



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 6V6W / pdb_00006v6w
Title : Crystal structure of antibody 438-B11 DSS mutant (Cys98A-100aA) in complex with an uncleaved prefusion optimized (UFO) soluble BG505 trimer and Fab 35O22
Authors : Kumar, S.; Wilson, I.A.
Deposited on : 2019-12-06
Resolution : 6.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

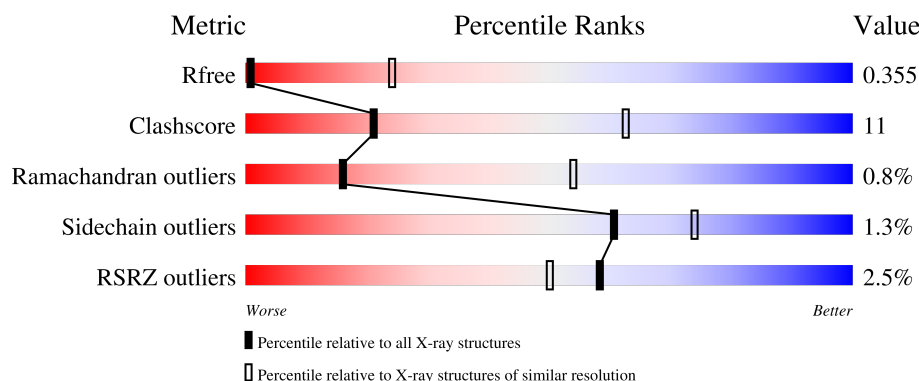
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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}	180053	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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 of 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 $\leq 5\%$. 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	243	2% 75% 23% .
1	D	243	2% 75% 23% .
2	B	216	% 69% 29% .
2	E	216	% 71% 26% ..
3	C	485	3% 67% 25% . 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	485	 % 69% 23% 7%
4	F	235	 4% 74% 21%
4	I	235	 4% 76% 18%
5	H	215	 % 75% 24%
5	J	215	 2% 75% 24%
6	K	140	 5% 75% 21%
6	T	140	 3% 75% 21%
7	L	4	 75% 25%
7	O	4	 75% 25%
8	M	2	 100%
8	P	2	 100%
9	N	5	 20% 60% 20%
9	Q	5	 20% 60% 20%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23434 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 35O22 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			
1	A	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 2 is a protein called 35O22 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			
2	B	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	453	Total	C	N	O	S	0	0	0
			3563	2234	630	671	28			
3	C	453	Total	C	N	O	S	0	0	0
			3563	2234	630	671	28			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	62	ASP	GLU	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	507	GLY	-	expression tag	UNP Q2N0S6
G	508	GLY	-	expression tag	UNP Q2N0S6
G	509	GLY	-	expression tag	UNP Q2N0S6
G	510	GLY	-	expression tag	UNP Q2N0S6
G	511	GLY	-	expression tag	UNP Q2N0S6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	512	SER	-	expression tag	UNP Q2N0S6
G	513	GLY	-	expression tag	UNP Q2N0S6
G	514	GLY	-	expression tag	UNP Q2N0S6
G	515	GLY	-	expression tag	UNP Q2N0S6
G	516	GLY	-	expression tag	UNP Q2N0S6
G	517	SER	-	expression tag	UNP Q2N0S6
C	62	ASP	GLU	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	507	GLY	-	expression tag	UNP Q2N0S6
C	508	GLY	-	expression tag	UNP Q2N0S6
C	509	GLY	-	expression tag	UNP Q2N0S6
C	510	GLY	-	expression tag	UNP Q2N0S6
C	511	GLY	-	expression tag	UNP Q2N0S6
C	512	SER	-	expression tag	UNP Q2N0S6
C	513	GLY	-	expression tag	UNP Q2N0S6
C	514	GLY	-	expression tag	UNP Q2N0S6
C	515	GLY	-	expression tag	UNP Q2N0S6
C	516	GLY	-	expression tag	UNP Q2N0S6
C	517	SER	-	expression tag	UNP Q2N0S6

- Molecule 4 is a protein called B11 DSS Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	226	Total	C	N	O	S	0	0	0
			1716	1091	291	328	6			
4	F	226	Total	C	N	O	S	0	0	0
			1716	1091	291	328	6			

- Molecule 5 is a protein called B11 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	213	Total	C	N	O	S	0	0	0
			1634	1022	281	327	4			
5	H	213	Total	C	N	O	S	0	0	0
			1634	1022	281	327	4			

- Molecule 6 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	134	Total	C	N	O	S	0	0	0
			1069	677	182	203	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	134	Total	C	N	O	S	0	0	0
			1069	677	182	203	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	?	-	ILE	deletion	UNP Q2N0S9
T	?	-	VAL	deletion	UNP Q2N0S9
T	?	-	GLN	deletion	UNP Q2N0S9
T	?	-	GLN	deletion	UNP Q2N0S9
T	?	-	GLN	deletion	UNP Q2N0S9
T	?	-	SER	deletion	UNP Q2N0S9
T	?	-	ASN	deletion	UNP Q2N0S9
T	?	-	LEU	deletion	UNP Q2N0S9
T	?	-	LEU	deletion	UNP Q2N0S9
T	?	-	ARG	deletion	UNP Q2N0S9
T	?	-	ALA	deletion	UNP Q2N0S9
T	?	-	ILE	deletion	UNP Q2N0S9
T	?	-	GLU	deletion	UNP Q2N0S9
T	547A	ASN	ALA	conflict	UNP Q2N0S9
T	547B	PRO	GLN	conflict	UNP Q2N0S9
T	547C	ASP	GLN	conflict	UNP Q2N0S9
T	547D	TRP	HIS	conflict	UNP Q2N0S9
T	547F	PRO	LEU	conflict	UNP Q2N0S9
T	547G	ASP	LYS	conflict	UNP Q2N0S9
T	547H	MET	LEU	conflict	UNP Q2N0S9
T	605	CYS	THR	conflict	UNP Q2N0S9
K	?	-	ILE	deletion	UNP Q2N0S9
K	?	-	VAL	deletion	UNP Q2N0S9
K	?	-	GLN	deletion	UNP Q2N0S9
K	?	-	GLN	deletion	UNP Q2N0S9
K	?	-	GLN	deletion	UNP Q2N0S9
K	?	-	SER	deletion	UNP Q2N0S9
K	?	-	ASN	deletion	UNP Q2N0S9
K	?	-	LEU	deletion	UNP Q2N0S9
K	?	-	LEU	deletion	UNP Q2N0S9
K	?	-	ARG	deletion	UNP Q2N0S9
K	?	-	ALA	deletion	UNP Q2N0S9
K	?	-	ILE	deletion	UNP Q2N0S9
K	?	-	GLU	deletion	UNP Q2N0S9
K	547A	ASN	ALA	conflict	UNP Q2N0S9
K	547B	PRO	GLN	conflict	UNP Q2N0S9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	547C	ASP	GLN	conflict	UNP Q2N0S9
K	547D	TRP	HIS	conflict	UNP Q2N0S9
K	547F	PRO	LEU	conflict	UNP Q2N0S9
K	547G	ASP	LYS	conflict	UNP Q2N0S9
K	547H	MET	LEU	conflict	UNP Q2N0S9
K	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 7 is an oligosaccharide called 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.



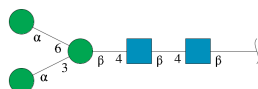
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	L	4	Total	C	N	O	0	0	0
			50	28	2	20			
7	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



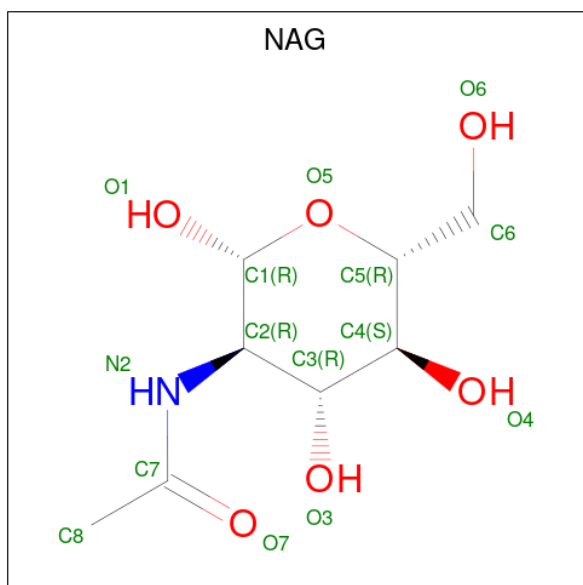
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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
9	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

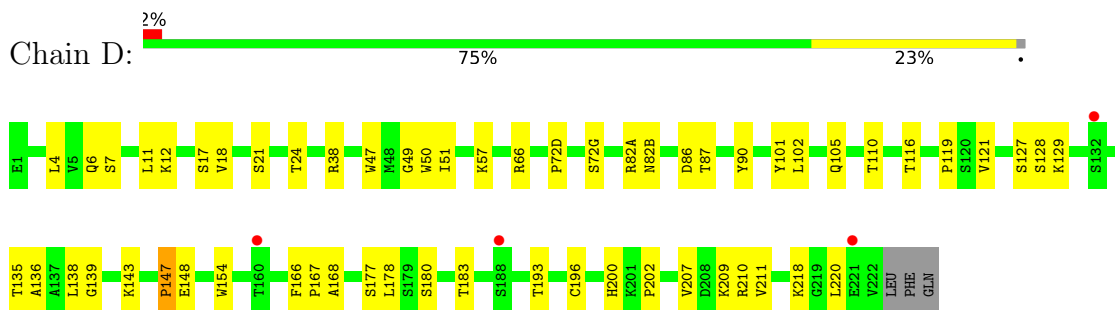
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	T	1	Total	C	N	O	0	0
			14	8	1	5		
10	T	1	Total	C	N	O	0	0
			14	8	1	5		
10	T	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	K	1	Total	C	N	O	0	0
			14	8	1	5		
10	K	1	Total	C	N	O	0	0
			14	8	1	5		
10	K	1	Total	C	N	O	0	0
			14	8	1	5		

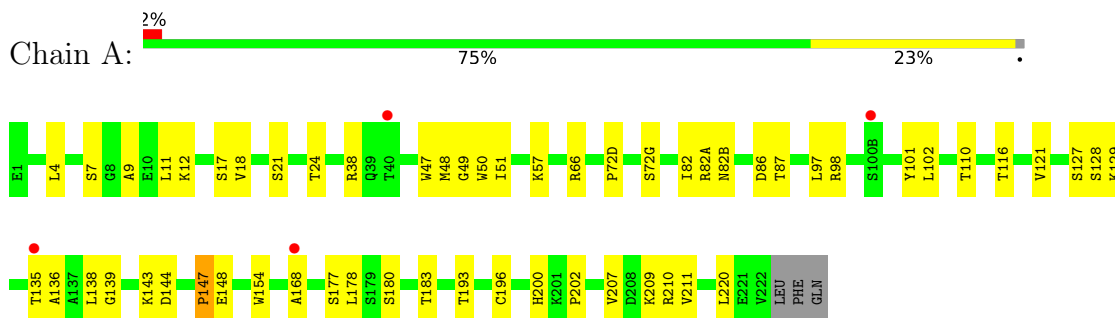
3 Residue-property plots

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.

