



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2017 – 08:19 PM EDT

PDB ID : 5GV3  
Title : Crystal structure of the membrane-distal domain of mouse lysosome-associated membrane protein 2 (LAMP-2)  
Authors : Tomabechi, Y.; Ehara, H.; Kukimoto-Niino, M.; Shirouzu, M.  
Deposited on : unknown  
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

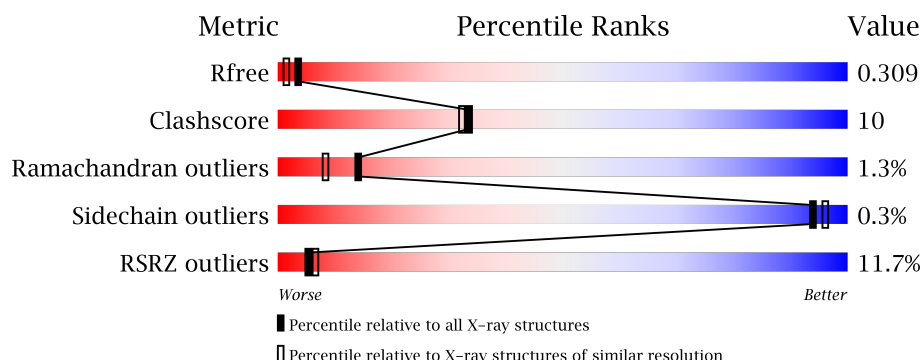
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	169	<div> <div>9%</div> <div>77%</div> <div>17%</div> <div>5%</div> </div>
1	B	169	<div> <div>13%</div> <div>76%</div> <div>20%</div> <div>••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	211	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2773 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 Lysosome-associated membrane glycoprotein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1261	802	205	248	6			
1	B	163	Total	C	N	O	S	0	0	0
			1275	809	209	251	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	-	expression tag	UNP P17047
A	190	GLY	-	expression tag	UNP P17047
A	191	SER	-	expression tag	UNP P17047
A	192	SER	-	expression tag	UNP P17047
A	193	LEU	-	expression tag	UNP P17047
B	25	ASP	-	expression tag	UNP P17047
B	190	GLY	-	expression tag	UNP P17047
B	191	SER	-	expression tag	UNP P17047
B	192	SER	-	expression tag	UNP P17047
B	193	LEU	-	expression tag	UNP P17047

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Zn	2	0
			6	6		
2	A	9	Total	Zn	3	0
			9	9		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

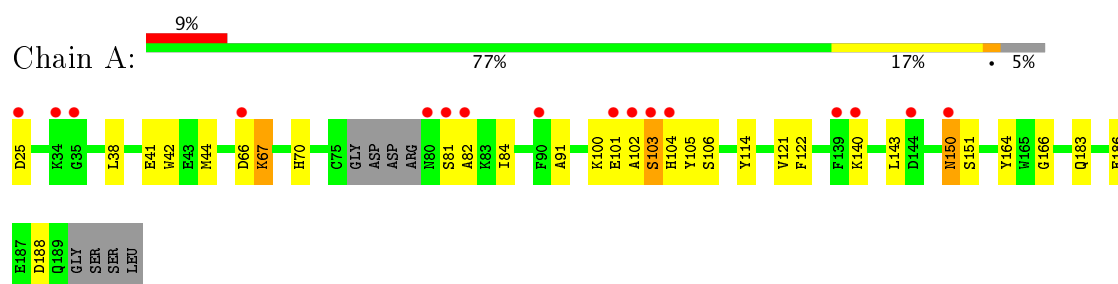
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	32	Total	O	0	0
			32	32		

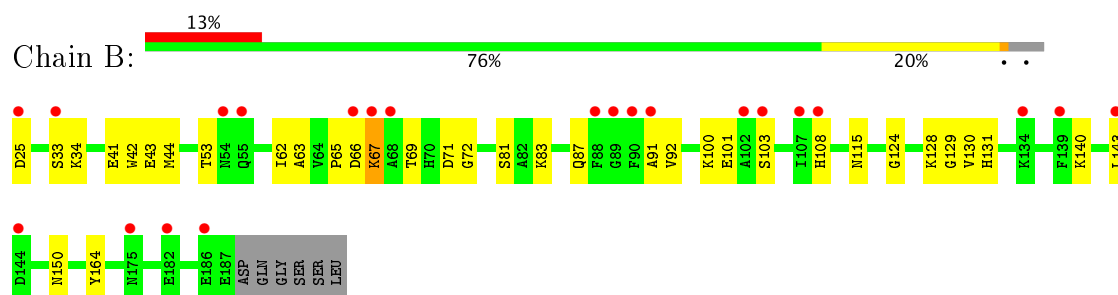
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Lysosome-associated membrane glycoprotein 2



