Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:23 AM BST

PDB ID	:	6N6B
Title	:	The complex crystal structure of neuraminidase from A/Minnesota/11/2010 with B10 antibody.
Authors	:	Yang, H.; Stevens, J.
Deposited on	:	2018-11-26
Resolution	:	2.30 Å(reported)

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

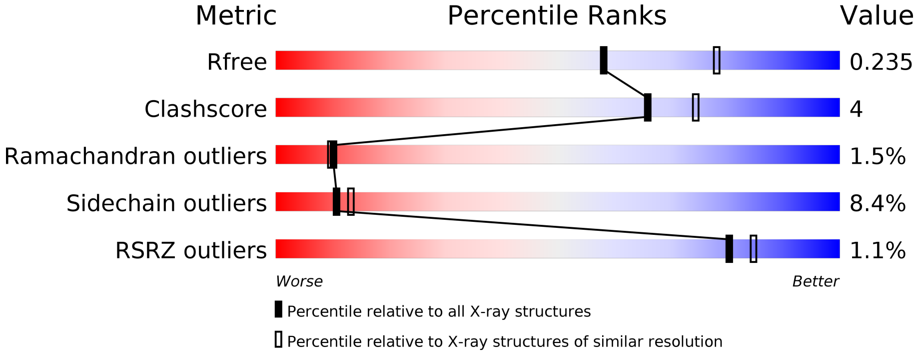
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

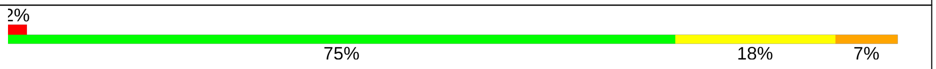
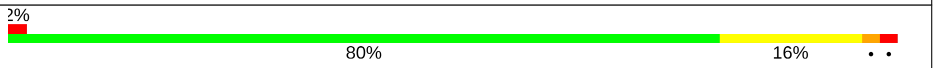
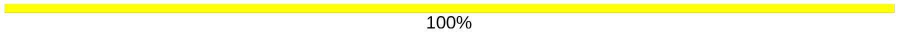
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 >=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 <=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	397	
2	K	221	
3	L	214	
4	B	5	

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6694 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3019	1876	536	584	23	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLY	-	expression tag	UNP A0A075ETL7
A	74	SER	-	expression tag	UNP A0A075ETL7
A	75	GLY	-	expression tag	UNP A0A075ETL7
A	76	ASP	-	expression tag	UNP A0A075ETL7
A	77	SER	-	expression tag	UNP A0A075ETL7
A	78	GLY	-	expression tag	UNP A0A075ETL7
A	79	SER	-	expression tag	UNP A0A075ETL7
A	80	PRO	-	expression tag	UNP A0A075ETL7
A	81	GLY	-	expression tag	UNP A0A075ETL7

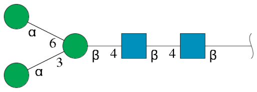
- Molecule 2 is a protein called B10 antibody Heavy Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	221	1693	1072	274	341	6	0	0	0

- Molecule 3 is a protein called B10 antibody Light Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1671	1037	285	341	8	0	0	0

- Molecule 4 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.

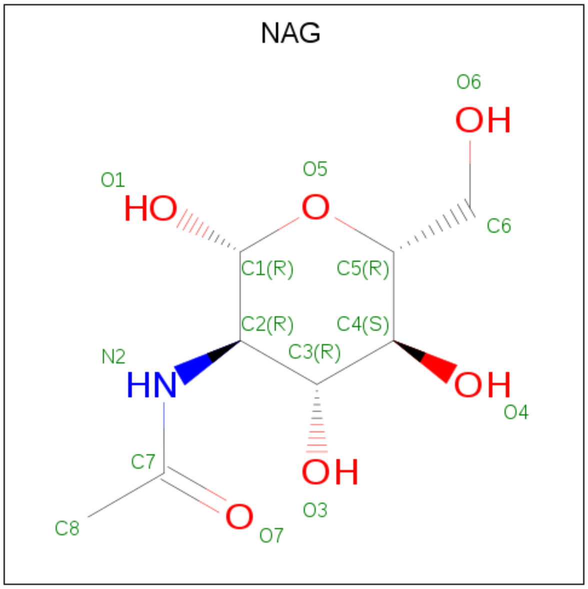


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	5	61	34	2	25	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	161	161	161	0	0
7	K	44	44	44	0	0