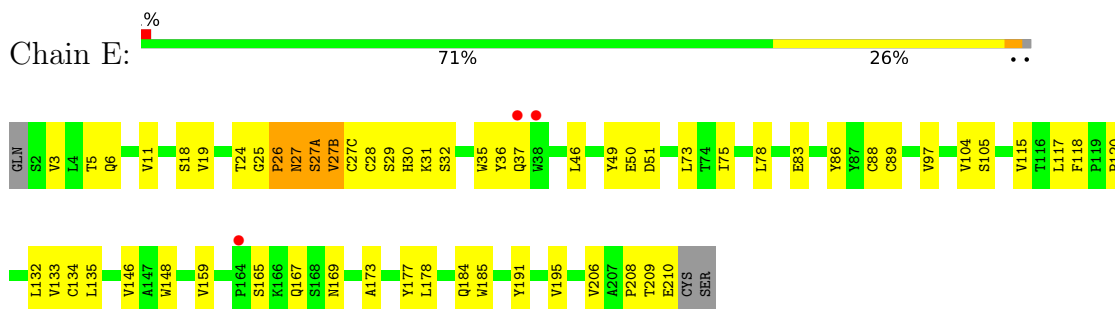
- Molecule 1: 35O22 Fab Heavy chain



- Molecule 1: 35O22 Fab Heavy chain

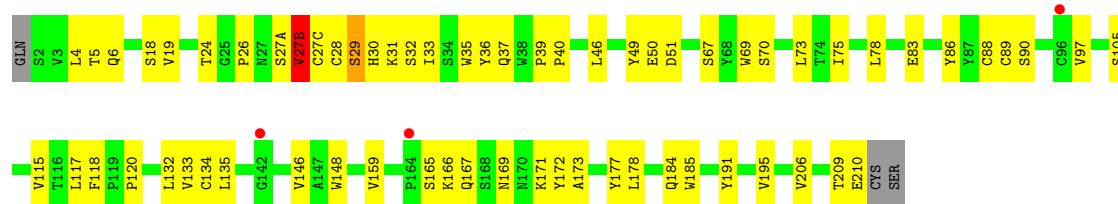


- Molecule 2: 35O22 Fab Light chain

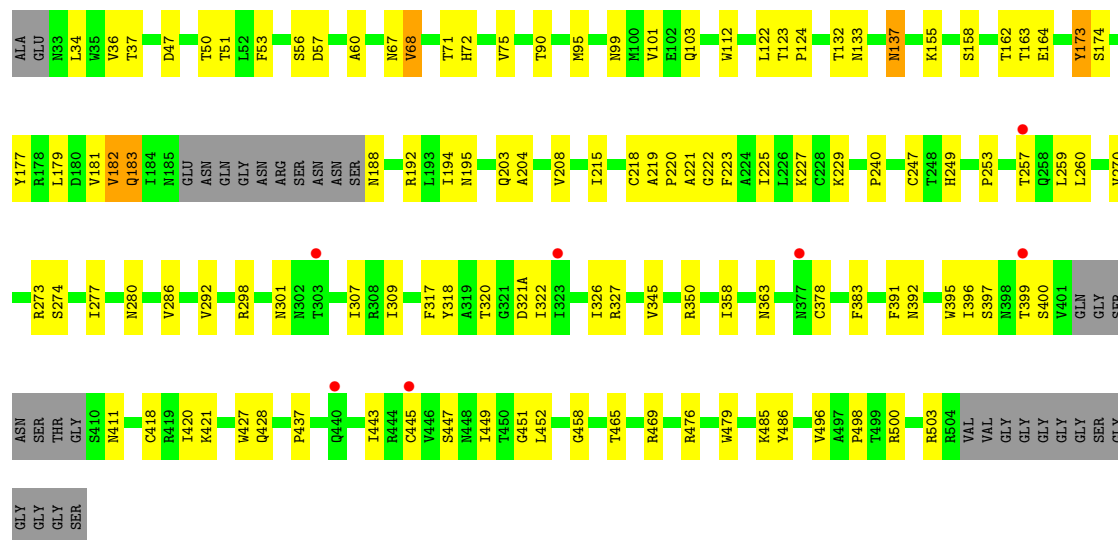


- Molecule 2: 35O22 Fab Light chain

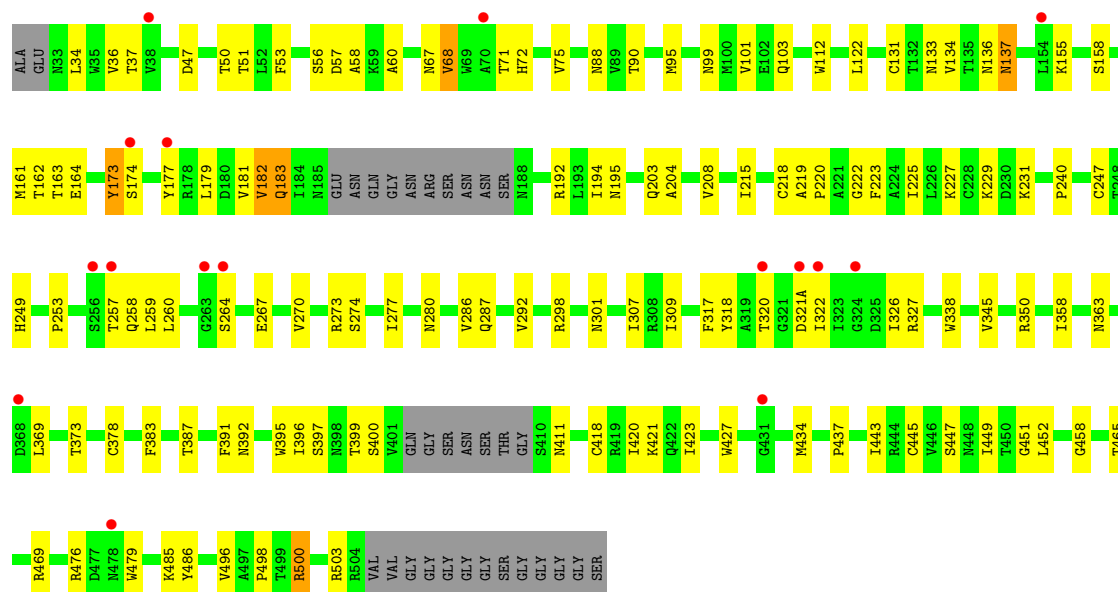




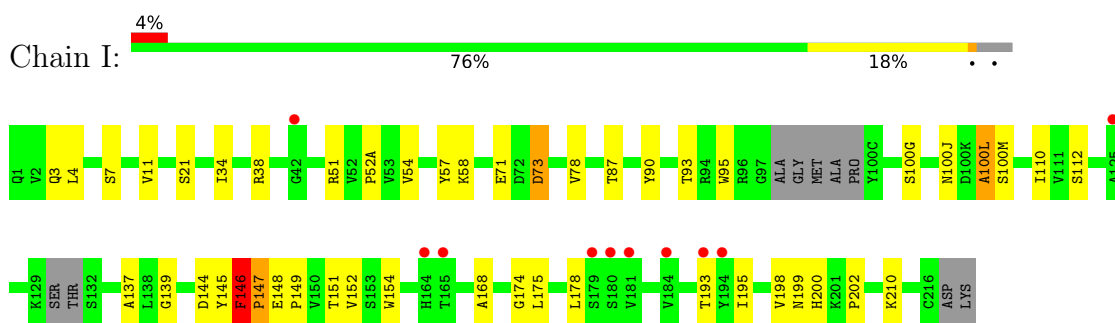
• Molecule 3: Envelope glycoprotein gp120



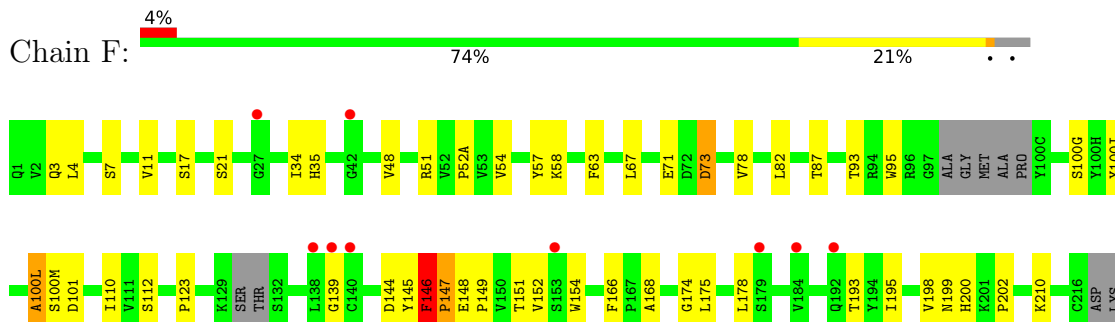
• Molecule 3: Envelope glycoprotein gp120



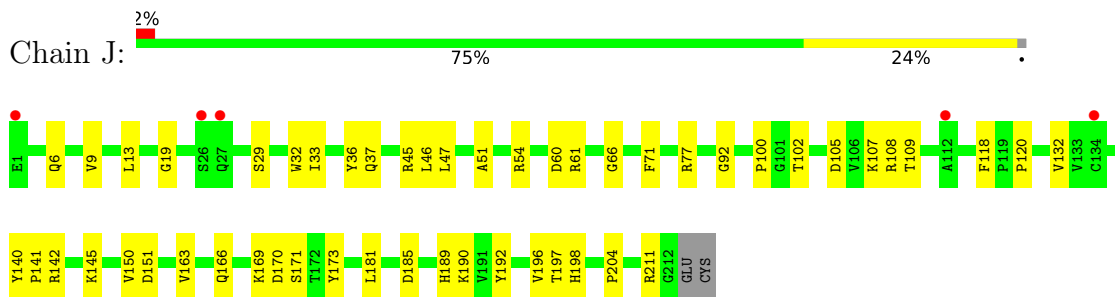
• Molecule 4: B11 DSS Fab heavy chain



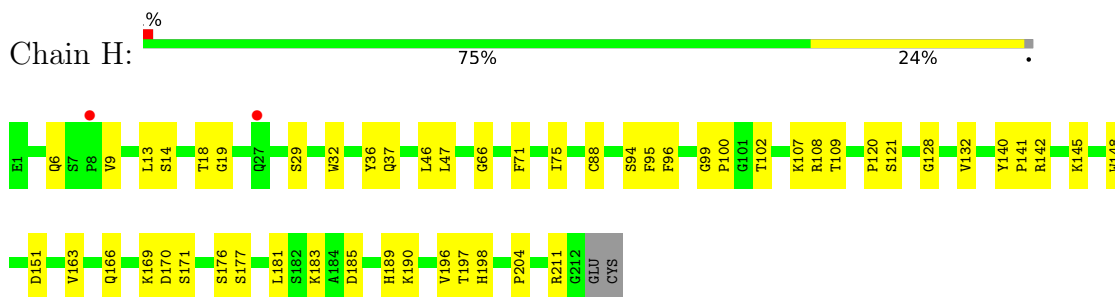
• Molecule 4: B11 DSS Fab heavy chain



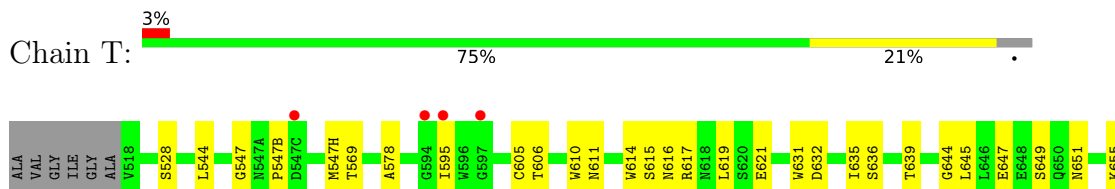
• Molecule 5: B11 Fab light chain



• Molecule 5: B11 Fab light chain



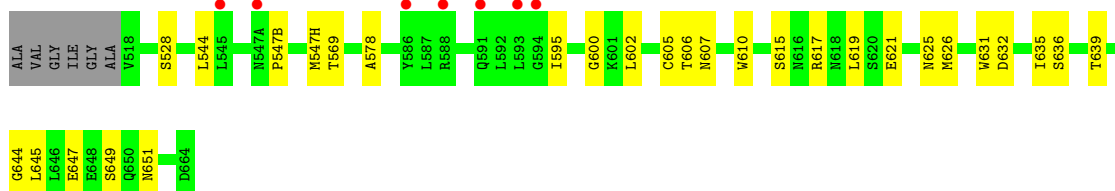
• Molecule 6: Envelope glycoprotein gp41





- Molecule 6: Envelope glycoprotein gp41

Chain K: 5% 75% 21%



- Molecule 7: 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 L: 75% 25%



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 75% 25%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 100%

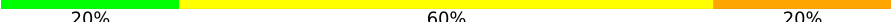


- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 20% 60% 20%



- Molecule 9: 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 Q:  20% 60% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	148.53Å 148.53Å 843.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.72 – 6.50 46.72 – 6.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (46.72-6.50) 97.2 (46.72-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 6.67Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.309 , 0.355 0.310 , 0.355	Depositor DCC
R_{free} test set	669 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	233.9	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 586.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.359 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	23434	wwPDB-VP
Average B, all atoms (Å ²)	279.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BMA, MAN, 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	0.14	0/1860	0.37	0/2533
1	D	0.13	0/1860	0.36	0/2533
2	B	0.25	0/1659	0.54	5/2269 (0.2%)
2	E	0.58	2/1659 (0.1%)	0.76	4/2269 (0.2%)
3	C	0.14	0/3637	0.35	0/4939
3	G	0.14	0/3637	0.35	0/4939
4	F	0.13	0/1760	0.35	0/2396
4	I	0.14	0/1760	0.36	0/2396
5	H	0.13	0/1669	0.37	0/2267
5	J	0.12	0/1669	0.36	0/2267
6	K	0.15	0/1092	0.33	0/1486
6	T	0.12	0/1092	0.32	0/1486
All	All	0.21	2/23354 (0.0%)	0.41	9/31780 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	26	PRO	N-CA	19.43	1.70	1.47
2	E	25	GLY	C-N	9.75	1.46	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	25	GLY	CA-C-N	18.45	139.67	119.92
2	E	25	GLY	C-N-CA	18.45	139.67	119.92
2	E	26	PRO	CA-N-CD	-9.00	99.40	112.00
2	E	27(A)	SER	N-CA-C	-6.68	103.93	111.07
2	B	29	SER	CA-C-N	6.58	134.10	121.54
2	B	29	SER	C-N-CA	6.58	134.10	121.54
2	B	27(A)	SER	N-CA-C	-6.56	96.82	110.80
2	B	27(B)	VAL	CA-CB-CG2	5.29	119.39	110.40
2	B	27(B)	VAL	N-CA-CB	5.27	119.92	111.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	146	PHE	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	1813	0	1784	40	0
1	D	1813	0	1784	37	0
2	B	1615	0	1544	70	0
2	E	1615	0	1544	61	0
3	C	3563	0	3500	85	0
3	G	3563	0	3500	77	0
4	F	1716	0	1692	40	0
4	I	1716	0	1692	32	0
5	H	1634	0	1588	32	0
5	J	1634	0	1588	29	0
6	K	1069	0	1034	23	0
6	T	1069	0	1034	22	0
7	L	50	0	43	0	0
7	O	50	0	43	0	0
8	M	28	0	25	0	0
8	P	28	0	25	0	0
9	N	61	0	52	2	0
9	Q	61	0	52	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	126	0	117	2	0
10	G	126	0	117	2	0
10	K	42	0	39	2	0
10	T	42	0	39	1	0
All	All	23434	0	22836	509	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 11.

