



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 04:17 PM EDT

PDB ID : 6OUS  
Title : Structure of fusion glycoprotein from human respiratory syncytial virus  
Authors : Su, H.P.  
Deposited on : 2019-05-05  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

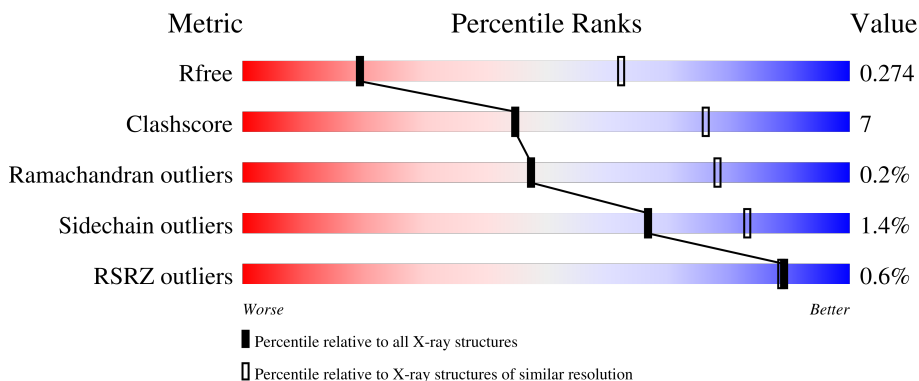
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.













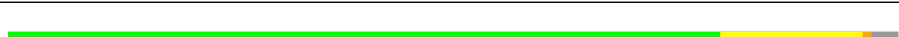
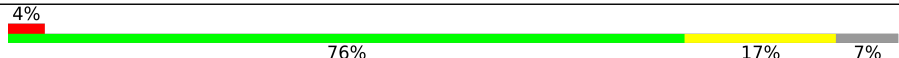









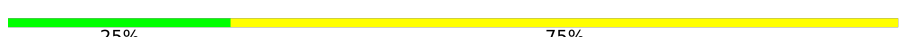



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	84	
1	C	84	
1	E	84	
1	G	84	
1	I	84	

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Mol	Chain	Length	Quality of chain
1	K	84	% 
2	B	414	
2	D	414	
2	F	414	
2	H	414	
2	J	414	
2	L	414	
3	M	231	
3	O	231	
3	Q	231	
3	S	231	
3	U	231	
3	W	231	
4	N	214	
4	P	214	
4	R	214	
4	T	214	
4	V	214	
4	X	214	
5	Y	4	
5	Z	4	
5	a	4	
5	b	4	
5	c	4	
5	d	4	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 41597 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 Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	73	Total 567	C 360	N 90	O 115	S 2	0	0	0
1	C	76	Total 583	C 369	N 94	O 117	S 3	0	0	0
1	E	73	Total 569	C 361	N 91	O 114	S 3	0	0	0
1	G	76	Total 581	C 367	N 93	O 118	S 3	0	0	0
1	I	78	Total 601	C 380	N 96	O 122	S 3	0	0	0
1	K	70	Total 546	C 347	N 87	O 109	S 3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
E	102	ALA	PRO	conflict	UNP P03420
G	102	ALA	PRO	conflict	UNP P03420
I	102	ALA	PRO	conflict	UNP P03420
K	102	ALA	PRO	conflict	UNP P03420

- Molecule 2 is a protein called Fusion glycoprotein F1 fused with Fibrin trimerization domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	404	Total 3057	C 1939	N 501	O 597	S 20	0	0	0
2	D	404	Total 3038	C 1920	N 501	O 597	S 20	0	0	0
2	F	401	Total 3056	C 1939	N 502	O 596	S 19	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	395	Total	C	N	O	S	0	0	0
			2977	1885	492	581	19			
2	J	389	Total	C	N	O	S	0	0	0
			2952	1866	489	577	20			
2	L	396	Total	C	N	O	S	0	0	0
			2982	1888	491	583	20			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	CYS	SER	conflict	UNP P03420
B	190	PHE	SER	conflict	UNP P03420
B	207	LEU	VAL	conflict	UNP P03420
B	290	CYS	SER	conflict	UNP P03420
B	379	VAL	ILE	conflict	UNP P03420
B	447	VAL	MET	conflict	UNP P03420
B	514	SER	-	linker	UNP P03420
B	515	ALA	-	linker	UNP P03420
B	516	ILE	-	linker	UNP P03420
B	517	GLY	-	linker	UNP P03420
B	546	GLY	-	expression tag	UNP M1E1E4
B	547	LEU	-	expression tag	UNP M1E1E4
B	548	VAL	-	expression tag	UNP M1E1E4
B	549	PRO	-	expression tag	UNP M1E1E4
B	550	ARG	-	expression tag	UNP M1E1E4
D	155	CYS	SER	conflict	UNP P03420
D	190	PHE	SER	conflict	UNP P03420
D	207	LEU	VAL	conflict	UNP P03420
D	290	CYS	SER	conflict	UNP P03420
D	379	VAL	ILE	conflict	UNP P03420
D	447	VAL	MET	conflict	UNP P03420
D	514	SER	-	linker	UNP P03420
D	515	ALA	-	linker	UNP P03420
D	516	ILE	-	linker	UNP P03420
D	517	GLY	-	linker	UNP P03420
D	546	GLY	-	expression tag	UNP M1E1E4
D	547	LEU	-	expression tag	UNP M1E1E4
D	548	VAL	-	expression tag	UNP M1E1E4
D	549	PRO	-	expression tag	UNP M1E1E4
D	550	ARG	-	expression tag	UNP M1E1E4
F	155	CYS	SER	conflict	UNP P03420
F	190	PHE	SER	conflict	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
F	207	LEU	VAL	conflict	UNP P03420
F	290	CYS	SER	conflict	UNP P03420
F	379	VAL	ILE	conflict	UNP P03420
F	447	VAL	MET	conflict	UNP P03420
F	514	SER	-	linker	UNP P03420
F	515	ALA	-	linker	UNP P03420
F	516	ILE	-	linker	UNP P03420
F	517	GLY	-	linker	UNP P03420
F	546	GLY	-	expression tag	UNP M1E1E4
F	547	LEU	-	expression tag	UNP M1E1E4
F	548	VAL	-	expression tag	UNP M1E1E4
F	549	PRO	-	expression tag	UNP M1E1E4
F	550	ARG	-	expression tag	UNP M1E1E4
H	155	CYS	SER	conflict	UNP P03420
H	190	PHE	SER	conflict	UNP P03420
H	207	LEU	VAL	conflict	UNP P03420
H	290	CYS	SER	conflict	UNP P03420
H	379	VAL	ILE	conflict	UNP P03420
H	447	VAL	MET	conflict	UNP P03420
H	514	SER	-	linker	UNP P03420
H	515	ALA	-	linker	UNP P03420
H	516	ILE	-	linker	UNP P03420
H	517	GLY	-	linker	UNP P03420
H	546	GLY	-	expression tag	UNP M1E1E4
H	547	LEU	-	expression tag	UNP M1E1E4
H	548	VAL	-	expression tag	UNP M1E1E4
H	549	PRO	-	expression tag	UNP M1E1E4
H	550	ARG	-	expression tag	UNP M1E1E4
J	155	CYS	SER	conflict	UNP P03420
J	190	PHE	SER	conflict	UNP P03420
J	207	LEU	VAL	conflict	UNP P03420
J	290	CYS	SER	conflict	UNP P03420
J	379	VAL	ILE	conflict	UNP P03420
J	447	VAL	MET	conflict	UNP P03420
J	514	SER	-	linker	UNP P03420
J	515	ALA	-	linker	UNP P03420
J	516	ILE	-	linker	UNP P03420
J	517	GLY	-	linker	UNP P03420
J	546	GLY	-	expression tag	UNP M1E1E4
J	547	LEU	-	expression tag	UNP M1E1E4
J	548	VAL	-	expression tag	UNP M1E1E4
J	549	PRO	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	550	ARG	-	expression tag	UNP M1E1E4
L	155	CYS	SER	conflict	UNP P03420
L	190	PHE	SER	conflict	UNP P03420
L	207	LEU	VAL	conflict	UNP P03420
L	290	CYS	SER	conflict	UNP P03420
L	379	VAL	ILE	conflict	UNP P03420
L	447	VAL	MET	conflict	UNP P03420
L	514	SER	-	linker	UNP P03420
L	515	ALA	-	linker	UNP P03420
L	516	ILE	-	linker	UNP P03420
L	517	GLY	-	linker	UNP P03420
L	546	GLY	-	expression tag	UNP M1E1E4
L	547	LEU	-	expression tag	UNP M1E1E4
L	548	VAL	-	expression tag	UNP M1E1E4
L	549	PRO	-	expression tag	UNP M1E1E4
L	550	ARG	-	expression tag	UNP M1E1E4

- Molecule 3 is a protein called RB1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	225	Total 1680	C 1061	N 281	O 332	S 6	0	0	0
3	O	224	Total 1669	C 1055	N 277	O 330	S 7	0	0	0
3	Q	229	Total 1701	C 1073	N 283	O 339	S 6	0	0	0
3	S	224	Total 1671	C 1055	N 279	O 331	S 6	0	0	0
3	U	215	Total 1583	C 1002	N 261	O 314	S 6	0	0	0
3	W	225	Total 1674	C 1057	N 279	O 331	S 7	0	0	0

- Molecule 4 is a protein called RB1 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	N	213	Total 1636	C 1028	N 275	O 328	S 5	0	0	0
4	P	213	Total 1630	C 1025	N 272	O 328	S 5	0	0	0
4	R	213	Total 1636	C 1028	N 275	O 328	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	213	Total	C	N	O	S	0	0	0
			1636	1028	275	328	5			
4	V	209	Total	C	N	O	S	0	0	0
			1580	995	265	315	5			
4	X	213	Total	C	N	O	S	0	0	0
			1636	1028	275	328	5			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	Z	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	a	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	b	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	c	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



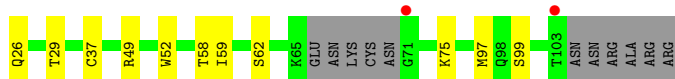


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	Total 14	8	1	5	0	0
6	F	1	Total 14	8	1	5	0	0
6	J	1	Total 14	8	1	5	0	0
6	L	1	Total 14	8	1	5	0	0

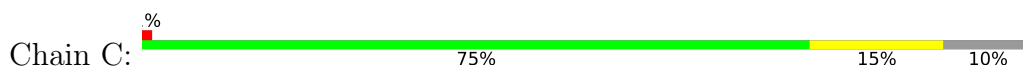
### 3 Residue-property plots [i](#)

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.

