



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:38 AM UTC

PDB ID : 6IBI / pdb\_00006ibi  
Title : Copper binding protein from *Laetisaria arvalis* (LaX325)  
Authors : Frandsen, K.E.H.; Tandrup, T.; Labourel, A.; Haon, M.; Berrin, J.-G.; Lo Leggio, L.  
Deposited on : 2018-11-30  
Resolution : 2.08 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

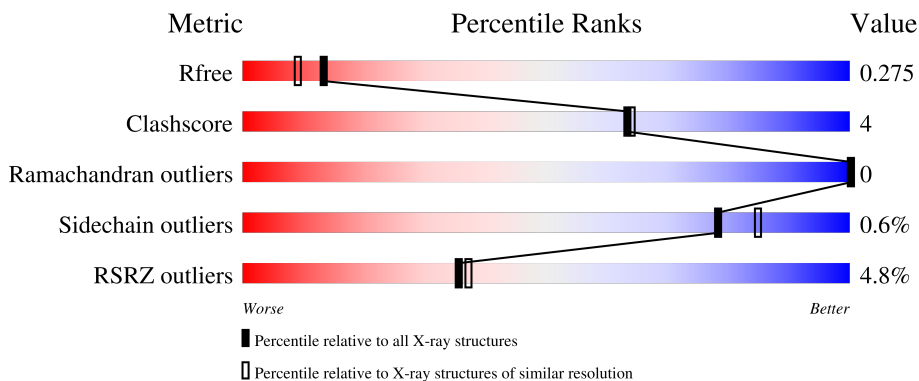
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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))
$R_{free}$	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	 2% 92% 6%
1	B	155	 3% 91% 5%
1	C	155	 2% 91% 8%
1	D	155	 12% 91% 5%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5546 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 Auxiliary activity CAZyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1172	727	204	235	6	0	4	0
1	B	150	1130	701	195	230	4	0	1	0
1	C	155	1191	737	211	237	6	0	3	0
1	D	149	1113	690	191	228	4	0	0	0

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



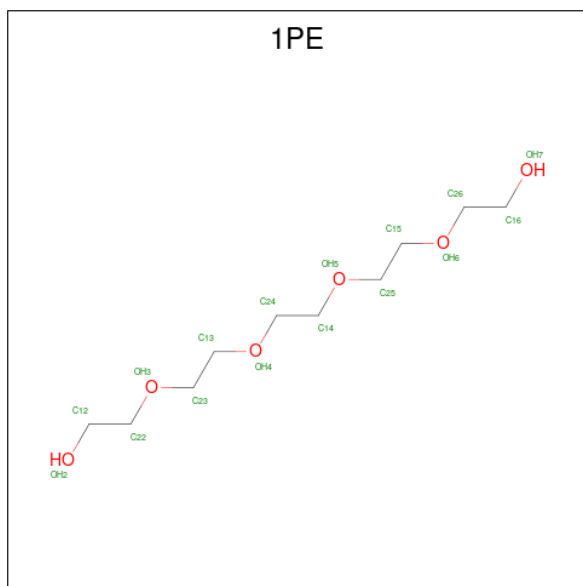
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



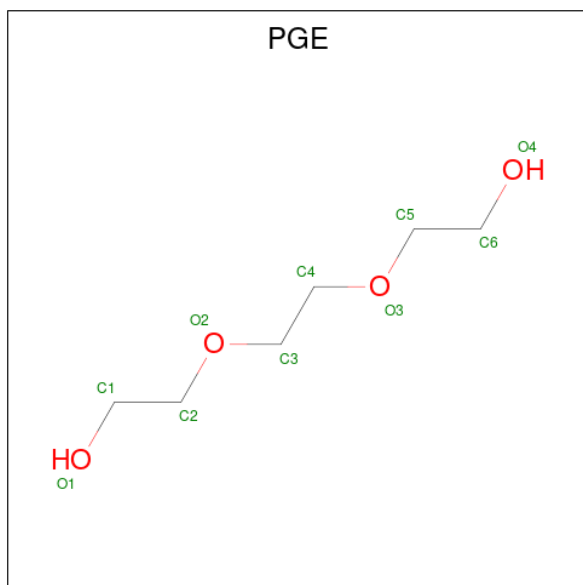
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			9	6	3		

