



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:41 PM GMT

PDB ID : 4Q26  
Title : Crystal Structure of Galectin-1 in Complex with N-Acetyllactosamine  
Authors : Grimm, C.; Bertleff-Zieschang, N.  
Deposited on : 2014-04-07  
Resolution : 1.40 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

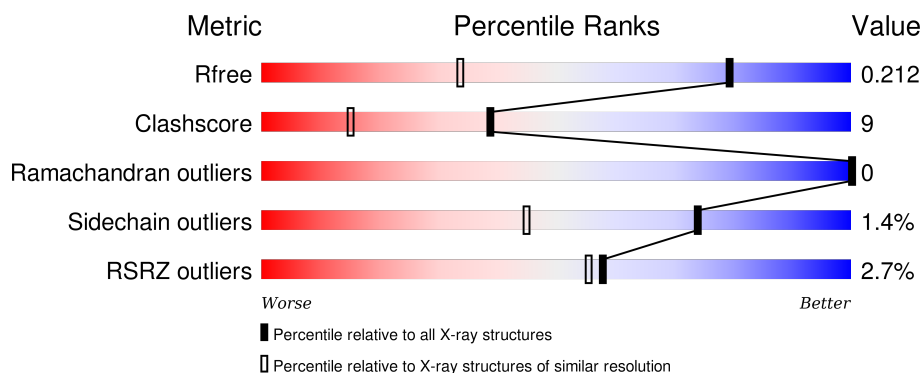
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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	136	<div> <div>87%</div> <div>10% ..</div> </div>
1	B	136	<div> <div>88%</div> <div>10% ..</div> </div>
1	G	136	<div> <div>7%</div> <div>80%</div> <div>16% ...</div> </div>
1	H	136	<div> <div>2%</div> <div>76%</div> <div>22% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NLC	A	201	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9095 atoms, of which 4195 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.

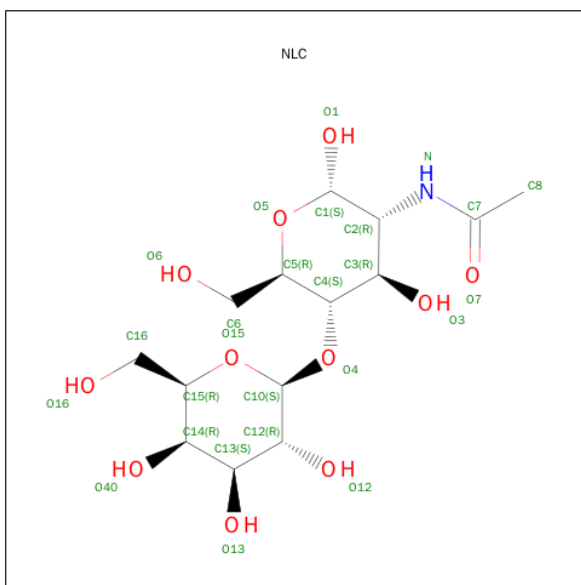
- Molecule 1 is a protein called Galectin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	133	Total	C	H	N	O	S	0	8	0
			2101	680	1025	184	203	9			
1	B	133	Total	C	H	N	O	S	0	5	0
			2084	675	1016	182	202	9			
1	G	133	Total	C	H	N	O	S	0	6	0
			2081	673	1013	183	202	10			
1	H	133	Total	C	H	N	O	S	0	8	0
			2116	684	1033	184	205	10			

There are 4 discrepancies between the modelled and reference sequences:

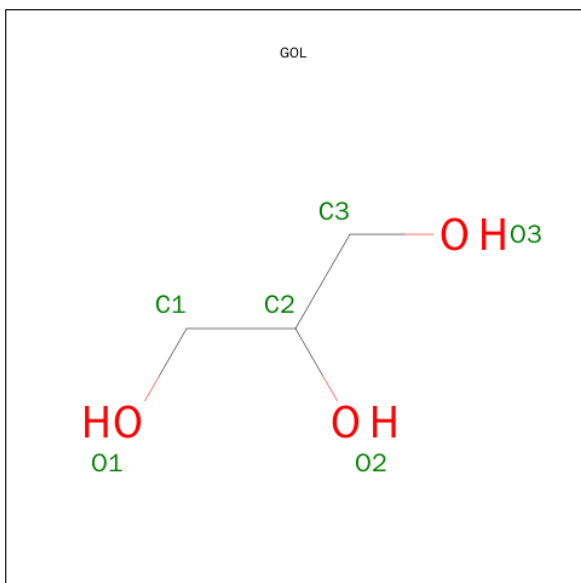
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P09382
B	-1	GLY	-	EXPRESSION TAG	UNP P09382
G	-1	GLY	-	EXPRESSION TAG	UNP P09382
H	-1	GLY	-	EXPRESSION TAG	UNP P09382