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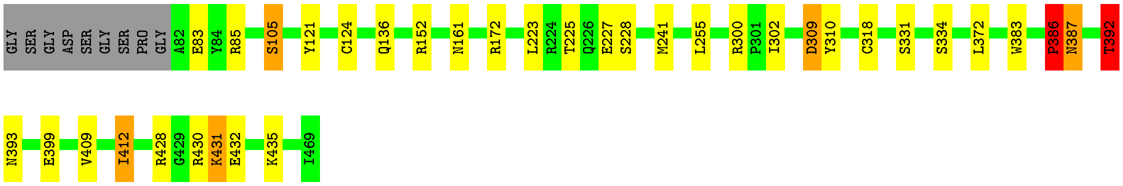
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	30	Total O 30 30	0	0

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.

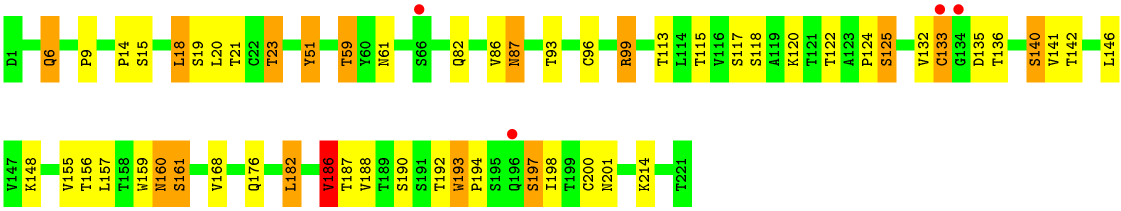
- Molecule 1: Neuraminidase

Chain A:



- Molecule 2: B10 antibody Heavy Chain Fab

Chain K:

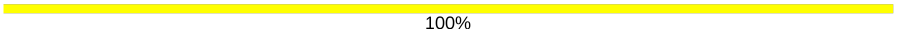


- Molecule 3: B10 antibody Light Chain Fab

Chain L:

- Molecule 4: 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 B:




NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	188.47Å 188.47Å 136.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.30) 97.5 (48.82-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.220 , 0.245 0.207 , 0.235	Depositor DCC
R_{free} test set	5115 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 20.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, 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	1.16	5/3091 (0.2%)	1.11	17/4190 (0.4%)
2	K	1.02	2/1739 (0.1%)	1.15	8/2384 (0.3%)
3	L	1.04	3/1710 (0.2%)	1.13	10/2325 (0.4%)
All	All	1.10	10/6540 (0.2%)	1.13	35/8899 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	K	0	3
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	52	SER	CB-OG	-7.52	1.32	1.42
3	L	60	ASP	CB-CG	6.74	1.66	1.51
1	A	227	GLU	CD-OE2	6.25	1.32	1.25
1	A	432	GLU	CG-CD	5.96	1.60	1.51
1	A	387	ASN	N-CA	5.85	1.58	1.46
3	L	163	TRP	CE3-CZ3	5.35	1.47	1.38
2	K	200	CYS	CB-SG	-5.32	1.73	1.81
2	K	19	SER	CB-OG	5.24	1.49	1.42
1	A	399	GLU	CG-CD	5.17	1.59	1.51
1	A	105	SER	CA-CB	5.04	1.60	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	99	ARG	NE-CZ-NH2	-16.41	112.09	120.30
2	K	99	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	A	85	ARG	NE-CZ-NH1	8.38	124.49	120.30
3	L	211	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	A	172	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	K	186	VAL	CB-CA-C	-7.74	96.69	111.40
1	A	309	ASP	C-N-CA	7.62	140.75	121.70
1	A	309	ASP	N-CA-C	7.26	130.60	111.00
3	L	60	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	310	TYR	N-CA-C	-7.00	92.10	111.00
1	A	309	ASP	O-C-N	-6.76	111.88	122.70
3	L	19	VAL	CB-CA-C	-6.62	98.83	111.40
1	A	309	ASP	CA-C-N	6.38	131.22	117.20
1	A	161	ASN	CB-CA-C	-6.27	97.85	110.40
1	A	85	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	K	99	ARG	CG-CD-NE	-6.17	98.84	111.80
2	K	140	SER	N-CA-C	6.07	127.38	111.00
3	L	1	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	A	152	ARG	NE-CZ-NH1	6.01	123.31	120.30
2	K	182	LEU	CA-CB-CG	5.99	129.07	115.30
2	K	99	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	300	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	409	VAL	CG1-CB-CG2	-5.90	101.46	110.90
1	A	428	ARG	NE-CZ-NH2	-5.90	117.35	120.30
3	L	45	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	428	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	412	ILE	CB-CA-C	-5.74	100.12	111.60
2	K	96	CYS	CA-CB-SG	5.72	124.29	114.00
3	L	90	GLN	N-CA-CB	-5.56	100.59	110.60
1	A	392	THR	CB-CA-C	-5.55	96.63	111.60
3	L	108	ARG	N-CA-C	5.53	125.94	111.00
1	A	386	PRO	C-N-CA	-5.51	107.92	121.70
3	L	52	SER	N-CA-CB	-5.43	102.36	110.50
3	L	28	ASP	CB-CG-OD2	-5.39	113.45	118.30
3	L	121	SER	N-CA-CB	5.32	118.49	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	ASP	Peptide
2	K	136	THR	Peptide
2	K	160	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	K	192	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3019	0	2862	12	0
2	K	1693	0	1636	23	0
3	L	1671	0	1583	15	0
4	B	61	0	52	0	0
5	A	1	0	0	0	0
6	A	14	0	13	0	0
7	A	161	0	0	3	0
7	K	44	0	0	2	0
7	L	30	0	0	0	0
All	All	6694	0	6146	49	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 4.

