



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:56 AM BST

PDB ID : 1QOO  
Title : lectin UEA-II complexed with NAG  
Authors : Loris, R.; De Greve, H.; Dao-Thi, M.-H.; Messens, J.; Imberty, A.; Wyns, L.  
Deposited on : 1999-11-15  
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

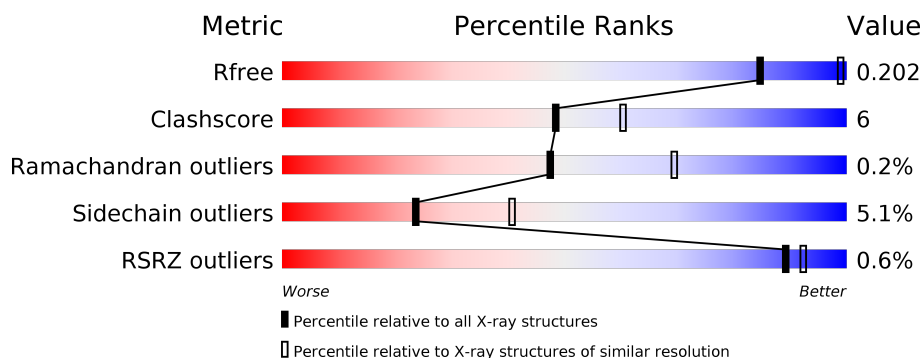
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	242	<div> <div>83%</div> <div>14%</div> <div>••</div> </div>
1	B	242	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>••</div> </div>
1	C	242	<div> <div>83%</div> <div>13%</div> <div>••</div> </div>
1	D	242	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>••</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7277 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 CHITIN BINDING LECTIN, UEA-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	1
			1783	1145	285	351	2			
1	B	237	Total	C	N	O	S	0	0	1
			1795	1153	287	353	2			
1	C	237	Total	C	N	O	S	0	0	1
			1795	1153	287	353	2			
1	D	237	Total	C	N	O	S	0	0	1
			1795	1153	287	353	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	ALA	conflict	GB AF190633
A	62	ILE	THR	conflict	GB AF190633
A	106	GLY	SER	conflict	GB AF190633
A	112	SER	ASN	conflict	GB AF190633
A	191	GLY	GLU	conflict	GB AF190633
A	229	VAL	ILE	conflict	GB AF190633
B	25	ASP	ALA	conflict	GB AF190633
B	62	ILE	THR	conflict	GB AF190633
B	106	GLY	SER	conflict	GB AF190633
B	112	SER	ASN	conflict	GB AF190633
B	191	GLY	GLU	conflict	GB AF190633
B	229	VAL	ILE	conflict	GB AF190633
C	25	ASP	ALA	conflict	GB AF190633
C	62	ILE	THR	conflict	GB AF190633
C	106	GLY	SER	conflict	GB AF190633
C	112	SER	ASN	conflict	GB AF190633
C	191	GLY	GLU	conflict	GB AF190633
C	229	VAL	ILE	conflict	GB AF190633
D	25	ASP	ALA	conflict	GB AF190633
D	62	ILE	THR	conflict	GB AF190633
D	106	GLY	SER	conflict	GB AF190633

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	112	SER	ASN	conflict	GB AF190633
D	191	GLY	GLU	conflict	GB AF190633
D	229	VAL	ILE	conflict	GB AF190633