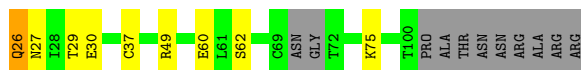
- Molecule 1: Fusion glycoprotein F2



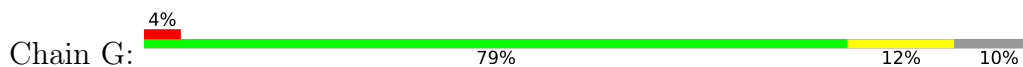
- Molecule 1: Fusion glycoprotein F2



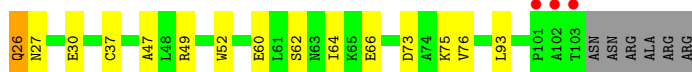
- Molecule 1: Fusion glycoprotein F2



- Molecule 1: Fusion glycoprotein F2

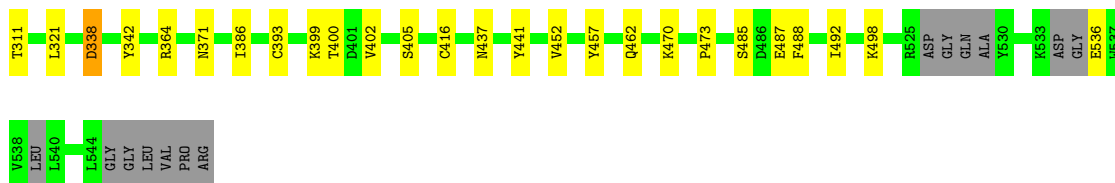


- Molecule 1: Fusion glycoprotein F2



- Molecule 1: Fusion glycoprotein F2

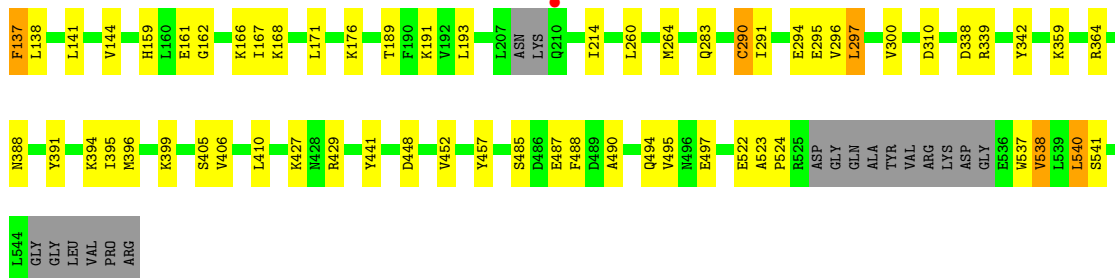
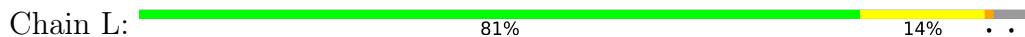




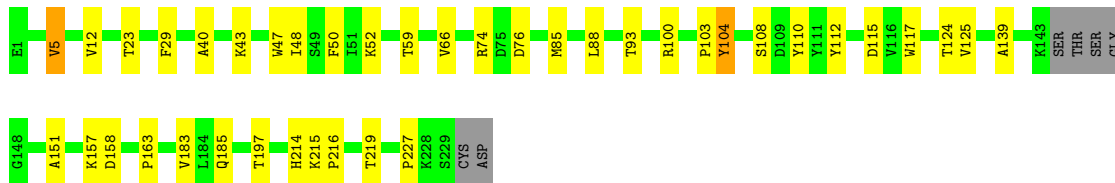
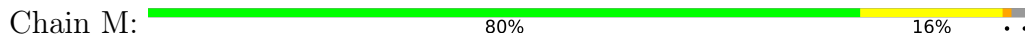
• Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



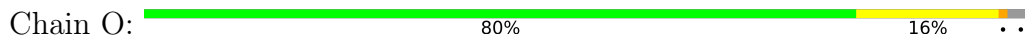
• Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



• Molecule 3: RB1 Fab Heavy Chain

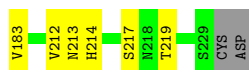
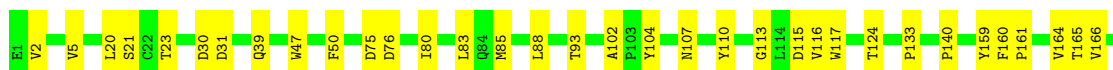
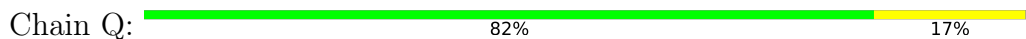


• Molecule 3: RB1 Fab Heavy Chain

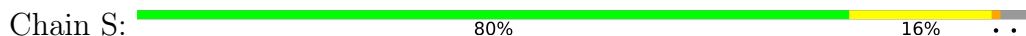




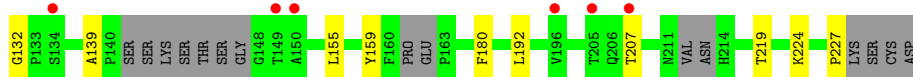
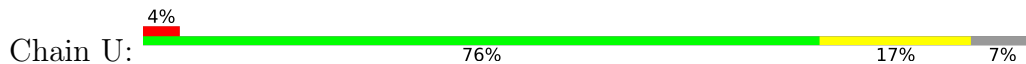
- Molecule 3: RB1 Fab Heavy Chain



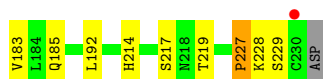
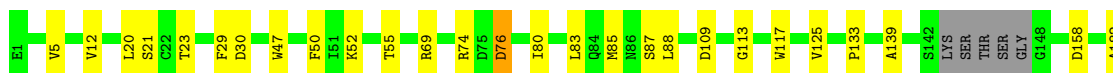
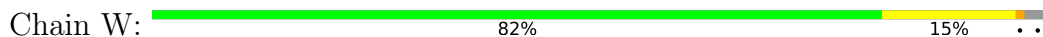
- Molecule 3: RB1 Fab Heavy Chain



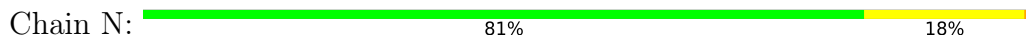
- Molecule 3: RB1 Fab Heavy Chain



- Molecule 3: RB1 Fab Heavy Chain

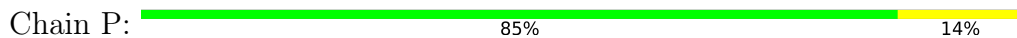


- Molecule 4: RB1 Fab Light chain

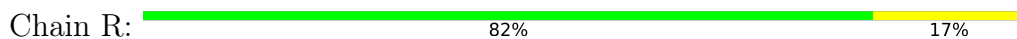




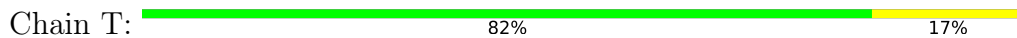
• Molecule 4: RB1 Fab Light chain



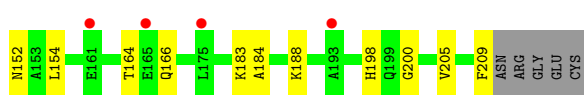
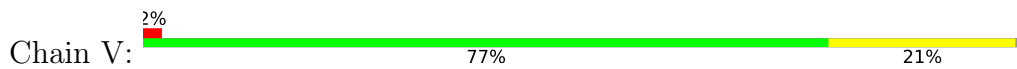
• Molecule 4: RB1 Fab Light chain