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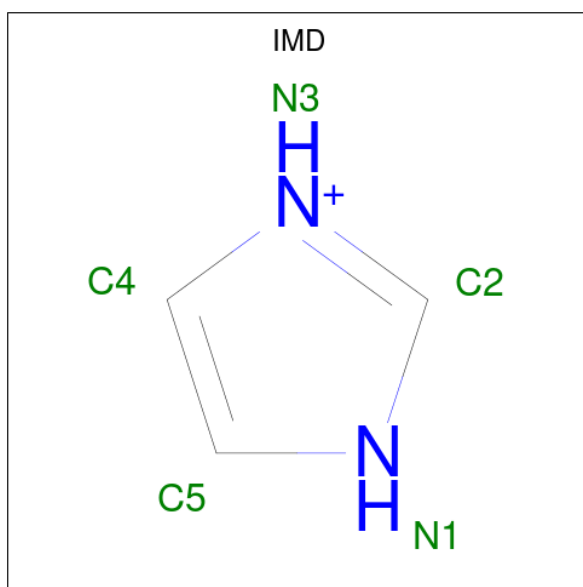
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N 5 3 2	0	0
6	C	1	Total C N 5 3 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	180	Total O 183 183	0	5
7	B	138	Total O 138 138	0	2
7	C	146	Total O 148 148	0	3
7	D	85	Total O 85 85	0	0

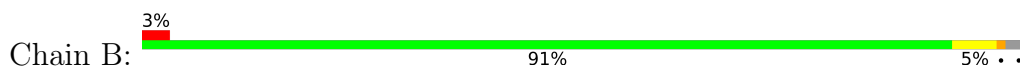
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

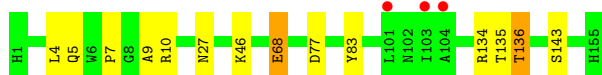
- Molecule 1: Auxiliary activity CAZyme



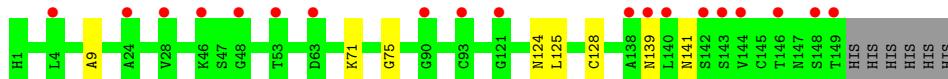
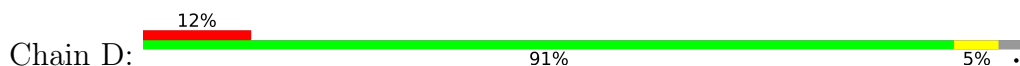
- Molecule 1: Auxiliary activity CAZyme



- Molecule 1: Auxiliary activity CAZyme



- Molecule 1: Auxiliary activity CAZyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.60Å 84.64Å 127.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.35 – 2.08 42.35 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.35-2.08) 99.5 (42.35-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.08Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.244 , 0.271 0.250 , 0.275	Depositor DCC
$R_{free}$ test set	2641 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.007 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: CU, 1PE, NAG, IMD, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.89	1/1213 (0.1%)	0.94	0/1657
1	B	0.84	0/1159	0.92	0/1584
1	C	0.83	0/1228	1.01	3/1676 (0.2%)
1	D	0.72	0/1138	0.92	0/1555
All	All	0.83	1/4738 (0.0%)	0.95	3/6472 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ASP	C-O	-5.37	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	THR	CA-CB-OG1	-6.17	100.35	109.60
1	C	68	GLU	CB-CG-CD	5.21	121.45	112.60
1	C	10	ARG	NE-CZ-NH1	-5.09	116.41	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	ARG	Sidechain
1	C	134	ARG	Sidechain