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

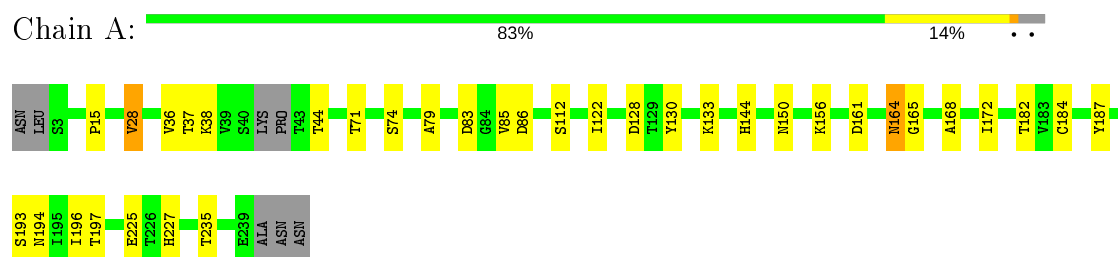


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

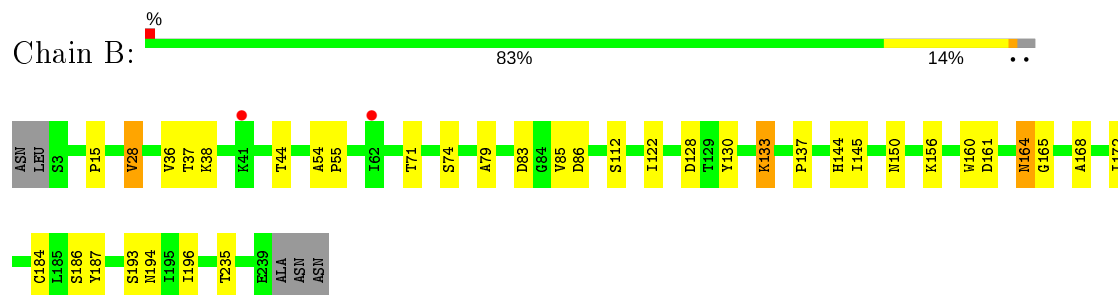
### 3 Residue-property plots [i](#)

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.

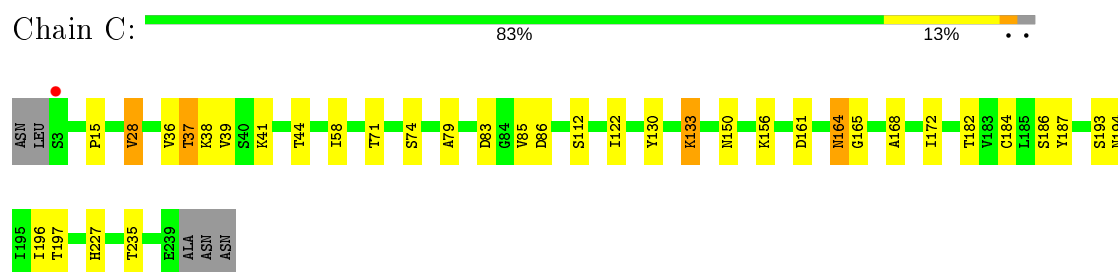
- Molecule 1: CHITIN BINDING LECTIN, UEA-II



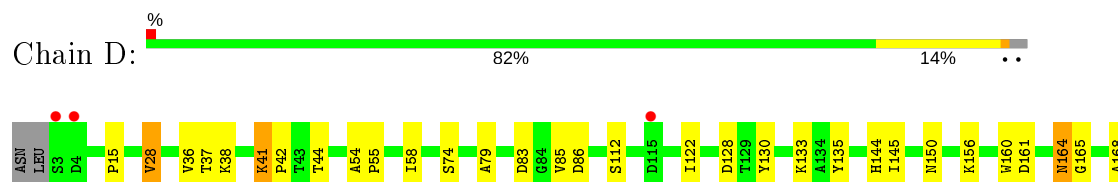
- Molecule 1: CHITIN BINDING LECTIN, UEA-II



- Molecule 1: CHITIN BINDING LECTIN, UEA-II



- Molecule 1: CHITIN BINDING LECTIN, UEA-II



T182	V183	C184	Y187	M194	I195	I196	T197	T235	E239	ALA	ASN	ASN
------	------	------	------	------	------	------	------	------	------	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.48Å 104.48Å 175.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.75 17.89 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.75) 98.3 (17.89-2.71)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.70Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.174 , 0.208 0.172 , 0.202	Depositor DCC
$R_{free}$ test set	2411 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7277	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: CA, MN, 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	0.41	0/1827	0.68	0/2489
1	B	0.40	0/1841	0.69	0/2511
1	C	0.40	0/1841	0.68	0/2511
1	D	0.41	0/1841	0.69	0/2511
All	All	0.41	0/7350	0.69	0/10022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1783	0	1721	22	0
1	B	1795	0	1731	22	0
1	C	1795	0	1731	25	0
1	D	1795	0	1731	24	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	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	29	0	28	0	0
4	B	14	0	13	0	0
4	C	29	0	28	0	0
4	D	29	0	28	0	0
All	All	7277	0	7011	86	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 6.