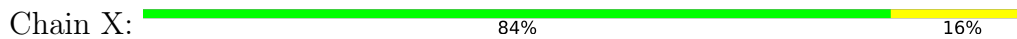
• Molecule 4: RB1 Fab Light chain

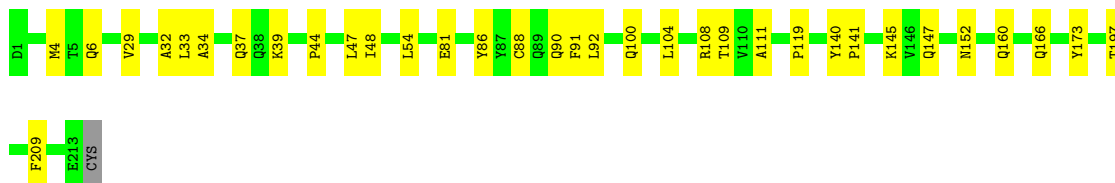


• Molecule 4: RB1 Fab Light chain



• Molecule 4: RB1 Fab Light chain





- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 25% 75%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.15Å 126.59Å 148.16Å 87.24° 79.15° 86.29°	Depositor
Resolution (Å)	49.86 – 3.40 49.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.86-3.40) 98.9 (49.85-3.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.245 , 0.275 0.245 , 0.274	Depositor DCC
$R_{free}$ test set	5767 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtrriage
Anisotropy	0.177	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 4.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	41597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, PCA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/566	0.53	0/767
1	C	0.27	0/582	0.50	0/788
1	E	0.27	0/567	0.50	0/766
1	G	0.27	0/580	0.48	0/788
1	I	0.27	0/601	0.48	0/815
1	K	0.28	0/543	0.49	0/732
2	B	0.29	0/3106	0.50	0/4223
2	D	0.28	0/3086	0.49	0/4198
2	F	0.28	0/3106	0.50	2/4221 (0.0%)
2	H	0.29	0/3020	0.52	1/4100 (0.0%)
2	J	0.29	0/2994	0.51	0/4061
2	L	0.31	1/3028 (0.0%)	0.52	1/4116 (0.0%)
3	M	0.28	0/1719	0.49	0/2337
3	O	0.33	0/1708	0.54	0/2323
3	Q	0.28	0/1741	0.50	0/2368
3	S	0.30	0/1710	0.51	0/2326
3	U	0.28	0/1617	0.51	0/2197
3	W	0.28	0/1713	0.49	0/2330
4	N	0.32	0/1671	0.59	2/2267 (0.1%)
4	P	0.34	1/1665 (0.1%)	0.53	1/2260 (0.0%)
4	R	0.28	0/1671	0.50	0/2267
4	T	0.28	0/1671	0.51	0/2267
4	V	0.27	0/1614	0.51	0/2195
4	X	0.28	0/1671	0.49	0/2267
All	All	0.29	2/41950 (0.0%)	0.51	7/56979 (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	P	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	290	CYS	CB-SG	5.57	1.91	1.82
4	P	49	PHE	CE2-CZ	5.34	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	108	ARG	NE-CZ-NH1	-10.06	115.27	120.30
2	H	155	CYS	CA-CB-SG	-9.40	97.08	114.00
2	F	505	PHE	CB-CG-CD1	7.79	126.25	120.80
4	N	108	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	L	297	LEU	CB-CG-CD1	-6.41	100.11	111.00
2	F	505	PHE	CB-CG-CD2	-6.12	116.52	120.80
4	P	49	PHE	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P	48	ILE	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	567	0	570	8	0
1	C	583	0	575	10	0
1	E	569	0	570	8	0
1	G	581	0	566	9	0
1	I	601	0	598	15	0
1	K	546	0	544	11	0
2	B	3057	0	3035	40	0
2	D	3038	0	2983	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3056	0	3036	53	0
2	H	2977	0	2950	41	0
2	J	2952	0	2935	50	0
2	L	2982	0	2943	45	0
3	M	1680	0	1644	24	0
3	O	1669	0	1631	29	0
3	Q	1701	0	1665	22	0
3	S	1671	0	1631	25	0
3	U	1583	0	1526	26	0
3	W	1674	0	1632	20	0
4	N	1636	0	1594	32	0
4	P	1630	0	1583	25	0
4	R	1636	0	1594	24	0
4	T	1636	0	1594	22	0
4	V	1580	0	1529	28	0
4	X	1636	0	1594	20	0
5	Y	50	0	43	0	0
5	Z	50	0	43	1	0
5	a	50	0	43	0	0
5	b	50	0	43	0	0
5	c	50	0	43	0	0
5	d	50	0	43	0	0
6	B	14	0	13	0	0
6	F	14	0	13	0	0
6	J	14	0	13	0	0
6	L	14	0	13	0	0
All	All	41597	0	40832	532	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 7.