## 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	1172	0	1069	8	0
1	B	1130	0	1034	6	0
1	C	1191	0	1080	12	0
1	D	1113	0	1015	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	84	0	77	1	0
3	B	84	0	78	2	0
3	C	84	0	78	4	0
3	D	70	0	65	0	0
4	A	16	0	19	1	0
4	B	7	0	9	0	0
4	C	7	0	9	0	0
4	D	10	0	12	1	0
5	A	10	0	14	2	0
6	B	5	0	5	1	0
6	C	5	0	5	1	0
7	A	183	0	0	3	0
7	B	138	0	0	3	0
7	C	148	0	0	4	0
7	D	85	0	0	2	0
All	All	5546	0	4569	38	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 (38) 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:127:GLN:C	1:A:128[C]:CYS:CA	2.52	0.81
1:A:128[C]:CYS:CA	1:A:129:ALA:N	2.44	0.80
5:A:209:PGE:O3	7:A:301:HOH:O	2.09	0.70
1:C:27:ASN:HD22	3:C:206:NAG:H83	1.61	0.65
1:D:124:ASN:C	1:D:125:LEU:HD12	2.25	0.61
1:C:135:THR:OG1	7:C:301:HOH:O	2.16	0.60
3:A:202:NAG:O4	7:A:302:HOH:O	2.17	0.58
1:C:83:TYR:OH	7:C:302:HOH:O	2.17	0.57
1:D:141:ASN:HB2	7:D:374:HOH:O	2.03	0.57
6:B:208:IMD:H4	7:B:375:HOH:O	2.05	0.56
1:A:95:PRO:HB3	4:A:208:1PE:H251	1.88	0.55
1:A:60:LEU:HD21	1:A:106:ILE:HD11	1.88	0.55
1:C:27:ASN:ND2	3:C:206:NAG:H83	2.21	0.55
1:C:4:LEU:HG	1:C:7:PRO:O	2.08	0.52
1:B:26[B]:ASN:OD1	3:B:206:NAG:H82	2.10	0.52
1:C:5[A]:GLN:HE22	1:C:46:LYS:HZ2	1.59	0.51
1:D:71:LYS:HE3	1:D:75:GLY:O	2.12	0.50
1:B:134:ARG:HD2	7:B:413:HOH:O	2.12	0.49
1:A:60:LEU:HD11	1:A:106:ILE:HD13	1.95	0.48
1:C:77:ASP:OD2	6:C:208:IMD:N3	2.47	0.47
1:B:127:GLN:NE2	7:B:310:HOH:O	2.47	0.46
1:D:71:LYS:CE	1:D:75:GLY:O	2.64	0.46
5:A:209:PGE:C4	7:A:301:HOH:O	2.63	0.45
4:D:207:1PE:H131	7:D:357:HOH:O	2.16	0.45
1:B:76:GLY:HA3	3:B:205:NAG:H5	2.00	0.44
1:C:5[A]:GLN:HE22	1:C:46:LYS:NZ	2.15	0.44
1:C:143:SER:HB3	3:C:207:NAG:H5	2.00	0.43
1:A:9:ALA:HA	1:A:128[A]:CYS:O	2.18	0.43
1:B:5:GLN:HB3	1:B:144:VAL:HG21	2.00	0.43
1:D:125:LEU:HD12	1:D:125:LEU:N	2.34	0.42
1:D:9:ALA:HA	1:D:128:CYS:O	2.19	0.42
1:B:9:ALA:HA	1:B:128:CYS:O	2.19	0.42
1:C:68:GLU:HG3	7:C:434:HOH:O	2.19	0.42
1:C:5[B]:GLN:NE2	7:C:313:HOH:O	2.53	0.41
1:A:60:LEU:HD21	1:A:106:ILE:CD1	2.50	0.41
3:C:206:NAG:H82	3:C:206:NAG:H2	1.92	0.41
1:A:50:ALA:HB1	1:A:51:PRO:HA	2.04	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	155/155 (100%)	153 (99%)	2 (1%)	0	100	100
1	B	149/155 (96%)	148 (99%)	1 (1%)	0	100	100
1	C	156/155 (101%)	154 (99%)	2 (1%)	0	100	100
1	D	147/155 (95%)	146 (99%)	1 (1%)	0	100	100
All	All	607/620 (98%)	601 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/125 (102%)	127 (100%)	0	100	100
