG22	1.81	0.60
1:B:275:LYS:HG3	1:D:264:GLU:OE1	2.03	0.59
1:A:265:ASN:C	1:C:272:LEU:HA	2.06	0.59
1:A:274:GLY:H	1:C:266:LYS:HG3	1.68	0.59
1:C:79:ILE:HD12	1:C:80:TRP:HD1	1.67	0.59
1:A:163:GLY:HA3	1:A:174:THR:HG22	1.85	0.59
1:D:44:ASP:HB3	1:D:56:LYS:HG3	1.86	0.57
1:B:266:LYS:HD3	1:D:273:GLU:CB	2.28	0.57
1:B:219:LEU:HD22	1:B:223:LEU:HD12	1.85	0.56
1:B:267:LEU:HG	1:D:271:ASN:O	2.06	0.55
1:B:261:GLU:O	1:B:262:ASP:HB2	2.06	0.55
1:B:269:ILE:C	1:D:270:PHE:HA	2.22	0.55
1:B:275:LYS:C	1:D:264:GLU:HB3	2.27	0.55
1:A:216:ARG:HB3	1:C:208:LYS:HD3	1.88	0.55
1:A:274:GLY:N	1:C:266:LYS:CB	2.45	0.54
1:A:276:ALA:C	1:C:265:ASN:C	2.41	0.54
1:B:268:ALA:N	1:D:270:PHE:C	2.55	0.54
1:A:266:LYS:HB2	1:C:270:PHE:O	2.08	0.54
1:A:276:ALA:HB1	1:C:265:ASN:HB2	1.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HG22	1:C:116:PRO:HD2	1.89	0.53
1:B:266:LYS:CB	1:D:273:GLU:HB2	2.37	0.53
1:A:274:GLY:N	1:C:266:LYS:HG3	2.23	0.53
1:C:70:ARG:HH21	1:C:130:LEU:HA	1.72	0.53
1:B:269:ILE:CA	1:D:270:PHE:HA	2.39	0.53
1:B:275:LYS:HB3	1:D:265:ASN:O	2.08	0.53
1:D:42:GLN:HB2	1:D:70:ARG:HB2	1.91	0.52
1:C:274:GLY:C	1:C:275:LYS:HE2	2.30	0.52
1:A:264:GLU:CG	1:C:275:LYS:O	2.57	0.51
1:C:114:LEU:HG	1:C:229:VAL:HG12	1.92	0.51
1:B:177:TRP:HE1	1:B:204:HIS:HE1	1.58	0.51
1:A:270:PHE:HD1	1:C:266:LYS:CE	2.21	0.51
1:B:266:LYS:HB3	1:D:273:GLU:H	1.69	0.51
1:C:153:GLY:H	1:C:156:ASP:HB2	1.75	0.51
1:A:276:ALA:C	1:C:265:ASN:O	2.46	0.51
1:B:141:GLN:HB3	1:B:224:PRO:HD3	1.94	0.50
1:D:160:ARG:HB2	1:D:177:TRP:O	2.11	0.50
1:C:266:LYS:HD3	1:C:269:ILE:CB	2.41	0.50
1:A:275:LYS:O	1:C:264:GLU:CG	2.56	0.50
1:B:264:GLU:CB	1:D:275:LYS:O	2.58	0.50
1:A:272:LEU:CD2	1:C:265:ASN:CB	2.79	0.50
1:B:273:GLU:HB2	1:D:266:LYS:CB	2.36	0.50
1:B:63:PRO:HB2	1:B:242:VAL:HB	1.94	0.50
1:A:274:GLY:N	1:C:266:LYS:CG	2.75	0.49
1:A:265:ASN:OD1	1:C:272:LEU:CB	2.37	0.49
1:B:273:GLU:HB2	1:D:266:LYS:HD3	1.93	0.49
1:D:97:ASN:HD22	1:D:184:ASN:ND2	2.11	0.49
1:B:98:LEU:HD21	1:B:110:LEU:HD22	1.94	0.49
1:A:276:ALA:O	1:C:265:ASN:O	2.25	0.48
1:B:70:ARG:HH21	1:B:130:LEU:HD23	1.76	0.48
1:B:270:PHE:C	1:D:268:ALA:N	2.67	0.48
1:C:68:LEU:HG	1:C:234:THR:HG22	1.95	0.48
1:A:26:LEU:HB2	1:B:30:THR:HB	1.94	0.48
1:A:265:ASN:CB	1:C:272:LEU:HD22	2.04	0.48
1:B:274:GLY:HA3	1:D:266:LYS:HG3	1.66	0.48
1:D:79:ILE:HG23	1:D:80:TRP:HD1	1.78	0.48
1:C:33:LYS:HD2	1:C:50:GLY:HA3	1.96	0.48
1:A:45:ALA:HB2	1:A:70:ARG:H	1.78	0.48