All (532) 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:F:487:GLU:OE2	2:F:498:LYS:NZ	1.84	1.09
4:N:108:ARG:NH1	4:N:171:SER:O	1.95	0.99
4:N:108:ARG:HH12	4:N:172:THR:HA	1.28	0.96
2:B:310:ASP:OD1	2:B:364:ARG:NH1	1.99	0.94
2:L:310:ASP:OD1	2:L:364:ARG:NH1	2.03	0.91
3:O:215:LYS:HG3	3:O:216:PRO:HD3	1.60	0.83
4:P:108:ARG:HH12	4:P:111:ALA:HB2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:310:ASP:OD1	2:J:364:ARG:NH1	2.15	0.80
4:N:108:ARG:NH2	4:N:140:TYR:HB2	1.97	0.80
2:D:176:LYS:NZ	2:D:263:ASP:OD2	2.12	0.78
4:P:29:VAL:HG13	4:P:92:LEU:HB2	1.68	0.76
4:T:108:ARG:HH12	4:T:111:ALA:HB2	1.52	0.75
2:H:386:ILE:HG13	2:H:492:ILE:HD11	1.67	0.74
2:J:487:GLU:OE2	2:J:498:LYS:NZ	2.17	0.73
2:H:293:LYS:HG2	2:H:294:GLU:OE2	1.89	0.73
4:X:108:ARG:HH12	4:X:111:ALA:HB2	1.54	0.70
2:J:530:TYR:O	2:L:538:VAL:HG21	1.90	0.70
2:B:522:GLU:HA	2:D:520:ILE:HD11	1.72	0.70
4:N:108:ARG:CZ	4:N:140:TYR:HB2	2.22	0.70
1:G:56:VAL:HG22	2:H:300:VAL:HG22	1.74	0.70
1:K:76:VAL:HG22	2:L:214:ILE:HD13	1.73	0.70
2:F:310:ASP:OD1	2:F:364:ARG:NH2	2.25	0.69
4:V:38:GLN:HB3	4:V:85:ALA:HB3	1.76	0.67
2:L:159:HIS:CG	2:L:291:ILE:HD11	2.29	0.67
2:J:205:PRO:O	2:J:208:ASN:ND2	2.23	0.66
2:F:386:ILE:HG13	2:F:492:ILE:HD11	1.78	0.66
4:P:29:VAL:HG12	4:P:32:ALA:HB3	1.76	0.66
1:K:29:THR:HG23	1:K:42:LYS:HG3	1.78	0.65
1:G:75:LYS:HD2	2:H:214:ILE:HG21	1.77	0.65
1:K:60:GLU:HG3	2:L:296:VAL:HG12	1.78	0.65
1:C:59:ILE:HB	2:D:297:LEU:HB3	1.78	0.65
2:D:310:ASP:OD1	2:D:364:ARG:NH1	2.30	0.65
3:W:228:LYS:HG2	3:W:229:SER:H	1.62	0.65
2:B:505:PHE:HD1	2:F:505:PHE:CE2	2.14	0.64
4:P:29:VAL:HA	4:P:92:LEU:HD22	1.80	0.64
2:H:488:PHE:CZ	2:J:488:PHE:HB3	2.32	0.64
1:I:93:LEU:HD22	2:J:289:MET:HE1	1.79	0.64
4:V:114:SER:HB2	4:V:137:ASN:HB3	1.78	0.64
2:H:310:ASP:OD1	2:H:364:ARG:NH1	2.28	0.64
2:J:530:TYR:HB3	2:L:538:VAL:HG23	1.80	0.63
2:B:168:LYS:NZ	2:B:294:GLU:O	2.31	0.63
1:I:93:LEU:HD22	2:J:289:MET:CE	2.29	0.63
1:G:97:MET:HG3	2:H:291:ILE:HA	1.80	0.62
4:N:108:ARG:HH12	4:N:172:THR:CA	2.08	0.62
1:K:31:GLU:OE2	1:K:42:LYS:NZ	2.28	0.62
3:O:100:ARG:NH2	3:O:115:ASP:OD2	2.27	0.62
3:M:5:VAL:HG23	3:M:23:THR:HB	1.83	0.61
3:W:29:PHE:O	3:W:74:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:108:ARG:CZ	4:N:172:THR:HG22	2.30	0.61
3:O:21:SER:HB3	3:O:80:ILE:HD11	1.82	0.61
3:O:102:ALA:HB2	3:O:115:ASP:HB2	1.83	0.61
2:D:432:ILE:HD11	2:D:447:VAL:HG22	1.81	0.61
2:H:470:LYS:NZ	3:S:30:ASP:HB2	2.16	0.60
2:J:487:GLU:HB3	2:J:490:ALA:HB2	1.82	0.60
2:J:406:VAL:HG13	2:L:144:VAL:HB	1.83	0.60
2:L:395:ILE:HD11	2:L:495:VAL:HG21	1.83	0.60
3:U:13:ARG:O	3:U:15:GLY:N	2.31	0.60
4:R:29:VAL:HA	4:R:92:LEU:HD22	1.82	0.60
2:D:293:LYS:HG2	2:D:294:GLU:HG3	1.83	0.60
3:O:85:MET:HB3	3:O:88:LEU:HD21	1.84	0.60
2:J:167:ILE:HG23	2:J:189:THR:HG21	1.82	0.60
4:T:147:GLN:HB3	4:T:154:LEU:HD21	1.83	0.59
2:F:505:PHE:HD1	2:F:505:PHE:O	1.85	0.59
2:L:429:ARG:NH2	4:X:92:LEU:O	2.35	0.59
2:F:321:LEU:HD11	2:F:473:PRO:HB3	1.84	0.59
4:N:33:LEU:HD11	4:N:88:CYS:HB2	1.85	0.59
2:B:206:ILE:HG21	2:B:214:ILE:HD13	1.84	0.58
2:J:325:ASN:H	2:J:331:ASN:ND2	2.01	0.58
2:L:399:LYS:NZ	2:L:485:SER:OG	2.36	0.58
3:M:40:ALA:HB3	3:M:43:LYS:HB2	1.84	0.58
3:O:5:VAL:HG23	3:O:23:THR:HB	1.85	0.58
3:Q:5:VAL:HG23	3:Q:23:THR:HB	1.86	0.58
2:F:505:PHE:CD1	2:F:505:PHE:C	2.77	0.58
1:I:30:GLU:HB2	2:J:410:LEU:HD12	1.86	0.58
2:D:494:GLN:O	2:D:497:GLU:HG2	2.04	0.57
3:S:185:GLN:HG2	3:S:189:LEU:O	2.03	0.57
3:Q:93:THR:HG23	3:Q:124:THR:HA	1.86	0.57
4:T:6:GLN:NE2	4:T:86:TYR:O	2.36	0.57
3:U:53:SER:O	3:U:57:GLY:HA3	2.02	0.57
2:D:176:LYS:HZ1	2:D:259:SER:HB3	1.69	0.57
2:F:470:LYS:NZ	3:Q:30:ASP:HB2	2.19	0.57
4:N:120:PRO:HD3	4:N:132:VAL:HG22	1.87	0.57
3:W:47:TRP:HZ2	3:W:50:PHE:HB2	1.70	0.57
3:Q:47:TRP:HZ2	3:Q:50:PHE:HB2	1.70	0.56
2:B:293:LYS:O	2:B:296:VAL:HG12	2.05	0.56
4:N:145:LYS:HB3	4:N:197:THR:HB	1.86	0.56
2:D:429:ARG:NE	3:O:110:TYR:HD1	2.03	0.56
2:J:493:SER:O	2:J:497:GLU:HG2	2.06	0.56
3:O:47:TRP:HZ2	3:O:50:PHE:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:432:ILE:HD11	2:J:447:VAL:HG22	1.88	0.56
3:Q:183:VAL:HG11	4:R:160:GLN:HG2	1.88	0.56
2:H:393:CYS:HB2	2:H:492:ILE:HD12	1.88	0.56
3:U:20:LEU:HD12	3:U:83:LEU:HD23	1.88	0.56
3:M:52:LYS:HE2	3:M:59:THR:HB	1.88	0.56
4:V:108:ARG:HG2	4:V:109:THR:H	1.69	0.55
3:O:11:LEU:HD21	3:O:13:ARG:HH21	1.70	0.55
3:O:75:ASP:HB3	3:O:80:ILE:HG22	1.87	0.55
4:X:145:LYS:HE2	4:X:147:GLN:OE1	2.07	0.55
3:M:93:THR:HG23	3:M:124:THR:HA	1.87	0.55
3:U:5:VAL:HG23	3:U:23:THR:HB	1.88	0.55
2:F:167:ILE:HG23	2:F:189:THR:HG21	1.88	0.55
2:L:523:ALA:HB1	2:L:524:PRO:HD2	1.88	0.55
2:H:386:ILE:HG13	2:H:492:ILE:CD1	2.36	0.55
2:B:252:LEU:HD21	2:B:260:LEU:HD12	1.89	0.55
2:H:163:GLU:OE2	2:H:182:SER:N	2.40	0.54
1:I:37:CYS:HB2	2:J:321:LEU:HD13	1.88	0.54
4:X:145:LYS:HB3	4:X:197:THR:HB	1.88	0.54
2:H:168:LYS:NZ	2:H:294:GLU:HB3	2.23	0.54
1:I:73:ASP:HB3	1:I:76:VAL:HB	1.89	0.54
3:W:139:ALA:HB1	3:W:227:PRO:HA	1.89	0.54
1:E:49:ARG:NH2	2:F:368:ASP:OD1	2.40	0.54
4:T:119:PRO:HB3	4:T:209:PHE:CE1	2.42	0.54
3:W:52:LYS:NZ	3:W:109:ASP:OD2	2.29	0.54
3:U:39:GLN:HB2	3:U:45:LEU:HD23	1.88	0.54
2:B:167:ILE:HG23	2:B:189:THR:HG21	1.90	0.54
1:E:37:CYS:HB2	2:F:321:LEU:HD13	1.89	0.54
4:X:29:VAL:HG12	4:X:32:ALA:HB3	1.89	0.54
1:A:75:LYS:HB2	2:B:214:ILE:HB	1.89	0.54
4:P:66:GLY:HA3	4:P:71:PHE:HA	1.88	0.54
4:V:108:ARG:HG2	4:V:109:THR:N	2.23	0.54
2:F:487:GLU:HB3	2:F:490:ALA:HB2	1.89	0.54
3:O:93:THR:HG23	3:O:124:THR:HA	1.89	0.54
4:T:120:PRO:HD3	4:T:132:VAL:HG22	1.90	0.54
3:S:183:VAL:HG11	4:T:160:GLN:HG2	1.90	0.53
3:M:47:TRP:HZ2	3:M:50:PHE:HB2	1.73	0.53
2:F:505:PHE:HD1	2:F:505:PHE:C	2.12	0.53
2:D:266:ILE:HD13	2:D:270:GLN:HB2	1.91	0.53
2:L:167:ILE:HG23	2:L:189:THR:HG21	1.90	0.53
3:M:29:PHE:O	3:M:74:ARG:NH2	2.41	0.53
4:N:5:THR:HA	4:N:100:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:39:GLN:OE1	4:R:38:GLN:NE2	2.41	0.53
1:K:30:GLU:OE1	2:L:441:TYR:OH	2.22	0.53
4:V:39:LYS:NZ	4:V:81:GLU:O	2.42	0.53
1:C:30:GLU:OE1	2:D:441:TYR:OH	2.19	0.53
2:L:168:LYS:HZ2	2:L:295:GLU:H	1.57	0.53
3:W:5:VAL:HG23	3:W:23:THR:HB	1.91	0.53
2:B:513:LEU:HG	2:B:516:ILE:HD12	1.91	0.53
2:D:360:VAL:O	2:D:361:GLN:NE2	2.41	0.53
3:M:139:ALA:HB1	3:M:227:PRO:HA	1.89	0.53
