



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:47 PM BST

PDB ID : 5OJM  
Title : Structure of a chimaeric beta3-alpha5 GABAA receptor in complex with nanobody Nb25  
Authors : Miller, P.S.; Scott, S.; Masiulis, S.; De Colibus, L.; Pardon, E.; Steyaert, J.; Aricescu, A.R.  
Deposited on : 2017-07-21  
Resolution : 3.30 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.

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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 : 1.8.5 (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

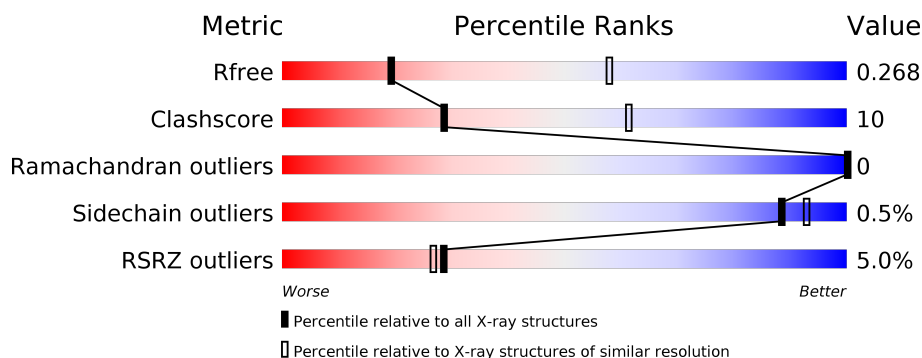
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	395	<div> <div>2%</div> <div>70% 14% 16%</div> </div>
1	B	395	<div> <div>3%</div> <div>68% 16% 16%</div> </div>
1	C	395	<div> <div>2%</div> <div>67% 16% 16%</div> </div>
1	D	395	<div> <div>0%</div> <div>66% 18% 16%</div> </div>
1	E	395	<div> <div>3%</div> <div>68% 16% 16%</div> </div>
2	K	125	<div> <div>17%</div> <div>83% 15% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	125	<div><div></div><div>18%83%15%</div><div></div></div>
2	M	125	<div><div></div><div>11%85%14%</div><div></div></div>
2	N	125	<div><div></div><div>10%86%13%</div><div></div></div>
2	O	125	<div><div></div><div>3%86%13%</div><div></div></div>
3	F	5	<div><div></div><div>100%</div><div></div></div>
3	G	5	<div><div></div><div>100%</div><div></div></div>
3	H	5	<div><div></div><div>80%20%</div><div></div></div>
4	I	6	<div><div></div><div>100%</div><div></div></div>
4	J	6	<div><div></div><div>50%50%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18538 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 Human GABAA receptor chimera beta3-alpha5, Gamma-aminobutyric acid receptor subunit beta-3, Gamma-aminobutyric acid receptor subunit alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2670	1736	442	476	16			
1	B	333	Total	C	N	O	S	0	0	0
			2692	1748	446	481	17			
1	C	330	Total	C	N	O	S	0	0	0
			2670	1736	442	476	16			
1	D	332	Total	C	N	O	S	0	0	0
			2684	1744	444	479	17			
1	E	330	Total	C	N	O	S	0	0	0
			2670	1736	442	476	16			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	SER	-	linker	UNP P31644
A	317	GLN	-	linker	UNP P31644
A	318	PRO	-	linker	UNP P31644
A	319	ALA	-	linker	UNP P31644
A	320	ARG	-	linker	UNP P31644
A	321	ALA	-	linker	UNP P31644
A	322	ALA	-	linker	UNP P31644
A	404	ILE	VAL	conflict	UNP P31644
A	428	THR	ALA	conflict	UNP P31644
A	432	GLY	-	expression tag	UNP P31644
A	433	THR	-	expression tag	UNP P31644
A	434	THR	-	expression tag	UNP P31644
A	435	GLU	-	expression tag	UNP P31644
A	436	THR	-	expression tag	UNP P31644
A	437	SER	-	expression tag	UNP P31644
A	438	GLN	-	expression tag	UNP P31644
A	439	VAL	-	expression tag	UNP P31644
A	440	ALA	-	expression tag	UNP P31644

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Chain	Residue	Modelled	Actual	Comment	Reference
A	441	PRO	-	expression tag	UNP P31644
A	442	ALA	-	expression tag	UNP P31644
B	316	SER	-	linker	UNP P31644
B	317	GLN	-	linker	UNP P31644
B	318	PRO	-	linker	UNP P31644
B	319	ALA	-	linker	UNP P31644
B	320	ARG	-	linker	UNP P31644
B	321	ALA	-	linker	UNP P31644
B	322	ALA	-	linker	UNP P31644
B	404	ILE	VAL	conflict	UNP P31644
B	428	THR	ALA	conflict	UNP P31644
B	432	GLY	-	expression tag	UNP P31644
B	433	THR	-	expression tag	UNP P31644
B	434	THR	-	expression tag	UNP P31644
B	435	GLU	-	expression tag	UNP P31644
B	436	THR	-	expression tag	UNP P31644
B	437	SER	-	expression tag	UNP P31644
B	438	GLN	-	expression tag	UNP P31644
B	439	VAL	-	expression tag	UNP P31644
B	440	ALA	-	expression tag	UNP P31644
B	441	PRO	-	expression tag	UNP P31644
B	442	ALA	-	expression tag	UNP P31644
C	316	SER	-	linker	UNP P31644
C	317	GLN	-	linker	UNP P31644
C	318	PRO	-	linker	UNP P31644
C	319	ALA	-	linker	UNP P31644
C	320	ARG	-	linker	UNP P31644
C	321	ALA	-	linker	UNP P31644
C	322	ALA	-	linker	UNP P31644
C	404	ILE	VAL	conflict	UNP P31644
C	428	THR	ALA	conflict	UNP P31644
C	432	GLY	-	expression tag	UNP P31644
C	433	THR	-	expression tag	UNP P31644
C	434	THR	-	expression tag	UNP P31644
C	435	GLU	-	expression tag	UNP P31644
C	436	THR	-	expression tag	UNP P31644
C	437	SER	-	expression tag	UNP P31644
C	438	GLN	-	expression tag	UNP P31644
C	439	VAL	-	expression tag	UNP P31644
C	440	ALA	-	expression tag	UNP P31644
C	441	PRO	-	expression tag	UNP P31644
C	442	ALA	-	expression tag	UNP P31644

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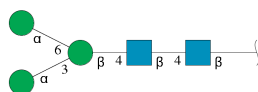
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Chain	Residue	Modelled	Actual	Comment	Reference
D	316	SER	-	linker	UNP P31644
D	317	GLN	-	linker	UNP P31644
D	318	PRO	-	linker	UNP P31644
D	319	ALA	-	linker	UNP P31644
D	320	ARG	-	linker	UNP P31644
D	321	ALA	-	linker	UNP P31644
D	322	ALA	-	linker	UNP P31644
D	404	ILE	VAL	conflict	UNP P31644
D	428	THR	ALA	conflict	UNP P31644
D	432	GLY	-	expression tag	UNP P31644
D	433	THR	-	expression tag	UNP P31644
D	434	THR	-	expression tag	UNP P31644
D	435	GLU	-	expression tag	UNP P31644
D	436	THR	-	expression tag	UNP P31644
D	437	SER	-	expression tag	UNP P31644
D	438	GLN	-	expression tag	UNP P31644
D	439	VAL	-	expression tag	UNP P31644
D	440	ALA	-	expression tag	UNP P31644
D	441	PRO	-	expression tag	UNP P31644
D	442	ALA	-	expression tag	UNP P31644
E	316	SER	-	linker	UNP P31644
E	317	GLN	-	linker	UNP P31644
E	318	PRO	-	linker	UNP P31644
E	319	ALA	-	linker	UNP P31644
E	320	ARG	-	linker	UNP P31644
E	321	ALA	-	linker	UNP P31644
E	322	ALA	-	linker	UNP P31644
E	404	ILE	VAL	conflict	UNP P31644
E	428	THR	ALA	conflict	UNP P31644
E	432	GLY	-	expression tag	UNP P31644
E	433	THR	-	expression tag	UNP P31644
E	434	THR	-	expression tag	UNP P31644
E	435	GLU	-	expression tag	UNP P31644
E	436	THR	-	expression tag	UNP P31644
E	437	SER	-	expression tag	UNP P31644
E	438	GLN	-	expression tag	UNP P31644
E	439	VAL	-	expression tag	UNP P31644
E	440	ALA	-	expression tag	UNP P31644
E	441	PRO	-	expression tag	UNP P31644
E	442	ALA	-	expression tag	UNP P31644

- Molecule 2 is a protein called Nanobody Nb25.