All (86) 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:D:161:ASP:H	1:D:194:ASN:HD21	1.32	0.78
1:C:161:ASP:H	1:C:194:ASN:HD21	1.34	0.76
1:B:161:ASP:H	1:B:194:ASN:HD21	1.33	0.76
1:A:161:ASP:H	1:A:194:ASN:HD21	1.34	0.76
1:D:182:THR:HG23	1:D:197:THR:HG22	1.70	0.73
1:C:182:THR:HG23	1:C:197:THR:HG22	1.71	0.70
1:A:193:SER:OG	1:C:197:THR:HG23	1.92	0.70
1:D:79:ALA:H	1:D:164:ASN:HD21	1.42	0.68
1:A:182:THR:HG23	1:A:197:THR:HG22	1.77	0.67
1:C:79:ALA:H	1:C:164:ASN:HD21	1.41	0.65
1:A:197:THR:HG23	1:C:193:SER:OG	1.96	0.65
1:A:79:ALA:H	1:A:164:ASN:HD21	1.44	0.65
1:B:79:ALA:H	1:B:164:ASN:HD21	1.44	0.64
1:B:85:VAL:HG12	1:B:130:TYR:HB2	1.80	0.64
1:D:85:VAL:HG12	1:D:130:TYR:HB2	1.80	0.63
1:C:85:VAL:HG12	1:C:130:TYR:HB2	1.81	0.61
1:D:41:LYS:CB	1:D:42:PRO:HD3	2.31	0.60
1:A:85:VAL:HG12	1:A:130:TYR:HB2	1.82	0.60
1:A:161:ASP:H	1:A:194:ASN:ND2	2.04	0.55
1:D:79:ALA:H	1:D:164:ASN:ND2	2.05	0.55
1:B:193:SER:OG	1:D:197:THR:HG23	2.08	0.54
1:C:79:ALA:H	1:C:164:ASN:ND2	2.04	0.54
1:A:197:THR:HG21	1:C:186:SER:HB2	1.90	0.53
1:B:161:ASP:H	1:B:194:ASN:ND2	2.03	0.53
1:B:79:ALA:H	1:B:164:ASN:ND2	2.07	0.53
1:A:79:ALA:H	1:A:164:ASN:ND2	2.07	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:CB	1:D:197:THR:HG21	2.39	0.52
1:D:161:ASP:H	1:D:194:ASN:ND2	2.04	0.52
1:A:197:THR:HG21	1:C:186:SER:CB	2.40	0.51
1:A:164:ASN:HD22	1:A:165:GLY:N	2.09	0.50
1:B:164:ASN:HD22	1:B:165:GLY:N	2.09	0.50
1:C:161:ASP:H	1:C:194:ASN:ND2	2.04	0.50
1:C:133:LYS:HE3	1:C:133:LYS:HA	1.92	0.50
1:B:186:SER:HB2	1:D:197:THR:HG21	1.94	0.49
1:B:15:PRO:HA	1:B:28:VAL:HG13	1.93	0.49
1:C:15:PRO:HA	1:C:28:VAL:HG13	1.94	0.48
1:D:164:ASN:HD22	1:D:165:GLY:N	2.11	0.48
1:A:15:PRO:HA	1:A:28:VAL:HG13	1.95	0.48
1:D:15:PRO:HA	1:D:28:VAL:HG13	1.96	0.48
1:D:156:LYS:HE2	1:D:196:ILE:HD11	1.96	0.47
1:C:156:LYS:HG2	1:C:196:ILE:HD11	1.97	0.47
1:B:156:LYS:HG2	1:B:196:ILE:HD11	1.96	0.47
1:C:164:ASN:HD22	1:C:165:GLY:N	2.12	0.47
1:D:168:ALA:HB2	1:D:187:TYR:CE1	2.49	0.47
1:B:156:LYS:HE2	1:B:196:ILE:HD11	1.96	0.46
1:A:156:LYS:HE2	1:A:196:ILE:HD11	1.97	0.46