- Molecule 2 is 2-(ACETYLAMINO)-2-DEOXY-4-O-BETA-D-GALACTOPYRANOSYL-ALPHA-D-GLUCOPYRANOSE (three-letter code: NLC) (formula: C<sub>14</sub>H<sub>25</sub>NO<sub>11</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 51	C 14	H 25	N 1	O 11	0	0
2	B	1	Total 51	C 14	H 25	N 1	O 11	0	0
2	G	1	Total 51	C 14	H 25	N 1	O 11	0	0
2	H	1	Total 51	C 14	H 25	N 1	O 11	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	H	O	0	0
			14	3	8	3		

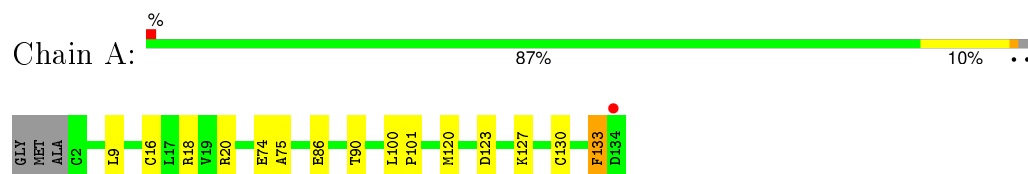
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	113	Total	O	0	0
			113	113		
4	G	133	Total	O	0	0
			133	133		
4	H	116	Total	O	0	0
			116	116		

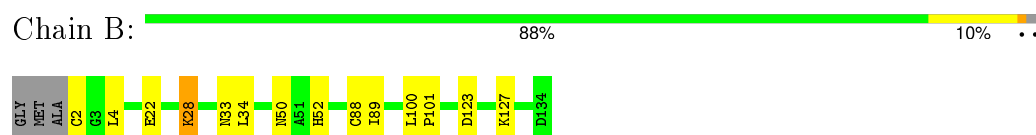
### 3 Residue-property plots [i](#)

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.

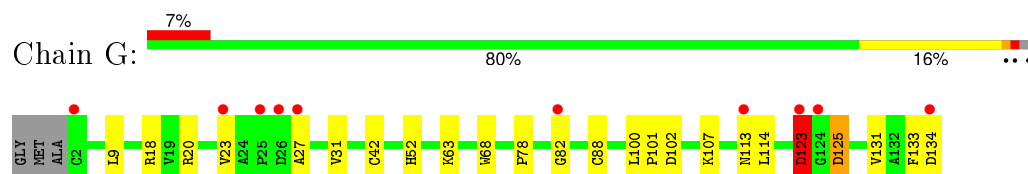
#### • Molecule 1: Galectin-1



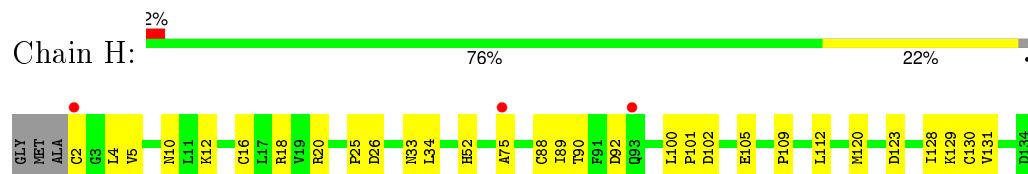
#### • Molecule 1: Galectin-1



#### • Molecule 1: Galectin-1



#### • Molecule 1: Galectin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.38 Å 85.52 Å 116.08 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 1.40 48.02 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.02-1.40) 99.2 (48.02-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.162 , 0.203 0.169 , 0.212	Depositor DCC
$R_{free}$ test set	2000 reflections (1.57%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 129682 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 40.39 % 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 2.7560e-04. 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: GOL, CME, NLC