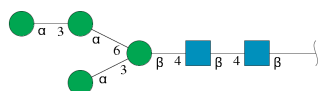
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	123	Total	C	N	O	S	0	0	0
			951	598	164	185	4			
2	L	123	Total	C	N	O	S	0	0	0
			951	598	164	185	4			
2	M	123	Total	C	N	O	S	0	0	0
			951	598	164	185	4			
2	N	123	Total	C	N	O	S	0	0	0
			951	598	164	185	4			
2	O	123	Total	C	N	O	S	0	0	0
			951	598	164	185	4			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



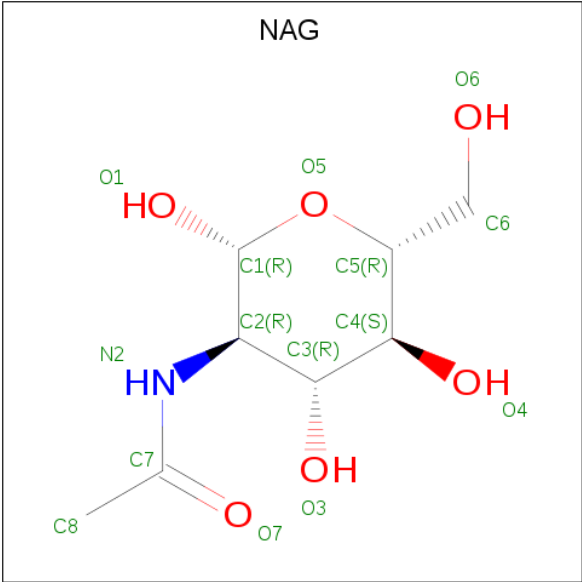
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



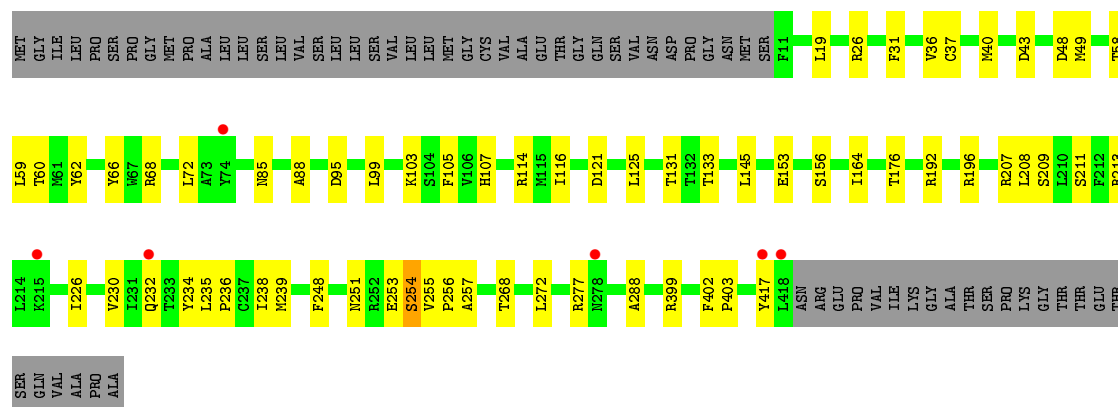
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 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>).

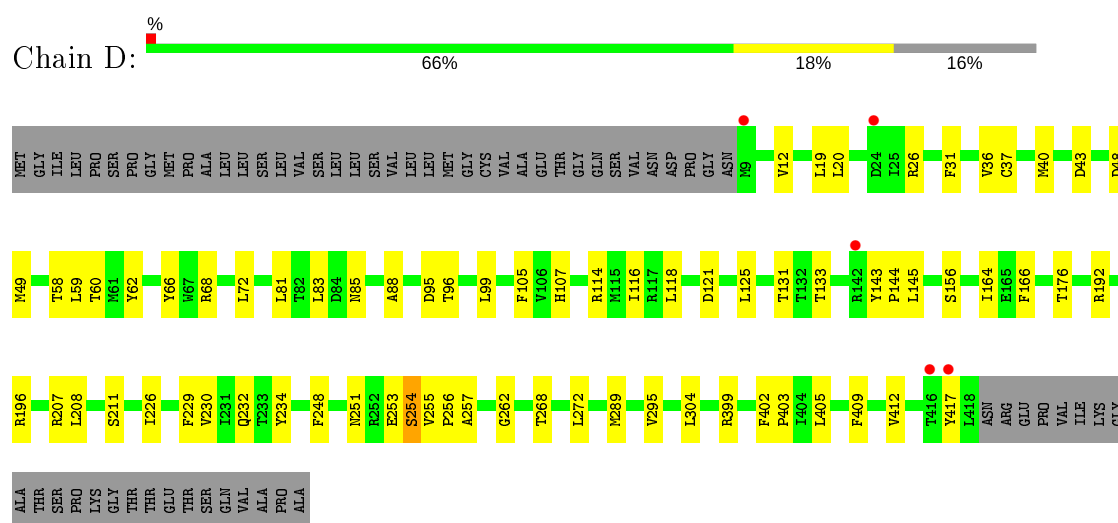


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

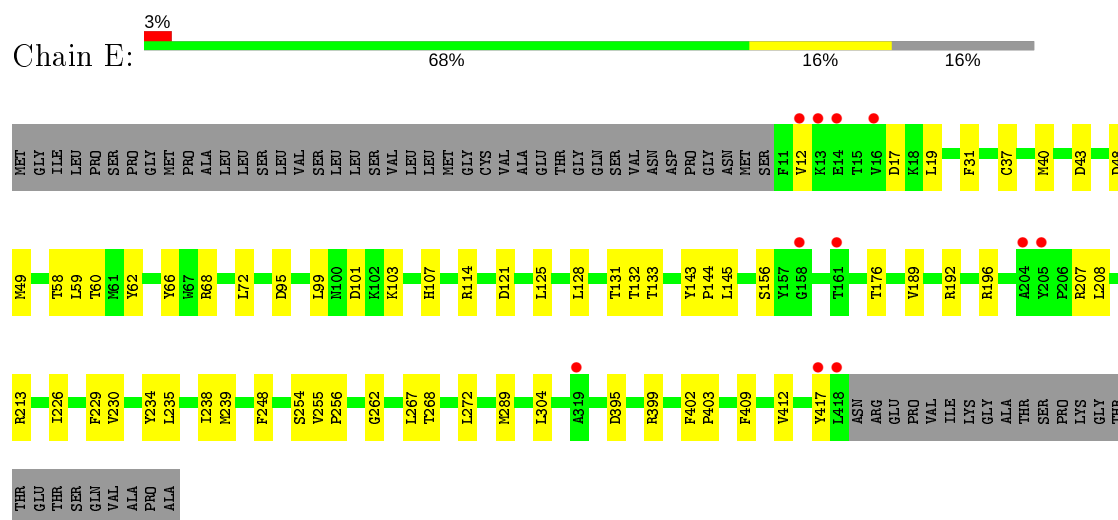




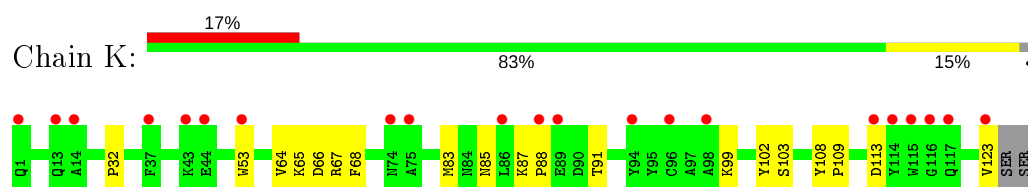
- Molecule 1: Human GABAA receptor chimera beta3-alpha5, Gamma-aminobutyric acid receptor subunit beta-3, Gamma-aminobutyric acid receptor subunit alpha-5



