



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 04:58 AM GMT

PDB ID : 3GXR  
Title : The crystal structure of g-type lysozyme from Atlantic cod (*Gadus morhua* L.) in complex with NAG oligomers sheds new light on substrate binding and the catalytic mechanism. Structure with NAG to 1.7  
Authors : Helland, R.; Larsen, R.L.; Finstad, S.; Kyomuhendo, P.; Larsen, A.N.  
Deposited on : 2009-04-02  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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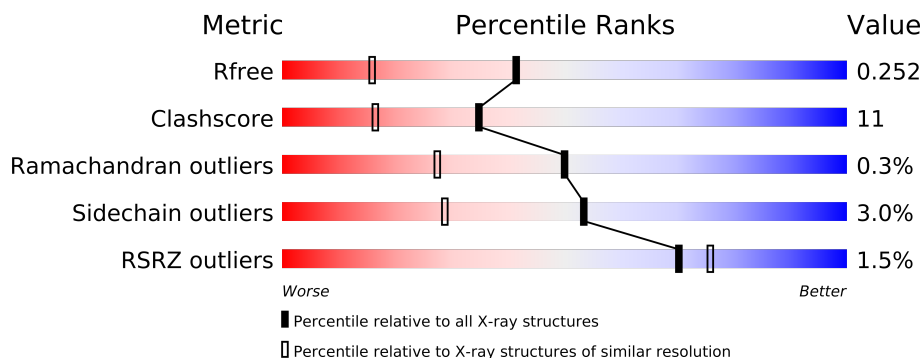
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	187	
1	B	187	
1	C	187	
1	D	187	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6211 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Goose-type lysozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1458	907	261	287	3			
1	B	183	Total	C	N	O	S	0	0	0
			1442	896	259	284	3			
1	C	174	Total	C	N	O	S	0	0	0
			1369	849	247	270	3			
1	D	186	Total	C	N	O	S	0	0	0
			1462	909	262	288	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	GLY	SEE REMARK 999	UNP B9TU22
B	147	ALA	GLY	SEE REMARK 999	UNP B9TU22
C	147	ALA	GLY	SEE REMARK 999	UNP B9TU22
D	147	ALA	GLY	SEE REMARK 999	UNP B9TU22

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			29	16	2	11		
2	D	2	Total	C	N	O	0	0
			29	16	2	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	GLY	SEE REMARK 999	UNP B9TU22
D	147	ALA	GLY	SEE REMARK 999	UNP B9TU22

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total 43	C 24	N 3	O 16	0	0
3	B	3	Total 43	C 24	N 3	O 16	0	0
3	D	3	Total 43	C 24	N 3	O 16	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	GLY	SEE REMARK 999	UNP B9TU22
B	147	ALA	GLY	SEE REMARK 999	UNP B9TU22
D	147	ALA	GLY	SEE REMARK 999	UNP B9TU22

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total 87	O 87	0	0
4	B	78	Total 78	O 78	0	0
4	C	67	Total 67	O 67	0	0
4	D	61	Total 61	O 61	0	0

### 3 Residue-property plots

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

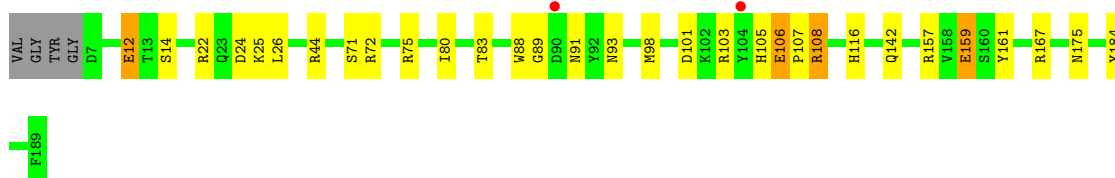
- Molecule 1: Goose-type lysozyme 1

Chain A: 