All (49) 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)
2:K:140:SER:O	2:K:188:VAL:O	1.97	0.81
2:K:6:GLN:HE21	2:K:6:GLN:H	1.39	0.71
2:K:133:CYS:HB3	2:K:135:ASP:OD2	1.94	0.67
3:L:120:PRO:O	3:L:121:SER:HB3	1.95	0.67
2:K:59:THR:HG21	7:K:337:HOH:O	1.96	0.66
2:K:6:GLN:NE2	2:K:6:GLN:H	1.93	0.66
3:L:13:THR:HG23	3:L:19:VAL:HG13	1.79	0.65
3:L:13:THR:HG21	3:L:19:VAL:HG22	1.81	0.63
2:K:23:THR:HG23	7:K:308:HOH:O	1.98	0.62
2:K:124:PRO:O	2:K:148:LYS:O	2.19	0.61
3:L:149:LYS:O	3:L:153:SER:O	2.18	0.60
1:A:223:LEU:HD11	1:A:241:MET:CE	2.32	0.59
3:L:150:ILE:HD12	3:L:155:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:107:ARG:O	3:L:108:ARG:O	2.21	0.58
1:A:223:LEU:HD11	1:A:241:MET:HE2	1.84	0.57
2:K:193:TRP:O	2:K:194:PRO:C	2.39	0.57
3:L:13:THR:CG2	3:L:19:VAL:HG13	2.36	0.56
2:K:87:ASN:C	2:K:87:ASN:HD22	2.09	0.55
2:K:142:THR:HG22	2:K:187:THR:OG1	2.08	0.54
2:K:18:LEU:CD1	2:K:20:LEU:HG	2.38	0.54
2:K:51:TYR:CE2	2:K:59:THR:HG23	2.43	0.53
3:L:135:PHE:C	3:L:136:LEU:HD23	2.30	0.52
1:A:392:THR:HB	1:A:393:ASN:OD1	2.11	0.51
1:A:318:CYS:O	1:A:386:PRO:O	2.29	0.50
1:A:334:SER:HA	1:A:387:ASN:HD21	1.76	0.50
1:A:255:LEU:HD12	1:A:255:LEU:N	2.27	0.50
2:K:159:TRP:CE2	2:K:186:VAL:HG22	2.48	0.49
1:A:435:LYS:HD2	7:A:755:HOH:O	2.14	0.47
1:A:430:ARG:HB3	1:A:431:LYS:HA	1.97	0.47
2:K:133:CYS:CB	2:K:135:ASP:OD2	2.62	0.47
3:L:33:VAL:HA	3:L:89:GLN:O	2.15	0.47
2:K:168:VAL:HG22	2:K:186:VAL:HG13	1.98	0.45
3:L:4:MET:SD	3:L:90:GLN:HB2	2.56	0.45
7:A:738:HOH:O	2:K:59:THR:HG22	2.17	0.45
7:A:738:HOH:O	2:K:59:THR:CG2	2.67	0.42
1:A:121:TYR:CG	1:A:228:SER:HA	2.54	0.42
3:L:135:PHE:O	3:L:136:LEU:HD23	2.18	0.42
1:A:302:ILE:HD13	1:A:383:TRP:CZ2	2.54	0.42
1:A:124:CYS:SG	1:A:412:ILE:HD11	2.60	0.42
2:K:132:VAL:HG12	2:K:133:CYS:HB2	2.01	0.41
2:K:157:LEU:HD23	2:K:157:LEU:C	2.40	0.41
2:K:160:ASN:HD21	2:K:198:ILE:HA	1.86	0.41
1:A:225:THR:HB	1:A:241:MET:HG2	2.02	0.41
2:K:160:ASN:HA	2:K:160:ASN:HD22	1.51	0.41
2:K:176:GLN:HG3	3:L:160:LEU:HD13	2.03	0.41
2:K:159:TRP:CZ2	2:K:186:VAL:HG22	2.56	0.41
3:L:198:HIS:HD2	3:L:200:THR:OG1	2.03	0.41
3:L:120:PRO:O	3:L:121:SER:CB	2.63	0.40
3:L:141:PRO:O	3:L:198:HIS:HE1	2.03	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	386/397 (97%)	367 (95%)	18 (5%)	1 (0%)	41	50
2	K	219/221 (99%)	199 (91%)	13 (6%)	7 (3%)	4	2
3	L	212/214 (99%)	201 (95%)	7 (3%)	4 (2%)	8	7
All	All	817/832 (98%)	767 (94%)	38 (5%)	12 (2%)	10	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	108	ARG
2	K	190	SER
1	A	386	PRO
2	K	197	SER
3	L	121	SER
2	K	125	SER
2	K	161	SER
3	L	150	ILE
2	K	141	VAL
3	L	68	GLU
2	K	14	PRO
2	K	193	TRP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/342 (98%)	329 (98%)	8 (2%)	49	66
2	K	195/195 (100%)	164 (84%)	31 (16%)	2	2
3	L	191/191 (100%)	169 (88%)	22 (12%)	5	6
All	All	723/728 (99%)	662 (92%)	61 (8%)	11	13