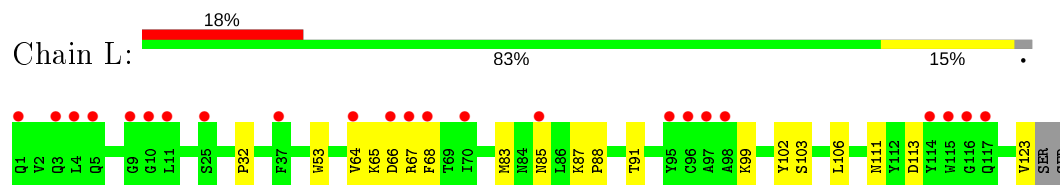
- Molecule 1: Human GABAA receptor chimera beta3-alpha5, Gamma-aminobutyric acid receptor subunit beta-3, Gamma-aminobutyric acid receptor subunit alpha-5



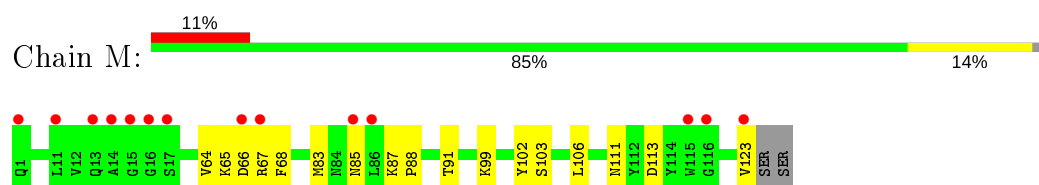
- Molecule 2: Nanobody Nb25



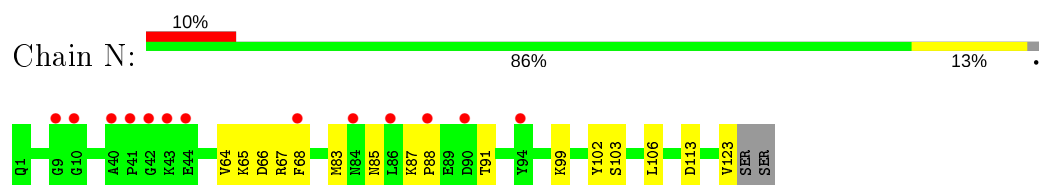
• Molecule 2: Nanobody Nb25



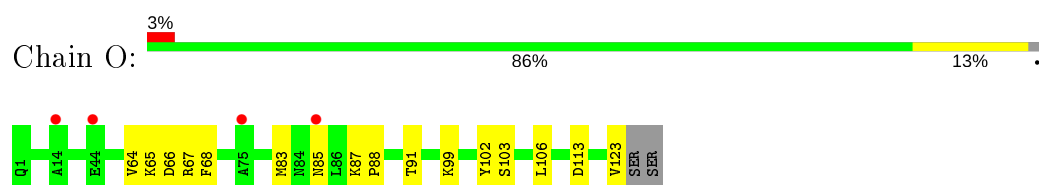
• Molecule 2: Nanobody Nb25



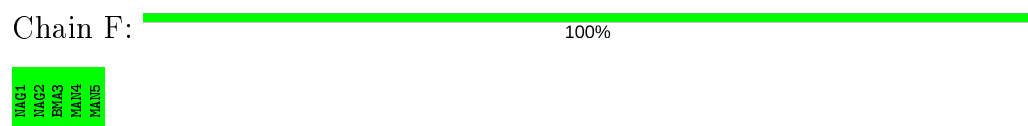
• Molecule 2: Nanobody Nb25



• Molecule 2: Nanobody Nb25

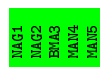


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 80% 20%



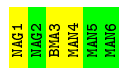
- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.35Å 139.94Å 191.50Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	48.88 – 3.30 48.88 – 3.28	Depositor EDS
% Data completeness (in resolution range)	73.6 (48.88-3.30) 99.1 (48.88-3.28)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0158, PHENIX (1.12rc)-2787-000)	Depositor
R, $R_{free}$	0.234 , 0.250 0.251 , 0.268	Depositor DCC
$R_{free}$ test set	3412 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.8	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 9.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	18538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: BMA, NAG, MAN

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	0.50	0/2737	0.44	0/3724
1	B	0.50	0/2759	0.43	0/3753
1	C	0.50	0/2737	0.44	0/3724
1	D	0.52	0/2751	0.44	0/3742
1	E	0.50	0/2737	0.44	0/3724
2	K	0.41	0/975	0.38	0/1321
2	L	0.38	0/975	0.37	0/1321
2	M	0.40	0/975	0.37	0/1321
2	N	0.41	0/975	0.37	0/1321
2	O	0.39	0/975	0.37	0/1321
All	All	0.48	0/18596	0.42	0/25272

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

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	2670	0	2678	60	0
1	B	2692	0	2698	70	0
1	C	2670	0	2678	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2684	0	2692	67	0
1	E	2670	0	2678	63	0
2	K	951	0	895	15	0
2	L	951	0	895	16	0
2	M	951	0	895	15	0
2	N	951	0	895	14	0
2	O	951	0	895	14	0
3	F	61	0	52	0	0
3	G	61	0	52	0	0
3	H	61	0	52	1	0
4	I	72	0	61	0	0
4	J	72	0	61	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
All	All	18538	0	18242	355	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 10.