1:D:156:LYS:HG2	1:D:196:ILE:HD11	1.98	0.46
1:C:168:ALA:HB2	1:C:187:TYR:CE1	2.51	0.46
1:C:156:LYS:HE2	1:C:196:ILE:HD11	1.98	0.45
1:A:79:ALA:N	1:A:164:ASN:HD21	2.14	0.45
1:B:133:LYS:HD3	1:B:137:PRO:HA	1.98	0.45
1:A:168:ALA:HB2	1:A:187:TYR:CE1	2.52	0.45
1:D:58:ILE:HA	1:D:58:ILE:HD12	1.85	0.45
1:C:122:ILE:H	1:C:150:ASN:ND2	2.14	0.45
1:D:122:ILE:H	1:D:150:ASN:ND2	2.15	0.45
1:A:122:ILE:H	1:A:150:ASN:ND2	2.15	0.45
1:A:156:LYS:HG2	1:A:196:ILE:HD11	1.98	0.45
1:B:168:ALA:HB2	1:B:187:TYR:CE1	2.52	0.45
1:B:122:ILE:H	1:B:150:ASN:ND2	2.16	0.44
1:C:133:LYS:CA	1:C:133:LYS:HE3	2.48	0.44
1:A:71:THR:HG22	1:A:172:ILE:HB	2.00	0.43
1:B:79:ALA:N	1:B:164:ASN:HD21	2.14	0.43
1:B:145:ILE:HG13	1:B:160:TRP:HB2	2.01	0.43
1:D:128:ASP:HB3	1:D:144:HIS:CE1	2.54	0.43
1:C:58:ILE:HA	1:C:58:ILE:HD12	1.86	0.42
1:D:135:TYR:CD1	1:D:135:TYR:N	2.86	0.42
1:B:71:THR:HG22	1:B:172:ILE:HB	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LYS:HE3	1:D:44:THR:CG2	2.49	0.42
1:A:38:LYS:HE3	1:A:44:THR:CG2	2.50	0.42
1:D:145:ILE:HG13	1:D:160:TRP:HB2	2.01	0.42
1:B:74:SER:HA	1:B:168:ALA:O	2.20	0.41
1:D:74:SER:HA	1:D:168:ALA:O	2.20	0.41
1:A:74:SER:HA	1:A:168:ALA:O	2.20	0.41
1:C:38:LYS:HE3	1:C:44:THR:CG2	2.49	0.41
1:D:79:ALA:N	1:D:164:ASN:HD21	2.13	0.41
1:C:37:THR:HG21	1:C:227:HIS:HD2	1.86	0.41
1:D:54:ALA:HA	1:D:55:PRO:HD3	1.93	0.41
1:B:128:ASP:HB3	1:B:144:HIS:CE1	2.56	0.40
1:B:38:LYS:HE3	1:B:44:THR:CG2	2.50	0.40
1:B:54:ALA:HA	1:B:55:PRO:HD3	1.91	0.40
1:C:79:ALA:N	1:C:164:ASN:HD21	2.12	0.40
1:C:74:SER:HA	1:C:168:ALA:O	2.22	0.40
1:C:71:THR:HG22	1:C:172:ILE:HB	2.03	0.40
1:A:128:ASP:HB3	1:A:144:HIS:CE1	2.56	0.40
1:A:225:GLU:OE2	1:A:227:HIS:HE1	2.05	0.40
1:C:39:VAL:HG23	1:C:39:VAL:O	2.22	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	231/242 (96%)	225 (97%)	6 (3%)	0	100	100
1	B	235/242 (97%)	227 (97%)	8 (3%)	0	100	100
1	C	235/242 (97%)	226 (96%)	8 (3%)	1 (0%)	34	53
1	D	235/242 (97%)	225 (96%)	9 (4%)	1 (0%)	34	53
All	All	936/968 (97%)	903 (96%)	31 (3%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41	LYS
1	C	41	LYS