1:A:196:ASN:HB2	1:A:216:ARG:HG3	1.95	0.47
1:C:114:LEU:HD23	1:C:227:VAL:HG21	1.96	0.47
1:A:75:THR:HG22	1:B:74:SER:OG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HH22	1:B:115:VAL:HG21	1.80	0.47
1:B:52:LEU:HB3	1:B:247:VAL:HB	1.97	0.47
1:D:144:ALA:HB3	1:D:165:ASP:HB2	1.96	0.47
1:D:51:LYS:HD2	1:D:248:LEU:HD22	1.96	0.47
1:D:68:LEU:HD12	1:D:124:LYS:HG2	1.97	0.47
1:A:270:PHE:CD1	1:C:266:LYS:HE3	2.50	0.46
1:D:92:THR:HB	1:D:252:PHE:HD1	1.80	0.46
1:A:272:LEU:O	1:A:276:ALA:O	2.29	0.46
1:B:68:LEU:HD12	1:B:124:LYS:HG2	1.96	0.46
1:B:237:LEU:HD12	2:B:301:GAL:H2	1.97	0.46
1:C:116:PRO:HB2	1:C:119:SER:HB2	1.97	0.46
1:C:272:LEU:N	1:C:276:ALA:H	2.13	0.46
1:B:186:GLU:HB2	1:B:203:VAL:HG23	1.98	0.46
1:B:275:LYS:O	1:D:264:GLU:HB3	2.04	0.45
1:A:52:LEU:HB3	1:A:247:VAL:HB	1.98	0.45
1:C:274:GLY:C	1:C:275:LYS:CE	2.85	0.45
1:A:266:LYS:C	1:C:276:ALA:H	2.19	0.45
1:A:275:LYS:O	1:C:264:GLU:CD	2.52	0.45
1:D:68:LEU:HD23	1:D:69:GLY:N	2.32	0.45
1:D:272:LEU:N	1:D:276:ALA:HB3	2.21	0.45
1:B:272:LEU:HD22	1:D:265:ASN:HB2	1.27	0.45
1:A:164:ILE:HD12	1:A:215:GLU:HB3	1.98	0.45
1:C:267:LEU:O	1:C:267:LEU:HD12	2.16	0.45
1:C:42:GLN:HB2	1:C:70:ARG:HB2	2.00	0.44
1:C:172:ILE:HD12	1:C:215:GLU:HG2	1.99	0.44
1:C:275:LYS:N	1:C:275:LYS:HE2	2.30	0.44
1:B:267:LEU:HG	1:D:271:ASN:C	2.05	0.44
1:C:266:LYS:CE	1:C:269:ILE:H	2.26	0.43
1:A:40:ILE:HD11	1:A:74:SER:HA	1.99	0.43
1:D:275:LYS:HE2	1:D:275:LYS:HB2	1.66	0.43
1:A:274:GLY:H	1:C:266:LYS:CG	2.31	0.43
1:B:67:SER:H	1:B:235:THR:HG1	1.66	0.43
1:B:42:GLN:HB2	1:B:70:ARG:HB2	2.01	0.43
1:A:107:ALA:HA	1:A:108:ASP:HA	1.64	0.42
1:A:153:GLY:H	1:A:156:ASP:HB2	1.83	0.42
1:C:70:ARG:HD3	1:C:72:PHE:CE2	2.55	0.42
1:A:63:PRO:HB2	1:A:242:VAL:HB	2.01	0.42
1:A:276:ALA:HA	1:C:264:GLU:HB3	2.00	0.42
1:C:107:ALA:HA	1:C:108:ASP:HA	1.65	0.42
1:A:274:GLY:H	1:C:266:LYS:CA	2.19	0.42
1:B:276:ALA:H	1:D:265:ASN:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:HG22	1:C:189:ILE:HB	2.01	0.42
1:B:276:ALA:O	1:D:265:ASN:HA	2.19	0.41
1:A:270:PHE:CE1	1:C:266:LYS:HE3	2.55	0.41
1:C:167:ASN:HD21	1:C:222:VAL:HG13	1.84	0.41
1:A:30:THR:OG1	1:B:26:LEU:HB2	2.20	0.41
1:D:107:ALA:HA	1:D:108:ASP:HA	1.84	0.41
1:A:166:VAL:HG21	1:A:217:VAL:HG21	2.01	0.41
1:A:141:GLN:HB3	1:A:224:PRO:HD3	2.03	0.41
1:B:266:LYS:CB	1:D:273:GLU:N	2.23	0.41
1:B:272:LEU:HD23	1:D:265:ASN:HB3	0.80	0.41
1:B:160:ARG:HB2	1:B:177:TRP:O	2.20	0.41
1:B:177:TRP:HE1	1:B:204:HIS:CE1	2.36	0.40