All (355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:OH	1:E:99:LEU:CD1	2.22	0.87
1:D:207:ARG:NH1	2:N:102:TYR:O	2.07	0.87
1:A:99:LEU:CD1	1:B:62:TYR:OH	2.24	0.86
1:B:143:TYR:OH	1:B:229:PHE:HE2	1.57	0.85
1:C:196:ARG:NH1	2:M:113:ASP:OD1	2.10	0.83
1:B:196:ARG:NH1	2:L:113:ASP:OD1	2.10	0.83
1:A:99:LEU:HD12	1:B:62:TYR:OH	1.79	0.82
1:D:99:LEU:CD1	1:E:62:TYR:OH	2.28	0.81
1:B:99:LEU:CD1	1:C:62:TYR:OH	2.28	0.81
1:C:99:LEU:CD1	1:D:62:TYR:OH	2.31	0.79
1:A:207:ARG:NH1	2:K:102:TYR:O	2.15	0.79
2:O:64:VAL:HG13	2:O:68:PHE:CD1	2.18	0.79
1:B:207:ARG:NH1	2:L:102:TYR:O	2.15	0.78
2:L:64:VAL:HG13	2:L:68:PHE:CD1	2.18	0.78
2:M:64:VAL:HG13	2:M:68:PHE:CD1	2.18	0.78
1:E:196:ARG:NH1	2:O:113:ASP:OD1	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:64:VAL:HG13	2:N:68:PHE:CD1	2.18	0.78
1:E:99:LEU:HD22	1:E:207:ARG:NH2	1.99	0.78
2:K:64:VAL:HG13	2:K:68:PHE:CD1	2.18	0.77
1:B:99:LEU:HD22	1:B:207:ARG:NH2	1.99	0.77
1:C:99:LEU:HD22	1:C:207:ARG:NH2	2.00	0.77
1:C:207:ARG:NH1	2:M:102:TYR:O	2.19	0.76
1:A:99:LEU:HD22	1:A:207:ARG:NH2	2.00	0.76
1:E:207:ARG:NH1	2:O:102:TYR:O	2.18	0.76
1:D:49:MET:HB3	1:D:58:THR:HG22	1.68	0.76
1:B:49:MET:HB3	1:B:58:THR:HG22	1.68	0.76
1:D:99:LEU:HD22	1:D:207:ARG:NH2	2.02	0.75
1:A:62:TYR:OH	1:E:99:LEU:HD12	1.87	0.75
1:D:99:LEU:HD12	1:E:62:TYR:OH	1.88	0.73
1:C:49:MET:HB3	1:C:58:THR:HG22	1.71	0.72
1:E:49:MET:HB3	1:E:58:THR:HG22	1.71	0.72
1:E:192:ARG:NH1	4:J:1:NAG:O7	2.25	0.70
1:D:196:ARG:NH1	2:N:113:ASP:OD1	2.23	0.70
1:A:49:MET:HB3	1:A:58:THR:HG22	1.71	0.70
1:B:99:LEU:HD12	1:C:62:TYR:OH	1.92	0.70
1:B:145:LEU:CD2	1:B:226:ILE:CD1	2.72	0.67
1:E:60:THR:OG1	1:E:131:THR:HG22	1.95	0.67
1:A:145:LEU:CD2	1:A:226:ILE:CD1	2.72	0.67
1:D:145:LEU:CD2	1:D:226:ILE:CD1	2.73	0.66
1:A:60:THR:OG1	1:A:131:THR:HG22	1.95	0.66
1:A:248:PHE:O	1:A:399:ARG:NE	2.28	0.66
1:C:145:LEU:CD2	1:C:226:ILE:CD1	2.73	0.66
1:C:99:LEU:HD12	1:D:62:TYR:OH	1.94	0.66
1:C:60:THR:OG1	1:C:131:THR:HG22	1.96	0.66
1:E:248:PHE:O	1:E:399:ARG:NE	2.29	0.66
1:C:248:PHE:O	1:C:399:ARG:NE	2.29	0.65
1:D:19:LEU:HD22	1:D:72:LEU:HA	1.79	0.65
1:B:60:THR:OG1	1:B:131:THR:HG22	1.97	0.65
1:C:153:GLU:OE1	1:C:209:SER:OG	2.14	0.65
1:D:248:PHE:O	1:D:399:ARG:NE	2.30	0.65
1:D:60:THR:OG1	1:D:131:THR:HG22	1.96	0.65
1:D:58:THR:HB	1:D:133:THR:HG22	1.79	0.64
1:E:145:LEU:CD2	1:E:226:ILE:CD1	2.74	0.64
2:O:91:THR:HG22	2:O:123:VAL:H	1.63	0.64
1:C:58:THR:CB	1:C:133:THR:HG22	2.29	0.63
1:D:40:MET:HG3	1:D:208:LEU:HD12	1.80	0.63
2:K:91:THR:HG22	2:K:123:VAL:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:HB	1:C:133:THR:HG22	1.80	0.63
2:L:91:THR:HG22	2:L:123:VAL:H	1.63	0.63
2:M:64:VAL:HG13	2:M:68:PHE:CG	2.33	0.63
1:E:40:MET:HG3	1:E:208:LEU:HD12	1.81	0.63
1:D:58:THR:CB	1:D:133:THR:HG22	2.29	0.62
1:A:58:THR:CB	1:A:133:THR:HG22	2.30	0.62
1:A:58:THR:HB	1:A:133:THR:HG22	1.80	0.62
1:B:143:TYR:OH	1:B:229:PHE:CE2	2.41	0.62
2:M:91:THR:HG22	2:M:123:VAL:H	1.65	0.62
2:O:64:VAL:HG13	2:O:68:PHE:CG	2.34	0.62
2:K:64:VAL:HG13	2:K:68:PHE:CG	2.34	0.61
1:D:99:LEU:HD12	1:E:62:TYR:HH	1.65	0.61
1:B:58:THR:HB	1:B:133:THR:HG22	1.83	0.61
2:L:64:VAL:HG13	2:L:68:PHE:CG	2.36	0.61
1:B:49:MET:HB3	1:B:58:THR:CG2	2.31	0.60
2:N:91:THR:HG22	2:N:123:VAL:H	1.65	0.60
2:N:64:VAL:HG13	2:N:68:PHE:CG	2.35	0.60
1:E:58:THR:CB	1:E:133:THR:HG22	2.32	0.60
1:A:164:ILE:HG23	1:A:206:PRO:HG3	1.81	0.60
1:D:68:ARG:NH1	1:D:121:ASP:OD1	2.34	0.60
1:E:68:ARG:NH1	1:E:121:ASP:OD1	2.35	0.60
1:C:68:ARG:NH1	1:C:121:ASP:OD1	2.34	0.60
1:B:68:ARG:NH1	1:B:121:ASP:OD1	2.34	0.59
1:A:68:ARG:NH1	1:A:121:ASP:OD1	2.35	0.59
1:C:145:LEU:CD2	1:C:226:ILE:HD13	2.31	0.59
1:A:62:TYR:OH	1:E:99:LEU:HD11	2.03	0.59
1:B:40:MET:HG3	1:B:208:LEU:HD12	1.85	0.59
1:C:232:GLN:O	1:C:236:PRO:HG2	2.03	0.59
1:D:49:MET:HB3	1:D:58:THR:CG2	2.33	0.58
1:B:58:THR:CB	1:B:133:THR:HG22	2.32	0.58
1:B:19:LEU:HD22	1:B:72:LEU:HA	1.84	0.58
1:C:40:MET:HG3	1:C:208:LEU:HD12	1.84	0.58
1:E:58:THR:HB	1:E:133:THR:HG22	1.84	0.58
1:E:145:LEU:CD2	1:E:226:ILE:HD13	2.33	0.58
1:E:49:MET:HB3	1:E:58:THR:CG2	2.34	0.58
1:E:99:LEU:HD22	1:E:207:ARG:CZ	2.33	0.58
1:C:99:LEU:HD22	1:C:207:ARG:CZ	2.33	0.58
1:A:196:ARG:NH1	2:K:113:ASP:OD1	2.37	0.57
2:O:67:ARG:NH2	2:O:85:ASN:O	2.37	0.57
1:C:255:VAL:N	1:C:256:PRO:HD2	2.19	0.57
1:B:255:VAL:N	1:B:256:PRO:HD2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:VAL:N	1:E:256:PRO:HD2	2.19	0.57
1:C:19:LEU:HD22	1:C:72:LEU:HA	1.86	0.57
1:B:145:LEU:HD23	1:B:226:ILE:CD1	2.35	0.57
1:D:255:VAL:N	1:D:256:PRO:HD2	2.19	0.57
1:E:19:LEU:HD22	1:E:72:LEU:HA	1.86	0.57
1:A:255:VAL:N	1:A:256:PRO:HD2	2.19	0.57
2:L:67:ARG:NH2	2:L:85:ASN:O	2.38	0.57
1:A:99:LEU:HD22	1:A:207:ARG:CZ	2.34	0.57
1:D:99:LEU:HD22	1:D:207:ARG:CZ	2.35	0.57
1:D:88:ALA:HB2	1:D:116:ILE:HD11	1.87	0.57
1:D:145:LEU:CD2	1:D:226:ILE:HD13	2.35	0.57
1:C:288:ALA:HB2	1:C:417:TYR:CE2	2.40	0.56
1:A:40:MET:HG3	1:A:208:LEU:HD12	1.86	0.56
1:E:235:LEU:HD23	1:E:238:ILE:HD11	1.86	0.56
2:M:67:ARG:NH2	2:M:85:ASN:O	2.38	0.56
2:N:67:ARG:NH2	2:N:85:ASN:O	2.38	0.56
2:K:67:ARG:NH2	2:K:85:ASN:O	2.38	0.56
1:E:226:ILE:HG22	1:E:226:ILE:O	2.06	0.55
1:C:226:ILE:HG22	1:C:226:ILE:O	2.06	0.55
1:B:277:ARG:HB3	1:C:232:GLN:HE21	1.71	0.55
1:B:145:LEU:CD2	1:B:226:ILE:HD13	2.37	0.54
1:B:145:LEU:CD2	1:B:226:ILE:HD11	2.37	0.54
1:D:68:ARG:NH1	1:D:121:ASP:O	2.37	0.54
1:A:145:LEU:HD23	1:A:226:ILE:CD1	2.37	0.54
1:A:226:ILE:HG22	1:A:226:ILE:O	2.07	0.54
2:N:65:LYS:O	2:N:66:ASP:HB2	2.08	0.54
1:A:248:PHE:O	1:A:399:ARG:NH2	2.40	0.54
1:C:145:LEU:HD23	1:C:226:ILE:CD1	2.38	0.54
1:A:49:MET:HB3	1:A:58:THR:CG2	2.36	0.54