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	0.85	1/1083 (0.1%)	0.93	2/1464 (0.1%)
1	B	0.78	0/1056	0.87	1/1424 (0.1%)
1	G	0.93	3/1063 (0.3%)	0.99	4/1435 (0.3%)
1	H	0.75	1/1079 (0.1%)	0.87	3/1456 (0.2%)
All	All	0.83	5/4281 (0.1%)	0.91	10/5779 (0.2%)

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	G	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	123	ASP	C-O	6.17	1.35	1.23
1	G	42	CYS	CB-SG	-5.22	1.73	1.81
1	G	125	ASP	CB-CG	5.05	1.62	1.51
1	A	86	GLU	CB-CG	-5.03	1.42	1.52
1	H	105	GLU	CB-CG	-5.00	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	125	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	133	PHE	N-CA-C	-6.05	94.65	111.00
1	G	20	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	B	123	ASP	CB-CG-OD2	-5.65	113.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	92	ASP	CB-CG-OD1	5.46	123.22	118.30
1	H	123	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	G	123	ASP	O-C-N	5.26	132.15	123.20
1	H	75	ALA	N-CA-C	5.18	124.98	111.00
1	A	123	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	G	107	LYS	CD-CE-NZ	5.03	123.26	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	123	ASP	Peptide
1	G	133	PHE	Peptide

## 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	1076	1025	1025	19	1
1	B	1068	1016	1033	14	0
1	G	1068	1013	1023	28	1
1	H	1083	1033	1046	30	5
2	A	26	25	25	0	0
2	B	26	25	25	1	0
2	G	26	25	25	0	0
2	H	26	25	25	1	0
3	G	6	8	8	1	0
4	A	133	0	0	3	1
4	B	113	0	0	3	1
4	G	133	0	0	11	0
4	H	116	0	0	5	5
All	All	4900	4195	4235	78	7

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 9.