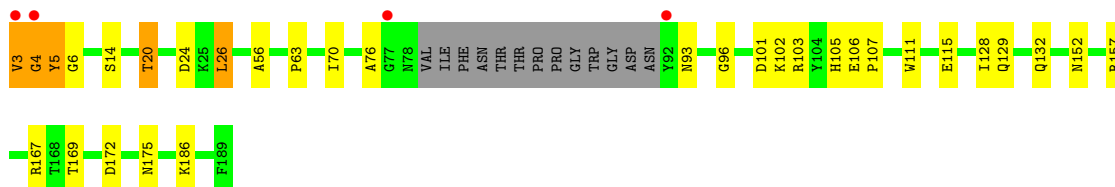
- Molecule 1: Goose-type lysozyme 1

Chain B: 



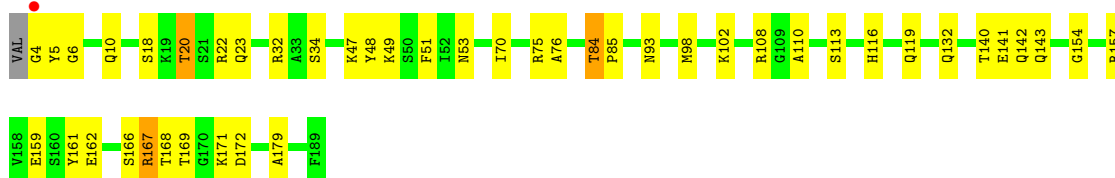
- Molecule 1: Goose-type lysozyme 1

Chain C: 