1:D:143:TYR:HH	1:D:229:PHE:HE1	1.56	0.54
1:C:248:PHE:O	1:C:399:ARG:NH2	2.41	0.54
2:M:65:LYS:O	2:M:66:ASP:HB2	2.07	0.54
1:A:145:LEU:CD2	1:A:226:ILE:HD13	2.38	0.53
1:B:226:ILE:HG22	1:B:226:ILE:O	2.07	0.53
1:C:277:ARG:HB3	1:D:232:GLN:HE21	1.73	0.53
1:B:99:LEU:HD22	1:B:207:ARG:CZ	2.38	0.53
2:N:68:PHE:HE2	2:N:83:MET:SD	2.31	0.53
1:B:103:LYS:HE3	1:C:105:PHE:CE2	2.44	0.53
2:K:68:PHE:CE2	2:K:83:MET:SD	3.02	0.53
1:C:49:MET:HB3	1:C:58:THR:CG2	2.36	0.53
1:D:226:ILE:HG22	1:D:226:ILE:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:PHE:O	1:D:399:ARG:NH2	2.41	0.53
2:O:68:PHE:HE2	2:O:83:MET:SD	2.32	0.53
2:L:65:LYS:O	2:L:66:ASP:HB2	2.09	0.53
2:L:68:PHE:CE2	2:L:83:MET:SD	3.03	0.53
2:N:68:PHE:CE2	2:N:83:MET:SD	3.03	0.53
2:K:68:PHE:HE2	2:K:83:MET:SD	2.31	0.52
2:L:68:PHE:HE2	2:L:83:MET:SD	2.31	0.52
1:C:230:VAL:HA	1:C:234:TYR:HB2	1.91	0.52
2:K:65:LYS:O	2:K:66:ASP:HB2	2.07	0.52
2:M:68:PHE:HE2	2:M:83:MET:SD	2.32	0.52
2:O:68:PHE:CE2	2:O:83:MET:SD	3.03	0.52
1:A:145:LEU:CD2	1:A:226:ILE:HD11	2.37	0.52
1:B:143:TYR:HH	1:B:229:PHE:HE2	0.74	0.52
2:M:68:PHE:CE2	2:M:83:MET:SD	3.03	0.52
2:O:65:LYS:O	2:O:66:ASP:HB2	2.08	0.52
1:E:48:ASP:HB2	1:E:58:THR:HG23	1.92	0.52
1:B:277:ARG:HB3	1:C:232:GLN:NE2	2.24	0.52
1:C:235:LEU:HD23	1:C:238:ILE:HD11	1.91	0.51
1:D:145:LEU:HD23	1:D:226:ILE:CD1	2.40	0.51
1:D:48:ASP:HB2	1:D:58:THR:CG2	2.40	0.51
1:E:248:PHE:O	1:E:399:ARG:NH2	2.42	0.51
2:O:91:THR:HG22	2:O:123:VAL:N	2.25	0.51
1:C:48:ASP:HB2	1:C:58:THR:CG2	2.41	0.51
1:E:68:ARG:NH1	1:E:121:ASP:O	2.38	0.51
2:L:91:THR:HG22	2:L:123:VAL:N	2.25	0.51
1:B:68:ARG:NH1	1:B:121:ASP:O	2.38	0.51
1:B:48:ASP:HB2	1:B:58:THR:HG23	1.93	0.51
2:M:91:THR:HG22	2:M:123:VAL:N	2.26	0.51
2:K:91:THR:HG22	2:K:123:VAL:N	2.26	0.51
1:B:48:ASP:HB2	1:B:58:THR:CG2	2.41	0.51
1:E:114:ARG:HB2	1:E:128:LEU:HD23	1.93	0.51
1:D:48:ASP:HB2	1:D:58:THR:HG23	1.92	0.50
1:D:230:VAL:HA	1:D:234:TYR:HB2	1.94	0.50
1:A:230:VAL:HA	1:A:234:TYR:HB2	1.92	0.50
1:E:145:LEU:HD23	1:E:226:ILE:CD1	2.40	0.50
1:E:143:TYR:HH	1:E:229:PHE:HE1	1.60	0.50
1:A:48:ASP:HB2	1:A:58:THR:CG2	2.42	0.50
1:D:66:TYR:CZ	1:D:125:LEU:HD13	2.47	0.50
1:C:48:ASP:HB2	1:C:58:THR:HG23	1.93	0.50
1:A:277:ARG:HB3	1:B:232:GLN:HE21	1.76	0.49
1:D:96:THR:HG22	1:D:166:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HB3	1:B:232:GLN:NE2	2.28	0.49
1:C:59:LEU:O	1:C:131:THR:HA	2.13	0.49
2:N:91:THR:HG22	2:N:123:VAL:N	2.26	0.49
1:D:226:ILE:HG22	1:D:230:VAL:HG23	1.94	0.49
1:B:230:VAL:HA	1:B:234:TYR:HB2	1.95	0.49
1:B:77:ILE:HG21	1:B:81:LEU:HD21	1.94	0.49
1:A:48:ASP:HB2	1:A:58:THR:HG23	1.93	0.49
1:E:48:ASP:HB2	1:E:58:THR:CG2	2.41	0.49
2:N:87:LYS:HB3	2:N:88:PRO:HD2	1.94	0.49
1:A:189:VAL:HG12	1:A:213:ARG:HB3	1.94	0.48
1:C:235:LEU:HA	1:C:238:ILE:HG12	1.94	0.48
1:C:66:TYR:CZ	1:C:125:LEU:HD13	2.48	0.48
1:D:59:LEU:O	1:D:131:THR:HA	2.13	0.48
2:K:87:LYS:HB3	2:K:88:PRO:HD2	1.94	0.48
1:C:251:ASN:OD1	1:C:253:GLU:HB2	2.13	0.48
1:B:59:LEU:O	1:B:131:THR:HA	2.14	0.48
1:E:230:VAL:HA	1:E:234:TYR:HB2	1.94	0.48
1:E:59:LEU:O	1:E:131:THR:HA	2.14	0.48
1:C:85:ASN:HB2	1:C:114:ARG:HG3	1.95	0.48
1:C:103:LYS:HE3	1:D:105:PHE:CE2	2.48	0.48
1:B:268:THR:O	1:B:272:LEU:HG	2.14	0.48
1:C:68:ARG:NH1	1:C:121:ASP:O	2.39	0.48
1:C:31:PHE:CE2	1:D:12:VAL:HG11	2.49	0.48
1:D:99:LEU:HD11	1:E:62:TYR:OH	2.14	0.48
1:A:62:TYR:HH	1:E:99:LEU:HD12	1.77	0.47
2:O:87:LYS:HB3	2:O:88:PRO:HD2	1.95	0.47
1:D:145:LEU:CD1	1:D:417:TYR:HB3	2.44	0.47
2:M:87:LYS:HB3	2:M:88:PRO:HD2	1.95	0.47
1:D:145:LEU:CD2	1:D:226:ILE:HD11	2.43	0.47
2:L:87:LYS:HB3	2:L:88:PRO:HD2	1.96	0.47
1:A:59:LEU:O	1:A:131:THR:HA	2.14	0.47
1:C:145:LEU:CD2	1:C:226:ILE:HD11	2.45	0.47
1:A:12:VAL:HG11	1:E:31:PHE:CE2	2.50	0.47
1:C:268:THR:O	1:C:272:LEU:HG	2.15	0.46
1:D:145:LEU:HD23	1:D:226:ILE:HG12	1.97	0.46
1:D:251:ASN:OD1	1:D:253:GLU:HB2	2.15	0.46
1:C:288:ALA:CB	1:C:417:TYR:CE2	2.99	0.46
1:E:235:LEU:HA	1:E:238:ILE:HG12	1.96	0.46
1:B:36:VAL:HB	1:B:164:ILE:HD13	1.97	0.46
1:D:107:HIS:NE2	1:D:131:THR:HG23	2.30	0.46
1:B:143:TYR:CZ	1:B:229:PHE:CE2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:CD1	1:B:417:TYR:HB3	2.46	0.46
1:B:79:LEU:HD12	1:B:81:LEU:HD23	1.97	0.46
1:A:66:TYR:CZ	1:A:125:LEU:HD13	2.51	0.46
1:A:143:TYR:HH	1:A:229:PHE:HE1	1.63	0.46
1:A:31:PHE:CE2	1:B:81:LEU:HD22	2.51	0.46
1:A:68:ARG:NH1	1:A:121:ASP:O	2.38	0.46
1:A:255:VAL:HB	1:B:254:SER:OG	2.15	0.46
1:B:107:HIS:NE2	1:B:131:THR:HG23	2.31	0.46
1:A:145:LEU:CD1	1:A:417:TYR:HB3	2.46	0.45
1:E:66:TYR:CZ	1:E:125:LEU:HD13	2.51	0.45
2:K:99:LYS:HG2	2:K:103:SER:HB2	1.99	0.45
2:O:68:PHE:CE2	2:O:83:MET:HB3	2.52	0.45
1:A:85:ASN:HB2	1:A:114:ARG:CG	2.47	0.45
1:C:26:ARG:NH1	1:D:20:LEU:HD12	2.31	0.45
1:E:268:THR:O	1:E:272:LEU:HG	2.16	0.45
1:E:145:LEU:CD1	1:E:417:TYR:HB3	2.46	0.45
1:B:66:TYR:CZ	1:B:125:LEU:HD13	2.51	0.45
4:J:3:BMA:H62	4:J:4:MAN:H2	1.77	0.45
2:K:68:PHE:CE2	2:K:83:MET:HB3	2.51	0.45
1:D:85:ASN:HB2	1:D:114:ARG:CG	2.46	0.45
2:N:68:PHE:CE2	2:N:83:MET:HB3	2.51	0.45
1:E:145:LEU:HD23	1:E:226:ILE:HG12	1.98	0.45
1:C:95:ASP:OD1	1:C:156:SER:HB2	2.16	0.45
1:D:85:ASN:HB2	1:D:114:ARG:HG3	1.98	0.45
2:M:68:PHE:CE2	2:M:83:MET:HB3	2.52	0.45
1:A:107:HIS:NE2	1:A:131:THR:HG23	2.31	0.44
1:D:192:ARG:HB2	1:D:211:SER:OG	2.17	0.44
1:E:226:ILE:HG22	1:E:230:VAL:HG23	2.00	0.44
1:B:144:PRO:HD3	1:B:289:MET:HB2	1.99	0.44
1:E:262:GLY:HA3	1:E:304:LEU:HD13	2.00	0.44
1:E:95:ASP:OD1	1:E:156:SER:HB2	2.17	0.44
1:B:95:ASP:OD1	1:B:156:SER:HB2	2.17	0.44
1:B:66:TYR:CE2	1:B:125:LEU:HD13	2.53	0.44
1:C:226:ILE:HG22	1:C:230:VAL:HG23	1.99	0.44
1:C:248:PHE:O	1:C:399:ARG:CZ	2.65	0.44