- Molecule 1: Lysosome-associated membrane glycoprotein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.61Å 103.93Å 129.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.49 – 2.10 48.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.49-2.10) 98.8 (48.21-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, $R_{free}$	0.269 , 0.307 0.270 , 0.309	Depositor DCC
$R_{free}$ test set	1980 reflections (8.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.035 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.45	1/1289 (0.1%)	0.65	0/1757
1	B	0.55	1/1304 (0.1%)	0.62	1/1778 (0.1%)
All	All	0.50	2/2593 (0.1%)	0.64	1/3535 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	GLU	CB-CG	11.71	1.74	1.52
1	A	150	ASN	CB-CG	5.44	1.63	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	43	GLU	CA-CB-CG	5.26	124.96	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	67	LYS	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	1261	0	1210	27	3
1	B	1275	0	1224	23	3
2	A	9	0	0	0	0
2	B	6	0	0	0	1
3	A	70	0	65	1	0
3	B	70	0	65	2	0
4	A	50	0	0	3	1
4	B	32	0	0	3	1
All	All	2773	0	2564	51	5

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 10.

All (51) 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:B:91:ALA:HB1	1:B:115:ASN:HB3	1.47	0.97
1:B:69:THR:HG23	1:B:87:GLN:OE1	1.71	0.90
1:B:42:TRP:HE1	1:B:44:MET:HE2	1.38	0.84
1:B:44:MET:SD	4:B:331:HOH:O	2.36	0.82
1:B:101:GLU:OE2	1:B:140:LYS:NZ	2.14	0.79
1:B:100:LYS:HE2	1:B:143:LEU:HD21	1.63	0.79
1:A:100:LYS:HE3	1:A:143:LEU:HD21	1.68	0.75
1:A:183:GLN:NE2	4:A:303:HOH:O	2.20	0.73
1:A:104:HIS:HB3	1:A:143:LEU:HD13	1.71	0.71
1:A:151:SER:OG	1:A:188:ASP:OD1	2.07	0.71
1:B:42:TRP:HE1	1:B:44:MET:CE	2.04	0.70
1:A:42:TRP:HE1	1:A:44:MET:CE	2.06	0.68
1:A:44:MET:HE1	1:A:164:TYR:HE1	1.60	0.67
1:A:102:ALA:HB3	1:A:140:LYS:HZ3	1.63	0.64
1:B:150:ASN:OD1	4:B:304:HOH:O	2.15	0.63
1:B:71:ASP:O	1:B:87:GLN:NE2	2.32	0.59
1:A:150:ASN:HA	1:A:166:GLY:HA2	1.84	0.59
1:A:186:GLU:OE1	4:A:302:HOH:O	2.17	0.59
3:A:210:NAG:H83	3:A:210:NAG:H3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:OD1	1:B:67:LYS:HG2	2.05	0.57
1:A:106:SER:HB3	1:A:140:LYS:NZ	2.21	0.56
1:A:102:ALA:HB3	1:A:140:LYS:NZ	2.21	0.56
1:A:42:TRP:HE1	1:A:44:MET:HE3	1.73	0.53
1:A:103:SER:C	1:A:140:LYS:HE3	2.30	0.52
1:B:81:SER:OG	3:B:209:NAG:H83	2.09	0.52
1:B:53:THR:N	1:B:124:GLY:O	2.42	0.51
1:B:103:SER:O	1:B:143:LEU:HB2	2.12	0.50
1:A:66:ASP:O	1:A:67:LYS:HG2	2.11	0.50
1:B:25:ASP:N	4:B:307:HOH:O	2.44	0.49
1:A:106:SER:HB3	1:A:140:LYS:HZ2	1.77	0.49
1:A:121:VAL:HG13	1:A:122:PHE:CD2	2.47	0.49
1:A:102:ALA:O	1:A:103:SER:OG	2.24	0.48
1:A:70:HIS:HE1	4:A:339:HOH:O	1.97	0.48
1:B:33:SER:HA	1:B:34:LYS:HA	1.58	0.47
1:B:72:GLY:O	1:B:83:LYS:HE3	2.14	0.47
1:A:44:MET:HE1	1:A:164:TYR:CE1	2.45	0.46
1:B:62:ILE:HD13	1:B:92:VAL:HG21	1.97	0.46
1:B:63:ALA:O	1:B:65:PRO:HD3	2.17	0.45
1:A:100:LYS:HG2	1:A:101:GLU:HG3	1.98	0.44
1:B:130:VAL:HG21	3:B:208:NAG:H82	1.99	0.44
1:A:91:ALA:O	1:A:114:TYR:HA	2.19	0.43
1:A:38:LEU:HD21	1:A:84:ILE:HD11	2.00	0.43
1:A:140:LYS:HD2	1:A:140:LYS:HA	1.61	0.42
1:B:42:TRP:NE1	1:B:44:MET:HE2	2.19	0.42
1:B:66:ASP:HA	1:B:67:LYS:HA	1.55	0.42
1:A:101:GLU:N	1:A:104:HIS:O	2.39	0.42
1:A:25:ASP:N	1:A:25:ASP:OD1	2.51	0.42
1:A:42:TRP:HE1	1:A:44:MET:HE2	1.82	0.42
1:B:128:LYS:HA	1:B:129:GLY:HA2	1.73	0.41
1:B:44:MET:HE1	1:B:164:TYR:HE1	1.85	0.41
1:A:105:TYR:HD2	1:A:143:LEU:HD12	1.86	0.41