All (509) 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:B:27(C):CYS:C	2:B:33:ILE:HD11	1.36	1.51
2:E:26:PRO:N	2:E:26:PRO:CA	1.70	1.48
2:B:27(C):CYS:O	2:B:33:ILE:HD11	1.22	1.32
2:E:3:VAL:CG2	2:E:26:PRO:HG3	1.69	1.22
2:B:28:CYS:SG	2:B:67:SER:O	1.99	1.19
2:E:26:PRO:HG2	2:E:27(B):VAL:HB	1.15	1.15
2:B:27(C):CYS:HB2	2:B:33:ILE:HD12	1.21	1.10
2:B:27(C):CYS:O	2:B:33:ILE:CD1	2.02	1.08
2:E:3:VAL:HG21	2:E:26:PRO:HG3	1.09	1.06
2:B:27(C):CYS:C	2:B:33:ILE:CD1	2.30	1.03
2:B:27(C):CYS:HB2	2:B:33:ILE:CD1	1.97	0.94
2:B:4:LEU:HD11	2:B:27(C):CYS:SG	2.12	0.90
3:C:90:THR:HG22	3:C:240:PRO:HA	1.53	0.89
2:E:3:VAL:CG2	2:E:26:PRO:CG	2.51	0.89
2:E:118:PHE:HB2	2:E:133:VAL:HB	1.57	0.86
2:B:27(C):CYS:CB	2:B:33:ILE:HD12	2.05	0.85
2:B:118:PHE:HB2	2:B:133:VAL:HB	1.58	0.84
2:B:27(C):CYS:HA	2:B:90:SER:OG	1.77	0.84
3:G:90:THR:HG22	3:G:240:PRO:HA	1.60	0.84
2:E:3:VAL:HB	2:E:26:PRO:HD3	1.61	0.80
2:B:27(C):CYS:HA	2:B:90:SER:CB	2.12	0.79
3:G:36:VAL:HG12	6:T:610:TRP:HE3	1.47	0.78
2:B:27(C):CYS:CA	2:B:33:ILE:HD11	2.16	0.76
3:C:496:VAL:O	6:K:631:TRP:NE1	2.19	0.74
3:C:36:VAL:HG12	6:K:610:TRP:HE3	1.53	0.74
3:C:51:THR:HB	6:K:578:ALA:HB2	1.69	0.74
4:F:146:PHE:HB3	4:F:147:PRO:HD2	1.70	0.74
1:A:72(G):SER:O	3:C:90:THR:OG1	2.05	0.72
3:G:181:VAL:HG13	3:G:183:GLN:H	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:VAL:HG13	3:C:183:GLN:H	1.55	0.72
1:D:72(G):SER:O	3:G:90:THR:OG1	2.07	0.72
2:E:26:PRO:HG2	2:E:27(B):VAL:CB	2.09	0.72
3:C:249:HIS:ND1	3:C:486:TYR:OH	2.19	0.71
1:D:66:ARG:NH2	1:D:82(B):ASN:O	2.24	0.71
4:I:146:PHE:HB3	4:I:147:PRO:HD2	1.71	0.71
3:G:496:VAL:O	6:T:631:TRP:NE1	2.23	0.70
1:D:116:THR:HG23	1:D:147:PRO:HG3	1.73	0.70
2:E:26:PRO:O	2:E:27(B):VAL:O	2.10	0.70
2:E:133:VAL:HG13	2:E:177:TYR:HE1	1.57	0.69
1:A:66:ARG:NH2	1:A:82(B):ASN:O	2.25	0.69
2:E:26:PRO:O	2:E:27(B):VAL:C	2.35	0.69
6:K:595:ILE:O	6:K:651:ASN:ND2	2.26	0.69
2:B:27(C):CYS:HA	2:B:90:SER:HB2	1.75	0.69
1:A:116:THR:HG23	1:A:147:PRO:HG3	1.73	0.68
4:I:146:PHE:O	4:I:148:GLU:N	2.21	0.68
4:F:146:PHE:O	4:F:148:GLU:N	2.20	0.67
2:B:27(C):CYS:CB	2:B:33:ILE:CD1	2.68	0.67
2:B:133:VAL:HG13	2:B:177:TYR:HE1	1.59	0.67
1:A:138:LEU:HB2	1:A:211:VAL:HG11	1.77	0.66
6:T:595:ILE:O	6:T:651:ASN:ND2	2.29	0.66
5:H:6:GLN:HG3	5:H:100:PRO:HD2	1.78	0.65
4:F:51:ARG:NH2	4:F:71:GLU:OE1	2.29	0.65
3:C:50:THR:O	3:C:103:GLN:NE2	2.29	0.65
3:C:181:VAL:HG11	3:C:192:ARG:HG2	1.79	0.65
2:E:3:VAL:HG21	2:E:26:PRO:CG	2.04	0.65
6:T:617:ARG:HH12	10:T:703:NAG:H83	1.62	0.65
2:B:5:THR:N	2:B:24:THR:O	2.31	0.64
2:B:27(C):CYS:CA	2:B:33:ILE:CD1	2.74	0.64
3:C:203:GLN:HE22	3:C:318:TYR:HD2	1.46	0.64
2:B:4:LEU:CD1	2:B:27(C):CYS:SG	2.85	0.64
3:C:181:VAL:HG12	3:C:192:ARG:H	1.62	0.64
3:C:292:VAL:HB	3:C:449:ILE:HB	1.80	0.64
1:D:127:SER:HB2	2:E:118:PHE:CE1	2.33	0.63
4:I:51:ARG:NH2	4:I:71:GLU:OE1	2.32	0.63
4:F:7:SER:HG	4:F:21:SER:HG	1.44	0.63
1:D:87:THR:HG23	1:D:110:THR:HA	1.80	0.63
2:E:89:CYS:SG	2:E:97:VAL:N	2.73	0.62
1:D:138:LEU:HB2	1:D:211:VAL:HG11	1.80	0.62
3:G:181:VAL:HG11	3:G:192:ARG:HG2	1.80	0.62
2:E:5:THR:N	2:E:24:THR:O	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:133:ASN:OD1	3:G:155:LYS:NZ	2.28	0.62
3:G:286:VAL:HB	3:G:452:LEU:HB2	1.80	0.62
2:B:27(C):CYS:HB3	2:B:90:SER:HB2	1.82	0.62
3:G:270:VAL:HG11	3:G:345:VAL:HG22	1.82	0.61
2:B:27(B):VAL:HG12	2:B:28:CYS:H	1.64	0.61
4:I:73:ASP:OD1	4:I:73:ASP:N	2.25	0.61
2:E:18:SER:HA	2:E:75:ILE:O	2.01	0.61
2:E:209:THR:HG23	2:E:210:GLU:HG3	1.82	0.61
1:D:148:GLU:HB2	1:D:202:PRO:HG2	1.82	0.61
3:G:50:THR:O	3:G:103:GLN:NE2	2.34	0.61
4:I:7:SER:OG	4:I:21:SER:OG	2.19	0.61
3:C:36:VAL:HG12	6:K:610:TRP:CE3	2.35	0.61
3:C:286:VAL:HB	3:C:452:LEU:HB2	1.82	0.61
5:J:6:GLN:HG3	5:J:100:PRO:HD2	1.83	0.60
6:K:617:ARG:HH12	10:K:703:NAG:H83	1.66	0.60
1:A:12:LYS:HG3	1:A:18:VAL:HB	1.83	0.60
2:E:3:VAL:HG23	2:E:26:PRO:CG	2.32	0.60
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.37	0.60
3:G:181:VAL:HG12	3:G:192:ARG:H	1.65	0.60
5:H:141:PRO:HG2	5:H:198:HIS:CE1	2.37	0.59
3:C:258:GLN:OE1	3:C:387:THR:HG21	2.02	0.59
3:G:292:VAL:HB	3:G:449:ILE:HB	1.84	0.59
2:E:27(B):VAL:O	2:E:27(B):VAL:HG12	2.02	0.59
3:C:222:GLY:N	6:K:544:LEU:O	2.35	0.59
3:C:60:ALA:HB1	3:C:71:THR:HG23	1.84	0.59
3:C:270:VAL:HG11	3:C:345:VAL:HG22	1.85	0.59
1:A:127:SER:HB2	2:B:118:PHE:HE1	1.68	0.58
2:B:6:GLN:NE2	2:B:88:CYS:SG	2.76	0.58
1:A:87:THR:HG23	1:A:110:THR:HA	1.84	0.58
6:K:528:SER:OG	9:Q:1:NAG:O7	2.18	0.58
3:G:221:ALA:HB2	6:T:547:GLY:H	1.69	0.58
5:J:141:PRO:HG2	5:J:198:HIS:CE1	2.38	0.58
1:A:66:ARG:NH2	1:A:86:ASP:OD2	2.36	0.58
3:C:137:ASN:HB2	10:C:618:NAG:H2	1.86	0.58
4:F:73:ASP:OD1	4:F:73:ASP:N	2.29	0.58
2:E:6:GLN:NE2	2:E:88:CYS:SG	2.77	0.58
4:F:7:SER:OG	4:F:21:SER:OG	2.19	0.58
1:A:127:SER:HB2	2:B:118:PHE:CE1	2.38	0.57
2:B:167:GLN:HG2	2:B:169:ASN:H	1.68	0.57
3:G:51:THR:HB	6:T:578:ALA:HB2	1.85	0.57
3:G:137:ASN:HB2	10:G:618:NAG:H2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:LYS:HG3	1:D:18:VAL:HB	1.85	0.57
1:D:66:ARG:NH2	1:D:86:ASP:OD2	2.37	0.57
3:C:204:ALA:HB3	3:C:437:PRO:HD3	1.87	0.57
3:G:322:ILE:HG21	3:G:326:ILE:HG22	1.86	0.57
3:C:162:THR:HG23	3:C:309:ILE:HG23	1.86	0.57
3:G:56:SER:O	3:G:56:SER:OG	2.22	0.56
3:C:133:ASN:OD1	3:C:155:LYS:NZ	2.31	0.56
3:G:307:ILE:HD11	3:G:317:PHE:HD2	1.69	0.56
1:A:129:LYS:HB3	1:A:135:THR:OG1	2.04	0.56
1:A:139:GLY:HA2	1:A:154:TRP:HH2	1.71	0.56
2:E:19:VAL:HG12	2:E:75:ILE:HB	1.87	0.56
2:E:167:GLN:HG2	2:E:169:ASN:H	1.70	0.56
1:A:128:SER:HA	1:A:220:LEU:HD13	1.86	0.56
1:A:139:GLY:HA3	1:A:180:SER:O	2.06	0.56
4:F:58:LYS:HG3	5:H:95:PHE:HE1	1.71	0.56
5:J:36:TYR:HE1	5:J:46:LEU:HD13	1.71	0.56
3:C:280:ASN:HD22	3:C:458:GLY:HA3	1.71	0.56
3:G:162:THR:HG23	3:G:309:ILE:HG23	1.88	0.55
3:C:112:TRP:HB3	3:C:427:TRP:HE1	1.71	0.55
2:E:132:LEU:HD12	2:E:178:LEU:HD23	1.86	0.55
3:C:53:PHE:CZ	6:K:547(B):PRO:HG3	2.42	0.55
2:E:29:SER:C	2:E:31:LYS:H	2.13	0.55
5:H:120:PRO:HD3	5:H:132:VAL:HG22	1.89	0.55
5:H:166:GLN:HE21	5:H:171:SER:HB3	1.72	0.55
1:A:148:GLU:HB2	1:A:202:PRO:HG2	1.86	0.55
3:G:203:GLN:HE22	3:G:318:TYR:HD2	1.55	0.55
5:J:120:PRO:HD3	5:J:132:VAL:HG22	1.89	0.55
2:B:28:CYS:SG	2:B:67:SER:C	2.84	0.55
3:C:307:ILE:HD11	3:C:317:PHE:HD2	1.71	0.55
3:C:391:PHE:O	3:C:392:ASN:ND2	2.40	0.55
2:E:117:LEU:HD23	2:E:206:VAL:HG13	1.88	0.55
5:J:145:LYS:HB3	5:J:197:THR:HB	1.88	0.55
2:B:37:GLN:HG3	2:B:86:TYR:HE1	1.70	0.55
2:E:3:VAL:HB	2:E:26:PRO:CD	2.34	0.55
2:E:35:TRP:CE2	2:E:73:LEU:HB2	2.42	0.55
3:G:112:TRP:HB3	3:G:427:TRP:HE1	1.71	0.55
3:G:60:ALA:HB1	3:G:71:THR:HG23	1.89	0.54
1:A:97:LEU:HD22	6:K:625:ASN:HB2	1.88	0.54
4:F:200:HIS:CD2	4:F:202:PRO:HD2	2.42	0.54
3:G:47:ASP:N	3:G:47:ASP:OD1	2.37	0.54
1:A:136:ALA:O	1:A:183:THR:HA	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27(B):VAL:O	2:B:31:LYS:HD2	2.06	0.54
3:C:181:VAL:HG23	3:C:194:ILE:HD11	1.89	0.54
2:E:32:SER:HB3	2:E:50:GLU:HA	1.89	0.54
4:I:200:HIS:CD2	4:I:202:PRO:HD2	2.42	0.54
5:H:145:LYS:HB3	5:H:197:THR:HB	1.89	0.54
2:B:132:LEU:HD12	2:B:178:LEU:HD23	1.89	0.54
3:C:447:SER:OG	10:C:615:NAG:O7	2.24	0.54
9:N:2:NAG:H83	9:N:2:NAG:H3	1.89	0.54
1:D:210:ARG:NH1	1:D:211:VAL:O	2.41	0.54
9:Q:2:NAG:H83	9:Q:2:NAG:H3	1.89	0.54
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.54
1:A:210:ARG:NH1	1:A:211:VAL:O	2.41	0.54
2:B:19:VAL:HG12	2:B:75:ILE:HB	1.88	0.54
2:B:83:GLU:HG3	2:B:105:SER:HA	1.90	0.54
5:H:142:ARG:HH22	5:H:163:VAL:HG21	1.73	0.54
3:C:34:LEU:HD12	3:C:498:PRO:HB2	1.90	0.53
4:I:87:THR:HG23	4:I:110:ILE:HA	1.90	0.53
3:C:179:LEU:HD22	3:C:421:LYS:HG3	1.90	0.53
4:F:100(I):TYR:O	5:H:96:PHE:HZ	1.91	0.53
2:B:209:THR:HG23	2:B:210:GLU:HG3	1.90	0.53
2:E:83:GLU:HG3	2:E:105:SER:HA	1.88	0.53
6:K:619:LEU:C	6:K:621:GLU:H	2.16	0.53
3:G:101:VAL:HG13	3:G:479:TRP:HB2	1.91	0.53
5:H:29:SER:HB2	5:H:32:TRP:CD1	2.44	0.53
3:G:260:LEU:HD12	3:G:451:GLY:HA3	1.89	0.53
5:J:29:SER:HB2	5:J:32:TRP:CD1	2.44	0.53
2:B:18:SER:HA	2:B:75:ILE:O	2.08	0.53
3:C:67:ASN:HB3	3:C:208:VAL:HG12	1.90	0.52
3:C:260:LEU:HD12	3:C:451:GLY:HA3	1.91	0.52
3:C:298:ARG:HB3	3:C:443:ILE:HB	1.91	0.52
5:H:128:GLY:HA2	5:H:183:LYS:HB2	1.91	0.52
3:G:34:LEU:HD12	3:G:498:PRO:HB2	1.90	0.52
3:G:177:TYR:CE1	3:G:420:ILE:HB	2.44	0.52
3:G:179:LEU:HD23	3:G:179:LEU:H	1.74	0.52
3:G:476:ARG:HA	3:G:479:TRP:HD1	1.74	0.52
3:C:322:ILE:HG21	3:C:326:ILE:HG22	1.92	0.52
4:F:123:PRO:O	5:H:121:SER:HB3	2.10	0.52
1:A:144:ASP:H	1:A:177:SER:HG	1.54	0.52
2:B:27(C):CYS:CB	2:B:90:SER:HB2	2.40	0.52
2:B:117:LEU:HD23	2:B:206:VAL:HG13	1.91	0.52
3:C:47:ASP:OD1	3:C:47:ASP:N	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:THR:HG23	4:F:110:ILE:HA	1.91	0.52
3:G:298:ARG:HB3	3:G:443:ILE:HB	1.92	0.52
1:D:128:SER:HA	1:D:220:LEU:HD13	1.91	0.52
3:G:181:VAL:HG23	3:G:194:ILE:HD11	1.91	0.52
3:G:218:CYS:HA	3:G:247:CYS:HA	1.91	0.52
1:D:129:LYS:HB3	1:D:135:THR:OG1	2.09	0.52
2:B:27(C):CYS:HA	2:B:90:SER:HG	1.72	0.52
3:C:218:CYS:HA	3:C:247:CYS:HA	1.92	0.52
3:C:258:GLN:OE1	3:C:387:THR:CG2	2.58	0.52
4:F:168:ALA:HB2	4:F:178:LEU:HD23	1.92	0.52
1:D:139:GLY:HA2	1:D:154:TRP:HH2	1.74	0.52
5:J:66:GLY:HA3	5:J:71:PHE:HA	1.92	0.52
1:D:7:SER:HB3	1:D:21:SER:H	1.75	0.52
1:D:72(D):PRO:HG2	3:G:240:PRO:HG3	1.92	0.52
3:C:476:ARG:HA	3:C:479:TRP:HD1	1.74	0.52
3:C:177:TYR:CE1	3:C:420:ILE:HB	2.44	0.51
2:E:6:GLN:HE22	2:E:88:CYS:H	1.57	0.51
3:G:280:ASN:HD22	3:G:458:GLY:HA3	1.75	0.51
5:H:36:TYR:HE1	5:H:46:LEU:HD13	1.75	0.51
2:E:133:VAL:HG13	2:E:177:TYR:CE1	2.43	0.51
3:G:36:VAL:HG12	6:T:610:TRP:CE3	2.36	0.51
2:B:89:CYS:SG	2:B:97:VAL:N	2.82	0.51
3:C:101:VAL:HG13	3:C:479:TRP:HB2	1.92	0.51
2:E:37:GLN:HG3	2:E:86:TYR:HE1	1.75	0.51
2:B:148:TRP:HD1	2:B:159:VAL:HG13	1.76	0.51
3:C:179:LEU:HD23	3:C:179:LEU:H	1.74	0.51
1:A:7:SER:HB3	1:A:21:SER:H	1.76	0.51
3:G:53:PHE:CZ	6:T:547(B):PRO:HG3	2.45	0.51
4:I:147:PRO:O	4:I:148:GLU:HG3	2.10	0.51
3:G:204:ALA:HB3	3:G:437:PRO:HD3	1.92	0.50
3:C:215:ILE:HD12	3:C:253:PRO:HG3	1.92	0.50
4:F:147:PRO:O	4:F:148:GLU:HG3	2.12	0.50
3:G:132:THR:OG1	3:G:188:ASN:OD1	2.29	0.50
5:J:37:GLN:HB2	5:J:47:LEU:HD11	1.94	0.50
2:B:27(C):CYS:CA	2:B:90:SER:HB2	2.41	0.50
1:D:139:GLY:HA3	1:D:180:SER:O	2.11	0.50
2:E:148:TRP:HB3	2:E:178:LEU:HD22	1.94	0.50
2:E:148:TRP:HD1	2:E:159:VAL:HG13	1.77	0.50
3:G:67:ASN:HB3	3:G:208:VAL:HG12	1.94	0.50
3:G:181:VAL:HG13	3:G:183:GLN:N	2.26	0.50
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:391:PHE:O	3:G:392:ASN:ND2	2.43	0.50
4:I:112:SER:OG	4:I:174:GLY:O	2.24	0.50
3:C:219:ALA:HB2	3:C:225:ILE:HG13	1.94	0.50
2:B:37:GLN:HG3	2:B:86:TYR:CE1	2.47	0.49
6:K:635:ILE:HG22	6:K:639:THR:HB	1.94	0.49
3:C:369:LEU:O	3:C:373:THR:OG1	2.26	0.49
6:T:619:LEU:C	6:T:621:GLU:H	2.19	0.49
2:E:3:VAL:CG2	2:E:26:PRO:CD	2.90	0.49
2:E:3:VAL:HG23	2:E:26:PRO:CD	2.43	0.49
3:C:112:TRP:HB3	3:C:427:TRP:NE1	2.27	0.49
3:G:447:SER:OG	10:G:615:NAG:O7	2.27	0.49
2:B:32:SER:HB3	2:B:50:GLU:HA	1.94	0.49
5:J:142:ARG:HH22	5:J:163:VAL:HG21	1.77	0.49
3:C:220:PRO:HG2	3:C:223:PHE:HD2	1.77	0.49
5:H:66:GLY:HA3	5:H:71:PHE:HA	1.94	0.49
1:D:47:TRP:CZ2	1:D:49:GLY:HA2	2.47	0.49
3:G:179:LEU:HD22	3:G:421:LYS:HG3	1.93	0.49
3:C:158:SER:HA	3:C:173:TYR:HA	1.94	0.49
3:G:257:THR:C	3:G:259:LEU:H	2.20	0.49
3:C:257:THR:C	3:C:259:LEU:H	2.20	0.49
3:G:215:ILE:HD12	3:G:253:PRO:HG3	1.93	0.49
1:D:218:LYS:NZ	2:E:210:GLU:OE1	2.32	0.48
2:E:19:VAL:HB	2:E:78:LEU:HD11	1.95	0.48
1:A:4:LEU:HD12	1:A:24:THR:HG22	1.94	0.48
4:F:112:SER:OG	4:F:174:GLY:O	2.26	0.48
1:D:11:LEU:HD22	1:D:147:PRO:HB3	1.95	0.48
1:D:136:ALA:O	1:D:183:THR:HA	2.13	0.48
1:A:11:LEU:HD22	1:A:147:PRO:HB3	1.95	0.48