All (78) 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:G:113:ASN:N	4:G:408:HOH:O	1.97	0.97
1:G:82:GLY:O	4:G:433:HOH:O	1.86	0.94
1:G:113:ASN:CA	4:G:408:HOH:O	2.18	0.91
1:H:120:MET:SD	4:H:389:HOH:O	2.28	0.91
1:A:16:CME:SD	1:A:90[B]:THR:HG23	2.11	0.90
1:A:74:GLU:OE1	4:A:406:HOH:O	1.89	0.88
1:B:50:ASN:OD1	4:B:386:HOH:O	1.92	0.87
1:H:25:PRO:O	1:H:26:ASP:HB2	1.75	0.85
1:B:2:CYS:N	4:B:380:HOH:O	2.12	0.82
1:H:16:CME:SD	1:H:90[B]:THR:CG2	2.68	0.81
1:G:123:ASP:O	1:G:123:ASP:OD2	2.00	0.80
1:A:9:LEU:HD23	1:B:4[A]:LEU:CD1	2.13	0.79
1:H:16:CME:SD	1:H:90[B]:THR:HG22	2.25	0.77
1:G:52:HIS:O	4:G:330:HOH:O	2.02	0.77
1:H:102:ASP:OD2	4:H:366:HOH:O	2.05	0.75
1:G:9:LEU:CD2	1:H:4[A]:LEU:CD1	2.66	0.73
1:G:123:ASP:OD1	4:G:390:HOH:O	2.07	0.72
1:G:114:LEU:N	4:G:408:HOH:O	2.20	0.70
1:G:123:ASP:O	1:G:123:ASP:CG	2.29	0.70
1:G:123:ASP:CG	4:G:390:HOH:O	2.30	0.69
1:H:25:PRO:O	1:H:26:ASP:CB	2.39	0.69
1:G:9:LEU:HD23	1:H:4[A]:LEU:HD12	1.77	0.66
1:H:120:MET:CE	4:H:389:HOH:O	2.43	0.66
1:G:114:LEU:O	4:G:424:HOH:O	2.15	0.65
1:H:16:CME:SD	1:H:90[B]:THR:HG23	2.38	0.62
1:B:34[A]:LEU:HD11	1:B:89:ILE:HD13	1.81	0.62
1:H:4[B]:LEU:C	1:H:4[B]:LEU:HD23	2.21	0.61
1:H:33:ASN:C	1:H:34[B]:LEU:HD12	2.24	0.58
1:A:20:ARG:HH22	1:A:130:CME:HZ3	1.69	0.58
1:H:18:ARG:HB3	1:H:130:CME:OH	2.04	0.58
1:G:9:LEU:HD23	1:H:4[A]:LEU:CD1	2.33	0.57
1:A:16:CME:SD	1:A:90[B]:THR:CG2	2.90	0.57
1:G:18:ARG:NH2	4:G:429:HOH:O	1.85	0.57
1:G:113:ASN:HA	4:G:408:HOH:O	1.96	0.56
1:A:9:LEU:CD2	1:B:4[A]:LEU:HD11	2.34	0.56
1:G:131[B]:VAL:CG2	1:H:131[B]:VAL:HG22	2.36	0.56
1:A:100[A]:LEU:HB3	1:A:101:PRO:HD2	1.87	0.55
1:A:9:LEU:HD22	1:A:133:PHE:CE1	2.42	0.55
1:A:9:LEU:HD23	1:B:4[A]:LEU:HD11	1.88	0.54
1:A:9:LEU:CD2	1:B:4[A]:LEU:CD1	2.84	0.54
3:G:201:GOL:H11	1:H:128:ILE:O	2.08	0.54
1:A:20:ARG:NH2	1:A:130:CME:HZ3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131[B]:VAL:HG23	1:H:131[B]:VAL:HG22	1.91	0.53
1:A:16:CME:HA	1:A:90[B]:THR:HG22	1.91	0.52
1:H:10:ASN:OD1	1:H:12:LYS:HE3	2.09	0.52
1:B:22:GLU:OE1	1:B:127:LYS:HE2	2.10	0.51
1:G:131[B]:VAL:HG22	1:H:131[B]:VAL:CG2	2.41	0.50
1:B:28:LYS:NZ	4:B:353:HOH:O	2.42	0.50
1:B:4[B]:LEU:HD23	1:B:4[B]:LEU:C	2.33	0.49
1:A:18:ARG:HB3	1:A:130:CME:HZ2	1.93	0.49
1:G:134:ASP:C	1:H:129:LYS:HE3	2.33	0.49
1:G:131[B]:VAL:CG2	1:H:131[B]:VAL:CG2	2.91	0.48
1:A:130:CME:HZ3	4:A:345:HOH:O	2.13	0.48
1:G:52:HIS:CE1	4:G:343:HOH:O	2.66	0.48
1:H:88:CME:SD	4:H:397:HOH:O	2.60	0.48
1:A:75:ALA:N	4:A:425:HOH:O	2.29	0.47
1:G:88:CME:OH	1:G:101:PRO:HA	2.14	0.47
1:H:34[A]:LEU:HD11	1:H:89:ILE:HD13	1.96	0.46
1:G:9:LEU:CD2	1:H:4[A]:LEU:HD12	2.39	0.46
1:A:100[B]:LEU:HB3	1:A:101:PRO:HD2	1.96	0.46
1:H:16:CME:SD	1:H:88:CME:HB2	2.56	0.46
1:B:88:CME:C	1:B:89:ILE:HG13	2.46	0.45
1:B:52:HIS:HB3	2:B:201:NLC:H3	1.98	0.45
1:H:34[B]:LEU:HD12	1:H:34[B]:LEU:N	2.32	0.45
1:A:120:MET:HB3	1:A:120:MET:HE3	1.74	0.45
1:B:100:LEU:HB3	1:B:101:PRO:HD2	1.98	0.45
1:A:130:CME:SD	1:A:130:CME:C	3.05	0.44
1:B:33:ASN:C	1:B:34[B]:LEU:HD12	2.38	0.43
1:G:23:VAL:HG12	1:G:27:ALA:HB2	2.00	0.43
1:H:112[A]:LEU:HB2	4:H:310:HOH:O	2.19	0.43
1:A:100[A]:LEU:HD23	1:A:100[A]:LEU:HA	1.67	0.43
1:H:100:LEU:HB3	1:H:101:PRO:HD2	2.01	0.43
1:G:63:LYS:HE3	1:G:68:TRP:CE2	2.54	0.42
1:G:78:PRO:HG2	1:G:101:PRO:HD2	2.01	0.42
1:H:52:HIS:HB3	2:H:201:NLC:H3	2.02	0.42
1:G:100:LEU:HB3	1:G:101:PRO:HD2	2.02	0.42
1:H:4[B]:LEU:HD23	1:H:5:VAL:N	2.34	0.41
1:G:31:VAL:HB	1:G:123:ASP:HB3	2.02	0.41