1:A:268:THR:O	1:A:272:LEU:HG	2.17	0.44
1:D:36:VAL:HB	1:D:164:ILE:HD13	1.98	0.44
2:M:99:LYS:HG2	2:M:103:SER:HB2	1.99	0.44
1:A:248:PHE:O	1:A:399:ARG:CZ	2.66	0.44
1:B:226:ILE:HG22	1:B:230:VAL:HG23	2.00	0.44
1:D:95:ASP:OD1	1:D:156:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:THR:O	1:D:272:LEU:HG	2.18	0.44
1:D:66:TYR:CE2	1:D:125:LEU:HD13	2.52	0.44
1:E:107:HIS:NE2	1:E:131:THR:HG23	2.33	0.44
2:O:99:LYS:HG2	2:O:103:SER:HB2	1.99	0.44
1:B:395:ASP:O	1:B:399:ARG:HG3	2.18	0.44
2:L:68:PHE:CE2	2:L:83:MET:HB3	2.52	0.44
1:A:145:LEU:HD23	1:A:226:ILE:HG12	1.99	0.44
1:A:58:THR:O	1:A:58:THR:HG23	2.18	0.44
1:D:31:PHE:CE2	1:E:12:VAL:HG11	2.53	0.44
2:L:99:LYS:HG2	2:L:103:SER:HB2	2.00	0.44
1:A:235:LEU:HA	1:A:235:LEU:HD23	1.89	0.43
1:A:95:ASP:OD1	1:A:156:SER:HB2	2.17	0.43
1:B:145:LEU:HD23	1:B:226:ILE:HD11	2.00	0.43
1:B:147:GLU:OE1	1:B:213:ARG:NH1	2.50	0.43
1:E:145:LEU:CD2	1:E:226:ILE:HD11	2.46	0.43
1:C:145:LEU:CD1	1:C:417:TYR:HB3	2.48	0.43
1:A:226:ILE:HG22	1:A:230:VAL:HG23	2.00	0.43
1:A:99:LEU:HD12	1:B:62:TYR:HH	1.82	0.43
1:C:402:PHE:HB2	1:C:403:PRO:HD3	2.00	0.43
1:E:402:PHE:HB2	1:E:403:PRO:HD3	2.00	0.43
1:C:58:THR:O	1:C:58:THR:HG23	2.18	0.43
2:M:99:LYS:HE2	2:M:106:LEU:HD23	2.00	0.43
1:B:192:ARG:HB2	1:B:211:SER:OG	2.17	0.43
2:N:99:LYS:HG2	2:N:103:SER:HB2	2.01	0.43
1:B:101:ASP:HB2	1:B:132:THR:HG23	2.01	0.43
1:B:79:LEU:CD1	1:B:81:LEU:HD23	2.49	0.43
1:D:248:PHE:O	1:D:399:ARG:CZ	2.67	0.43
2:L:99:LYS:HE2	2:L:106:LEU:HD23	2.01	0.43
2:O:99:LYS:HE2	2:O:106:LEU:HD23	2.01	0.43
1:A:99:LEU:HD11	1:B:62:TYR:OH	2.15	0.43
1:B:85:ASN:HB2	1:B:114:ARG:HG3	2.00	0.43
1:A:262:GLY:HA3	1:A:304:LEU:HD13	2.01	0.43
1:C:107:HIS:NE2	1:C:131:THR:HG23	2.33	0.43
1:B:199:VAL:HB	2:L:111:ASN:HD21	1.84	0.43
1:E:66:TYR:CE2	1:E:125:LEU:HD13	2.54	0.43
1:A:192:ARG:HB2	1:A:211:SER:OG	2.19	0.42
1:D:144:PRO:HD3	1:D:289:MET:HB2	2.00	0.42
1:B:248:PHE:HB3	1:B:399:ARG:HG2	1.99	0.42
1:E:238:ILE:HG13	1:E:239:MET:N	2.33	0.42
1:A:101:ASP:HB2	1:A:132:THR:HG23	2.01	0.42
1:C:66:TYR:CE2	1:C:125:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LEU:HD11	1:D:118:LEU:HD12	2.01	0.42
1:B:145:LEU:HD23	1:B:226:ILE:HG12	2.02	0.42
1:D:262:GLY:HA3	1:D:304:LEU:HD13	2.02	0.42
1:C:31:PHE:CE2	1:D:81:LEU:HD22	2.54	0.42
1:D:58:THR:O	1:D:58:THR:HG23	2.19	0.42
1:B:402:PHE:HB2	1:B:403:PRO:HD3	2.01	0.42
1:E:43:ASP:HA	1:E:176:THR:OG1	2.20	0.42
1:E:248:PHE:O	1:E:399:ARG:CZ	2.67	0.41
1:B:280:LEU:HB3	1:B:281:PRO:HD2	2.02	0.41
1:C:88:ALA:HB2	1:C:116:ILE:HD11	2.02	0.41
1:C:255:VAL:N	1:C:256:PRO:CD	2.83	0.41
1:D:145:LEU:HD22	1:D:226:ILE:HD11	2.02	0.41
1:A:66:TYR:CE2	1:A:125:LEU:HD13	2.54	0.41
1:C:192:ARG:HB2	1:C:211:SER:OG	2.20	0.41
1:A:255:VAL:N	1:A:256:PRO:CD	2.83	0.41
1:C:254:SER:HB3	1:C:257:ALA:HB3	2.02	0.41
1:E:144:PRO:HD3	1:E:289:MET:HB2	2.03	0.41
1:B:85:ASN:HB2	1:B:114:ARG:CG	2.49	0.41
1:E:101:ASP:HB2	1:E:132:THR:HG23	2.02	0.41
1:E:189:VAL:CG1	1:E:213:ARG:HB3	2.50	0.41
1:C:36:VAL:HB	1:C:164:ILE:HD13	2.02	0.41
1:D:405:LEU:HA	1:D:405:LEU:HD23	1.90	0.41
1:A:267:LEU:HD22	1:B:268:THR:HG21	2.01	0.41
1:C:145:LEU:HD23	1:C:226:ILE:HG12	2.01	0.41
1:D:26:ARG:NH2	1:E:17:ASP:OD1	2.48	0.41
2:K:108:TYR:HA	2:K:109:PRO:HD3	1.86	0.41
1:C:85:ASN:HB2	1:C:114:ARG:CG	2.50	0.41
1:E:58:THR:HG23	1:E:58:THR:O	2.20	0.41
1:B:58:THR:HG23	1:B:58:THR:O	2.19	0.41
1:A:43:ASP:HA	1:A:176:THR:OG1	2.21	0.41
1:B:255:VAL:N	1:B:256:PRO:CD	2.84	0.41
1:D:402:PHE:HB2	1:D:403:PRO:HD3	2.02	0.41
1:D:145:LEU:HD12	1:D:417:TYR:HB3	2.03	0.41
1:A:268:THR:HG21	1:E:267:LEU:HD22	2.03	0.41
1:E:395:ASP:O	1:E:399:ARG:HG3	2.21	0.41
2:L:32:PRO:HB2	2:L:53:TRP:HB2	2.03	0.41
1:B:262:GLY:HA3	1:B:304:LEU:HD13	2.03	0.41
1:D:254:SER:HB3	1:D:257:ALA:HB3	2.02	0.41
1:D:409:PHE:O	1:D:412:VAL:HG22	2.20	0.41
1:E:235:LEU:HD23	1:E:235:LEU:HA	1.91	0.41
2:N:99:LYS:HE2	2:N:106:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD13	1:B:417:TYR:HB3	2.03	0.40
1:B:99:LEU:HD11	1:C:62:TYR:OH	2.15	0.40
1:D:295:VAL:HG11	1:D:409:PHE:CZ	2.57	0.40
1:D:43:ASP:HA	1:D:176:THR:OG1	2.21	0.40
1:A:105:PHE:CE2	1:E:103:LYS:HE3	2.56	0.40
1:C:238:ILE:HG13	1:C:239:MET:N	2.36	0.40
1:C:43:ASP:HA	1:C:176:THR:OG1	2.21	0.40
2:M:103:SER:O	2:M:111:ASN:HB3	2.22	0.40
1:E:409:PHE:O	1:E:412:VAL:HG22	2.21	0.40
1:C:213:ARG:HB2	3:H:1:NAG:H81	2.02	0.40
2:K:32:PRO:HB2	2:K:53:TRP:HB2	2.03	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	328/395 (83%)	319 (97%)	9 (3%)	0	100	100
1	B	331/395 (84%)	322 (97%)	9 (3%)	0	100	100
1	C	328/395 (83%)	320 (98%)	8 (2%)	0	100	100
1	D	330/395 (84%)	320 (97%)	10 (3%)	0	100	100
1	E	328/395 (83%)	318 (97%)	10 (3%)	0	100	100
2	K	121/125 (97%)	115 (95%)	6 (5%)	0	100	100
2	L	121/125 (97%)	115 (95%)	6 (5%)	0	100	100
2	M	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
2	N	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
2	O	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
All	All	2250/2600 (86%)	2177 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	293/346 (85%)	291 (99%)	2 (1%)	84	90
1	B	296/346 (86%)	295 (100%)	1 (0%)	92	96
1	C	293/346 (85%)	291 (99%)	2 (1%)	84	90
1	D	295/346 (85%)	293 (99%)	2 (1%)	84	90
1	E	293/346 (85%)	291 (99%)	2 (1%)	84	90
2	K	97/99 (98%)	97 (100%)	0	100	100
2	L	97/99 (98%)	97 (100%)	0	100	100
2	M	97/99 (98%)	97 (100%)	0	100	100
2	N	97/99 (98%)	97 (100%)	0	100	100
2	O	97/99 (98%)	97 (100%)	0	100	100
All	All	1955/2225 (88%)	1946 (100%)	9 (0%)	88	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	CYS
1	A	254	SER
1	B	37	CYS
1	C	37	CYS
1	C	254	SER
1	D	37	CYS
1	D	254	SER
1	E	37	CYS
1	E	254	SER