4:F:139:GLY:HA2	4:F:154:TRP:CH2	2.49	0.48
4:I:146:PHE:HB3	4:I:147:PRO:CD	2.43	0.48
2:B:6:GLN:HE22	2:B:88:CYS:H	1.60	0.48
2:B:24:THR:HA	2:B:27(C):CYS:SG	2.53	0.48
2:E:26:PRO:CG	2:E:27(B):VAL:HB	2.10	0.48
3:C:72:HIS:O	6:K:547(H):MET:HE3	2.14	0.48
5:J:151:ASP:OD2	5:J:189:HIS:ND1	2.39	0.48
5:H:37:GLN:HB2	5:H:47:LEU:HD11	1.94	0.48
3:G:37:THR:HG22	6:T:605:CYS:HA	1.96	0.48
3:G:274:SER:HB3	3:G:277:ILE:HG12	1.95	0.48
5:J:196:VAL:O	5:J:204:PRO:HA	2.14	0.48
4:F:93:THR:HB	4:F:100(M):SER:HB3	1.94	0.48
4:F:193:THR:HG23	4:F:210:LYS:HE3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:SER:O	3:C:287:GLN:NE2	2.43	0.47
3:C:363:ASN:O	3:C:469:ARG:NH1	2.44	0.47
2:E:6:GLN:NE2	2:E:88:CYS:H	2.11	0.47
2:B:24:THR:HB	2:B:70:SER:HB2	1.96	0.47
2:B:184:GLN:O	2:B:191:TYR:OH	2.33	0.47
4:F:139:GLY:HA2	4:F:154:TRP:HH2	1.79	0.47
3:G:158:SER:HA	3:G:173:TYR:HA	1.96	0.47
4:I:193:THR:HG23	4:I:210:LYS:HE3	1.96	0.47
3:G:181:VAL:HG22	3:G:182:VAL:H	1.80	0.47
2:E:27:ASN:N	2:E:27:ASN:HD22	2.12	0.47
6:T:651:ASN:HB3	6:T:655:LYS:HD3	1.97	0.47
2:B:133:VAL:HG13	2:B:177:TYR:CE1	2.46	0.47
3:C:163:THR:OG1	3:C:164:GLU:N	2.47	0.47
5:H:196:VAL:O	5:H:204:PRO:HA	2.15	0.47
3:G:222:GLY:N	6:T:544:LEU:O	2.48	0.47
4:I:195:ILE:HG22	4:I:210:LYS:HA	1.97	0.47
2:E:146:VAL:HG22	2:E:195:VAL:HG22	1.96	0.47
3:C:37:THR:HG22	6:K:605:CYS:HA	1.97	0.47
2:E:27:ASN:N	2:E:27:ASN:ND2	2.60	0.46
6:T:528:SER:OG	9:N:1:NAG:O7	2.27	0.46
3:G:72:HIS:O	6:T:547(H):MET:HE3	2.16	0.46
2:B:27(B):VAL:HG12	2:B:28:CYS:N	2.30	0.46
2:E:36:TYR:HE1	2:E:46:LEU:HD13	1.80	0.46
3:G:219:ALA:HB2	3:G:225:ILE:HG13	1.98	0.46
1:D:47:TRP:HZ2	1:D:50:TRP:CD1	2.34	0.46
3:G:112:TRP:HB3	3:G:427:TRP:NE1	2.31	0.46
5:J:37:GLN:OE1	5:J:45:ARG:NH2	2.45	0.46
3:C:181:VAL:HG13	3:C:183:GLN:N	2.27	0.46
3:C:383:PHE:HB3	3:C:418:CYS:SG	2.56	0.46
1:A:47:TRP:HZ2	1:A:50:TRP:CD1	2.34	0.46
6:T:632:ASP:O	6:T:636:SER:OG	2.29	0.46
2:B:120:PRO:HD2	2:B:185:TRP:CH2	2.50	0.46
3:C:321(A):ASP:N	3:C:321(A):ASP:OD1	2.49	0.46
4:F:146:PHE:HB3	4:F:147:PRO:CD	2.42	0.46
4:I:34:ILE:HG21	4:I:78:VAL:HG21	1.98	0.46
4:I:145:TYR:HE2	4:I:148:GLU:HA	1.81	0.46
1:A:51:ILE:HG13	1:A:57:LYS:HB3	1.98	0.46
1:A:101:TYR:CD2	1:A:102:LEU:HG	2.51	0.45
2:B:146:VAL:HG22	2:B:195:VAL:HG22	1.98	0.45
4:F:34:ILE:HG21	4:F:78:VAL:HG21	1.96	0.45
2:E:24:THR:HA	2:E:28:CYS:SG	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:184:GLN:O	2:E:191:TYR:OH	2.33	0.45
5:J:166:GLN:HE21	5:J:171:SER:HB3	1.81	0.45
3:C:395:TRP:CZ3	3:C:400:SER:HB3	2.51	0.45
3:C:220:PRO:HG2	3:C:223:PHE:CD2	2.51	0.45
3:C:274:SER:HB3	3:C:277:ILE:HG12	1.97	0.45
5:J:54:ARG:NH1	5:J:60:ASP:HA	2.32	0.45
2:E:37:GLN:HG3	2:E:86:TYR:CE1	2.51	0.45
2:E:165:SER:O	2:E:173:ALA:N	2.49	0.45
2:E:185:TRP:CE2	2:E:208:PRO:HB3	2.51	0.45
3:G:179:LEU:HD13	3:G:421:LYS:HE3	1.98	0.45
4:F:144:ASP:HA	4:F:175:LEU:HB3	1.99	0.45
6:K:600:GLY:O	6:K:602:LEU:N	2.43	0.45
1:A:72(D):PRO:HG2	3:C:240:PRO:HG3	1.99	0.45
2:B:19:VAL:HB	2:B:78:LEU:HD11	1.98	0.45
3:C:95:MET:SD	3:C:273:ARG:HD3	2.56	0.45
3:C:181:VAL:HG22	3:C:182:VAL:H	1.81	0.45
5:H:181:LEU:HD23	5:H:185:ASP:HB3	1.99	0.45
6:T:645:LEU:O	6:T:649:SER:HB3	2.17	0.45
2:B:115:VAL:HA	2:B:135:LEU:O	2.17	0.45
3:C:161:MET:HE2	3:C:309:ILE:HD13	1.99	0.45
3:G:95:MET:SD	3:G:273:ARG:HD3	2.56	0.44
5:J:105:ASP:OD1	5:J:173:TYR:OH	2.35	0.44
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.99	0.44
2:B:118:PHE:HE2	2:B:135:LEU:HD12	1.82	0.44
3:C:179:LEU:HD13	3:C:421:LYS:HE3	1.97	0.44
3:C:503:ARG:NH2	6:K:606:THR:HA	2.33	0.44
3:G:383:PHE:HB3	3:G:418:CYS:SG	2.57	0.44
3:G:395:TRP:CZ3	3:G:400:SER:HB3	2.51	0.44
2:B:148:TRP:HB3	2:B:178:LEU:HD22	1.97	0.44
6:K:645:LEU:O	6:K:649:SER:HB3	2.18	0.44
2:B:165:SER:O	2:B:173:ALA:N	2.48	0.44
1:D:168:ALA:HA	1:D:178:LEU:HB3	1.98	0.44
3:G:321(A):ASP:OD1	3:G:321(A):ASP:N	2.50	0.44
6:T:644:GLY:HA2	6:T:647:GLU:HG2	1.99	0.44
2:B:29:SER:C	2:B:31:LYS:N	2.75	0.44
5:H:169:LYS:HG2	5:H:170:ASP:N	2.32	0.44
1:D:101:TYR:CD2	1:D:102:LEU:HG	2.53	0.44
3:G:249:HIS:HD1	3:G:486:TYR:HH	0.57	0.44
4:I:11:VAL:HG22	4:I:110:ILE:HB	1.99	0.44
4:I:146:PHE:C	4:I:148:GLU:H	2.19	0.44
5:J:181:LEU:HD23	5:J:185:ASP:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:363:ASN:O	3:G:469:ARG:NH1	2.50	0.44
2:E:35:TRP:CZ2	2:E:73:LEU:HB2	2.53	0.44
2:E:134:CYS:HB2	2:E:148:TRP:CH2	2.53	0.44
3:G:163:THR:OG1	3:G:164:GLU:N	2.46	0.44
5:J:107:LYS:HA	5:J:140:TYR:OH	2.18	0.44
4:F:147:PRO:HB2	4:F:149:PRO:HD3	1.99	0.44
4:I:147:PRO:HB2	4:I:149:PRO:HD3	2.00	0.44
6:T:615:SER:O	6:T:617:ARG:N	2.51	0.44
1:A:38:ARG:NH1	1:A:86:ASP:OD1	2.48	0.44
2:E:29:SER:C	2:E:31:LYS:N	2.76	0.43
2:E:36:TYR:CE1	2:E:46:LEU:HD13	2.53	0.43
4:I:58:LYS:HA	4:I:58:LYS:HD2	1.78	0.43
4:I:137:ALA:HB3	5:J:118:PHE:HZ	1.83	0.43
1:A:38:ARG:HB3	1:A:48:MET:SD	2.58	0.43
5:H:13:LEU:HD21	5:H:19:GLY:HA3	2.00	0.43
1:D:121:VAL:HB	1:D:207:VAL:HG11	2.00	0.43
1:A:196:CYS:SG	1:A:209:LYS:HB2	2.58	0.43
2:B:6:GLN:NE2	2:B:88:CYS:H	2.15	0.43
2:E:115:VAL:HA	2:E:135:LEU:O	2.18	0.43
5:J:29:SER:HB2	5:J:32:TRP:HD1	1.82	0.43
4:F:195:ILE:HG22	4:F:210:LYS:HA	2.01	0.43
1:D:51:ILE:HG13	1:D:57:LYS:HB3	2.00	0.43
1:D:196:CYS:SG	1:D:209:LYS:HB2	2.59	0.43
2:E:120:PRO:HD2	2:E:185:TRP:CH2	2.53	0.43
4:F:152:VAL:HG22	4:F:198:VAL:HG22	2.00	0.43
5:H:88:CYS:O	5:H:99:GLY:N	2.51	0.43
1:D:4:LEU:HD12	1:D:24:THR:HG22	2.00	0.43
3:C:396:ILE:HG22	3:C:397:SER:H	1.84	0.43
5:H:108:ARG:HG2	5:H:109:THR:N	2.34	0.43
5:J:169:LYS:HG2	5:J:170:ASP:N	2.33	0.43
1:A:9:ALA:HB1	1:A:148:GLU:HG3	1.99	0.43
3:C:286:VAL:O	3:C:451:GLY:HA2	2.18	0.43
4:F:11:VAL:HG22	4:F:110:ILE:HB	2.01	0.43
5:H:6:GLN:NE2	5:H:102:THR:OG1	2.50	0.43
4:I:93:THR:HB	4:I:100(M):SER:HB3	1.99	0.43
5:J:108:ARG:HG2	5:J:109:THR:N	2.33	0.43
4:I:38:ARG:HB2	4:I:90:TYR:CD1	2.53	0.43
6:T:611:ASN:HB3	6:T:614:TRP:CD2	2.54	0.43
3:C:131:CYS:HB3	3:C:155:LYS:HB3	2.00	0.43
4:I:100(J):ASN:HB3	5:J:92:GLY:O	2.18	0.43
5:J:61:ARG:HD2	5:J:77:ARG:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:TRP:CD1	2:B:159:VAL:HG13	2.54	0.43
6:K:644:GLY:HA2	6:K:647:GLU:HG2	2.01	0.43
3:G:72:HIS:NE2	6:T:547(H):MET:SD	2.92	0.43
3:G:396:ILE:HG22	3:G:397:SER:H	1.83	0.43
3:C:423:ILE:HA	3:C:434:MET:O	2.18	0.43
4:F:101:ASP:HB3	5:H:46:LEU:HD23	2.01	0.43
4:F:151:THR:HG23	4:F:199:ASN:HB3	2.00	0.43
6:K:615:SER:O	6:K:617:ARG:N	2.51	0.43
1:D:119:PRO:HD3	1:D:200:HIS:ND1	2.34	0.42
3:G:286:VAL:O	3:G:451:GLY:HA2	2.19	0.42
4:I:144:ASP:HA	4:I:175:LEU:HB3	2.01	0.42
6:K:617:ARG:NH1	6:K:626:MET:SD	2.92	0.42
3:G:399:THR:OG1	3:G:400:SER:N	2.52	0.42
3:C:338:TRP:HZ2	3:C:391:PHE:HE1	1.67	0.42
4:F:100(I):TYR:HE2	5:H:94:SER:HA	1.83	0.42
5:H:107:LYS:HA	5:H:140:TYR:OH	2.19	0.42
5:H:151:ASP:OD2	5:H:189:HIS:ND1	2.42	0.42
4:I:151:THR:HG23	4:I:199:ASN:HB3	2.00	0.42
2:B:26:PRO:O	2:B:27(B):VAL:N	2.52	0.42
6:K:632:ASP:O	6:K:636:SER:OG	2.28	0.42
1:A:147:PRO:HG2	1:A:200:HIS:CE1	2.54	0.42
2:B:167:GLN:N	2:B:171:LYS:O	2.49	0.42
4:F:95:TRP:CZ3	4:F:100(L):ALA:HB3	2.55	0.42
3:G:227:LYS:HA	3:G:485:LYS:O	2.20	0.42
4:I:139:GLY:HA2	4:I:154:TRP:HH2	1.84	0.42
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.54	0.42
3:G:220:PRO:HG2	3:G:223:PHE:HD2	1.83	0.42
3:G:503:ARG:NH2	6:T:606:THR:HA	2.35	0.42
4:I:139:GLY:HA2	4:I:154:TRP:CH2	2.54	0.42
4:I:152:VAL:HG22	4:I:198:VAL:HG22	2.01	0.42
3:C:231:LYS:HD2	3:C:267:GLU:HB3	2.02	0.42
2:E:3:VAL:CB	2:E:26:PRO:HG3	2.43	0.42
5:J:6:GLN:NE2	5:J:102:THR:OG1	2.52	0.42
5:J:13:LEU:HD21	5:J:19:GLY:HA3	2.01	0.42
2:B:24:THR:HB	2:B:70:SER:CB	2.50	0.42
5:H:148:TRP:NE1	5:H:177:SER:OG	2.44	0.42
1:D:193:THR:HG23	1:D:210:ARG:NE	2.35	0.42
1:A:143:LYS:NZ	1:A:144:ASP:OD2	2.53	0.42
2:B:36:TYR:HE1	2:B:46:LEU:HD13	1.84	0.42
3:C:503:ARG:HB3	6:K:607:ASN:HD21	1.85	0.42
4:F:54:VAL:HG21	4:F:100(G):SER:OG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:ARG:NH2	3:C:396:ILE:O	2.53	0.41
4:F:166:PHE:CZ	5:H:176:SER:HB2	2.55	0.41
4:F:168:ALA:HA	4:F:178:LEU:HB3	2.02	0.41
4:I:54:VAL:HG21	4:I:100(G):SER:OG	2.21	0.41
1:A:143:LYS:HA	1:A:177:SER:HB3	2.01	0.41
4:F:17:SER:HA	4:F:82:LEU:O	2.20	0.41
4:F:145:TYR:HE2	4:F:148:GLU:HA	1.85	0.41
5:H:190:LYS:HG2	5:H:211:ARG:HB3	2.02	0.41
1:D:166:PHE:HA	1:D:167:PRO:HD3	1.92	0.41
4:I:168:ALA:HB2	4:I:178:LEU:HD23	2.02	0.41
2:B:24:THR:HG21	2:B:69:TRP:HZ3	1.86	0.41
3:C:500:ARG:H	3:C:500:ARG:HD3	1.85	0.41
4:F:3:GLN:HG2	4:F:4:LEU:N	2.35	0.41
4:F:35:HIS:HB2	4:F:93:THR:OG1	2.21	0.41
1:A:98:ARG:HH12	3:C:88:ASN:HB3	1.85	0.41
1:A:127:SER:CB	2:B:118:PHE:CE1	3.02	0.41
6:T:635:ILE:HG22	6:T:639:THR:HB	2.01	0.41
3:C:34:LEU:HD22	10:K:702:NAG:H81	2.01	0.41
4:F:58:LYS:HA	4:F:58:LYS:HD2	1.76	0.41
5:H:36:TYR:CE1	5:H:46:LEU:HD13	2.55	0.41
2:E:185:TRP:NE1	2:E:208:PRO:HB3	2.34	0.41
3:G:56:SER:N	3:G:75:VAL:O	2.48	0.41
1:A:121:VAL:HB	1:A:207:VAL:HG11	2.01	0.41
4:F:48:VAL:HA	4:F:63:PHE:HE2	1.86	0.41
1:D:17:SER:HB3	1:D:82(A):ARG:HG2	2.02	0.41
1:D:38:ARG:NH1	1:D:86:ASP:OD1	2.51	0.41
3:G:174:SER:HB3	3:G:320:THR:O	2.20	0.41
4:I:3:GLN:HG2	4:I:4:LEU:N	2.36	0.41
5:J:150:VAL:HG13	5:J:192:TYR:HE1	1.86	0.41
3:C:134:VAL:HG13	3:C:136:ASN:H	1.85	0.41
1:D:86:ASP:O	1:D:90:TYR:OH	2.39	0.41
3:G:358:ILE:HG23	3:G:465:THR:HB	2.03	0.41
4:I:95:TRP:CZ3	4:I:100(L):ALA:HB3	2.55	0.41
1:A:66:ARG:HE	1:A:82:ILE:HD11	1.85	0.41
3:C:399:THR:OG1	3:C:400:SER:N	2.52	0.41
1:D:6:GLN:H	1:D:105:GLN:NE2	2.19	0.41
3:G:220:PRO:HG2	3:G:223:PHE:CD2	2.56	0.41
5:J:33:ILE:O	5:J:51:ALA:N	2.54	0.41
2:B:29:SER:O	2:B:31:LYS:N	2.54	0.41
2:B:39:PRO:HA	2:B:40:PRO:HD3	1.95	0.41
3:C:122:LEU:HD11	3:C:203:GLN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:LYS:HA	3:C:485:LYS:O	2.21	0.41
5:H:18:THR:HA	5:H:75:ILE:O	2.21	0.41
2:E:3:VAL:CB	2:E:26:PRO:CD	3.00	0.41
3:G:122:LEU:HD11	3:G:203:GLN:HB2	2.02	0.41
3:C:56:SER:C	3:C:58:ALA:H	2.29	0.41
4:F:63:PHE:HB3	4:F:67:LEU:HB2	2.03	0.41
2:E:49:TYR:C	2:E:51:ASP:H	2.28	0.40
3:G:53:PHE:CZ	3:G:220:PRO:HB3	2.56	0.40
4:I:51:ARG:HG3	4:I:57:TYR:HB3	2.02	0.40
5:J:36:TYR:CE1	5:J:46:LEU:HD13	2.54	0.40
1:A:193:THR:HG23	1:A:210:ARG:NE	2.36	0.40
3:C:174:SER:HB3	3:C:320:THR:O	2.21	0.40
3:C:358:ILE:HG23	3:C:465:THR:HB	2.01	0.40
5:H:29:SER:HB2	5:H:32:TRP:HD1	1.85	0.40
1:D:147:PRO:HG2	1:D:200:HIS:CE1	2.56	0.40
4:F:51:ARG:HG3	4:F:57:TYR:HB3	2.03	0.40
3:G:350:ARG:NH2	3:G:396:ILE:O	2.54	0.40
5:J:190:LYS:HG2	5:J:211:ARG:HB3	2.02	0.40
2:B:49:TYR:C	2:B:51:ASP:H	2.29	0.40
2:B:166:LYS:HA	2:B:172:TYR:HD1	1.86	0.40
3:C:56:SER:N	3:C:75:VAL:O	2.48	0.40
5:H:14:SER:OG	5:H:107:LYS:HB3	2.22	0.40
1:D:127:SER:CB	2:E:118:PHE:CE1	3.04	0.40
1:D:143:LYS:HA	1:D:177:SER:HB3	2.02	0.40
1:A:17:SER:HB3	1:A:82(A):ARG:HG2	2.03	0.40
6:K:635:ILE:O	6:K:639:THR:N	2.54	0.40
2:E:11:VAL:O	2:E:104:VAL:HA	2.21	0.40
3:G:123:THR:N	3:G:124:PRO:HD2	2.37	0.40
3:G:428:GLN:OE1	3:G:428:GLN:N	2.53	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	238/243 (98%)	223 (94%)	14 (6%)	1 (0%)	30	67
1	D	238/243 (98%)	223 (94%)	14 (6%)	1 (0%)	30	67
2	B	211/216 (98%)	186 (88%)	23 (11%)	2 (1%)	14	51
2	E	211/216 (98%)	190 (90%)	20 (10%)	1 (0%)	24	63
3	C	447/485 (92%)	404 (90%)	40 (9%)	3 (1%)	18	56
3	G	447/485 (92%)	403 (90%)	41 (9%)	3 (1%)	18	56
4	F	220/235 (94%)	199 (90%)	17 (8%)	4 (2%)	6	34
4	I	220/235 (94%)	199 (90%)	17 (8%)	4 (2%)	6	34
5	H	211/215 (98%)	190 (90%)	20 (10%)	1 (0%)	24	63
5	J	211/215 (98%)	189 (90%)	21 (10%)	1 (0%)	24	63
6	K	132/140 (94%)	116 (88%)	15 (11%)	1 (1%)	16	54
6	T	132/140 (94%)	117 (89%)	13 (10%)	2 (2%)	8	40
All	All	2918/3068 (95%)	2639 (90%)	255 (9%)	24 (1%)	16	54