- Molecule 1: Goose-type lysozyme 1

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.19Å 75.52Å 78.29Å 90.00° 93.25° 90.00°	Depositor
Resolution (Å)	34.00 – 1.70 34.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.00-1.70) 99.2 (34.00-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.204 , 0.252 0.203 , 0.252	Depositor DCC
$R_{free}$ test set	3526 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 69939 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	1.01	1/1489 (0.1%)	0.95	3/2011 (0.1%)
1	B	1.02	2/1472 (0.1%)	0.89	1/1988 (0.1%)
1	C	0.94	2/1394 (0.1%)	0.89	2/1876 (0.1%)
1	D	0.98	0/1493	0.85	0/2016
All	All	0.99	5/5848 (0.1%)	0.90	6/7891 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	GLU	CG-CD	6.94	1.62	1.51
1	B	12	GLU	CG-CD	6.40	1.61	1.51
1	A	173	TYR	CD2-CE2	6.30	1.48	1.39
1	B	184	TYR	CD2-CE2	5.34	1.47	1.39
1	C	106	GLU	CD-OE2	5.33	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASN	N-CA-C	7.01	129.93	111.00
1	C	5	TYR	N-CA-C	6.33	128.09	111.00
1	A	103	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	6	GLY	N-CA-C	-5.42	99.54	113.10
1	B	72	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	5	TYR	CA-C-N	5.16	126.52	116.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1458	0	1397	19	0
1	B	1442	0	1385	30	0
1	C	1369	0	1319	28	0
1	D	1462	0	1400	43	0
2	A	29	0	27	0	0
2	D	29	0	27	4	0
3	A	43	0	39	3	0
3	B	43	0	39	7	0
3	D	43	0	39	1	0
4	A	87	0	0	1	0
4	B	78	0	0	2	0
4	C	67	0	0	4	0
4	D	61	0	0	7	0
All	All	6211	0	5672	124	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:ASN:HB3	4:D:244:HOH:O	1.59	1.01
1:B:101:ASP:OD1	1:B:103:ARG:HD3	1.74	0.87
1:C:4:GLY:HA3	1:C:5:TYR:HB2	1.56	0.86
1:D:98:MET:H	1:D:116:HIS:HE1	1.21	0.84
1:B:98:MET:H	1:B:116:HIS:HE1	1.30	0.80
1:D:98:MET:H	1:D:116:HIS:CE1	2.03	0.77
1:B:98:MET:H	1:B:116:HIS:CE1	2.02	0.77
1:A:101:ASP:OD1	1:A:103:ARG:HD3	1.84	0.77
1:D:23:GLN:HE21	1:D:75:ARG:HH11	1.31	0.77
1:D:169:THR:HG21	3:D:301:NAG:H61	1.66	0.76
1:B:12:GLU:HG2	1:B:161:TYR:OH	1.87	0.75
1:C:4:GLY:CA	1:C:5:TYR:HB2	2.17	0.73
1:D:20:THR:HG23	1:D:172:ASP:OD2	1.88	0.73
3:B:302:NAG:C7	3:B:303:NAG:O6	2.38	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:ASN:ND2	1:A:103:ARG:HD2	2.05	0.70
1:B:108:ARG:HH11	1:B:108:ARG:HG2	1.56	0.69
1:A:91:ASN:O	1:A:91:ASN:CG	2.28	0.69
1:D:159:GLU:OE2	1:D:167:ARG:NH1	2.25	0.69
1:D:20:THR:CG2	1:D:172:ASP:OD2	2.41	0.68
1:A:23:GLN:HG3	3:A:302:NAG:O7	1.95	0.67
3:B:302:NAG:H82	3:B:303:NAG:O6	1.94	0.67