3:W:30:ASP:OD2	3:W:76:ASP:HB3	2.09	0.53
2:H:487:GLU:OE2	2:H:498:LYS:NZ	2.37	0.52
2:L:388:ASN:OD1	2:L:391:TYR:N	2.42	0.52
3:M:214:HIS:CD2	3:M:216:PRO:HD2	2.43	0.52
4:X:39:LYS:NZ	4:X:81:GLU:O	2.27	0.52
2:F:171:LEU:HD11	2:F:189:THR:HG22	1.91	0.52
2:J:221:ILE:O	2:J:225:GLN:HG2	2.09	0.52
4:R:105:GLU:OE1	4:R:173:TYR:OH	2.18	0.52
4:T:186:TYR:O	4:T:192:TYR:OH	2.27	0.52
3:S:104:TYR:N	3:S:110:TYR:O	2.39	0.52
1:A:97:MET:SD	2:B:292:ILE:HG22	2.50	0.52
4:V:66:GLY:HA3	4:V:71:PHE:HA	1.92	0.52
2:J:432:ILE:HD13	3:U:104:TYR:HB3	1.92	0.52
2:J:473:PRO:HG2	2:J:476:ASN:ND2	2.25	0.52
2:H:206:ILE:HG21	2:H:214:ILE:HD12	1.91	0.51
3:U:159:TYR:OH	3:U:192:LEU:HD23	2.10	0.51
3:O:39:GLN:OE1	4:P:38:GLN:NE2	2.40	0.51
3:U:47:TRP:HZ2	3:U:50:PHE:HB2	1.74	0.51
3:O:47:TRP:CZ2	3:O:50:PHE:HB2	2.45	0.51
4:V:37:GLN:HB2	4:V:47:LEU:HD11	1.93	0.51
1:E:30:GLU:OE1	2:F:441:TYR:OH	2.18	0.51
3:M:157:LYS:HZ2	4:N:131:SER:HG	1.55	0.51
3:U:207:THR:HG22	3:U:224:LYS:HE3	1.92	0.51
4:N:39:LYS:NZ	4:N:81:GLU:O	2.27	0.51
2:B:171:LEU:HD11	2:B:189:THR:HG22	1.93	0.51
3:S:47:TRP:HZ2	3:S:50:PHE:HB2	1.75	0.51
4:V:147:GLN:HB3	4:V:154:LEU:HD21	1.93	0.51
3:W:85:MET:HB3	3:W:88:LEU:HD21	1.93	0.51
2:F:426:ASN:ND2	2:F:446:GLY:O	2.43	0.51
2:H:536:GLU:N	2:L:522:GLU:OE2	2.44	0.51
4:V:83:PHE:HD1	4:V:104:LEU:HB3	1.76	0.51
2:B:445:LYS:NZ	2:B:465:LYS:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:VAL:HB	2:F:406:VAL:HG13	1.93	0.50
4:P:107:LYS:NZ	4:V:205:VAL:HG22	2.25	0.50
3:Q:117:TRP:CE3	4:R:44:PRO:HD2	2.47	0.50
1:G:30:GLU:OE1	2:H:441:TYR:OH	2.24	0.50
2:H:321:LEU:HD11	2:H:473:PRO:HB3	1.92	0.50
2:L:538:VAL:O	2:L:540:LEU:N	2.40	0.50
4:P:114:SER:HB2	4:P:137:ASN:HB3	1.93	0.50
4:P:119:PRO:HB3	4:P:209:PHE:CE1	2.46	0.50
4:V:12:SER:HB2	4:V:107:LYS:HG3	1.94	0.50
1:A:59:ILE:HG23	2:B:193:LEU:HB3	1.93	0.50
2:F:386:ILE:O	2:F:492:ILE:HD13	2.12	0.50
3:O:173:LEU:HD21	3:O:196:VAL:HG21	1.93	0.50
4:R:155:GLN:HB3	4:R:158:ASN:HD21	1.76	0.50
3:S:21:SER:HB3	3:S:80:ILE:HD11	1.94	0.50
2:J:530:TYR:HB3	2:L:538:VAL:CG2	2.41	0.50
3:M:85:MET:HB3	3:M:88:LEU:HD21	1.92	0.50
2:F:526:ASP:OD1	2:F:526:ASP:N	2.44	0.50
4:T:25:THR:HG22	4:T:69:THR:O	2.10	0.50
2:B:445:LYS:HZ3	2:B:465:LYS:HD3	1.77	0.50
4:P:12:SER:HB3	4:P:107:LYS:HG3	1.93	0.50
3:Q:85:MET:HB3	3:Q:88:LEU:HD21	1.94	0.50
3:U:53:SER:HA	3:U:74:ARG:HH12	1.76	0.50
4:V:108:ARG:HE	4:V:109:THR:HG22	1.77	0.50
4:X:48:ILE:HG12	4:X:54:LEU:HD12	1.92	0.50
2:B:427:LYS:HG2	2:B:448:ASP:OD2	2.11	0.50
2:D:206:ILE:HG21	2:D:214:ILE:HD13	1.94	0.50
1:I:62:SER:OG	2:J:200:ASP:OD1	2.30	0.50
4:T:122:ASP:O	4:T:126:LYS:HG3	2.12	0.50
2:H:161:GLU:OE1	2:H:161:GLU:N	2.41	0.50
4:V:119:PRO:HB3	4:V:209:PHE:CE1	2.47	0.50
2:F:470:LYS:HE3	3:Q:31:ASP:HB2	1.92	0.49
2:H:162:GLY:O	2:H:166:LYS:HG3	2.12	0.49
2:H:169:SER:HA	2:H:172:LEU:HD13	1.94	0.49
2:H:218:GLU:OE2	1:I:75:LYS:NZ	2.34	0.49
1:C:59:ILE:HD12	2:D:297:LEU:HD23	1.94	0.49
2:D:176:LYS:HG3	2:D:189:THR:O	2.12	0.49
3:M:112:TYR:CG	4:N:49:PHE:HD2	2.29	0.49
3:S:158:ASP:OD2	3:S:185:GLN:NE2	2.45	0.49
4:V:35:TRP:HB2	4:V:48:ILE:HB	1.94	0.49
1:I:60:GLU:OE2	2:J:296:VAL:HB	2.12	0.49
2:L:138:LEU:HB3	2:L:141:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:426:ASN:ND2	2:D:446:GLY:O	2.40	0.49
3:S:133:PRO:HB3	3:S:159:TYR:HB3	1.94	0.49
2:H:400:THR:HG22	2:H:402:VAL:HG13	1.93	0.49
4:R:108:ARG:NH2	4:R:111:ALA:HB2	2.28	0.49
2:H:405:SER:HB3	2:H:457:TYR:CE1	2.48	0.49
1:K:97:MET:SD	2:L:291:ILE:HG23	2.53	0.49
2:L:137:PHE:HE1	2:L:339:ARG:HH21	1.59	0.49
4:X:119:PRO:HB3	4:X:209:PHE:CE1	2.48	0.49
2:J:323:THR:HG23	2:J:475:ILE:HG12	1.94	0.49
3:O:133:PRO:HB3	3:O:159:TYR:HB3	1.93	0.48
4:P:37:GLN:HB2	4:P:47:LEU:HD11	1.95	0.48
3:S:17:SER:OG	3:S:86:ASN:OD1	2.24	0.48
4:V:48:ILE:HG12	4:V:54:LEU:HD12	1.95	0.48
2:F:393:CYS:HB2	2:F:492:ILE:CD1	2.43	0.48
4:X:6:GLN:NE2	4:X:86:TYR:O	2.41	0.48
3:S:75:ASP:HB3	3:S:80:ILE:HG22	1.95	0.48
1:A:59:ILE:HB	2:B:297:LEU:HB3	1.96	0.48
2:B:406:VAL:HG13	2:D:144:VAL:HB	1.93	0.48
2:D:405:SER:HB3	2:D:457:TYR:CE1	2.48	0.48
3:U:180:PHE:CD2	4:V:164:THR:HG23	2.49	0.48
3:W:12:VAL:HG13	3:W:125:VAL:HG22	1.95	0.48
3:W:133:PRO:HD2	3:W:219:THR:HG21	1.96	0.48
3:O:12:VAL:HG13	3:O:125:VAL:HG22	1.94	0.48
4:V:29:VAL:HG12	4:V:32:ALA:HB3	1.94	0.48
2:B:279:GLN:HB2	2:D:241:ALA:HA	1.95	0.48
3:O:158:ASP:OD1	3:O:185:GLN:NE2	2.42	0.48
4:P:107:LYS:HZ3	4:V:205:VAL:HG22	1.79	0.48
1:I:75:LYS:HE3	2:J:217:ILE:HB	1.95	0.48
4:N:48:ILE:HG13	4:N:54:LEU:HD12	1.96	0.48
4:R:108:ARG:HG2	4:R:109:THR:N	2.29	0.48
2:B:523:ALA:HB3	2:D:532:ARG:HG2	1.96	0.48
2:H:171:LEU:HD11	2:H:189:THR:HG22	1.95	0.47
4:T:29:VAL:HA	4:T:92:LEU:HD22	1.96	0.47
2:B:338:ASP:OD1	2:B:338:ASP:N	2.47	0.47
4:N:29:VAL:HA	4:N:92:LEU:HD22	1.96	0.47
4:N:66:GLY:HA3	4:N:71:PHE:HA	1.96	0.47
3:Q:21:SER:HB3	3:Q:80:ILE:HD11	1.96	0.47
2:F:514:SER:HA	2:F:515:ALA:HA	1.59	0.47
1:K:30:GLU:HB2	2:L:410:LEU:HD12	1.97	0.47
3:W:69:ARG:NH2	3:W:87:SER:O	2.46	0.47
3:O:112:TYR:CD1	3:O:113:GLY:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:16:ARG:CB	3:U:87:SER:H	2.27	0.47
1:C:29:THR:HG22	1:C:30:GLU:N	2.29	0.47
2:H:167:ILE:HG23	2:H:189:THR:HG21	1.97	0.47
2:H:393:CYS:HB2	2:H:492:ILE:CD1	2.45	0.47
2:L:338:ASP:HB2	2:L:342:TYR:OH	2.14	0.47
3:M:158:ASP:OD1	3:M:185:GLN:NE2	2.45	0.47
2:F:312:PRO:HG2	2:F:344:ASP:OD2	2.15	0.47
2:L:162:GLY:O	2:L:166:LYS:HG3	2.14	0.47
2:L:523:ALA:HB2	2:L:537:TRP:NE1	2.30	0.47
3:M:47:TRP:CZ2	3:M:50:PHE:HB2	2.50	0.47
3:M:112:TYR:CG	4:N:49:PHE:CD2	3.03	0.47
4:P:35:TRP:HB2	4:P:48:ILE:HB	1.97	0.47
2:B:321:LEU:HD11	2:B:473:PRO:HB3	1.96	0.47
2:D:520:ILE:HG22	2:D:521:PRO:O	2.15	0.47
2:F:427:LYS:HG2	2:F:448:ASP:OD2	2.15	0.47
3:M:183:VAL:HG11	4:N:160:GLN:HG2	1.96	0.47
3:Q:102:ALA:HB2	3:Q:115:ASP:CG	2.35	0.47
3:W:20:LEU:HD12	3:W:83:LEU:HD23	1.97	0.47
2:D:321:LEU:HD11	2:D:473:PRO:HB3	1.97	0.46
2:J:338:ASP:OD1	2:J:338:ASP:N	2.48	0.46
2:J:405:SER:HB3	2:J:457:TYR:CE1	2.50	0.46
3:O:104:TYR:HA	3:O:112:TYR:HD2	1.80	0.46
3:Q:75:ASP:HB3	3:Q:80:ILE:HG22	1.97	0.46
4:R:108:ARG:HH21	4:R:111:ALA:HB2	1.80	0.46
3:U:104:TYR:HA	3:U:112:TYR:HD2	1.79	0.46
2:J:171:LEU:HD13	2:J:191:LYS:HB2	1.96	0.46
4:P:33:LEU:HD13	4:P:34:ALA:N	2.29	0.46
2:F:148:ILE:HB	2:F:288:ILE:HD11	1.98	0.46