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	147	PRO
2	B	30	HIS
4	F	147	PRO
6	K	569	THR
3	G	301	ASN
6	T	569	THR
2	B	27(B)	VAL
3	C	301	ASN
2	E	30	HIS
3	G	411	ASN
3	C	411	ASN
3	G	68	VAL
4	I	52(A)	PRO
4	I	100(L)	ALA
3	C	68	VAL
4	F	52(A)	PRO
4	F	100(L)	ALA
4	I	146	PHE
5	J	9	VAL
6	T	616	ASN
4	F	146	PHE
5	H	9	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	147	PRO
1	A	147	PRO

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	203/206 (98%)	203 (100%)	0	100	100
1	D	203/206 (98%)	203 (100%)	0	100	100
2	B	186/189 (98%)	186 (100%)	0	100	100
2	E	186/189 (98%)	182 (98%)	4 (2%)	45	64
3	C	405/424 (96%)	392 (97%)	13 (3%)	34	56
3	G	405/424 (96%)	392 (97%)	13 (3%)	34	56
4	F	193/199 (97%)	191 (99%)	2 (1%)	68	78
4	I	193/199 (97%)	191 (99%)	2 (1%)	68	78
5	H	183/185 (99%)	183 (100%)	0	100	100
5	J	183/185 (99%)	183 (100%)	0	100	100
6	K	116/118 (98%)	116 (100%)	0	100	100
6	T	116/118 (98%)	116 (100%)	0	100	100
All	All	2572/2642 (97%)	2538 (99%)	34 (1%)	61	74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	27	ASN
2	E	27(A)	SER
2	E	27(B)	VAL
2	E	27(C)	CYS
3	G	57	ASP
3	G	68	VAL
3	G	99	ASN
3	G	137	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	173	TYR
3	G	182	VAL
3	G	183	GLN
3	G	195	ASN
3	G	229	LYS
3	G	327	ARG
3	G	378	CYS
3	G	445	CYS
3	G	500	ARG
4	I	73	ASP
4	I	146	PHE
3	C	57	ASP
3	C	68	VAL
3	C	99	ASN
3	C	137	ASN
3	C	173	TYR
3	C	182	VAL
3	C	183	GLN
3	C	195	ASN
3	C	229	LYS
3	C	327	ARG
3	C	378	CYS
3	C	445	CYS
3	C	500	ARG
4	F	73	ASP
4	F	146	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	164	HIS
2	E	6	GLN
2	E	27	ASN
3	G	203	GLN
3	G	293	GLN
3	G	300	ASN
3	G	352	HIS
3	G	392	ASN
3	G	432	GLN
4	I	100(J)	ASN
4	I	192	GLN
5	J	198	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	HIS
2	B	6	GLN
3	C	293	GLN
3	C	432	GLN
4	F	192	GLN
5	H	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 ⓘ

22 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	$\# Z > 2$
7	NAG	L	1	3,7	14,14,15	0.22	0	17,19,21	0.53	0
7	NAG	L	2	7	14,14,15	0.21	0	17,19,21	0.40	0
7	BMA	L	3	7	11,11,12	0.78	0	15,15,17	0.72	0
7	MAN	L	4	7	11,11,12	0.92	0	15,15,17	1.03	1 (6%)
8	NAG	M	1	3,8	14,14,15	0.28	0	17,19,21	0.51	0
8	NAG	M	2	8	14,14,15	0.25	0	17,19,21	0.47	0
9	NAG	N	1	3,9	14,14,15	0.22	0	17,19,21	0.50	0
9	NAG	N	2	9	14,14,15	0.43	0	17,19,21	1.38	2 (11%)
9	BMA	N	3	9	11,11,12	0.71	0	15,15,17	0.70	0
9	MAN	N	4	9	11,11,12	0.70	0	15,15,17	0.99	2 (13%)
9	MAN	N	5	9	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
7	NAG	O	1	3,7	14,14,15	0.22	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	O	2	7	14,14,15	0.19	0	17,19,21	0.40	0
7	BMA	O	3	7	11,11,12	0.76	0	15,15,17	0.70	0
7	MAN	O	4	7	11,11,12	0.92	0	15,15,17	1.01	1 (6%)
8	NAG	P	1	3,8	14,14,15	0.27	0	17,19,21	0.50	0
8	NAG	P	2	8	14,14,15	0.26	0	17,19,21	0.44	0
9	NAG	Q	1	3,9	14,14,15	0.22	0	17,19,21	0.53	0
9	NAG	Q	2	9	14,14,15	0.42	0	17,19,21	1.37	2 (11%)
9	BMA	Q	3	9	11,11,12	0.74	0	15,15,17	0.71	0
9	MAN	Q	4	9	11,11,12	0.70	0	15,15,17	1.01	2 (13%)
9	MAN	Q	5	9	11,11,12	0.70	0	15,15,17	1.01	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	L	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1
7	MAN	L	4	7	-	2/2/19/22	0/1/1/1
8	NAG	M	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	1/6/23/26	0/1/1/1
9	NAG	N	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	N	2	9	-	5/6/23/26	0/1/1/1
9	BMA	N	3	9	-	1/2/19/22	0/1/1/1
9	MAN	N	4	9	-	2/2/19/22	0/1/1/1
9	MAN	N	5	9	-	2/2/19/22	0/1/1/1
7	NAG	O	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	2/2/19/22	0/1/1/1
8	NAG	P	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
9	NAG	Q	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	6/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	1/2/19/22	0/1/1/1
9	MAN	Q	4	9	-	2/2/19/22	0/1/1/1
9	MAN	Q	5	9	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	2	NAG	C2-N2-C7	4.70	129.20	122.90
9	N	2	NAG	C2-N2-C7	4.69	129.19	122.90
7	O	4	MAN	C1-O5-C5	2.74	115.86	112.19
7	L	4	MAN	C1-O5-C5	2.72	115.83	112.19
9	Q	4	MAN	O2-C2-C3	-2.32	105.35	110.15
9	Q	5	MAN	O2-C2-C3	-2.26	105.48	110.15
9	N	2	NAG	C1-C2-N2	2.24	113.96	110.43
9	N	4	MAN	O2-C2-C3	-2.23	105.53	110.15
9	Q	2	NAG	C1-C2-N2	2.22	113.93	110.43
9	Q	5	MAN	C1-O5-C5	2.20	115.13	112.19
9	Q	4	MAN	C1-O5-C5	2.18	115.11	112.19
9	N	4	MAN	C1-O5-C5	2.17	115.09	112.19
9	N	5	MAN	O2-C2-C3	-2.16	105.68	110.15
9	N	5	MAN	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	4	MAN	C4-C5-C6-O6
7	O	4	MAN	C4-C5-C6-O6
9	N	2	NAG	C8-C7-N2-C2
9	N	2	NAG	O7-C7-N2-C2
9	Q	2	NAG	C8-C7-N2-C2
9	Q	2	NAG	O7-C7-N2-C2
9	N	4	MAN	O5-C5-C6-O6
9	Q	4	MAN	O5-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6
7	L	4	MAN	O5-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
9	N	3	BMA	O5-C5-C6-O6
9	Q	3	BMA	O5-C5-C6-O6
8	M	1	NAG	O5-C5-C6-O6
8	P	1	NAG	C4-C5-C6-O6
8	M	1	NAG	C4-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