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	105	SER
1	A	136	GLN
1	A	331	SER
1	A	372	LEU
1	A	386	PRO
1	A	392	THR
1	A	431	LYS
2	K	6	GLN
2	K	9	PRO
2	K	15	SER
2	K	18	LEU
2	K	21	THR
2	K	23	THR
2	K	51	TYR
2	K	59	THR
2	K	61	ASN
2	K	82	GLN
2	K	86	VAL
2	K	87	ASN
2	K	93	THR
2	K	99	ARG
2	K	113	THR
2	K	115	THR
2	K	117	SER
2	K	118	SER
2	K	120	LYS
2	K	122	THR
2	K	125	SER
2	K	133	CYS
2	K	146	LEU

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Mol	Chain	Res	Type
2	K	155	VAL
2	K	156	THR
2	K	161	SER
2	K	182	LEU
2	K	186	VAL
2	K	197	SER
2	K	201	ASN
2	K	214	LYS
3	L	17	ASP
3	L	19	VAL
3	L	29	VAL
3	L	52	SER
3	L	53	THR
3	L	60	ASP
3	L	90	GLN
3	L	114	THR
3	L	121	SER
3	L	126	THR
3	L	142	LYS
3	L	145	ASN
3	L	149	LYS
3	L	155	ARG
3	L	169	LYS
3	L	178	THR
3	L	193	THR
3	L	197	THR
3	L	201	SER
3	L	202	THR
3	L	208	SER
3	L	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	136	GLN
1	A	150	HIS
1	A	168	HIS
1	A	199	ASN
1	A	358	ASN
1	A	385	ASN
1	A	387	ASN

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Mol	Chain	Res	Type
2	K	6	GLN
2	K	61	ASN
2	K	87	ASN
2	K	110	GLN
2	K	160	ASN
2	K	169	HIS
2	K	176	GLN
3	L	138	ASN
3	L	198	HIS

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 ⓘ

5 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	$\#\|Z\| > 2$
4	NAG	B	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	1.55	4 (23%)
4	NAG	B	2	4	14,14,15	0.97	2 (14%)	17,19,21	1.63	5 (29%)
4	BMA	B	3	4	11,11,12	1.30	2 (18%)	15,15,17	2.35	6 (40%)
4	MAN	B	4	4	11,11,12	1.32	1 (9%)	15,15,17	1.84	6 (40%)
4	MAN	B	5	4	11,11,12	1.23	2 (18%)	15,15,17	3.96	9 (60%)