1	B	121/125 (97%)	120 (99%)	1 (1%)	73	80
1	C	128/125 (102%)	127 (99%)	1 (1%)	73	80
1	D	118/125 (94%)	117 (99%)	1 (1%)	73	80
All	All	494/500 (99%)	491 (99%)	3 (1%)	78	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	ILE
1	C	136	THR
1	D	139	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	B	124	ASN
1	B	127	GLN
1	C	78	GLN
1	C	124	ASN
1	C	127	GLN
1	D	78	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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	NAG	C	206	1	14,14,15	0.87	0	17,19,21	0.76	0
4	1PE	D	207	-	9,9,15	0.51	0	8,8,14	0.65	0
3	NAG	B	202	1	14,14,15	0.92	0	17,19,21	0.62	0
4	1PE	A	210	-	8,8,15	0.71	0	7,7,14	0.67	0
6	IMD	B	208	-	5,5,5	0.89	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	204	1	14,14,15	1.00	0	17,19,21	0.66	0
3	NAG	B	206	1	14,14,15	0.75	0	17,19,21	0.63	0
3	NAG	C	204	1	14,14,15	1.21	2 (14%)	17,19,21	1.33	3 (17%)
3	NAG	A	203	1	14,14,15	1.10	1 (7%)	17,19,21	0.58	0
3	NAG	D	205	1	14,14,15	0.59	0	17,19,21	0.45	0
4	1PE	A	208	-	6,6,15	0.63	0	5,5,14	0.64	0
3	NAG	B	203	1	14,14,15	0.67	0	17,19,21	0.50	0
3	NAG	D	202	1	14,14,15	0.49	0	17,19,21	0.65	0
3	NAG	A	204	1	14,14,15	0.92	0	17,19,21	0.86	0
3	NAG	A	207	1	14,14,15	1.15	1 (7%)	17,19,21	0.44	0
4	1PE	C	209	-	6,6,15	0.51	0	5,5,14	0.60	0
4	1PE	B	209	-	6,6,15	0.42	0	5,5,14	0.44	0
3	NAG	D	206	1	14,14,15	1.14	1 (7%)	17,19,21	0.55	0
3	NAG	A	202	1	14,14,15	0.80	0	17,19,21	0.71	0
3	NAG	C	202	1	14,14,15	0.84	1 (7%)	17,19,21	0.69	0
5	PGE	A	209	-	9,9,9	0.46	0	8,8,8	0.55	0
6	IMD	C	208	-	5,5,5	0.64	0	5,5,5	0.68	0
3	NAG	A	206	1	14,14,15	0.65	0	17,19,21	0.84	0
3	NAG	C	205	1	14,14,15	1.04	1 (7%)	17,19,21	0.73	0
3	NAG	B	205	1	14,14,15	0.82	0	17,19,21	0.77	1 (5%)
3	NAG	C	207	1	14,14,15	0.59	0	17,19,21	0.62	0
3	NAG	C	203	1	14,14,15	1.16	1 (7%)	17,19,21	0.68	0
3	NAG	D	204	1	14,14,15	0.76	1 (7%)	17,19,21	0.52	0
3	NAG	D	203	1	14,14,15	0.67	0	17,19,21	0.76	0
3	NAG	A	205	1	14,14,15	0.92	0	17,19,21	0.56	0
3	NAG	B	207	1	14,14,15	0.75	0	17,19,21	0.50	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	NAG	C	206	1	-	4/6/23/26	0/1/1/1
4	1PE	D	207	-	-	3/7/7/13	-
3	NAG	B	202	1	-	1/6/23/26	0/1/1/1
4	1PE	A	210	-	-	3/6/6/13	-
6	IMD	B	208	-	-	-	0/1/1/1
3	NAG	B	204	1	-	1/6/23/26	0/1/1/1
3	NAG	B	206	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	204	1	-	3/6/23/26	0/1/1/1
3	NAG	A	203	1	-	0/6/23/26	0/1/1/1