1:C:128:ILE:O	1:C:132:GLN:HG3	1.95	0.66
1:B:24:ASP:OD1	4:B:288:HOH:O	2.13	0.66
1:B:108:ARG:HH11	1:B:108:ARG:CG	2.09	0.65
1:C:3:VAL:O	1:C:4:GLY:C	2.35	0.64
1:A:10:GLN:HE22	1:B:44:ARG:HH11	1.45	0.64
1:D:23:GLN:HE21	1:D:75:ARG:NH1	1.96	0.62
1:C:129:GLN:NE2	4:C:217:HOH:O	2.31	0.62
1:B:106:GLU:HB3	1:B:108:ARG:NH2	2.15	0.61
1:C:56:ALA:HB1	1:C:63:PRO:HD3	1.83	0.61
1:D:116:HIS:HD2	4:D:190:HOH:O	1.83	0.61
1:A:110:ALA:HB3	1:A:113:SER:HB3	1.83	0.61
1:D:49:LYS:NZ	1:D:53:ASN:HD21	1.99	0.60
1:D:4:GLY:HA3	1:D:132:GLN:HE22	1.67	0.60
1:D:166:SER:O	1:D:171:LYS:HD2	2.01	0.59
1:D:98:MET:N	1:D:116:HIS:HE1	1.99	0.58
3:B:302:NAG:C8	3:B:303:NAG:O6	2.52	0.58
1:D:166:SER:O	1:D:171:LYS:CD	2.51	0.58
1:B:142:GLN:HG2	1:B:161:TYR:CE1	2.39	0.58
1:B:101:ASP:OD2	1:B:103:ARG:NH1	2.37	0.58
1:B:93:ASN:ND2	1:B:103:ARG:HD2	2.20	0.57
1:C:20:THR:CG2	1:C:172:ASP:OD2	2.52	0.57
1:A:49:LYS:HE2	1:A:189:PHE:OXT	2.05	0.57
1:B:159:GLU:HG3	4:B:280:HOH:O	2.04	0.57
1:C:3:VAL:O	1:C:6:GLY:HA2	2.05	0.56
1:D:157:ARG:NH2	2:D:202:NAG:O6	2.38	0.56
1:B:89:GLY:HA3	3:B:301:NAG:C8	2.35	0.56
1:C:20:THR:HG23	1:C:172:ASP:OD2	2.05	0.56
1:D:140:THR:HA	1:D:143:GLN:HE21	1.70	0.56
1:B:80:ILE:CG2	3:B:301:NAG:C8	2.85	0.55
1:B:14:SER:H	1:B:175:ASN:ND2	2.04	0.55
1:B:98:MET:N	1:B:116:HIS:HE1	2.02	0.55
1:C:152:ASN:HD21	1:C:169:THR:H	1.54	0.55
1:C:4:GLY:CA	1:C:5:TYR:CB	2.84	0.55
1:D:4:GLY:CA	1:D:132:GLN:HE22	2.20	0.55
1:A:91:ASN:O	1:A:91:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:166:SER:O	1:D:171:LYS:HE3	2.07	0.53
1:B:14:SER:H	1:B:175:ASN:HD22	1.54	0.53
2:D:201:NAG:H62	4:D:223:HOH:O	2.07	0.53
1:D:108:ARG:H	1:D:119:GLN:HE22	1.56	0.53
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.23	0.53
1:A:10:GLN:NE2	1:B:44:ARG:HH11	2.06	0.53
2:D:201:NAG:C6	4:D:223:HOH:O	2.55	0.53
1:D:32:ARG:HG3	4:D:218:HOH:O	2.09	0.52
1:B:91:ASN:CB	4:D:244:HOH:O	2.34	0.51
1:A:169:THR:HG21	3:A:301:NAG:H61	1.92	0.51
1:C:102:LYS:HE3	4:C:205:HOH:O	2.11	0.51
1:C:14:SER:H	1:C:175:ASN:ND2	2.10	0.50
1:A:14:SER:H	1:A:175:ASN:ND2	2.08	0.50
1:D:5:TYR:N	1:D:6:GLY:HA2	2.26	0.50
1:C:102:LYS:CE	4:C:205:HOH:O	2.59	0.50
1:B:157:ARG:HG2	1:B:167:ARG:HG3	1.94	0.49
1:B:22:ARG:NH2	1:B:25:LYS:HG2	2.27	0.49
1:C:157:ARG:HG2	1:C:167:ARG:NH2	2.26	0.49
1:D:157:ARG:HG2	1:D:167:ARG:NH2	2.28	0.49
1:C:101:ASP:OD1	1:C:103:ARG:HD3	2.13	0.49
3:B:302:NAG:C7	3:B:303:NAG:HO6	2.26	0.48
1:D:110:ALA:HB3	1:D:113:SER:HB3	1.96	0.48
1:D:140:THR:HA	1:D:143:GLN:NE2	2.28	0.48
1:C:152:ASN:ND2	1:C:169:THR:H	2.12	0.47