1:A:79:ILE:HD13	1:A:223:LEU:HD13	2.02	0.40
1:B:266:LYS:O	1:D:269:ILE:O	2.39	0.40
1:D:53:ARG:HG2	1:D:246:GLU:HG2	2.03	0.40
1:A:272:LEU:HD23	1:C:265:ASN:HB3	1.98	0.40
1:C:272:LEU:CA	1:C:276:ALA:C	2.69	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	251/281 (89%)	226 (90%)	23 (9%)	2 (1%)	19	9
1	B	251/281 (89%)	238 (95%)	12 (5%)	1 (0%)	34	25
1	C	246/281 (88%)	226 (92%)	20 (8%)	0	100	100
1	D	246/281 (88%)	233 (95%)	11 (4%)	2 (1%)	19	9
All	All	994/1124 (88%)	923 (93%)	66 (7%)	5 (0%)	29	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	D	153	GLY
1	D	106	PRO
1	B	106	PRO
1	A	106	PRO

### 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	210/237 (89%)	210 (100%)	0	100	100
1	B	211/237 (89%)	206 (98%)	5 (2%)	49	43
1	C	208/237 (88%)	208 (100%)	0	100	100
1	D	208/237 (88%)	206 (99%)	2 (1%)	76	75
All	All	837/948 (88%)	830 (99%)	7 (1%)	81	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ARG
1	B	108	ASP
1	B	115	VAL
1	B	149	THR
1	B	175	THR
1	D	59	GLU
1	D	260	LYS

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	120	GLN
1	B	78	GLN
1	B	184	ASN
1	B	204	HIS
1	C	135	ASN

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Mol	Chain	Res	Type
1	C	204	HIS
1	C	265	ASN
1	D	184	ASN
1	D	196	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z  > 2$
3	EDO	B	303	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	B	302	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	D	302	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	A	302	-	3,3,3	0.46	0	2,2,2	0.32	0
6	PEG	D	304	-	6,6,6	0.44	0	5,5,5	0.29	0
6	PEG	B	305	-	6,6,6	0.43	0	5,5,5	0.34	0
2	GAL	C	301	-	12,12,12	0.55	0	17,17,17	0.63	0
2	GAL	B	301	-	12,12,12	0.53	0	17,17,17	0.55	0
2	GAL	D	301	-	12,12,12	0.54	0	17,17,17	0.54	0
6	PEG	B	304	-	6,6,6	0.44	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GAL	A	301	-	12,12,12	0.55	0	17,17,17	0.59	0
3	EDO	D	303	-	3,3,3	0.45	0	2,2,2	0.35	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	EDO	B	303	-	-	1/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
6	PEG	D	304	-	-	1/4/4/4	-
6	PEG	B	305	-	-	2/4/4/4	-
2	GAL	C	301	-	-	1/2/22/22	0/1/1/1
2	GAL	B	301	-	-	0/2/22/22	0/1/1/1
2	GAL	D	301	-	-	1/2/22/22	0/1/1/1
6	PEG	B	304	-	-	3/4/4/4	-
2	GAL	A	301	-	-	1/2/22/22	0/1/1/1
3	EDO	D	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	305	PEG	O2-C3-C4-O4
3	A	302	EDO	O1-C1-C2-O2