3	NAG	D	205	1	-	0/6/23/26	0/1/1/1
4	1PE	A	208	-	-	0/4/4/13	-
3	NAG	B	203	1	-	0/6/23/26	0/1/1/1
3	NAG	D	202	1	-	2/6/23/26	0/1/1/1
3	NAG	A	204	1	-	0/6/23/26	0/1/1/1
3	NAG	A	207	1	-	1/6/23/26	0/1/1/1
4	1PE	C	209	-	-	3/4/4/13	-
4	1PE	B	209	-	-	2/4/4/13	-
3	NAG	D	206	1	-	3/6/23/26	0/1/1/1
3	NAG	A	202	1	-	0/6/23/26	0/1/1/1
3	NAG	C	202	1	-	0/6/23/26	0/1/1/1
5	PGE	A	209	-	-	2/7/7/7	-
6	IMD	C	208	-	-	-	0/1/1/1
3	NAG	A	206	1	-	0/6/23/26	0/1/1/1
3	NAG	C	205	1	-	3/6/23/26	0/1/1/1
3	NAG	B	205	1	-	1/6/23/26	0/1/1/1
3	NAG	C	207	1	-	4/6/23/26	0/1/1/1
3	NAG	C	203	1	-	0/6/23/26	0/1/1/1
3	NAG	D	204	1	-	0/6/23/26	0/1/1/1
3	NAG	D	203	1	-	0/6/23/26	0/1/1/1
3	NAG	A	205	1	-	0/6/23/26	0/1/1/1
3	NAG	B	207	1	-	4/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	207	NAG	C1-C2	3.80	1.57	1.52
3	D	206	NAG	C2-N2	3.13	1.51	1.46
3	C	203	NAG	C2-N2	-3.00	1.41	1.46
3	C	204	NAG	C3-C2	-2.82	1.46	1.52
3	C	204	NAG	C4-C5	2.60	1.58	1.53
3	A	203	NAG	O5-C1	2.44	1.47	1.43
3	D	204	NAG	C1-C2	2.20	1.55	1.52
3	C	205	NAG	O5-C5	2.08	1.47	1.43
3	C	202	NAG	C1-C2	2.03	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	204	NAG	O5-C1-C2	-3.30	106.18	111.29
3	C	204	NAG	C4-C3-C2	-2.44	107.44	111.02
3	C	204	NAG	C1-C2-N2	2.42	114.24	110.43
3	B	205	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	204	NAG	C1-C2-N2-C7
3	C	206	NAG	C8-C7-N2-C2
3	C	206	NAG	O7-C7-N2-C2
3	C	205	NAG	O7-C7-N2-C2
3	C	206	NAG	O5-C5-C6-O6
3	C	207	NAG	O5-C5-C6-O6
3	C	205	NAG	C8-C7-N2-C2
3	C	206	NAG	C4-C5-C6-O6
3	B	206	NAG	C4-C5-C6-O6
3	C	207	NAG	C4-C5-C6-O6
3	B	206	NAG	O5-C5-C6-O6
3	C	204	NAG	C4-C5-C6-O6
4	A	210	1PE	OH4-C13-C23-OH3
3	D	202	NAG	C4-C5-C6-O6
3	C	204	NAG	O5-C5-C6-O6
3	D	202	NAG	O5-C5-C6-O6
3	C	207	NAG	C8-C7-N2-C2
3	C	207	NAG	O7-C7-N2-C2
4	B	209	1PE	OH4-C13-C23-OH3
4	B	209	1PE	OH2-C12-C22-OH3
3	B	207	NAG	C4-C5-C6-O6
4	D	207	1PE	OH6-C15-C25-OH5
5	A	209	PGE	O1-C1-C2-O2
4	A	210	1PE	C23-C13-OH4-C24
3	C	205	NAG	O5-C5-C6-O6
4	A	210	1PE	C12-C22-OH3-C23
3	B	207	NAG	O5-C5-C6-O6
4	D	207	1PE	C14-C24-OH4-C13
4	D	207	1PE	C24-C14-OH5-C25
4	C	209	1PE	OH6-C15-C25-OH5
4	C	209	1PE	C25-C15-OH6-C26
3	A	207	NAG	C8-C7-N2-C2
3	B	207	NAG	C3-C2-N2-C7
3	D	206	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	202	NAG	C4-C5-C6-O6
3	B	205	NAG	C4-C5-C6-O6
3	B	204	NAG	C4-C5-C6-O6
3	B	207	NAG	C1-C2-N2-C7
3	D	206	NAG	C1-C2-N2-C7
4	C	209	1PE	C16-C26-OH6-C15
3	D	206	NAG	O5-C5-C6-O6
5	A	209	PGE	C6-C5-O3-C4