2:L:487:GLU:HB3	2:L:490:ALA:HB2	1.97	0.46
3:U:2:VAL:HG11	3:U:116:VAL:HG11	1.98	0.46
2:D:293:LYS:O	2:D:296:VAL:HG12	2.15	0.46
3:O:102:ALA:HB3	3:O:112:TYR:CZ	2.50	0.46
4:T:24:ARG:HG3	4:T:70:VAL:HG22	1.98	0.46
2:D:405:SER:HB2	2:D:452:VAL:HG21	1.97	0.46
2:L:405:SER:HB3	2:L:457:TYR:CE1	2.50	0.46
2:L:427:LYS:HG2	2:L:448:ASP:OD2	2.16	0.46
2:L:494:GLN:O	2:L:497:GLU:HG2	2.16	0.46
3:Q:47:TRP:CZ2	3:Q:50:PHE:HB2	2.50	0.46
3:W:47:TRP:CZ2	3:W:50:PHE:HB2	2.51	0.46
2:F:283:GLN:HB3	2:F:359:LYS:HE2	1.96	0.46
2:F:338:ASP:HB2	2:F:342:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:405:SER:HB3	2:F:457:TYR:CE1	2.51	0.46
2:F:449:THR:HB	2:F:456:LEU:HD11	1.97	0.46
2:F:361:GLN:HE21	2:F:361:GLN:HA	1.80	0.46
3:M:100:ARG:NH1	3:M:115:ASP:OD2	2.49	0.46
2:F:266:ILE:HD13	2:F:270:GLN:HB2	1.98	0.46
3:M:48:ILE:HG23	3:M:66:VAL:HG21	1.97	0.46
4:T:113:PRO:HB3	4:T:139:PHE:HB3	1.98	0.46
3:U:93:THR:HA	3:U:123:VAL:O	2.16	0.46
3:U:139:ALA:HB1	3:U:227:PRO:HA	1.98	0.46
3:O:54:LYS:HB3	3:O:54:LYS:HE2	1.70	0.45
2:F:137:PHE:HD1	2:F:339:ARG:HE	1.63	0.45
4:P:38:GLN:O	4:P:84:ALA:HB1	2.16	0.45
3:S:93:THR:HG23	3:S:124:THR:HA	1.98	0.45
2:J:530:TYR:CD2	2:L:538:VAL:HB	2.51	0.45
2:L:290:CYS:SG	2:L:300:VAL:HG23	2.56	0.45
3:M:104:TYR:N	3:M:110:TYR:O	2.40	0.45
4:N:33:LEU:HG	4:N:34:ALA:N	2.32	0.45
4:P:12:SER:CB	4:P:107:LYS:HG3	2.47	0.45
4:R:37:GLN:HB2	4:R:47:LEU:HD11	1.98	0.45
3:S:5:VAL:HG23	3:S:23:THR:HB	1.98	0.45
4:T:25:THR:HG21	4:T:29:VAL:CG2	2.46	0.45
3:U:131:LYS:HD3	3:U:132:GLY:O	2.17	0.45
4:X:4:MET:O	4:X:100:GLN:NE2	2.47	0.45
2:B:494:GLN:O	2:B:497:GLU:HG2	2.16	0.45
2:F:252:LEU:HD21	2:F:260:LEU:HD12	1.98	0.45
2:F:327:LYS:NZ	2:F:329:GLY:H	2.14	0.45
2:J:272:LYS:HB2	2:J:272:LYS:HE3	1.66	0.45
2:L:523:ALA:HB2	2:L:537:TRP:CD1	2.52	0.45
4:N:140:TYR:CG	4:N:141:PRO:HA	2.52	0.45
3:O:112:TYR:CD1	3:O:112:TYR:C	2.90	0.45
3:Q:133:PRO:HB3	3:Q:159:TYR:HB3	1.97	0.45
4:X:108:ARG:HG2	4:X:109:THR:N	2.32	0.45
2:B:519:TYR:HB2	2:D:519:TYR:CZ	2.51	0.45
1:I:64:ILE:HD11	2:J:200:ASP:OD1	2.16	0.45
1:C:46:SER:HG	2:D:311:THR:H	1.63	0.45
2:H:144:VAL:HB	2:L:406:VAL:HG13	1.98	0.45
1:I:47:ALA:HB2	2:J:364:ARG:HD2	1.98	0.45
1:K:49:ARG:NH1	1:K:52:TRP:CE2	2.85	0.45
2:L:161:GLU:OE1	2:L:161:GLU:N	2.47	0.45
4:P:39:LYS:HD2	4:P:84:ALA:HB2	1.97	0.45
3:W:158:ASP:OD1	3:W:185:GLN:NE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:LYS:NZ	2:D:259:SER:HB3	2.32	0.45
4:P:13:ALA:HA	4:P:107:LYS:HD2	1.97	0.45
3:Q:20:LEU:HD12	3:Q:83:LEU:HD23	1.98	0.45
4:T:42:LYS:HA	4:T:42:LYS:HD3	1.82	0.45
3:W:21:SER:HB3	3:W:80:ILE:HD11	1.98	0.45
2:F:246:PRO:HB3	2:F:283:GLN:HA	1.99	0.45
2:H:470:LYS:HE3	3:S:31:ASP:HB2	1.99	0.45
2:J:338:ASP:HB2	2:J:342:TYR:OH	2.17	0.45
4:V:184:ALA:O	4:V:188:LYS:HG3	2.17	0.45
4:X:37:GLN:HB2	4:X:47:LEU:HD11	1.98	0.45
1:A:49:ARG:NH1	1:A:52:TRP:CE2	2.84	0.45
1:E:26:PCA:HB2	1:E:27:ASN:H	1.46	0.45
3:O:12:VAL:O	3:O:125:VAL:HA	2.17	0.45
4:X:166:GLN:HG3	4:X:173:TYR:CZ	2.52	0.45
2:B:246:PRO:HB3	2:B:283:GLN:HA	1.99	0.44
3:O:214:HIS:HB3	3:O:219:THR:OG1	2.16	0.44
2:H:204:LEU:N	2:H:205:PRO:HD2	2.32	0.44
3:S:52:LYS:O	3:S:74:ARG:NH1	2.50	0.44
2:B:176:LYS:HE3	2:B:190:PHE:CE2	2.52	0.44
2:D:415:SER:HB3	2:D:417:TYR:CE2	2.52	0.44
3:U:16:ARG:O	3:U:86:ASN:HA	2.16	0.44
2:B:292:ILE:HG21	2:B:292:ILE:HD13	1.70	0.44
2:H:338:ASP:HB3	2:H:342:TYR:OH	2.17	0.44
4:R:119:PRO:HB3	4:R:209:PHE:CE1	2.53	0.44
3:S:214:HIS:CD2	3:S:216:PRO:HD2	2.53	0.44
3:U:4:LEU:HD11	3:U:116:VAL:HG23	1.98	0.44
2:J:237:PHE:CE2	2:J:251:MET:SD	3.11	0.44
2:J:415:SER:HB3	2:J:417:TYR:CE2	2.52	0.44
3:M:12:VAL:HG13	3:M:125:VAL:HG22	1.98	0.44
3:M:103:PRO:HB3	3:M:108:SER:O	2.18	0.44
3:S:4:LEU:HD22	3:S:24:VAL:HG22	1.99	0.44
3:U:18:LEU:HD23	3:U:85:MET:CE	2.48	0.44
1:K:58:THR:HA	2:L:297:LEU:O	2.18	0.44
3:M:215:LYS:HB3	3:M:215:LYS:HE2	1.75	0.44
3:S:102:ALA:HB2	3:S:115:ASP:CG	2.38	0.44
4:N:184:ALA:O	4:N:188:LYS:HG3	2.18	0.43
3:S:12:VAL:HG13	3:S:125:VAL:HG22	2.00	0.43
2:B:424:ALA:O	2:B:432:ILE:HG13	2.19	0.43
2:J:426:ASN:OD1	2:J:427:LYS:N	2.51	0.43
3:U:47:TRP:CZ2	3:U:50:PHE:HB2	2.53	0.43
3:U:155:LEU:HD12	3:U:192:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:400:THR:HG22	2:F:402:VAL:HG13	2.00	0.43
2:H:405:SER:HB2	2:H:452:VAL:HG21	2.01	0.43
4:N:108:ARG:NH2	4:N:172:THR:HG22	2.33	0.43
4:R:210:ASN:HB2	4:R:213:GLU:OE1	2.18	0.43
4:X:34:ALA:O	4:X:88:CYS:HA	2.19	0.43
2:B:449:THR:HB	2:B:456:LEU:HD11	1.99	0.43
2:D:176:LYS:HD3	2:D:190:PHE:CD2	2.53	0.43
2:F:415:SER:HB3	2:F:417:TYR:CE2	2.53	0.43
2:J:294:GLU:HA	2:J:295:GLU:HA	1.58	0.43
4:R:34:ALA:O	4:R:88:CYS:HA	2.18	0.43
4:V:38:GLN:O	4:V:84:ALA:HB1	2.18	0.43
1:G:75:LYS:HD2	2:H:214:ILE:CG2	2.46	0.43
1:I:49:ARG:NH1	1:I:52:TRP:CE2	2.87	0.43
2:J:351:PHE:CE2	2:J:353:PRO:HG3	2.53	0.43
2:D:338:ASP:HB3	2:D:342:TYR:OH	2.18	0.43
2:L:283:GLN:HB3	2:L:359:LYS:HE2	2.00	0.43
3:U:85:MET:HB3	3:U:88:LEU:HD21	2.00	0.43
1:C:49:ARG:NH1	1:C:52:TRP:CE2	2.87	0.43
2:L:291:ILE:HD13	2:L:291:ILE:HG21	1.75	0.43
4:P:108:ARG:HG2	4:P:109:THR:N	2.33	0.43
3:S:141:SER:OG	3:S:142:SER:N	2.50	0.43
2:D:183:ASN:OD1	2:D:185:VAL:HG12	2.18	0.43
2:H:416:CYS:O	2:H:437:ASN:HA	2.18	0.43
4:N:19:VAL:HG22	4:N:75:ILE:HB	2.01	0.43
4:X:33:LEU:HD13	4:X:34:ALA:N	2.34	0.43
2:B:318:THR:HG23	2:B:339:ARG:HB3	2.00	0.43
1:C:76:VAL:HA	1:C:79:ILE:HG22	2.01	0.43
2:D:312:PRO:HG2	2:D:344:ASP:OD2	2.19	0.43
2:L:294:GLU:HA	2:L:295:GLU:HA	1.55	0.43
4:N:33:LEU:HG	4:N:34:ALA:H	1.83	0.43
4:T:108:ARG:HG2	4:T:109:THR:N	2.34	0.43
2:D:316:LEU:HD23	2:D:338:ASP:O	2.19	0.43
1:E:60:GLU:HA	2:F:296:VAL:HG23	2.00	0.43
4:T:37:GLN:HB2	4:T:47:LEU:HD11	2.01	0.43
2:J:318:THR:HG23	2:J:339:ARG:HB3	2.01	0.42
4:N:113:PRO:HB3	4:N:139:PHE:HB3	2.01	0.42
3:U:29:PHE:O	3:U:74:ARG:NH2	2.51	0.42
2:D:522:GLU:HB3	2:F:520:ILE:HG22	2.02	0.42
2:F:327:LYS:HZ3	2:F:329:GLY:H	1.66	0.42
2:F:388:ASN:OD1	2:F:389:PRO:HD2	2.19	0.42
1:K:77:LYS:HD2	1:K:77:LYS:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:2:VAL:HG12	3:Q:116:VAL:HG11	2.02	0.42
4:T:25:THR:HG21	4:T:29:VAL:HG23	2.01	0.42
4:T:61:ARG:NE	4:T:82:ASP:OD2	2.46	0.42
4:V:11:LEU:HD21	4:V:19:VAL:HB	2.00	0.42
2:H:150:SER:O	2:H:153:ALA:HB3	2.19	0.42
5:Z:1:NAG:H5	5:Z:2:NAG:C7	2.49	0.42