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ARG:NH2	4:H:321:HOH:O[4_455]	0.72	1.48
1:H:20:ARG:CZ	4:H:321:HOH:O[4_455]	1.33	0.87
1:H:20:ARG:HH22	4:H:321:HOH:O[4_455]	0.95	0.65
1:A:75:ALA:HB1	1:G:102:ASP:HB3[1_655]	1.33	0.27
4:A:375:HOH:O	4:B:361:HOH:O[4_554]	1.96	0.24
1:H:20:ARG:HH21	4:H:321:HOH:O[4_455]	1.40	0.20
1:H:20:ARG:NH1	4:H:321:HOH:O[4_455]	2.06	0.14

## 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	136/136 (100%)	133 (98%)	3 (2%)	0	100	100
1	B	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
1	G	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
1	H	136/136 (100%)	133 (98%)	3 (2%)	0	100	100
All	All	539/544 (99%)	528 (98%)	11 (2%)	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	113/107 (106%)	112 (99%)	1 (1%)	84	63
1	B	110/107 (103%)	109 (99%)	1 (1%)	84	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	112/107 (105%)	110 (98%)	2 (2%)	66	32
1	H	114/107 (106%)	112 (98%)	2 (2%)	66	32
All	All	449/428 (105%)	443 (99%)	6 (1%)	74	48

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	B	28	LYS
1	G	123	ASP
1	G	125	ASP
1	H	2	CYS
1	H	109	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	A	130	1	7,9,10	0.86	0	6,9,11	3.27	4 (66%)
1	CME	A	16	1	7,9,10	0.89	0	6,9,11	1.99	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CME	A	88	1	7,9,10	1.09	0	6,9,11	1.98	2 (33%)
1	CME	B	130	1	7,9,10	0.82	0	6,9,11	3.47	4 (66%)
1	CME	B	16	1	7,9,10	0.73	0	6,9,11	2.34	2 (33%)
1	CME	B	88	1	7,9,10	0.95	0	6,9,11	1.27	2 (33%)
1	CME	G	130	1	7,9,10	0.75	0	6,9,11	2.55	3 (50%)
1	CME	G	16	1	7,9,10	1.07	0	6,9,11	1.33	1 (16%)
1	CME	G	88	1	7,9,10	0.99	0	6,9,11	1.56	1 (16%)
1	CME	H	130	1	7,9,10	0.85	0	6,9,11	3.51	4 (66%)
1	CME	H	16	1	7,9,10	0.77	0	6,9,11	2.06	1 (16%)
1	CME	H	88	1	7,9,10	0.86	0	6,9,11	1.13	1 (16%)