1:C:24:ASP:HB3	1:C:26:LEU:HD13	1.96	0.47
1:D:20:THR:HG21	1:D:172:ASP:OD2	2.15	0.47
1:A:91:ASN:HA	1:A:92:TYR:HA	1.84	0.46
1:D:171:LYS:HD3	1:D:171:LYS:HA	1.80	0.46
1:C:70:ILE:CG2	1:C:76:ALA:HA	2.46	0.46
1:A:145:LYS:NZ	1:A:175:ASN:HD21	2.14	0.45
1:D:34:SER:CB	1:D:179:ALA:HB3	2.47	0.45
1:D:34:SER:HB3	1:D:179:ALA:HB3	1.99	0.45
1:C:70:ILE:HG22	1:C:76:ALA:HA	1.98	0.44
1:A:39:GLN:HG2	1:D:51:PHE:CZ	2.53	0.44
1:B:91:ASN:CG	4:D:244:HOH:O	2.55	0.44
1:C:20:THR:HG21	1:C:172:ASP:OD2	2.17	0.44
1:D:132:GLN:HG2	1:D:143:GLN:CD	2.36	0.44
1:D:166:SER:O	1:D:171:LYS:CE	2.64	0.44
1:D:84:THR:HA	1:D:85:PRO:HA	1.70	0.44
1:C:93:ASN:CG	1:C:103:ARG:HD2	2.38	0.43
1:B:157:ARG:HD2	1:B:167:ARG:CZ	2.48	0.43
1:D:142:GLN:HG2	1:D:161:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:93:ASN:ND2	1:D:102:LYS:HE2	2.33	0.43
1:C:115:GLU:HG3	4:C:234:HOH:O	2.19	0.43
1:A:5:TYR:HA	4:A:223:HOH:O	2.18	0.43
1:A:93:ASN:HD22	1:A:103:ARG:HD2	1.80	0.42
1:D:154:GLY:HA3	2:D:201:NAG:C7	2.50	0.42
1:B:105:HIS:O	1:B:107:PRO:HD3	2.19	0.42
3:A:301:NAG:H1	3:A:302:NAG:H61	2.01	0.42
1:C:96:GLY:HA2	1:C:111:TRP:HB2	2.02	0.42
1:B:71:SER:O	1:B:75:ARG:HD2	2.19	0.42
1:B:83:THR:HG21	1:B:88:TRP:O	2.20	0.42
1:A:95:PHE:CD2	1:A:107:PRO:HB2	2.54	0.42
1:A:34:SER:CB	1:A:179:ALA:HB3	2.50	0.42
1:D:4:GLY:HA3	1:D:5:TYR:HA	1.47	0.41
1:C:186:LYS:HB2	1:C:186:LYS:HE3	1.88	0.41
1:C:3:VAL:O	1:C:4:GLY:O	2.38	0.41
1:B:89:GLY:HA3	3:B:301:NAG:C7	2.50	0.41
1:D:168:THR:O	1:D:171:LYS:NZ	2.43	0.41
1:D:4:GLY:HA3	1:D:132:GLN:NE2	2.34	0.41
1:C:93:ASN:HB3	1:C:103:ARG:HD2	2.03	0.41
1:D:132:GLN:HG2	1:D:143:GLN:NE2	2.36	0.41
1:D:10:GLN:HB2	1:D:141:GLU:HG2	2.02	0.41
1:D:93:ASN:HD22	1:D:102:LYS:HE2	1.86	0.40
1:C:105:HIS:O	1:C:107:PRO:HD3	2.21	0.40
1:A:7:ASP:N	1:A:141:GLU:OE2	2.47	0.40
1:D:47:LYS:HE2	1:D:48:TYR:CZ	2.57	0.40
1:D:70:ILE:CG2	1:D:76:ALA:HA	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	183/187 (98%)	177 (97%)	5 (3%)	1 (0%)	38	17
1	B	181/187 (97%)	177 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	170/187 (91%)	163 (96%)	6 (4%)	1 (1%)	33	13
1	D	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
All	All	718/748 (96%)	697 (97%)	19 (3%)	2 (0%)	50	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	C	4	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/154 (99%)	148 (97%)	5 (3%)	50	25
1	B	152/154 (99%)	148 (97%)	4 (3%)	59	35
1	C	143/154 (93%)	140 (98%)	3 (2%)	66	45
1	D	153/154 (99%)	147 (96%)	6 (4%)	43	18
All	All	601/616 (98%)	583 (97%)	18 (3%)	53	29