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

Mol	Chain	Res	Type
1	E	85	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 ⓘ

27 monosaccharides 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	$\# Z  > 2$
3	NAG	F	1	1,3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.48	0
3	BMA	F	3	3	11,11,12	0.19	0	15,15,17	0.39	0
3	MAN	F	4	3	11,11,12	0.28	0	15,15,17	0.32	0
3	MAN	F	5	3	11,11,12	0.25	0	15,15,17	0.38	0
3	NAG	G	1	1,3	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	G	2	3	14,14,15	0.20	0	17,19,21	0.50	0
3	BMA	G	3	3	11,11,12	0.40	0	15,15,17	0.74	0
3	MAN	G	4	3	11,11,12	0.28	0	15,15,17	0.31	0
3	MAN	G	5	3	11,11,12	0.37	0	15,15,17	0.31	0
3	NAG	H	1	1,3	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.46	0
3	BMA	H	3	3	11,11,12	0.37	0	15,15,17	0.57	0
3	MAN	H	4	3	11,11,12	0.17	0	15,15,17	0.26	0
3	MAN	H	5	3	11,11,12	0.25	0	15,15,17	0.55	0
4	NAG	I	1	1,4	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	0.41	0
4	BMA	I	3	4	11,11,12	0.26	0	15,15,17	0.35	0
4	MAN	I	4	4	11,11,12	0.44	0	15,15,17	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	I	5	4	11,11,12	0.52	0	15,15,17	0.60	0
4	MAN	I	6	4	11,11,12	0.25	0	15,15,17	0.25	0
4	NAG	J	1	1,4	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	J	2	4	14,14,15	0.24	0	17,19,21	0.39	0
4	BMA	J	3	4	11,11,12	0.34	0	15,15,17	0.37	0
4	MAN	J	4	4	11,11,12	0.32	0	15,15,17	0.46	0
4	MAN	J	5	4	11,11,12	0.31	0	15,15,17	0.35	0
4	MAN	J	6	4	11,11,12	0.45	0	15,15,17	0.49	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	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	MAN	J	6	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	3	BMA	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
4	J	3	BMA	1	0
4	J	1	NAG	1	0
4	J	4	MAN	1	0