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
1	CME	A	130	1	-	0/5/8/10	0/0/0/0
1	CME	A	16	1	-	0/5/8/10	0/0/0/0
1	CME	A	88	1	-	0/5/8/10	0/0/0/0
1	CME	B	130	1	-	0/5/8/10	0/0/0/0
1	CME	B	16	1	-	0/5/8/10	0/0/0/0
1	CME	B	88	1	-	0/5/8/10	0/0/0/0
1	CME	G	130	1	-	0/5/8/10	0/0/0/0
1	CME	G	16	1	-	0/5/8/10	0/0/0/0
1	CME	G	88	1	-	0/5/8/10	0/0/0/0
1	CME	H	130	1	-	0/5/8/10	0/0/0/0
1	CME	H	16	1	-	0/5/8/10	0/0/0/0
1	CME	H	88	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	130	CME	CZ-CE-SD	-6.37	97.60	113.16
1	B	130	CME	CZ-CE-SD	-5.32	100.15	113.16
1	A	16	CME	CZ-CE-SD	-3.53	104.54	113.16
1	A	130	CME	CB-SG-SD	-3.39	97.36	103.95
1	B	130	CME	CB-SG-SD	-2.88	98.36	103.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	CME	OH-CZ-CE	-2.83	99.52	111.15
1	G	130	CME	CZ-CE-SD	-2.63	106.74	113.16
1	G	130	CME	O-C-CA	-2.52	118.97	125.72
1	A	130	CME	O-C-CA	-2.37	119.36	125.72
1	G	16	CME	O-C-CA	-2.33	119.48	125.72
1	H	88	CME	O-C-CA	-2.08	120.15	125.72
1	B	88	CME	O-C-CA	-2.03	120.27	125.72
1	A	16	CME	O-C-CA	-2.02	120.29	125.72
1	B	16	CME	CZ-CE-SD	2.01	118.07	113.16
1	B	88	CME	CB-SG-SD	2.20	108.22	103.95
1	A	16	CME	OH-CZ-CE	2.37	120.88	111.15
1	A	130	CME	OH-CZ-CE	2.78	122.58	111.15
1	H	130	CME	OH-CZ-CE	2.99	123.44	111.15
1	G	88	CME	CB-SG-SD	3.02	109.82	103.95
1	A	88	CME	CE-SD-SG	3.15	118.35	103.75
1	B	130	CME	OH-CZ-CE	3.23	124.43	111.15
1	H	130	CME	CB-SG-SD	3.34	110.45	103.95
1	H	130	CME	CE-SD-SG	3.51	120.02	103.75
1	H	16	CME	CB-SG-SD	4.53	112.76	103.95
1	G	130	CME	CE-SD-SG	4.79	126.00	103.75
1	B	16	CME	CB-SG-SD	4.85	113.38	103.95
1	B	130	CME	CE-SD-SG	4.89	126.45	103.75
1	A	130	CME	CE-SD-SG	6.07	131.93	103.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	130	CME	5	0
1	A	16	CME	3	0
1	B	88	CME	1	0
1	G	88	CME	1	0
1	H	130	CME	1	0
1	H	16	CME	4	0
1	H	88	CME	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NLC	A	201	-	27,27,27	1.57	4 (14%)	34,39,39	1.07	2 (5%)
2	NLC	B	201	-	27,27,27	1.84	7 (25%)	34,39,39	1.84	8 (23%)
3	GOL	G	201	-	5,5,5	0.55	0	5,5,5	0.86	0
2	NLC	G	202	-	27,27,27	2.02	8 (29%)	34,39,39	1.42	6 (17%)
2	NLC	H	201	-	27,27,27	1.41	4 (14%)	34,39,39	1.58	6 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NLC	A	201	-	-	0/12/52/52	0/2/2/2
2	NLC	B	201	-	-	0/12/52/52	0/2/2/2
3	GOL	G	201	-	-	0/4/4/4	0/0/0/0
2	NLC	G	202	-	-	0/12/52/52	0/2/2/2
2	NLC	H	201	-	-	0/12/52/52	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	202	NLC	C3-C2	-3.66	1.45	1.53
2	B	201	NLC	C14-C13	-3.36	1.43	1.52
2	B	201	NLC	C3-C4	-2.93	1.44	1.52
2	G	202	NLC	C14-C13	-2.70	1.45	1.52
2	A	201	NLC	C3-C2	-2.65	1.47	1.53
2	G	202	NLC	O5-C5	-2.65	1.37	1.44
2	G	202	NLC	C3-C4	-2.39	1.45	1.52
2	B	201	NLC	C3-C2	-2.33	1.48	1.53
2	B	201	NLC	C4-C5	-2.32	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	NLC	C3-C4	-2.05	1.46	1.52
2	G	202	NLC	O4-C10	2.17	1.47	1.41
2	B	201	NLC	C14-C15	2.31	1.58	1.53
2	H	201	NLC	O15-C15	2.46	1.50	1.44
2	A	201	NLC	O3-C3	2.49	1.48	1.43