All (5) 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:A:41:GLU:OE2	2:B:206:ZN:ZN[4_566]	1.63	0.57
1:A:150:ASN:ND2	1:B:41:GLU:OE2[4_566]	2.07	0.13
4:A:335:HOH:O	4:B:312:HOH:O[4_566]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:OD1	1:B:25:ASP:OD2[4_566]	2.16	0.04
1:B:101:GLU:OE2	1:B:131:HIS:ND1[8_566]	2.19	0.01

## 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	157/169 (93%)	146 (93%)	7 (4%)	4 (2%)	6	2
1	B	161/169 (95%)	147 (91%)	14 (9%)	0	100	100
All	All	318/338 (94%)	293 (92%)	21 (7%)	4 (1%)	14	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	SER
1	A	67	LYS
1	A	82	ALA
1	A	81	SER

### 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	144/150 (96%)	144 (100%)	0	100	100
1	B	145/150 (97%)	144 (99%)	1 (1%)	87	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	289/300 (96%)	288 (100%)	1 (0%)	94	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	HIS

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

Mol	Chain	Res	Type
1	A	168	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 15 are monoatomic - leaving 10 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	A	210	1	14,14,15	0.57	0	15,19,21	1.30	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	211	1	14,14,15	0.32	0	15,19,21	0.48	0
3	NAG	A	212	1	14,14,15	0.26	0	15,19,21	0.70	0
3	NAG	A	213	1	14,14,15	0.59	0	15,19,21	0.49	0
3	NAG	A	214	1	14,14,15	0.38	0	15,19,21	0.45	0
3	NAG	B	207	1	14,14,15	0.48	0	15,19,21	0.59	0
3	NAG	B	208	1	14,14,15	0.30	0	15,19,21	0.67	1 (6%)
3	NAG	B	209	1	14,14,15	0.46	0	15,19,21	0.83	1 (6%)
3	NAG	B	210	1	14,14,15	0.18	0	15,19,21	0.54	0
3	NAG	B	211	1	14,14,15	0.45	0	15,19,21	0.36	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	A	210	1	-	0/6/23/26	0/1/1/1
3	NAG	A	211	1	-	0/6/23/26	0/1/1/1
3	NAG	A	212	1	-	0/6/23/26	0/1/1/1
3	NAG	A	213	1	-	0/6/23/26	0/1/1/1
3	NAG	A	214	1	-	0/6/23/26	0/1/1/1
3	NAG	B	207	1	-	0/6/23/26	0/1/1/1
3	NAG	B	208	1	-	0/6/23/26	0/1/1/1
3	NAG	B	209	1	-	0/6/23/26	0/1/1/1
3	NAG	B	210	1	-	0/6/23/26	0/1/1/1
3	NAG	B	211	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	209	NAG	C1-C2-N2	2.07	114.02	110.49
3	B	208	NAG	C1-O5-C5	2.18	115.17	112.17
3	A	210	NAG	C2-N2-C7	3.99	128.76	122.94