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	86	PRO
1	A	91	ASN
1	A	92	TYR
1	A	185	LYS
1	B	26	LEU
1	B	106	GLU
1	B	108	ARG
1	B	159	GLU
1	C	3	VAL
1	C	20	THR
1	C	26	LEU

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Mol	Chain	Res	Type
1	D	18	SER
1	D	20	THR
1	D	22	ARG
1	D	84	THR
1	D	162	GLU
1	D	167	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	53	ASN
1	A	91	ASN
1	A	93	ASN
1	A	99	GLN
1	A	175	ASN
1	B	23	GLN
1	B	54	ASN
1	B	78	ASN
1	B	93	ASN
1	B	105	HIS
1	B	116	HIS
1	B	143	GLN
1	B	175	ASN
1	C	23	GLN
1	C	39	GLN
1	C	54	ASN
1	C	99	GLN
1	C	152	ASN
1	C	175	ASN
1	D	23	GLN
1	D	53	ASN
1	D	93	ASN
1	D	99	GLN
1	D	116	HIS
1	D	119	GLN
1	D	132	GLN
1	D	143	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

13 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	201	2	15,15,15	0.67	0	21,21,21	1.73	5 (23%)
2	NAG	A	202	2	14,14,15	1.09	1 (7%)	15,19,21	2.05	4 (26%)
3	NAG	A	301	3	15,15,15	1.08	1 (6%)	21,21,21	1.04	1 (4%)
3	NAG	A	302	3	14,14,15	1.49	2 (14%)	15,19,21	1.23	1 (6%)
3	NAG	A	303	3	14,14,15	0.68	0	15,19,21	2.01	3 (20%)
3	NAG	B	301	3	15,15,15	0.72	0	21,21,21	1.76	5 (23%)
3	NAG	B	302	3	14,14,15	0.90	1 (7%)	15,19,21	1.93	4 (26%)
3	NAG	B	303	3	14,14,15	0.67	0	15,19,21	1.49	3 (20%)
2	NAG	D	201	2	15,15,15	0.74	0	21,21,21	2.34	6 (28%)
2	NAG	D	202	2	14,14,15	0.85	0	15,19,21	1.07	1 (6%)
3	NAG	D	301	3	15,15,15	0.80	0	21,21,21	1.52	5 (23%)
3	NAG	D	302	3	14,14,15	0.94	0	15,19,21	1.69	2 (13%)
3	NAG	D	303	3	14,14,15	0.60	0	15,19,21	1.69	2 (13%)

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	NAG	A	201	2	-	0/6/26/26	0/1/1/1
2	NAG	A	202	2	-	0/6/22/26	0/1/1/1
3	NAG	A	301	3	-	0/6/26/26	0/1/1/1
3	NAG	A	302	3	-	0/6/22/26	0/1/1/1
3	NAG	A	303	3	-	0/6/22/26	0/1/1/1
3	NAG	B	301	3	-	0/6/26/26	0/1/1/1
3	NAG	B	302	3	-	0/6/22/26	0/1/1/1
3	NAG	B	303	3	-	0/6/22/26	0/1/1/1
2	NAG	D	201	2	-	0/6/26/26	0/1/1/1
2	NAG	D	202	2	-	0/6/22/26	0/1/1/1
3	NAG	D	301	3	-	0/6/26/26	0/1/1/1
3	NAG	D	302	3	-	0/6/22/26	0/1/1/1
3	NAG	D	303	3	-	0/6/22/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	NAG	C6-C5	4.08	1.56	1.50
2	A	202	NAG	C6-C5	2.83	1.54	1.50
3	A	301	NAG	C1-C2	2.32	1.55	1.53
3	B	302	NAG	C6-C5	2.28	1.54	1.50
3	A	302	NAG	C2-N2	2.08	1.49	1.45