1:A:58:THR:HA	2:B:297:LEU:O	2.19	0.42
2:B:164:VAL:CG2	2:B:291:ILE:HD11	2.50	0.42
2:L:396:MET:HG3	2:L:488:PHE:HA	2.01	0.42
4:R:33:LEU:HD13	4:R:34:ALA:N	2.34	0.42
3:W:113:GLY:HA2	4:X:91:PHE:CE1	2.54	0.42
4:X:140:TYR:CG	4:X:141:PRO:HA	2.54	0.42
1:G:46:SER:HG	2:H:311:THR:H	1.67	0.42
4:N:108:ARG:NH1	4:N:171:SER:C	2.68	0.42
4:N:158:ASN:HB3	4:N:179:LEU:HD12	2.02	0.42
4:R:66:GLY:HA3	4:R:71:PHE:HA	2.01	0.42
1:A:62:SER:HB3	2:B:196:LYS:HA	2.00	0.42
3:W:183:VAL:HG11	4:X:160:GLN:HG2	2.01	0.42
1:I:62:SER:HB2	2:J:196:LYS:HA	2.01	0.42
4:T:88:CYS:O	4:T:99:GLY:N	2.52	0.42
2:B:204:LEU:N	2:B:205:PRO:HD2	2.35	0.42
1:E:30:GLU:HB2	2:F:410:LEU:HD12	2.02	0.42
2:F:393:CYS:HB2	2:F:492:ILE:HD11	2.01	0.42
4:N:108:ARG:HG2	4:N:109:THR:N	2.34	0.42
4:T:19:VAL:HG22	4:T:75:ILE:HB	2.01	0.42
2:H:292:ILE:HD12	2:H:297:LEU:HD13	2.02	0.41
2:J:246:PRO:HB3	2:J:283:GLN:HA	2.01	0.41
2:L:260:LEU:O	2:L:264:MET:HG3	2.20	0.41
2:L:394:LYS:HE3	2:L:394:LYS:HB3	1.93	0.41
3:W:182:ALA:HA	3:W:192:LEU:HB3	2.01	0.41
1:E:62:SER:HB3	2:F:196:LYS:HA	2.02	0.41
2:F:204:LEU:N	2:F:205:PRO:HD2	2.36	0.41
2:F:338:ASP:N	2:F:338:ASP:OD1	2.51	0.41
2:J:405:SER:HB2	2:J:452:VAL:HG21	2.02	0.41
3:O:40:ALA:HB3	3:O:43:LYS:HB2	2.02	0.41
4:P:7:SER:HA	4:P:8:PRO:HA	1.83	0.41
3:Q:160:PHE:HA	3:Q:161:PRO:HA	1.86	0.41
4:R:7:SER:HA	4:R:8:PRO:HA	1.83	0.41
2:D:293:LYS:HG2	2:D:294:GLU:N	2.35	0.41
1:G:62:SER:HB3	2:H:196:LYS:HA	2.02	0.41
1:I:75:LYS:HB2	2:J:214:ILE:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:240:ASN:HB2	2:J:244:THR:HG22	2.01	0.41
2:J:416:CYS:O	2:J:437:ASN:HA	2.20	0.41
3:O:117:TRP:CE3	4:P:44:PRO:HD2	2.55	0.41
4:V:21:ILE:HD12	4:V:73:LEU:HD23	2.02	0.41
2:F:503:LEU:HD23	2:F:503:LEU:HA	1.88	0.41
2:J:251:MET:HG3	2:J:299:TYR:CE2	2.55	0.41
3:M:151:ALA:HB2	3:M:197:THR:HG22	2.02	0.41
3:S:215:LYS:HE2	3:S:215:LYS:HB3	1.72	0.41
4:V:106:ILE:H	4:V:166:GLN:HE22	1.67	0.41
2:B:338:ASP:HB2	2:B:342:TYR:OH	2.20	0.41
3:M:117:TRP:CE3	4:N:44:PRO:HD2	2.56	0.41
4:N:75:ILE:HG21	4:N:78:LEU:HD23	2.01	0.41
3:W:117:TRP:CE3	4:X:44:PRO:HD2	2.56	0.41
2:D:167:ILE:HG23	2:D:189:THR:HG21	2.02	0.41
2:F:494:GLN:HA	2:F:497:GLU:HG2	2.03	0.41
2:J:445:LYS:HE3	4:V:56:THR:HG23	2.03	0.41
4:N:7:SER:HA	4:N:8:PRO:HA	1.85	0.41
3:S:117:TRP:CE3	4:T:44:PRO:HD2	2.56	0.41
4:T:61:ARG:CZ	4:T:79:GLN:HG3	2.51	0.41
1:A:37:CYS:HB2	2:B:321:LEU:HD13	2.03	0.41
2:B:416:CYS:O	2:B:437:ASN:HA	2.21	0.41
2:H:159:HIS:HA	2:H:291:ILE:HD13	2.03	0.41
2:L:405:SER:HB2	2:L:452:VAL:HG21	2.03	0.41
4:V:38:GLN:NE2	4:V:42:LYS:O	2.54	0.41
3:W:214:HIS:ND1	3:W:217:SER:OG	2.36	0.41
1:C:47:ALA:HB2	2:D:364:ARG:HD2	2.03	0.41
2:F:424:ALA:O	2:F:432:ILE:HG13	2.21	0.41
2:J:432:ILE:CD1	3:U:104:TYR:HB3	2.50	0.41
1:K:59:ILE:HG23	2:L:193:LEU:HB3	2.02	0.41
4:P:120:PRO:HD3	4:P:132:VAL:HG22	2.02	0.41
3:Q:113:GLY:HA2	4:R:91:PHE:CE1	2.56	0.41
4:R:82:ASP:O	4:R:86:TYR:OH	2.30	0.41
2:L:161:GLU:HG3	4:V:18:ARG:HH12	1.84	0.41
2:L:171:LEU:HD13	2:L:191:LYS:HB2	2.02	0.41
3:O:113:GLY:HA2	4:P:91:PHE:CE1	2.56	0.41
4:R:48:ILE:HG12	4:R:54:LEU:HD12	2.03	0.41
4:R:108:ARG:HG2	4:R:109:THR:H	1.85	0.41
4:R:108:ARG:HD2	4:R:170:ASP:O	2.21	0.41
3:U:53:SER:HA	3:U:74:ARG:NH1	2.36	0.41
4:V:125:LEU:O	4:V:183:LYS:HD2	2.21	0.41
1:C:28:ILE:HG22	2:D:410:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:PHE:CD1	2:H:441:TYR:HB2	2.56	0.41
2:J:162:GLY:O	2:J:166:LYS:HG3	2.21	0.41
3:O:113:GLY:HA2	4:P:91:PHE:CZ	2.56	0.41
3:Q:166:VAL:HG22	3:Q:212:VAL:HG22	2.03	0.41
3:Q:214:HIS:ND1	3:Q:217:SER:OG	2.38	0.41
4:R:12:SER:OG	4:R:105:GLU:OE2	2.26	0.41
4:R:113:PRO:HB3	4:R:139:PHE:HB3	2.02	0.41
3:S:20:LEU:HD12	3:S:83:LEU:HD23	2.02	0.41
2:B:227:ASN:O	2:B:231:LEU:HG	2.21	0.40
1:C:58:THR:HA	2:D:297:LEU:O	2.21	0.40
1:E:75:LYS:NZ	2:F:217:ILE:HB	2.36	0.40
3:S:173:LEU:HD21	3:S:196:VAL:HG21	2.03	0.40
2:D:283:GLN:HB3	2:D:359:LYS:HE2	2.03	0.40
4:R:19:VAL:HG22	4:R:75:ILE:HB	2.03	0.40
3:S:12:VAL:O	3:S:125:VAL:HA	2.21	0.40
3:S:47:TRP:CZ2	3:S:50:PHE:HB2	2.53	0.40
2:F:164:VAL:HG21	2:F:293:LYS:HD3	2.03	0.40
2:F:416:CYS:O	2:F:437:ASN:HA	2.21	0.40
2:H:462:GLN:HG2	2:J:156:LYS:NZ	2.35	0.40
3:M:112:TYR:CD1	4:N:49:PHE:CD2	3.10	0.40
3:O:200:SER:O	3:O:203:LEU:HD12	2.21	0.40
4:V:198:HIS:CE1	4:V:200:GLY:H	2.39	0.40
4:X:86:TYR:HE2	4:X:104:LEU:HD12	1.87	0.40
2:B:487:GLU:HB3	2:B:490:ALA:HB2	2.03	0.40
2:J:171:LEU:HD11	2:J:189:THR:HG22	2.03	0.40
4:P:35:TRP:CD2	4:P:73:LEU:HB2	2.57	0.40
3:Q:165:THR:OG1	3:Q:213:ASN:HB3	2.21	0.40
2:D:280:ILE:HG21	2:D:366:PHE:CG	2.56	0.40
2:F:543:PHE:HA	2:F:544:LEU:HA	1.76	0.40
1:G:97:MET:C	1:G:99:SER:H	2.24	0.40
2:H:399:LYS:NZ	2:H:485:SER:HB3	2.36	0.40
1:I:26:PCA:HA	1:I:27:ASN:HA	1.82	0.40
3:Q:104:TYR:N	3:Q:110:TYR:O	2.48	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	69/84 (82%)	66 (96%)	3 (4%)	0	100	100
1	C	72/84 (86%)	69 (96%)	2 (3%)	1 (1%)	11	37
1	E	69/84 (82%)	65 (94%)	4 (6%)	0	100	100
1	G	72/84 (86%)	68 (94%)	3 (4%)	1 (1%)	11	37
1	I	76/84 (90%)	72 (95%)	4 (5%)	0	100	100
1	K	64/84 (76%)	62 (97%)	2 (3%)	0	100	100
2	B	400/414 (97%)	376 (94%)	23 (6%)	1 (0%)	41	72
2	D	400/414 (97%)	378 (94%)	19 (5%)	3 (1%)	19	51
2	F	397/414 (96%)	372 (94%)	24 (6%)	1 (0%)	41	72
2	H	385/414 (93%)	366 (95%)	19 (5%)	0	100	100
2	J	381/414 (92%)	362 (95%)	18 (5%)	1 (0%)	41	72
2	L	390/414 (94%)	365 (94%)	25 (6%)	0	100	100
3	M	221/231 (96%)	212 (96%)	8 (4%)	1 (0%)	29	61
3	O	220/231 (95%)	210 (96%)	10 (4%)	0	100	100
3	Q	227/231 (98%)	214 (94%)	12 (5%)	1 (0%)	34	67
3	S	220/231 (95%)	208 (94%)	12 (6%)	0	100	100
3	U	205/231 (89%)	197 (96%)	8 (4%)	0	100	100
3	W	221/231 (96%)	209 (95%)	11 (5%)	1 (0%)	29	61
4	N	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
4	P	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
4	R	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
4	T	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
4	V	207/214 (97%)	200 (97%)	7 (3%)	0	100	100
4	X	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
All	All	5351/5658 (95%)	5076 (95%)	264 (5%)	11 (0%)	47	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	531	VAL
1	C	67	ASN
2	D	295	GLU
2	F	294	GLU
2	B	542	THR
1	G	98	GLN
2	D	294	GLU
2	D	517	GLY
3	Q	140	PRO
3	W	227	PRO
3	M	163	PRO