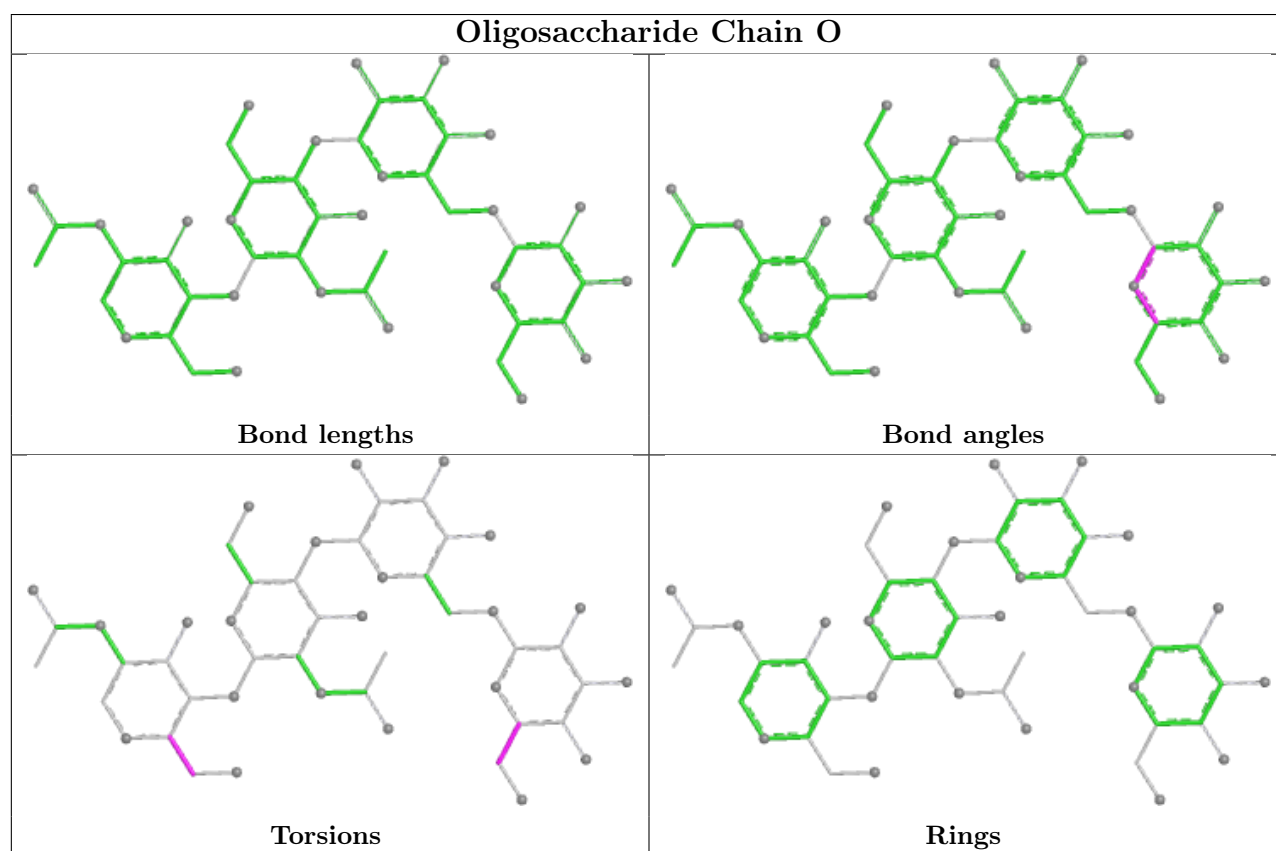
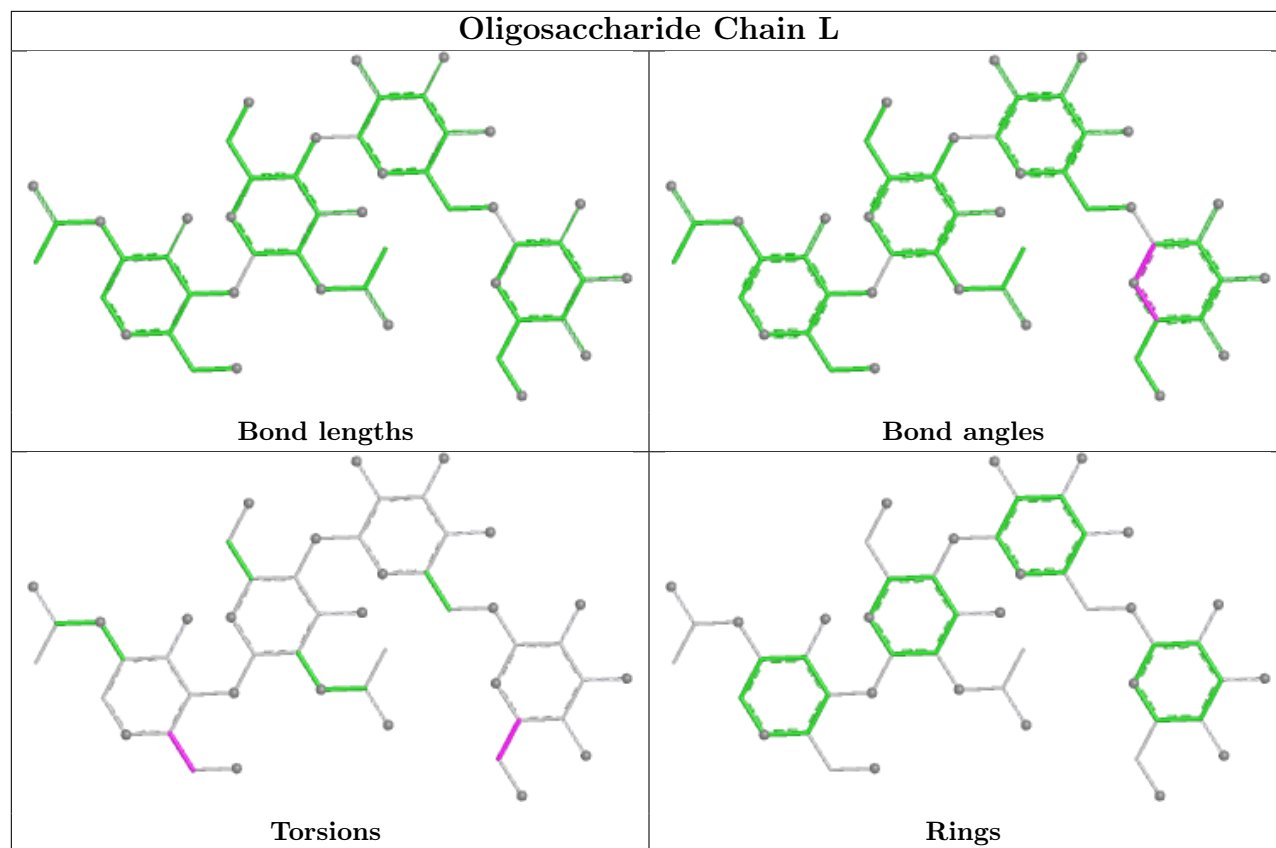
Mol	Chain	Res	Type	Atoms
7	L	1	NAG	O5-C5-C6-O6
9	Q	4	MAN	C4-C5-C6-O6
9	N	4	MAN	C4-C5-C6-O6
9	Q	2	NAG	C4-C5-C6-O6
9	N	5	MAN	C4-C5-C6-O6
9	Q	5	MAN	C4-C5-C6-O6
8	M	2	NAG	C1-C2-N2-C7
9	N	2	NAG	C1-C2-N2-C7
9	Q	2	NAG	C1-C2-N2-C7
9	N	2	NAG	C3-C2-N2-C7
9	Q	2	NAG	C3-C2-N2-C7
9	Q	1	NAG	C4-C5-C6-O6
9	N	5	MAN	O5-C5-C6-O6
9	Q	5	MAN	O5-C5-C6-O6
9	Q	1	NAG	O5-C5-C6-O6

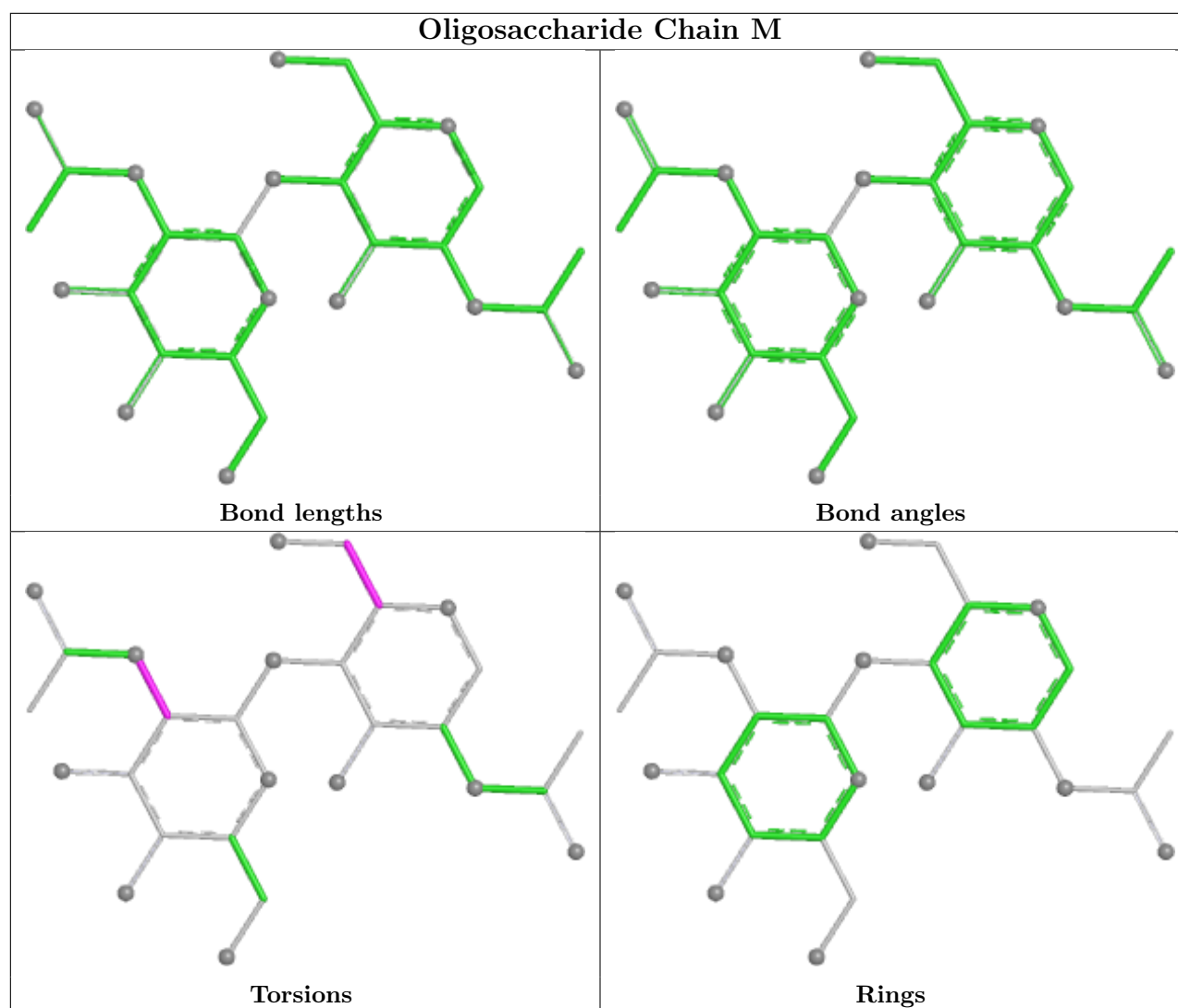
There are no ring outliers.

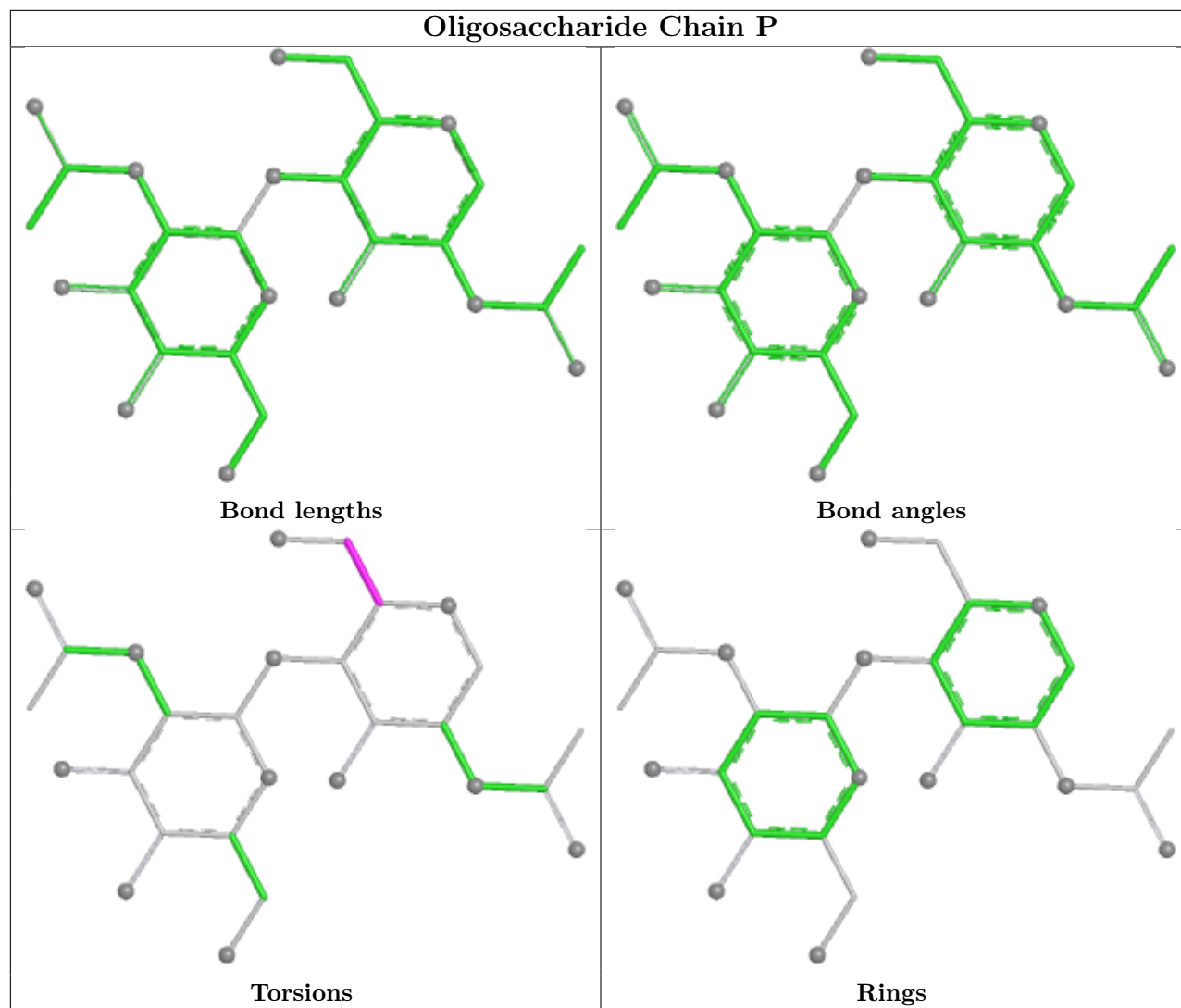
4 monomers are involved in 4 short contacts:

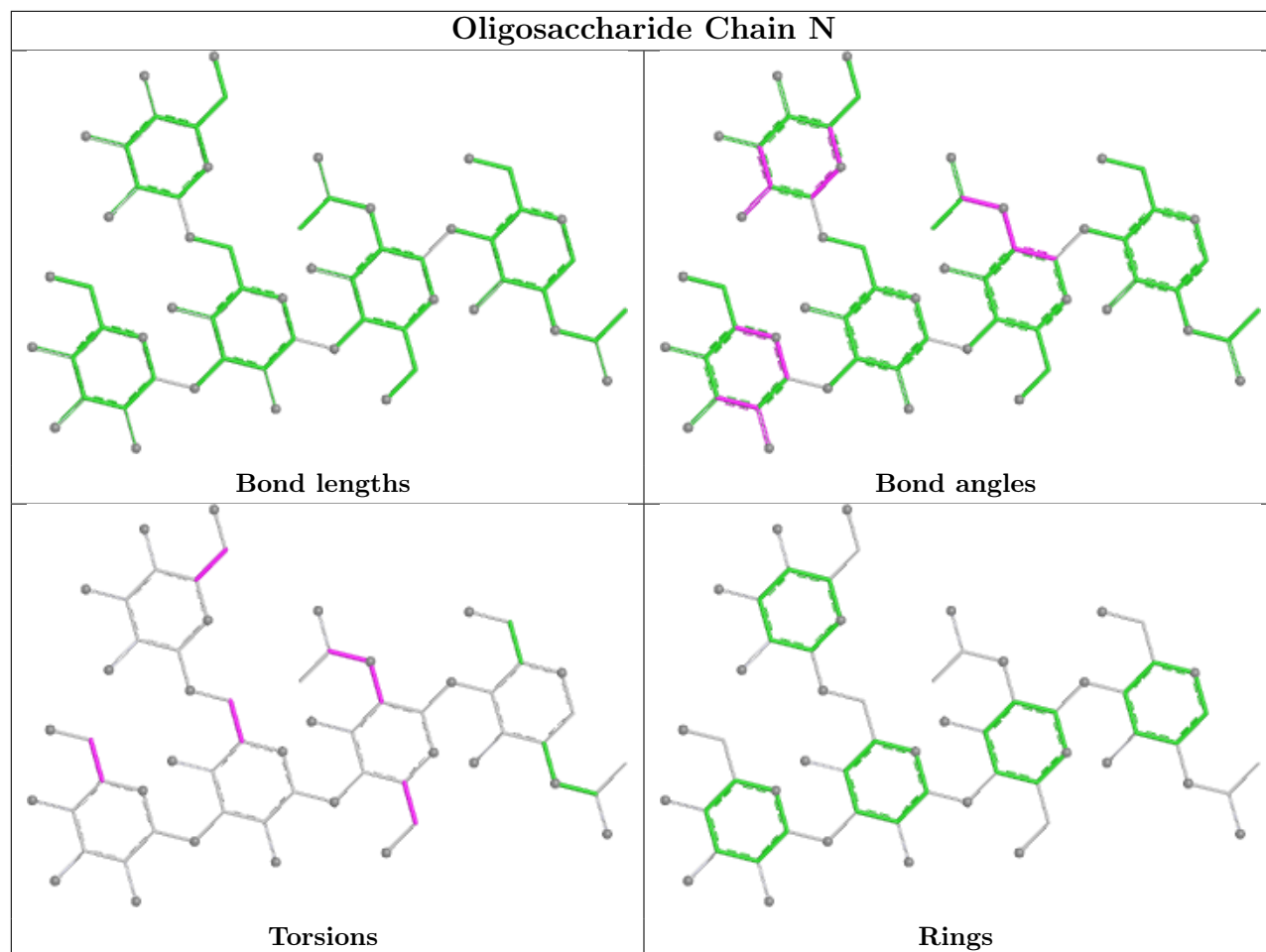
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	1	NAG	1	0
9	N	2	NAG	1	0
9	Q	2	NAG	1	0
9	N	1	NAG	1	0