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	NAG	O6-C6-C5	-6.26	103.13	112.42
2	D	201	NAG	C1-O5-C5	5.85	123.88	113.40
2	A	202	NAG	O5-C1-C2	5.31	114.99	109.61
2	D	201	NAG	O5-C5-C4	5.27	119.52	109.76
3	B	302	NAG	O5-C1-C2	-5.21	104.33	109.61
3	B	301	NAG	O5-C1-C2	4.33	114.00	109.61
2	D	201	NAG	C6-C5-C4	-4.21	102.83	113.00
3	D	303	NAG	O5-C1-C2	3.86	113.52	109.61
3	B	303	NAG	O6-C6-C5	-3.84	106.71	112.42
3	D	302	NAG	C1-C2-N2	-3.80	106.43	110.85
3	D	302	NAG	O5-C1-C2	-3.80	105.76	109.61
2	A	201	NAG	C3-C4-C5	3.79	116.96	110.20
2	A	202	NAG	O6-C6-C5	-3.69	106.93	112.42
3	B	302	NAG	O6-C6-C5	-3.65	107.00	112.42
3	B	301	NAG	C3-C2-N2	-3.65	102.82	110.56
3	D	303	NAG	C1-C2-C3	-3.53	105.54	110.59
2	D	201	NAG	O3-C3-C4	-3.42	102.69	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	NAG	C1-C2-N2	-3.41	106.88	110.85
2	D	201	NAG	O5-C1-C2	3.16	112.81	109.61
2	A	201	NAG	C6-C5-C4	-3.12	105.46	113.00
3	D	301	NAG	O5-C5-C4	2.81	114.97	109.76
3	A	303	NAG	C1-C2-N2	-2.64	107.78	110.85
2	D	202	NAG	C1-C2-N2	-2.57	107.86	110.85
2	A	201	NAG	O7-C7-C8	-2.55	117.07	122.04
2	D	201	NAG	C3-C4-C5	2.40	114.49	110.20
2	A	202	NAG	O7-C7-C8	-2.39	117.37	122.04
3	B	302	NAG	C1-C2-C3	2.38	114.01	110.59
3	D	301	NAG	C1-C2-C3	2.38	114.01	110.59
3	B	303	NAG	O5-C1-C2	2.31	111.95	109.61
2	A	202	NAG	O7-C7-N2	2.29	126.69	121.90
2	A	201	NAG	C1-O5-C5	2.25	117.44	113.40
3	B	301	NAG	C4-C3-C2	-2.25	107.24	110.44
3	A	301	NAG	C1-C2-N2	2.24	113.45	110.85
3	A	302	NAG	C1-C2-C3	-2.18	107.47	110.59
2	A	201	NAG	C3-C2-N2	2.16	115.13	110.56
3	B	303	NAG	O1-C1-C2	-2.15	104.48	109.27
3	B	302	NAG	C2-N2-C7	-2.15	117.27	123.02
3	B	301	NAG	C1-C2-N2	2.12	113.31	110.85
3	B	301	NAG	C1-O5-C5	-2.10	109.65	113.40
3	D	301	NAG	O5-C5-C6	2.09	111.49	106.34
3	A	303	NAG	O3-C3-C2	-2.05	108.25	111.86
3	D	301	NAG	O5-C1-C2	2.04	111.68	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	185/187 (98%)	0.00	1 (0%) 88 92	12, 19, 29, 35	0
1	B	183/187 (97%)	-0.03	2 (1%) 77 83	12, 19, 31, 37	0
1	C	174/187 (93%)	0.01	4 (2%) 57 63	13, 21, 35, 46	0
1	D	186/187 (99%)	0.05	1 (0%) 88 92	12, 20, 33, 41	0
All	All	728/748 (97%)	0.01	8 (1%) 70 83	12, 20, 33, 46	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	TYR	5.2
1	D	4	GLY	5.2
1	C	4	GLY	4.4
1	C	3	VAL	2.9
1	A	84	THR	2.7
1	B	90	ASP	2.5
1	B	104	TYR	2.4
1	C	77	GLY	2.3

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	303	14/15	0.59	27.76	4,12,18,18	14
3	NAG	B	302	14/15	0.49	15.17	8,12,14,16	14
2	NAG	D	201	15/15	0.26	14.84	12,16,19,20	15
2	NAG	D	202	14/15	0.24	11.83	9,12,18,21	14
3	NAG	B	301	15/15	0.46	7.91	5,12,14,14	15
3	NAG	D	301	15/15	0.18	4.69	8,13,17,18	15
3	NAG	D	302	14/15	0.17	2.87	13,15,19,20	14
3	NAG	A	303	14/15	0.13	1.22	16,23,31,35	0
3	NAG	A	301	15/15	0.10	0.87	13,16,20,22	0
3	NAG	D	303	14/15	0.14	0.57	12,16,19,22	14
3	NAG	A	302	14/15	0.10	-0.09	15,18,27,28	0
2	NAG	A	202	14/15	0.08	-0.16	16,21,28,31	0
2	NAG	A	201	15/15	0.08	-0.55	22,25,33,33	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.