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	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	1/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	MAN	B	5	4	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5	MAN	O4-C4	2.86	1.49	1.43
4	B	4	MAN	O2-C2	2.70	1.49	1.43
4	B	5	MAN	O5-C5	2.43	1.48	1.43
4	B	1	NAG	C1-C2	2.32	1.55	1.52
4	B	3	BMA	O5-C5	2.24	1.48	1.43
4	B	3	BMA	C6-C5	2.14	1.59	1.51
4	B	2	NAG	C1-C2	2.06	1.55	1.52
4	B	2	NAG	C4-C5	2.03	1.57	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	5	MAN	C1-C2-C3	8.14	119.67	109.67
4	B	5	MAN	C2-C3-C4	6.23	121.67	110.89
4	B	5	MAN	O4-C4-C5	5.81	123.72	109.30
4	B	5	MAN	O3-C3-C2	-5.47	99.53	109.99
4	B	3	BMA	C6-C5-C4	5.04	124.81	113.00
4	B	3	BMA	O4-C4-C3	-4.46	100.05	110.35
4	B	5	MAN	O5-C1-C2	3.97	116.89	110.77
4	B	1	NAG	O5-C1-C2	-3.70	105.44	111.29
4	B	5	MAN	O5-C5-C4	3.64	119.69	110.83
4	B	5	MAN	C3-C4-C5	-3.53	103.95	110.24
4	B	4	MAN	O5-C5-C6	3.44	112.59	107.20
4	B	4	MAN	O2-C2-C1	3.15	115.60	109.15
4	B	5	MAN	O2-C2-C3	-2.93	104.27	110.14
4	B	3	BMA	O3-C3-C2	-2.92	104.40	109.99
4	B	3	BMA	O4-C4-C5	2.91	116.53	109.30
4	B	2	NAG	C3-C4-C5	-2.90	105.06	110.24
4	B	1	NAG	C1-O5-C5	2.78	115.96	112.19
4	B	5	MAN	O4-C4-C3	-2.67	104.17	110.35
4	B	4	MAN	O5-C1-C2	2.57	114.74	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	BMA	O5-C1-C2	-2.48	106.94	110.77
4	B	2	NAG	C2-N2-C7	2.48	126.43	122.90
4	B	1	NAG	O5-C5-C6	2.38	110.93	107.20
4	B	3	BMA	O5-C5-C4	-2.37	105.06	110.83
4	B	2	NAG	C1-O5-C5	-2.32	109.04	112.19
4	B	4	MAN	O2-C2-C3	2.31	114.76	110.14
4	B	2	NAG	O7-C7-C8	-2.13	118.10	122.06
4	B	4	MAN	C1-O5-C5	2.11	115.05	112.19
4	B	4	MAN	C2-C3-C4	2.08	114.49	110.89
4	B	2	NAG	O4-C4-C3	-2.05	105.61	110.35
4	B	1	NAG	O4-C4-C3	-2.02	105.68	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\|>2$
6	NAG	A	507	1	14,14,15	1.41	2 (14%)	17,19,21	2.92	9 (52%)

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
6	NAG	A	507	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	507	NAG	O4-C4	3.44	1.51	1.43
6	A	507	NAG	O5-C1	-2.12	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	507	NAG	C3-C4-C5	-5.78	99.92	110.24
6	A	507	NAG	O5-C5-C6	-4.61	99.97	107.20
6	A	507	NAG	O4-C4-C5	4.49	120.45	109.30
6	A	507	NAG	C1-O5-C5	3.97	117.57	112.19
6	A	507	NAG	C6-C5-C4	3.55	121.33	113.00
6	A	507	NAG	O3-C3-C4	3.14	117.60	110.35
6	A	507	NAG	C1-C2-N2	-3.06	105.27	110.49
6	A	507	NAG	O4-C4-C3	2.64	116.46	110.35
6	A	507	NAG	O3-C3-C2	-2.55	104.19	109.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (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, 95th 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($\AA^2$)	Q<0.9
1	A	388/397 (97%)	-0.32	0	100	100	16, 25, 40, 67	0
2	K	221/221 (100%)	-0.10	4 (1%)	68	74	22, 42, 69, 104	0
3	L	214/214 (100%)	-0.15	5 (2%)	60	67	25, 43, 70, 100	0
All	All	823/832 (98%)	-0.22	9 (1%)	80	85	16, 32, 65, 104	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	202	THR	3.1
3	L	152	GLY	2.6
2	K	133	CYS	2.5
2	K	196	GLN	2.5
3	L	153	SER	2.3
2	K	66	SER	2.2
3	L	15	VAL	2.1
3	L	157	ASN	2.0
2	K	134	GLY	2.0

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

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

6.3 Carbohydrates (i)

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, 95th 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^2)	Q<0.9
4	MAN	B	5	11/12	0.88	0.21	43,54,65,69	0
4	MAN	B	4	11/12	0.91	0.14	27,28,30,33	0
4	BMA	B	3	11/12	0.97	0.10	25,28,34,52	0
4	NAG	B	1	14/15	0.97	0.11	25,27,45,61	0
4	NAG	B	2	14/15	0.98	0.09	24,26,28,30	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^{th} 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^2)	Q<0.9
6	NAG	A	507	14/15	0.93	0.15	31,40,46,49	0
5	CA	A	501	1/1	0.99	0.11	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.