2	A	201	NLC	C1-C2	2.50	1.56	1.53
2	H	201	NLC	O3-C3	2.69	1.49	1.43
2	G	202	NLC	C4-C5	2.93	1.61	1.52
2	B	201	NLC	O3-C3	2.96	1.49	1.43
2	H	201	NLC	C8-C7	3.07	1.57	1.50
2	G	202	NLC	O3-C3	3.33	1.50	1.43
2	A	201	NLC	O15-C15	4.31	1.55	1.44
2	B	201	NLC	C1-C2	5.13	1.59	1.53
2	G	202	NLC	O5-C1	5.36	1.53	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	NLC	O3-C3-C2	-4.84	99.54	109.57
2	B	201	NLC	O3-C3-C2	-4.69	99.86	109.57
2	G	202	NLC	O3-C3-C2	-3.40	102.53	109.57
2	G	202	NLC	O13-C13-C12	-3.32	102.88	110.36
2	B	201	NLC	O13-C13-C12	-3.16	103.23	110.36
2	H	201	NLC	O13-C13-C12	-3.07	103.43	110.36
2	H	201	NLC	O15-C15-C14	-2.96	104.02	109.67
2	G	202	NLC	C10-O4-C4	-2.83	110.47	118.00
2	A	201	NLC	O13-C13-C12	-2.49	104.75	110.36
2	G	202	NLC	C2-N-C7	-2.44	116.80	123.21
2	B	201	NLC	C13-C14-C15	-2.38	105.99	110.23
2	B	201	NLC	C8-C7-N	-2.34	111.61	116.10
2	H	201	NLC	O5-C5-C6	-2.32	100.36	106.38
2	H	201	NLC	C8-C7-N	-2.24	111.80	116.10
2	B	201	NLC	O3-C3-C4	-2.10	104.91	109.89
2	G	202	NLC	C1-O5-C5	-2.06	109.59	113.54
2	G	202	NLC	O7-C7-N	2.09	126.11	121.84
2	A	201	NLC	C16-C15-C14	2.25	118.62	112.99
2	H	201	NLC	O7-C7-C8	2.52	126.71	122.07
2	B	201	NLC	O40-C14-C13	2.67	116.37	110.36
2	B	201	NLC	O7-C7-C8	3.65	128.79	122.07
2	B	201	NLC	C10-O4-C4	3.75	127.98	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	NLC	1	0
3	G	201	GOL	1	0
2	H	201	NLC	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	130/136 (95%)	-0.24	1 (0%) 87 86	18, 25, 41, 60	0
1	B	130/136 (95%)	-0.19	0 100 100	16, 26, 43, 58	0
1	G	130/136 (95%)	0.11	10 (7%) 16 14	18, 27, 55, 71	0
1	H	130/136 (95%)	-0.18	3 (2%) 64 62	18, 29, 45, 60	0
All	All	520/544 (95%)	-0.13	14 (2%) 58 55	16, 26, 46, 71	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	27	ALA	4.7
1	G	134	ASP	4.2
1	G	25	PRO	4.2
1	G	113	ASN	3.8
1	H	2	CYS	3.2
1	G	2	CYS	3.2
1	G	124	GLY	3.0
1	G	23	VAL	2.9
1	G	123	ASP	2.9
1	H	93	GLN	2.3
1	H	75	ALA	2.2
1	G	82	GLY	2.2
1	G	26	ASP	2.1
1	A	134	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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
1	CME	A	16	10/11	0.96	0.07	-	27,38,49,59	0
1	CME	H	16	10/11	0.92	0.15	-	28,38,69,72	0
1	CME	G	88	10/11	0.94	0.11	-	19,29,67,69	0
1	CME	G	16	10/11	0.92	0.10	-	29,36,57,58	0
1	CME	B	130	10/11	0.90	0.12	-	14,30,61,66	0
1	CME	H	88	10/11	0.92	0.10	-	22,28,59,62	0
1	CME	H	130	10/11	0.93	0.13	-	21,31,77,81	0
1	CME	G	130	10/11	0.94	0.12	-	18,24,66,67	0
1	CME	A	130	10/11	0.94	0.13	-	15,21,61,75	0
1	CME	B	16	10/11	0.93	0.13	-	20,29,55,64	0
1	CME	B	88	10/11	0.96	0.07	-	20,26,47,54	0
1	CME	A	88	10/11	0.94	0.10	-	20,26,44,56	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	NLC	A	201	26/26	0.93	0.10	2.08	19,28,36,42	0
3	GOL	G	201	6/6	0.80	0.16	1.03	34,43,63,66	11
2	NLC	G	202	26/26	0.93	0.10	1.01	18,27,40,49	0
2	NLC	H	201	26/26	0.96	0.07	-0.01	15,22,28,31	0
2	NLC	B	201	26/26	0.97	0.07	-0.29	14,20,24,28	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.