## 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	$\# Z  > 2$
5	NAG	B	501	1	14,14,15	0.26	0	17,19,21	0.49	0
5	NAG	A	501	1	14,14,15	0.34	0	17,19,21	0.41	0
5	NAG	D	501	1	14,14,15	0.34	0	17,19,21	0.50	0
5	NAG	C	501	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	E	501	1	14,14,15	0.22	0	17,19,21	0.63	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
5	NAG	B	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	C	501	1	-	1/6/23/26	0/1/1/1
5	NAG	E	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	501	NAG	C4-C5-C6-O6
5	E	501	NAG	O5-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	C	501	NAG	C4-C5-C6-O6

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 ⓘ

### 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	330/395 (83%)	-0.20	7 (2%) 63 62	30, 58, 101, 133	0
1	B	333/395 (84%)	0.03	10 (3%) 50 49	31, 62, 94, 138	0
1	C	330/395 (83%)	-0.05	6 (1%) 68 67	31, 61, 104, 137	0
1	D	332/395 (84%)	-0.15	5 (1%) 73 72	28, 51, 85, 155	0
1	E	330/395 (83%)	0.03	11 (3%) 46 44	26, 54, 89, 141	0
2	K	123/125 (98%)	0.91	21 (17%) 1 1	54, 101, 132, 151	0
2	L	123/125 (98%)	0.80	23 (18%) 1 1	78, 125, 168, 182	0
2	M	123/125 (98%)	0.43	14 (11%) 5 4	58, 97, 129, 150	0
2	N	123/125 (98%)	0.39	13 (10%) 6 6	52, 102, 141, 153	0
2	O	123/125 (98%)	-0.23	4 (3%) 46 44	60, 91, 117, 123	0
All	All	2270/2600 (87%)	0.07	114 (5%) 28 27	26, 65, 129, 182	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	68	PHE	6.1
2	L	115	TRP	6.1
1	A	127	GLY	5.8
2	L	116	GLY	5.7
2	L	117	GLN	5.5
2	K	88	PRO	5.1
2	N	43	LYS	5.1
1	B	417	TYR	4.7
1	E	204	ALA	4.6
2	K	1	GLN	4.6
2	N	44	GLU	4.3
2	K	115	TRP	4.2
2	L	85	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	M	1	GLN	3.9
2	L	4	LEU	3.9
2	L	1	GLN	3.8
1	D	417	TYR	3.8
1	B	278	ASN	3.8
2	L	98	ALA	3.7
2	M	86	LEU	3.7
2	K	114	TYR	3.6
1	C	278	ASN	3.6
2	K	96	CYS	3.6
2	L	96	CYS	3.6
2	L	114	TYR	3.5
2	K	75	ALA	3.5
2	M	123	VAL	3.5
2	N	68	PHE	3.4
2	K	74	ASN	3.3
2	M	11	LEU	3.3
2	N	41	PRO	3.3
2	N	88	PRO	3.3
2	N	10	GLY	3.2
1	C	215	LYS	3.2
1	C	232	GLN	3.2
2	M	13	GLN	3.2
2	K	123	VAL	3.1
1	E	14	GLU	3.1
2	K	14	ALA	3.0
1	A	66	TYR	3.0
2	L	10	GLY	3.0
1	B	113	ASN	3.0
2	M	15	GLY	2.9
1	E	13	LYS	2.9
2	K	44	GLU	2.9
2	M	115	TRP	2.8
2	K	43	LYS	2.8
2	K	53	TRP	2.8
2	L	70	ILE	2.8
2	L	11	LEU	2.7
2	M	85	ASN	2.7
1	E	417	TYR	2.7
2	L	9	GLY	2.7
1	A	125	LEU	2.6
1	B	159	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	40	ALA	2.6
2	L	67	ARG	2.6
1	E	158	GLY	2.6
1	A	115	MET	2.6
2	K	89	GLU	2.6
2	K	116	GLY	2.6
2	N	42	GLY	2.6
1	B	77	ILE	2.6
2	M	14	ALA	2.6
2	O	14	ALA	2.5
1	A	126	TYR	2.5
2	O	75	ALA	2.5
2	L	37	PHE	2.5
2	M	66	ASP	2.5
1	D	9	MET	2.4
2	L	95	TYR	2.4
2	L	3	GLN	2.4
2	M	16	GLY	2.4
1	D	416	THR	2.4
2	N	86	LEU	2.4
1	C	417	TYR	2.4
2	L	97	ALA	2.4
1	E	12	VAL	2.4
2	N	94	TYR	2.4
2	L	64	VAL	2.4
2	L	66	ASP	2.3
2	N	84	ASN	2.3
2	K	98	ALA	2.3
1	D	142	ARG	2.3
2	M	67	ARG	2.3
2	L	5	GLN	2.3
1	B	14	GLU	2.3
1	C	74	TYR	2.2
2	K	13	GLN	2.2
2	K	94	TYR	2.2
2	K	113	ASP	2.2
2	K	117	GLN	2.2
1	B	145	LEU	2.2
2	N	90	ASP	2.2
1	D	24	ASP	2.1
2	K	86	LEU	2.1
1	B	45	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	313	PHE	2.1
1	E	16	VAL	2.1
2	O	44	GLU	2.1
2	L	25	SER	2.1
2	N	9	GLY	2.1
1	E	205	TYR	2.1
1	C	418	LEU	2.1
2	M	116	GLY	2.1
1	B	114	ARG	2.1
1	A	159	TYR	2.1
1	A	64	GLN	2.0
2	K	37	PHE	2.0
1	E	319	ALA	2.0
1	E	418	LEU	2.0
1	E	161	THR	2.0
2	O	85	ASN	2.0
2	M	17	SER	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	G	5	11/12	0.60	0.32	98,114,118,120	0
3	MAN	H	5	11/12	0.61	0.26	113,123,130,133	0
3	MAN	F	5	11/12	0.72	0.23	102,109,116,117	0
4	MAN	J	4	11/12	0.76	0.35	112,120,129,139	0
4	MAN	I	4	11/12	0.76	0.24	104,123,129,138	0
4	MAN	I	5	11/12	0.77	0.19	121,129,137,141	0
3	BMA	H	3	11/12	0.81	0.12	104,113,127,138	0
3	BMA	F	3	11/12	0.83	0.14	86,96,110,122	0
3	MAN	H	4	11/12	0.84	0.42	105,120,130,132	0
3	BMA	G	3	11/12	0.85	0.13	101,108,113,121	0
3	MAN	G	4	11/12	0.88	0.15	98,108,114,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	J	3	11/12	0.90	0.15	78,83,90,105	0
4	MAN	J	5	11/12	0.90	0.17	93,115,122,123	0
4	MAN	I	6	11/12	0.90	0.20	108,123,134,135	0
4	BMA	I	3	11/12	0.91	0.11	93,99,114,118	0
4	MAN	J	6	11/12	0.91	0.15	80,86,92,94	0
4	NAG	I	2	14/15	0.92	0.15	53,64,74,87	0
3	NAG	G	1	14/15	0.93	0.16	71,77,81,84	0
3	MAN	F	4	11/12	0.93	0.12	93,99,112,112	0
3	NAG	F	2	14/15	0.93	0.18	65,69,73,79	0
4	NAG	J	1	14/15	0.94	0.13	66,68,74,77	0
3	NAG	H	2	14/15	0.95	0.10	65,78,87,99	0
3	NAG	F	1	14/15	0.95	0.14	54,59,63,71	0
4	NAG	J	2	14/15	0.95	0.15	56,70,77,80	0
3	NAG	G	2	14/15	0.95	0.13	84,88,98,101	0
4	NAG	I	1	14/15	0.96	0.16	46,49,53,55	0
3	NAG	H	1	14/15	0.96	0.16	68,75,81,85	0

## 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	501	14/15	0.86	0.27	122,141,148,149	0
5	NAG	D	501	14/15	0.92	0.20	93,102,115,117	0
5	NAG	E	501	14/15	0.92	0.15	101,108,114,117	0
5	NAG	C	501	14/15	0.93	0.13	140,153,164,166	0
5	NAG	B	501	14/15	0.94	0.17	96,100,112,119	0

## 6.5 Other polymers

There are no such residues in this entry.