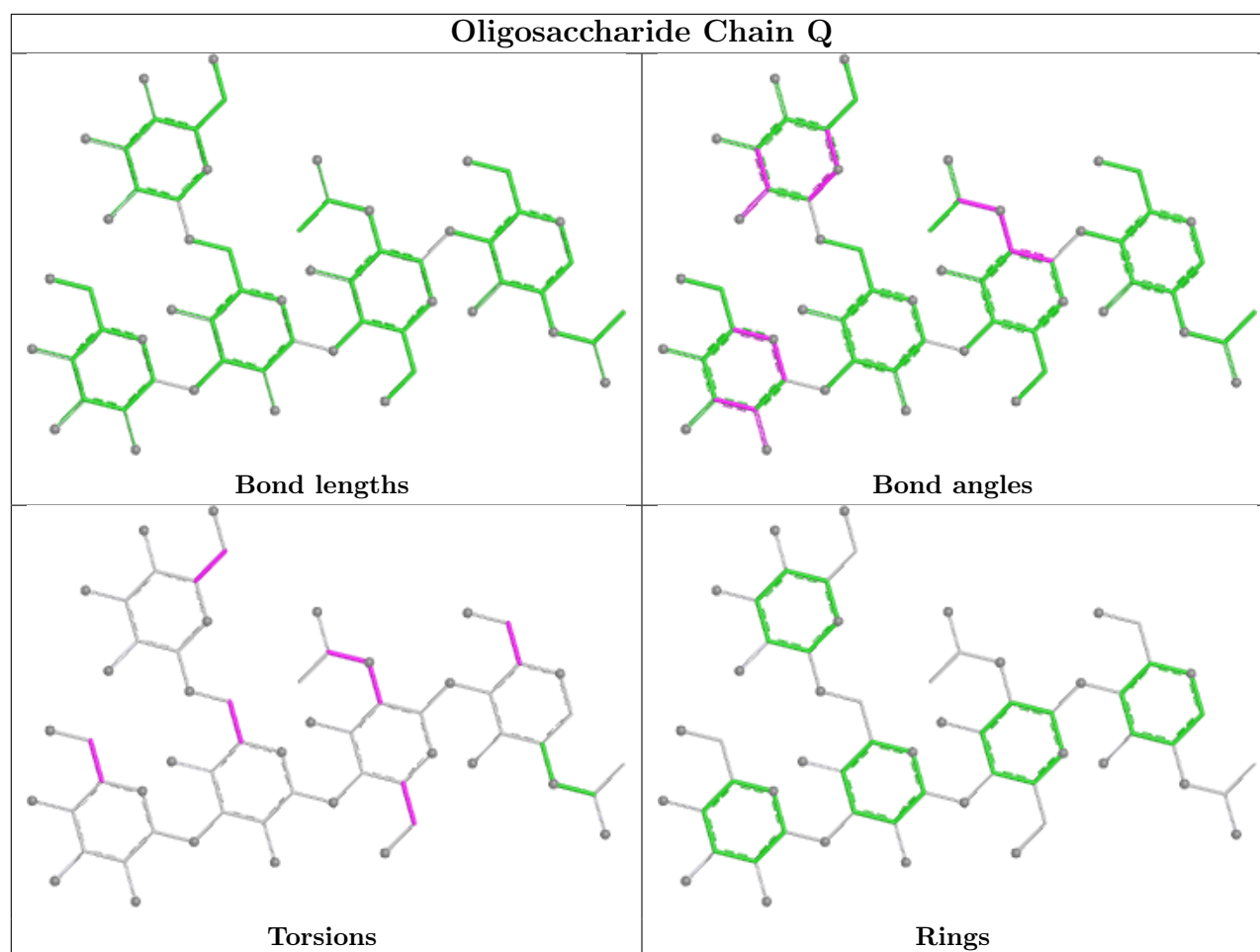
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
10	NAG	T	702	6	14,14,15	0.32	0	17,19,21	0.38	0
10	NAG	C	613	3	14,14,15	0.28	0	17,19,21	0.41	0
10	NAG	T	701	6	14,14,15	0.27	0	17,19,21	0.47	0
10	NAG	G	615	3	14,14,15	0.37	0	17,19,21	0.60	0
10	NAG	K	703	6	14,14,15	0.42	0	17,19,21	0.58	0
10	NAG	G	612	3	14,14,15	0.37	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	G	613	3	14,14,15	0.25	0	17,19,21	0.43	0
10	NAG	G	617	3	14,14,15	0.35	0	17,19,21	0.53	0
10	NAG	C	617	3	14,14,15	0.34	0	17,19,21	0.50	0
10	NAG	G	620	3	14,14,15	0.27	0	17,19,21	0.45	0
10	NAG	C	615	3	14,14,15	0.34	0	17,19,21	0.61	0
10	NAG	C	620	3	14,14,15	0.26	0	17,19,21	0.45	0
10	NAG	G	614	3	14,14,15	0.25	0	17,19,21	0.49	0
10	NAG	C	614	3	14,14,15	0.22	0	17,19,21	0.50	0
10	NAG	C	612	3	14,14,15	0.35	0	17,19,21	0.44	0
10	NAG	T	703	6	14,14,15	0.46	0	17,19,21	0.57	0
10	NAG	K	701	6	14,14,15	0.27	0	17,19,21	0.47	0
10	NAG	G	616	3	14,14,15	0.31	0	17,19,21	0.60	0
10	NAG	C	616	3	14,14,15	0.30	0	17,19,21	0.59	0
10	NAG	G	619	3	14,14,15	0.32	0	17,19,21	0.58	0
10	NAG	C	618	3	14,14,15	0.51	0	17,19,21	0.58	0
10	NAG	C	619	3	14,14,15	0.35	0	17,19,21	0.60	0
10	NAG	K	702	6	14,14,15	0.33	0	17,19,21	0.38	0
10	NAG	G	618	3	14,14,15	0.54	0	17,19,21	0.57	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
10	NAG	T	702	6	-	2/6/23/26	0/1/1/1
10	NAG	C	613	3	-	1/6/23/26	0/1/1/1
10	NAG	T	701	6	-	2/6/23/26	0/1/1/1
10	NAG	G	615	3	-	4/6/23/26	0/1/1/1
10	NAG	K	703	6	-	2/6/23/26	0/1/1/1
10	NAG	G	612	3	-	3/6/23/26	0/1/1/1
10	NAG	G	613	3	-	1/6/23/26	0/1/1/1
10	NAG	G	617	3	-	0/6/23/26	0/1/1/1
10	NAG	C	617	3	-	0/6/23/26	0/1/1/1
10	NAG	G	620	3	-	2/6/23/26	0/1/1/1
10	NAG	C	615	3	-	4/6/23/26	0/1/1/1
10	NAG	C	620	3	-	2/6/23/26	0/1/1/1
10	NAG	G	614	3	-	2/6/23/26	0/1/1/1
10	NAG	C	614	3	-	2/6/23/26	0/1/1/1
10	NAG	C	612	3	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	T	703	6	-	2/6/23/26	0/1/1/1
10	NAG	K	701	6	-	3/6/23/26	0/1/1/1
10	NAG	G	616	3	-	2/6/23/26	0/1/1/1
10	NAG	C	616	3	-	2/6/23/26	0/1/1/1
10	NAG	G	619	3	-	3/6/23/26	0/1/1/1
10	NAG	C	618	3	-	2/6/23/26	0/1/1/1
10	NAG	C	619	3	-	3/6/23/26	0/1/1/1
10	NAG	K	702	6	-	2/6/23/26	0/1/1/1
10	NAG	G	618	3	-	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 (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	T	701	NAG	O5-C5-C6-O6
10	K	701	NAG	O5-C5-C6-O6
10	G	615	NAG	O5-C5-C6-O6
10	C	615	NAG	O5-C5-C6-O6
10	G	614	NAG	C4-C5-C6-O6
10	C	614	NAG	C4-C5-C6-O6
10	G	615	NAG	C4-C5-C6-O6
10	C	615	NAG	C4-C5-C6-O6
10	T	703	NAG	O5-C5-C6-O6
10	T	701	NAG	C4-C5-C6-O6
10	K	701	NAG	C4-C5-C6-O6
10	G	612	NAG	C8-C7-N2-C2
10	G	612	NAG	O7-C7-N2-C2
10	G	620	NAG	C8-C7-N2-C2
10	G	620	NAG	O7-C7-N2-C2
10	C	612	NAG	C8-C7-N2-C2
10	C	612	NAG	O7-C7-N2-C2
10	C	620	NAG	C8-C7-N2-C2
10	C	620	NAG	O7-C7-N2-C2
10	T	703	NAG	C4-C5-C6-O6
10	C	614	NAG	O5-C5-C6-O6
10	G	614	NAG	O5-C5-C6-O6
10	K	703	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	K	703	NAG	C4-C5-C6-O6
10	T	702	NAG	C4-C5-C6-O6
10	T	702	NAG	O5-C5-C6-O6
10	G	619	NAG	O5-C5-C6-O6
10	C	619	NAG	O5-C5-C6-O6
10	K	702	NAG	C4-C5-C6-O6
10	G	612	NAG	O5-C5-C6-O6
10	K	702	NAG	O5-C5-C6-O6
10	C	612	NAG	O5-C5-C6-O6
10	G	616	NAG	C1-C2-N2-C7
10	C	616	NAG	C1-C2-N2-C7
10	G	615	NAG	C3-C2-N2-C7
10	G	618	NAG	C3-C2-N2-C7
10	G	619	NAG	C3-C2-N2-C7
10	C	615	NAG	C3-C2-N2-C7
10	C	618	NAG	C3-C2-N2-C7
10	C	619	NAG	C3-C2-N2-C7
10	G	615	NAG	C1-C2-N2-C7
10	G	618	NAG	C1-C2-N2-C7
10	G	619	NAG	C1-C2-N2-C7
10	C	615	NAG	C1-C2-N2-C7
10	C	618	NAG	C1-C2-N2-C7
10	C	619	NAG	C1-C2-N2-C7
10	K	701	NAG	C1-C2-N2-C7
10	G	616	NAG	C3-C2-N2-C7
10	C	616	NAG	C3-C2-N2-C7
10	G	613	NAG	C4-C5-C6-O6
10	C	613	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	615	NAG	1	0
10	K	703	NAG	1	0
10	C	615	NAG	1	0
10	T	703	NAG	1	0
10	C	618	NAG	1	0
10	K	702	NAG	1	0
10	G	618	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å ²)	Q<0.9
1	A	240/243 (98%)	-0.12	4 (1%) 69 59	209, 293, 422, 436	0
1	D	240/243 (98%)	-0.27	4 (1%) 69 59	195, 301, 440, 465	0
2	B	213/216 (98%)	-0.12	3 (1%) 73 62	221, 295, 398, 412	0
2	E	213/216 (98%)	-0.07	3 (1%) 73 62	219, 290, 423, 441	0
3	C	453/485 (93%)	0.07	16 (3%) 47 43	201, 255, 314, 383	0
3	G	453/485 (93%)	0.01	7 (1%) 72 60	190, 254, 305, 355	0
4	F	226/235 (96%)	0.12	9 (3%) 42 41	230, 272, 325, 360	0
4	I	226/235 (96%)	0.06	10 (4%) 39 39	229, 267, 316, 366	0
5	H	213/215 (99%)	-0.18	2 (0%) 81 70	239, 287, 327, 371	0
5	J	213/215 (99%)	-0.14	5 (2%) 61 53	239, 279, 322, 361	0
6	K	134/140 (95%)	-0.03	7 (5%) 33 35	202, 239, 281, 313	0
6	T	134/140 (95%)	-0.10	4 (2%) 52 46	191, 235, 283, 316	0
All	All	2958/3068 (96%)	-0.05	74 (2%) 58 50	190, 269, 398, 465	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	399	THR	5.0
3	C	174	SER	4.9
5	J	26	SER	4.8
4	I	180	SER	4.7
3	C	324	GLY	4.6
2	B	142	GLY	4.6
5	J	27	GLN	4.6
4	I	179	SER	4.5
6	T	597	GLY	4.3
4	I	165	THR	4.2
4	I	193	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	139	GLY	4.2
6	K	591	GLN	4.0
4	F	140	CYS	3.9
6	T	594	GLY	3.8
3	C	321(A)	ASP	3.5
4	F	138	LEU	3.5
3	C	70	ALA	3.2
6	K	547(A)	ASN	3.1
5	J	134	CYS	3.1
3	C	368	ASP	3.1
2	B	164	PRO	3.1
1	A	168	ALA	3.1
1	A	40	THR	3.1
6	K	588	ARG	3.1
4	F	184	VAL	3.0
3	C	322	ILE	2.9
4	I	164	HIS	2.9
4	I	42	GLY	2.9
3	G	323	ILE	2.8
4	I	125	ALA	2.8
4	F	42	GLY	2.7
3	C	257	THR	2.7
2	E	37	GLN	2.7
1	D	221	GLU	2.7
1	D	132	SER	2.6
5	H	8	PRO	2.6
3	C	264	SER	2.6
3	C	263	GLY	2.6
3	C	177	TYR	2.6
1	D	188	SER	2.6
6	T	547(C)	ASP	2.5
2	E	38	TRP	2.5
3	C	38	VAL	2.5
5	J	112	ALA	2.5
4	F	192	GLN	2.4
3	C	154	LEU	2.4
3	C	320	THR	2.4
6	K	586	TYR	2.4
5	H	27	GLN	2.3
2	B	96	CYS	2.3
6	K	545	LEU	2.3
6	K	593	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	153	SER	2.3
3	G	445	CYS	2.3
1	A	100(B)	SER	2.2
3	C	478	ASN	2.2
4	I	194	TYR	2.2
3	G	440	GLN	2.2
4	F	27	GLY	2.2
4	I	184	VAL	2.2
3	G	303	THR	2.2
4	F	179	SER	2.2
6	T	595	ILE	2.2
4	I	181	VAL	2.1
3	G	377	ASN	2.1
1	D	160	THR	2.1
3	C	431	GLY	2.1
3	G	257	THR	2.1
5	J	1	GLU	2.1
6	K	594	GLY	2.0
1	A	135	THR	2.0
2	E	164	PRO	2.0
3	C	256	SER	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.

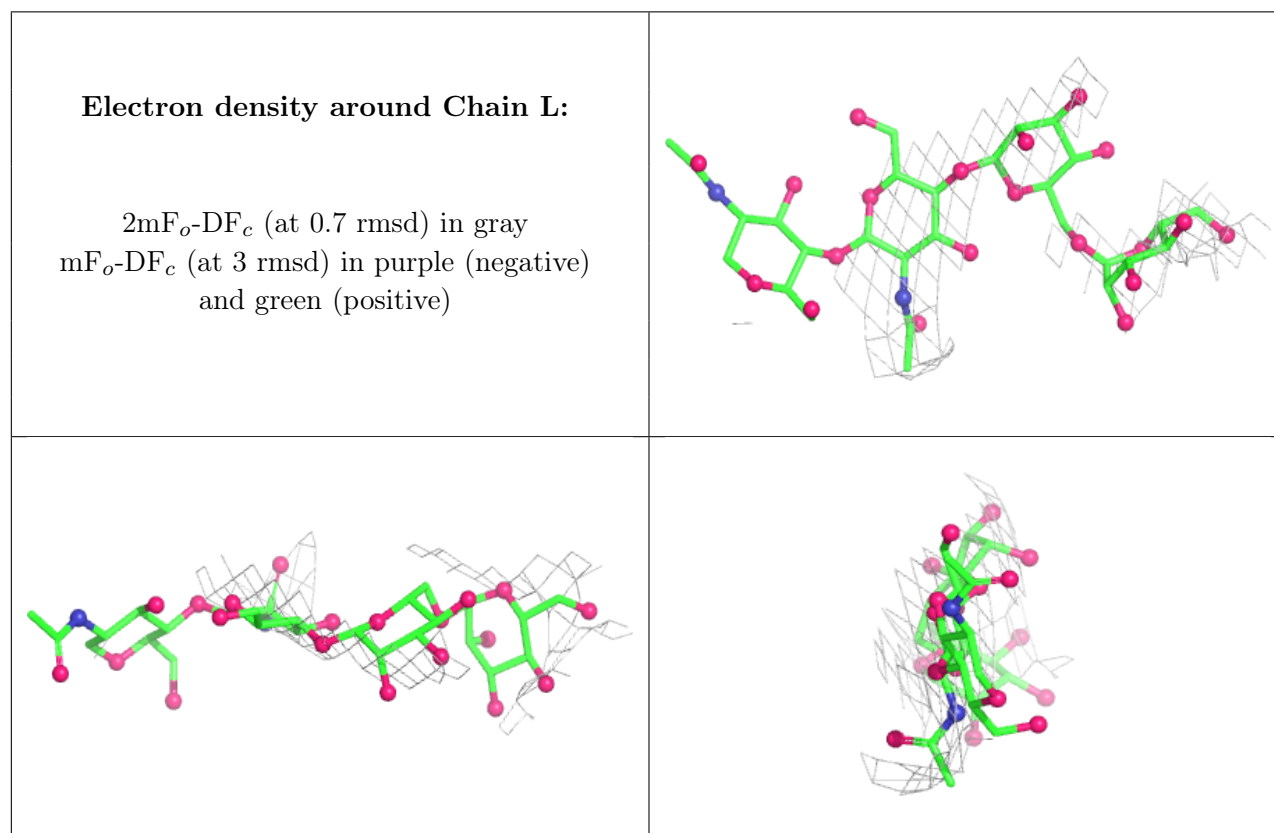
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	L	1	14/15	-	-	233,235,239,240	0
7	NAG	L	2	14/15	-	-	234,236,239,242	0
7	BMA	L	3	11/12	-	-	236,236,238,238	0
7	MAN	L	4	11/12	-	-	239,240,242,243	0
7	NAG	O	2	14/15	0.89	0.06	237,239,242,244	0
9	NAG	Q	2	14/15	0.94	0.08	285,287,289,290	0
9	NAG	Q	1	14/15	0.95	0.10	277,279,282,283	0

Continued on next page...