6	B	304	PEG	O1-C1-C2-O2
6	B	304	PEG	O2-C3-C4-O4
3	D	303	EDO	O1-C1-C2-O2
6	D	304	PEG	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2
2	D	301	GAL	C4-C5-C6-O6
2	A	301	GAL	C4-C5-C6-O6
6	B	304	PEG	C4-C3-O2-C2
2	C	301	GAL	C4-C5-C6-O6
6	B	305	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	GAL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	253/281 (90%)	0.82	26 (10%) 6 6	23, 41, 62, 63	14 (5%)
1	B	253/281 (90%)	-0.15	5 (1%) 65 67	12, 18, 32, 32	14 (5%)
1	C	250/281 (88%)	-0.03	4 (1%) 72 73	19, 25, 31, 41	14 (5%)
1	D	250/281 (88%)	-0.12	5 (2%) 65 67	15, 22, 26, 36	14 (5%)
All	All	1006/1124 (89%)	0.13	40 (3%) 38 40	12, 24, 53, 63	56 (5%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	267	LEU	5.8
1	A	128	LEU	5.2
1	A	164	ILE	5.1
1	B	269	ILE	5.0
1	C	269	ILE	5.0
1	A	136	TYR	4.7
1	A	151	TYR	4.3
1	A	236	GLY	3.9
1	A	167	ASN	3.8
1	C	265	ASN	3.7
1	A	130	LEU	3.7
1	A	242	VAL	3.4
1	B	273	GLU	3.3
1	D	273	GLU	3.2
1	D	264	GLU	3.1
1	A	162	ILE	3.1
1	A	232	SER	3.0
1	C	151	TYR	2.9
1	A	267	LEU	2.8
1	A	269	ILE	2.7
1	B	272	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	PHE	2.7
1	B	276	ALA	2.7
1	C	264	GLU	2.6
1	A	241	TYR	2.6
1	A	155	TRP	2.6
1	A	172	ILE	2.6
1	A	124	LYS	2.4
1	B	275	LYS	2.4
1	A	83	THR	2.3
1	D	269	ILE	2.3
1	A	237	LEU	2.3
1	A	166	VAL	2.3
1	A	147	PHE	2.3
1	A	55	THR	2.2
1	A	211	PHE	2.2
1	A	54	ILE	2.1
1	A	258	ILE	2.0
1	A	143	VAL	2.0
1	D	275	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GAL	A	301	12/12	0.83	0.20	24,25,25,25	12
2	GAL	D	301	12/12	0.84	0.18	24,24,25,25	12
2	GAL	C	301	12/12	0.87	0.18	26,27,27,27	12
3	EDO	A	302	4/4	0.88	0.17	36,36,36,37	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	303	1/1	0.91	0.14	78,78,78,78	0
2	GAL	B	301	12/12	0.91	0.18	20,20,21,21	12
6	PEG	B	304	7/7	0.93	0.13	31,31,31,31	0
3	EDO	B	303	4/4	0.94	0.16	29,29,29,30	0
3	EDO	D	302	4/4	0.95	0.11	26,26,26,26	0
6	PEG	B	305	7/7	0.96	0.11	22,22,22,22	0
6	PEG	D	304	7/7	0.97	0.10	18,19,19,20	0
5	MN	C	303	1/1	0.97	0.07	65,65,65,65	0
3	EDO	B	302	4/4	0.97	0.09	18,19,19,19	0
4	CA	D	305	1/1	0.97	0.10	22,22,22,22	0
3	EDO	D	303	4/4	0.97	0.10	27,27,27,27	0
5	MN	A	304	1/1	0.98	0.05	41,41,41,41	0
4	CA	C	302	1/1	0.98	0.09	24,24,24,24	0
4	CA	B	306	1/1	0.99	0.11	27,27,27,27	0
5	MN	B	307	1/1	0.99	0.07	38,38,38,38	0
5	MN	D	306	1/1	0.99	0.03	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.