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	206	NAG	3	0
4	D	207	1PE	1	0
6	B	208	IMD	1	0
3	B	206	NAG	1	0
4	A	208	1PE	1	0
3	A	202	NAG	1	0
5	A	209	PGE	2	0
6	C	208	IMD	1	0
3	B	205	NAG	1	0
3	C	207	NAG	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	153/155 (98%)	0.34	3 (1%) 65 67	21, 35, 51, 100	4 (2%)
1	B	150/155 (96%)	0.50	4 (2%) 56 58	24, 38, 59, 102	1 (0%)
1	C	155/155 (100%)	0.50	3 (1%) 66 69	17, 39, 67, 85	3 (1%)
1	D	149/155 (96%)	1.12	19 (12%) 7 8	37, 51, 83, 107	0
All	All	607/620 (97%)	0.61	29 (4%) 35 37	17, 40, 70, 107	8 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	THR	4.1
1	B	138	ALA	3.7
1	D	138	ALA	3.7
1	D	142	SER	3.1
1	D	28	VAL	3.1
1	D	140	LEU	3.1
1	A	152	HIS	3.0
1	D	144	VAL	2.9
1	A	153	HIS	2.9
1	C	104	ALA	2.9
1	A	151	HIS	2.9
1	D	139	ASN	2.7
1	C	103	ILE	2.5
1	D	143	SER	2.4
1	D	24	ALA	2.3
1	B	140	LEU	2.3
1	D	121	GLY	2.3
1	B	144	VAL	2.3
1	D	148	SER	2.2
1	D	146	THR	2.2
1	D	48	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	53	THR	2.2
1	C	101	LEU	2.1
1	D	90	GLY	2.1
1	B	100	SER	2.1
1	D	4	LEU	2.1
1	D	46	LYS	2.1
1	D	93	CYS	2.1
1	D	63	ASP	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	207	14/15	0.40	0.17	86,113,127,131	0
3	NAG	B	206	14/15	0.42	0.17	89,120,128,128	0
3	NAG	D	206	14/15	0.52	0.18	79,104,114,115	0
3	NAG	C	207	14/15	0.60	0.18	85,103,112,115	0
3	NAG	C	205	14/15	0.62	0.18	69,96,101,102	0
4	1PE	A	210	9/16	0.68	0.27	76,88,96,98	0
3	NAG	B	205	14/15	0.71	0.19	71,99,107,119	0
3	NAG	C	206	14/15	0.72	0.21	63,70,74,76	14
4	1PE	C	209	7/16	0.78	0.20	69,74,76,79	0
3	NAG	C	204	14/15	0.79	0.15	57,62,66,71	0
4	1PE	B	209	7/16	0.81	0.16	51,60,67,74	0
3	NAG	A	206	14/15	0.81	0.14	73,84,89,93	0
5	PGE	A	209	10/10	0.83	0.21	68,82,100,100	0
3	NAG	D	202	14/15	0.84	0.13	54,58,68,76	0
3	NAG	A	207	14/15	0.84	0.14	68,74,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	204	14/15	0.85	0.14	58,65,76,81	0
3	NAG	D	205	14/15	0.86	0.12	64,72,81,89	0
6	IMD	B	208	5/5	0.86	0.21	61,68,72,73	0
3	NAG	D	203	14/15	0.87	0.10	57,62,67,73	0
4	1PE	D	207	10/16	0.87	0.17	63,66,78,78	0
3	NAG	C	202	14/15	0.89	0.11	39,44,54,66	0
6	IMD	C	208	5/5	0.89	0.16	70,71,72,73	0
4	1PE	A	208	7/16	0.90	0.12	55,59,64,64	0
3	NAG	A	204	14/15	0.91	0.10	35,40,48,51	0
3	NAG	A	205	14/15	0.92	0.10	34,40,42,55	0
3	NAG	B	203	14/15	0.92	0.09	43,49,58,62	0
3	NAG	B	204	14/15	0.92	0.09	39,42,46,52	0
3	NAG	A	203	14/15	0.93	0.09	30,34,40,41	0
3	NAG	C	203	14/15	0.94	0.07	26,29,33,36	0
3	NAG	B	202	14/15	0.95	0.08	32,40,44,46	0
3	NAG	A	202	14/15	0.96	0.07	27,32,36,38	0
2	CU	D	201	1/1	0.97	0.04	71,71,71,71	0
2	CU	B	201	1/1	0.99	0.03	41,41,41,41	0
2	CU	C	201	1/1	0.99	0.03	35,35,35,35	0
2	CU	A	201	1/1	1.00	0.02	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.