Continued from previous page...

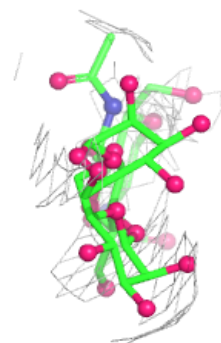
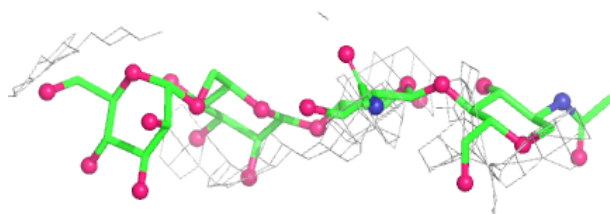
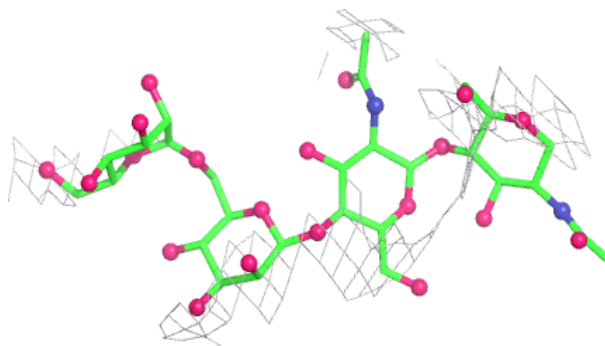
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	N	2	14/15	0.96	0.09	283,284,286,287	0
8	NAG	M	2	14/15	0.96	0.13	245,248,248,250	0
8	NAG	P	1	14/15	0.96	0.18	241,242,244,244	0
9	NAG	N	1	14/15	0.97	0.08	275,277,279,280	0
7	MAN	O	4	11/12	0.97	0.07	241,243,245,246	0
7	NAG	O	1	14/15	0.98	0.08	236,238,242,242	0
8	NAG	P	2	14/15	0.98	0.06	248,250,251,252	0
9	BMA	N	3	11/12	-	-	291,293,296,297	0
9	MAN	N	4	11/12	-	-	293,294,297,298	0
9	MAN	N	5	11/12	-	-	300,302,305,306	0
7	BMA	O	3	11/12	0.98	0.05	238,239,240,241	0
8	NAG	M	1	14/15	0.99	0.19	238,239,241,241	0
9	BMA	Q	3	11/12	-	-	294,296,299,300	0
9	MAN	Q	4	11/12	-	-	295,297,300,301	0
9	MAN	Q	5	11/12	-	-	303,305,308,309	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

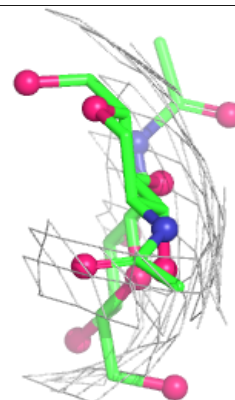
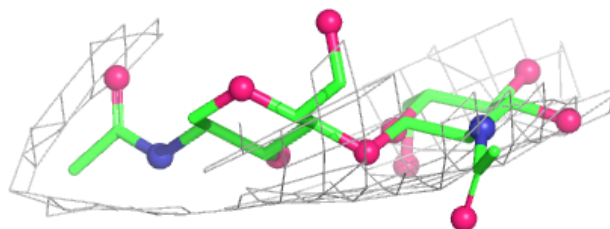
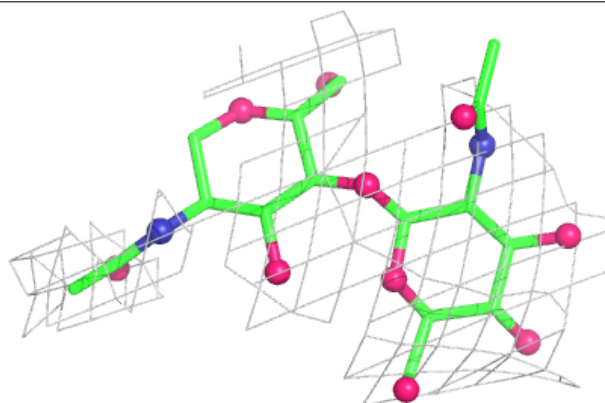


Electron density around Chain O:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

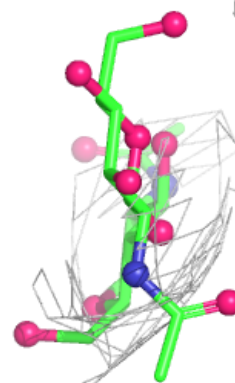
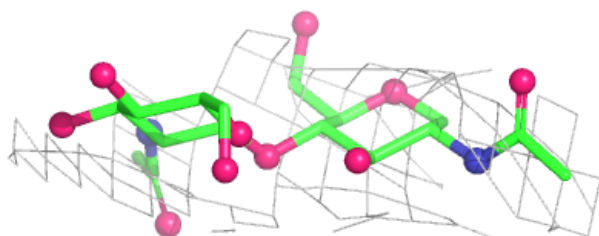
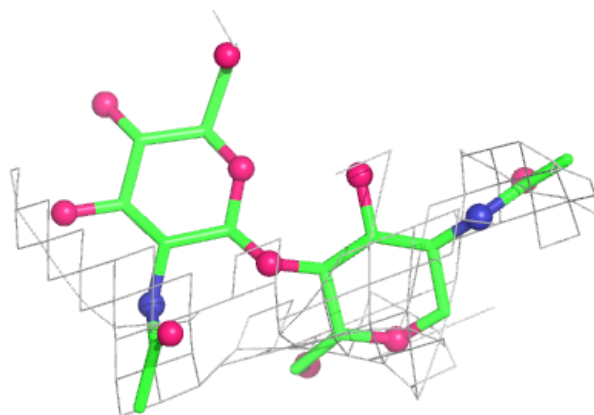
**Electron density around Chain M:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



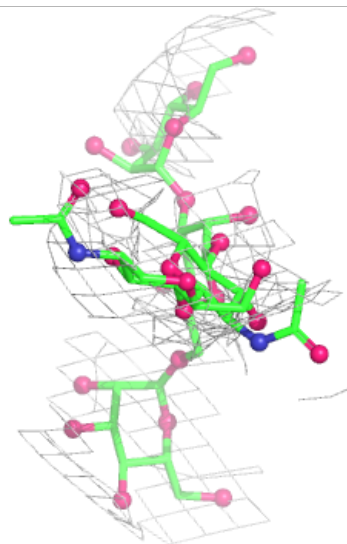
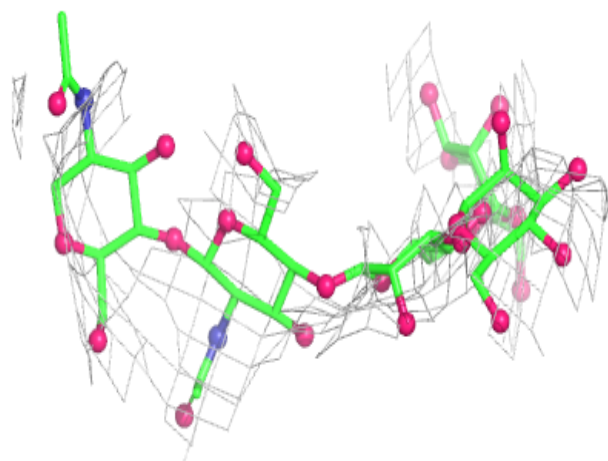
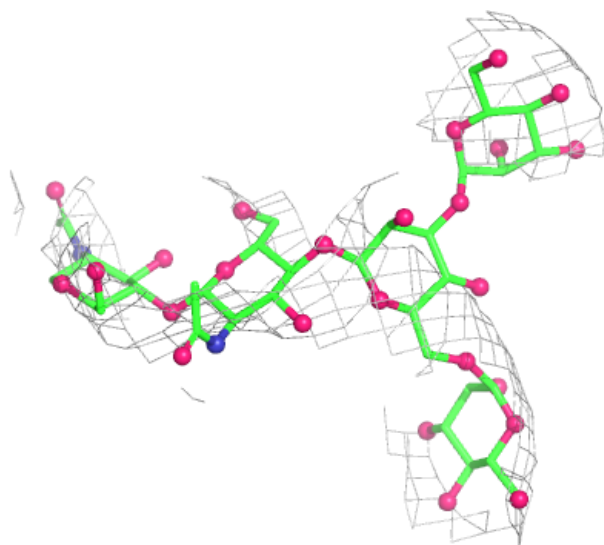
Electron density around Chain P:

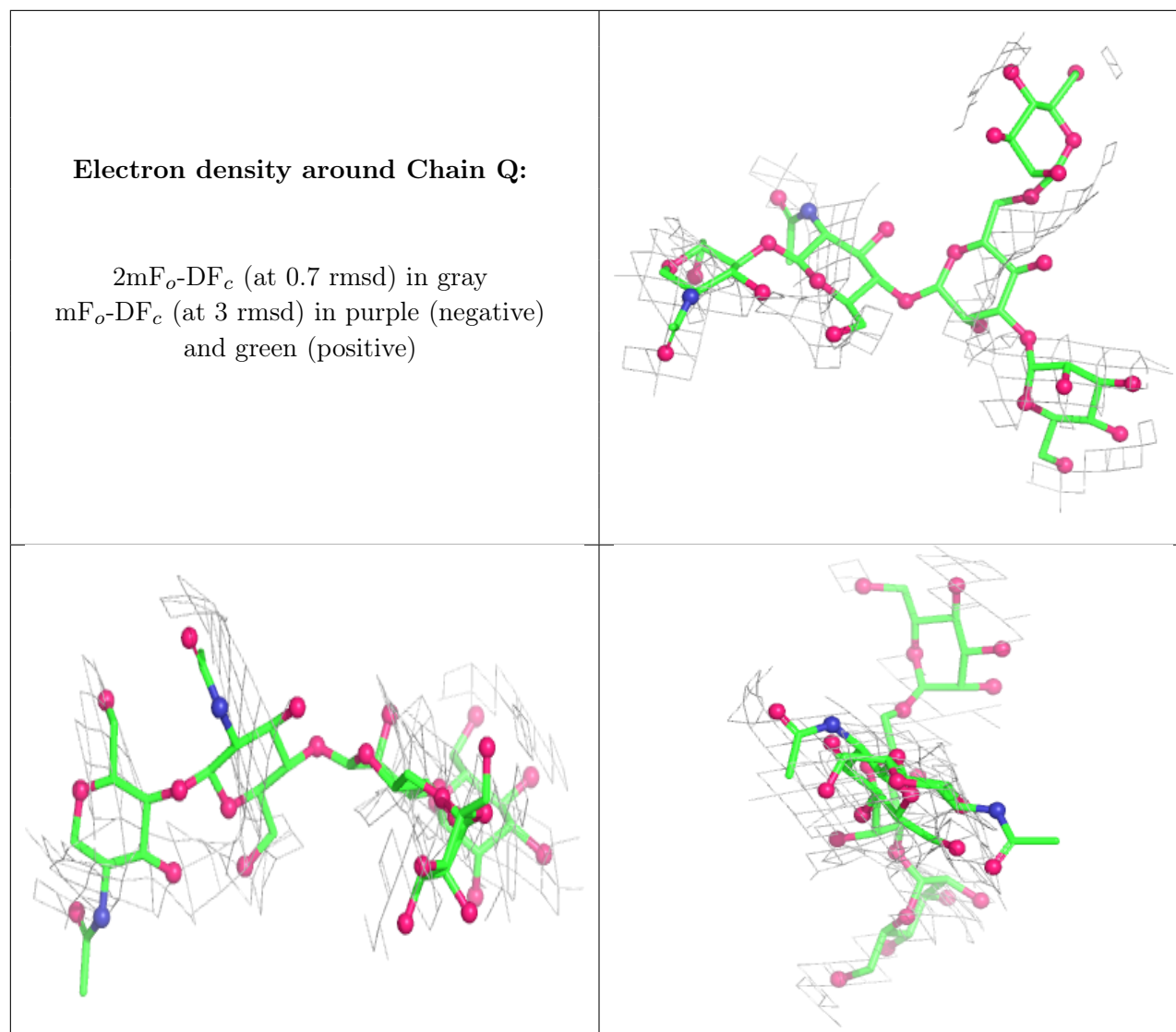
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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, 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
10	NAG	C	612	14/15	0.91	0.09	256,259,263,263	0
10	NAG	G	612	14/15	0.94	0.12	253,256,260,260	0
10	NAG	C	615	14/15	0.94	0.10	236,238,240,240	0
10	NAG	C	614	14/15	0.95	0.09	242,247,250,251	0
10	NAG	C	619	14/15	0.95	0.12	279,281,284,285	0
10	NAG	K	702	14/15	0.95	0.11	286,289,291,291	0
10	NAG	G	616	14/15	0.96	0.12	277,280,283,283	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	G	618	14/15	0.96	0.15	248,257,262,262	0
10	NAG	C	616	14/15	0.96	0.12	280,283,286,286	0
10	NAG	T	702	14/15	0.96	0.12	283,286,288,289	0
10	NAG	C	620	14/15	0.96	0.09	269,276,280,281	0
10	NAG	G	614	14/15	0.96	0.10	239,244,247,248	0
10	NAG	C	613	14/15	0.97	0.15	233,235,238,239	0
10	NAG	T	703	14/15	0.97	0.13	278,282,285,286	0
10	NAG	K	701	14/15	0.97	0.11	284,286,288,289	0
10	NAG	C	617	14/15	0.97	0.10	233,236,239,240	0
10	NAG	K	703	14/15	0.97	0.13	281,285,288,289	0
10	NAG	G	613	14/15	0.98	0.15	231,232,235,236	0
10	NAG	G	620	14/15	0.98	0.07	267,273,277,278	0
10	NAG	C	618	14/15	0.98	0.16	251,260,264,265	0
10	NAG	T	701	14/15	0.98	0.12	281,283,285,287	0
10	NAG	G	615	14/15	0.99	0.08	234,235,237,237	0
10	NAG	G	619	14/15	0.99	0.12	277,278,281,282	0
10	NAG	G	617	14/15	0.99	0.13	231,233,236,237	0

6.5 Other polymers [i](#)

There are no such residues in this entry.