### 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	197/205 (96%)	187 (95%)	10 (5%)	24	41
1	B	198/205 (97%)	188 (95%)	10 (5%)	24	41
1	C	198/205 (97%)	188 (95%)	10 (5%)	24	41
1	D	198/205 (97%)	188 (95%)	10 (5%)	24	41
All	All	791/820 (96%)	751 (95%)	40 (5%)	24	41

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	36	VAL
1	A	37	THR
1	A	83	ASP
1	A	86	ASP
1	A	112	SER
1	A	133	LYS
1	A	164	ASN
1	A	184	CYS
1	A	235	THR
1	B	28	VAL
1	B	36	VAL
1	B	37	THR
1	B	83	ASP
1	B	86	ASP
1	B	112	SER
1	B	133	LYS
1	B	164	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	184	CYS
1	B	235	THR
1	C	28	VAL
1	C	36	VAL
1	C	37	THR
1	C	83	ASP
1	C	86	ASP
1	C	112	SER
1	C	133	LYS
1	C	164	ASN
1	C	184	CYS
1	C	235	THR
1	D	28	VAL
1	D	36	VAL
1	D	37	THR
1	D	83	ASP
1	D	86	ASP
1	D	112	SER
1	D	133	LYS
1	D	164	ASN
1	D	184	CYS
1	D	235	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	120	ASN
1	A	150	ASN
1	A	164	ASN
1	A	194	ASN
1	A	220	ASN
1	A	227	HIS
1	A	237	ASN
1	B	35	GLN
1	B	120	ASN
1	B	150	ASN
1	B	164	ASN
1	B	194	ASN
1	B	220	ASN
1	B	227	HIS
1	B	237	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	35	GLN
1	C	120	ASN
1	C	150	ASN
1	C	164	ASN
1	C	194	ASN
1	C	220	ASN
1	C	227	HIS
1	C	237	ASN
1	D	35	GLN
1	D	120	ASN
1	D	150	ASN
1	D	164	ASN
1	D	194	ASN
1	D	220	ASN
1	D	227	HIS
1	D	237	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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
4	NAG	A	501	-	15,15,15	0.40	0	21,21,21	0.67	0
4	NAG	B	401	1	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
4	NAG	C	401	1	14,14,15	0.60	0	17,19,21	1.09	1 (5%)
4	NAG	D	401	1	14,14,15	0.61	0	17,19,21	1.05	2 (11%)
4	NAG	A	401	1	14,14,15	0.58	0	17,19,21	1.28	2 (11%)
4	NAG	C	501	-	15,15,15	0.50	0	21,21,21	0.68	0
4	NAG	D	501	-	15,15,15	0.55	0	21,21,21	0.66	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
4	NAG	A	501	-	-	2/6/26/26	0/1/1/1
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	D	401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	501	-	-	0/6/26/26	0/1/1/1
4	NAG	D	501	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	NAG	C2-N2-C7	-2.97	118.68	122.90
4	A	401	NAG	C4-C3-C2	-2.80	106.92	111.02
4	B	401	NAG	C2-N2-C7	-2.80	118.92	122.90
4	C	401	NAG	C4-C3-C2	-2.75	107.00	111.02
4	D	401	NAG	C2-N2-C7	-2.65	119.13	122.90
4	D	401	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	501	NAG	C4-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	501	NAG	O5-C5-C6-O6
4	C	401	NAG	C1-C2-N2-C7
4	A	501	NAG	O5-C5-C6-O6
4	C	401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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	235/242 (97%)	-0.71	0	100   100	8, 19, 46, 62	0
1	B	237/242 (97%)	-0.65	2 (0%)	86   90	8, 19, 46, 62	0
1	C	237/242 (97%)	-0.66	1 (0%)	92   95	9, 20, 49, 62	0
1	D	237/242 (97%)	-0.64	3 (1%)	77   84	9, 20, 48, 63	0
All	All	946/968 (97%)	-0.66	6 (0%)	89   92	8, 19, 47, 63	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	ILE	3.5
1	D	4	ASP	3.4
1	D	115	ASP	2.6
1	D	3	SER	2.4
1	C	3	SER	2.2
1	B	41	LYS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	401	14/15	0.75	0.32	53,64,77,82	0
4	NAG	A	401	14/15	0.83	0.26	51,63,74,74	0
4	NAG	D	401	14/15	0.86	0.30	58,64,67,68	0
4	NAG	B	401	14/15	0.87	0.24	43,51,61,63	0
3	CA	A	302	1/1	0.90	0.16	26,26,26,26	0
4	NAG	D	501	15/15	0.90	0.32	20,38,50,56	0
4	NAG	C	501	15/15	0.92	0.24	21,31,48,51	0
3	CA	D	308	1/1	0.94	0.10	26,26,26,26	0
4	NAG	A	501	15/15	0.95	0.14	16,25,43,45	0
3	CA	C	306	1/1	0.95	0.19	28,28,28,28	0
3	CA	B	304	1/1	0.98	0.07	21,21,21,21	0
2	MN	D	307	1/1	0.98	0.11	22,22,22,22	0
2	MN	B	303	1/1	0.98	0.10	15,15,15,15	0
2	MN	C	305	1/1	0.98	0.08	15,15,15,15	0
2	MN	A	301	1/1	0.99	0.09	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.