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
3	A	210	NAG	1	0
3	B	208	NAG	1	0
3	B	209	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	161/169 (95%)	0.87	16 (9%) <b>8</b> <b>10</b>	37, 51, 72, 92	0
1	B	163/169 (96%)	0.98	22 (13%) <b>3</b> <b>5</b>	39, 54, 79, 98	0
All	All	324/338 (95%)	0.92	38 (11%) <b>5</b> <b>6</b>	37, 53, 78, 98	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ASP	9.7
1	A	103	SER	7.6
1	A	90	PHE	7.2
1	B	67	LYS	6.4
1	B	88	PHE	5.9
1	A	82	ALA	4.4
1	B	33	SER	4.2
1	B	89	GLY	4.1
1	A	101	GLU	4.1
1	B	90	PHE	4.0
1	B	143	LEU	3.7
1	B	55	GLN	3.5
1	A	66	ASP	3.4
1	A	140	LYS	3.4
1	A	25	ASP	3.3
1	B	25	ASP	3.3
1	B	103	SER	3.2
1	A	80	ASN	3.0
1	A	34	LYS	3.0
1	B	107	ILE	3.0
1	B	144	ASP	2.9
1	B	108	HIS	2.9
1	B	139	PHE	2.8
1	A	81	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	54	ASN	2.7
1	B	68	ALA	2.6
1	A	102	ALA	2.6
1	B	186	GLU	2.5
1	A	144	ASP	2.4
1	B	175	ASN	2.4
1	B	91	ALA	2.3
1	A	150	ASN	2.3
1	B	134	LYS	2.3
1	A	35	GLY	2.3
1	B	182	GLU	2.2
1	A	104	HIS	2.1
1	B	102	ALA	2.1
1	A	139	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	NAG	B	211	14/15	0.75	0.23	3.39	43,63,68,77	0
3	NAG	B	209	14/15	0.80	0.19	1.69	60,70,82,85	0
3	NAG	A	211	14/15	0.87	0.17	0.37	40,52,67,73	0
3	NAG	A	210	14/15	0.84	0.16	0.16	46,54,64,74	0
3	NAG	B	210	14/15	0.88	0.15	-0.22	42,50,58,62	0
3	NAG	A	214	14/15	0.94	0.15	-0.40	43,53,66,69	0
2	ZN	B	203	1/1	0.95	0.08	-1.67	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	206	1/1	0.36	0.36	-	64,64,64,64	1
2	ZN	B	201	1/1	0.98	0.02	-	38,38,38,38	0
2	ZN	B	202	1/1	0.94	0.06	-	48,48,48,48	0
3	NAG	A	212	14/15	0.47	0.27	-	73,89,104,106	0
2	ZN	A	209	1/1	-	-	-	79,79,79,79	1
2	ZN	A	207	1/1	0.68	0.24	-	102,102,102,102	1
3	NAG	B	208	14/15	0.81	0.12	-	68,79,84,85	0
2	ZN	A	204	1/1	-	-	-	68,68,68,68	1
2	ZN	B	204	1/1	0.53	0.14	-	93,93,93,93	1
2	ZN	A	202	1/1	0.94	0.07	-	49,49,49,49	1
2	ZN	B	206	1/1	-	-	-	60,60,60,60	1
2	ZN	A	208	1/1	0.87	0.46	-	69,69,69,69	1
2	ZN	A	203	1/1	0.24	0.14	-	90,90,90,90	1
3	NAG	A	213	14/15	0.52	0.28	-	70,86,92,93	0
2	ZN	B	205	1/1	-	-	-	90,90,90,90	1
3	NAG	B	207	14/15	0.71	0.20	-	57,71,82,83	0
2	ZN	A	201	1/1	0.94	0.09	-	45,45,45,45	0
2	ZN	A	205	1/1	-	-	-	80,80,80,80	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.