### 5.3.2 Protein sidechains [i](#)

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	63/74 (85%)	61 (97%)	2 (3%)	39	67
1	C	63/74 (85%)	63 (100%)	0	100	100
1	E	63/74 (85%)	62 (98%)	1 (2%)	62	81
1	G	63/74 (85%)	63 (100%)	0	100	100
1	I	66/74 (89%)	65 (98%)	1 (2%)	65	82
1	K	60/74 (81%)	60 (100%)	0	100	100
2	B	350/373 (94%)	346 (99%)	4 (1%)	73	86
2	D	344/373 (92%)	343 (100%)	1 (0%)	92	97
2	F	350/373 (94%)	344 (98%)	6 (2%)	60	80
2	H	339/373 (91%)	331 (98%)	8 (2%)	49	74
2	J	340/373 (91%)	333 (98%)	7 (2%)	53	76
2	L	340/373 (91%)	335 (98%)	5 (2%)	65	82
3	M	187/194 (96%)	183 (98%)	4 (2%)	53	76
3	O	186/194 (96%)	183 (98%)	3 (2%)	62	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	190/194 (98%)	186 (98%)	4 (2%)	53	76
3	S	186/194 (96%)	183 (98%)	3 (2%)	62	81
3	U	173/194 (89%)	169 (98%)	4 (2%)	50	74
3	W	186/194 (96%)	184 (99%)	2 (1%)	73	86
4	N	185/187 (99%)	182 (98%)	3 (2%)	62	81
4	P	184/187 (98%)	184 (100%)	0	100	100
4	R	185/187 (99%)	183 (99%)	2 (1%)	73	86
4	T	185/187 (99%)	182 (98%)	3 (2%)	62	81
4	V	176/187 (94%)	174 (99%)	2 (1%)	73	86
4	X	185/187 (99%)	183 (99%)	2 (1%)	73	86
All	All	4649/4968 (94%)	4582 (99%)	67 (1%)	67	83

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	99	SER
2	B	176	LYS
2	B	500	ASN
2	B	510	ASP
2	B	539	LEU
2	D	137	PHE
1	E	29	THR
2	F	161	GLU
2	F	264	MET
2	F	361	GLN
2	F	505	PHE
2	F	506	ILE
2	F	521	PRO
2	H	155	CYS
2	H	176	LYS
2	H	264	MET
2	H	290	CYS
2	H	291	ILE
2	H	296	VAL
2	H	338	ASP
2	H	371	ASN
1	I	66	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	137	PHE
2	J	206	ILE
2	J	331	ASN
2	J	371	ASN
2	J	429	ARG
2	J	475	ILE
2	J	530	TYR
2	L	137	PHE
2	L	176	LYS
2	L	538	VAL
2	L	540	LEU
2	L	541	SER
3	M	5	VAL
3	M	76	ASP
3	M	104	TYR
3	M	219	THR
4	N	36	TYR
4	N	90	GLN
4	N	109	THR
3	O	76	ASP
3	O	104	TYR
3	O	203	LEU
3	Q	76	ASP
3	Q	107	ASN
3	Q	164	VAL
3	Q	219	THR
4	R	90	GLN
4	R	109	THR
3	S	17	SER
3	S	30	ASP
3	S	76	ASP
4	T	90	GLN
4	T	109	THR
4	T	152	ASN
3	U	5	VAL
3	U	76	ASP
3	U	107	ASN
3	U	219	THR
4	V	90	GLN
4	V	152	ASN
3	W	55	THR
3	W	76	ASP

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Mol	Chain	Res	Type
4	X	90	GLN
4	X	152	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	500	ASN
2	H	462	GLN
4	R	152	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	PCA	A	26	1	7,8,9	1.79	1 (14%)	9,10,12	2.31	5 (55%)
1	PCA	E	26	1	7,8,9	1.80	1 (14%)	9,10,12	2.12	5 (55%)
1	PCA	C	26	1,2	7,8,9	1.82	1 (14%)	9,10,12	2.06	5 (55%)
1	PCA	I	26	1	7,8,9	1.83	1 (14%)	9,10,12	2.19	6 (66%)
1	PCA	G	26	1	7,8,9	1.84	1 (14%)	9,10,12	2.18	5 (55%)
1	PCA	K	26	1	7,8,9	1.82	1 (14%)	9,10,12	2.27	5 (55%)

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
1	PCA	A	26	1	-	0/0/11/13	0/1/1/1
1	PCA	E	26	1	-	0/0/11/13	0/1/1/1
1	PCA	C	26	1,2	-	0/0/11/13	0/1/1/1
1	PCA	I	26	1	-	0/0/11/13	0/1/1/1
1	PCA	G	26	1	-	0/0/11/13	0/1/1/1
1	PCA	K	26	1	-	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	26	PCA	CD-N	4.75	1.47	1.34
1	I	26	PCA	CD-N	4.73	1.47	1.34
1	K	26	PCA	CD-N	4.71	1.47	1.34
1	C	26	PCA	CD-N	4.67	1.46	1.34
1	E	26	PCA	CD-N	4.64	1.46	1.34
1	A	26	PCA	CD-N	4.58	1.46	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PCA	CB-CA-C	-3.47	107.93	112.70
1	K	26	PCA	OE-CD-CG	-3.24	121.11	126.76
1	A	26	PCA	OE-CD-CG	-3.22	121.15	126.76
1	I	26	PCA	OE-CD-CG	-3.15	121.27	126.76
1	K	26	PCA	CA-N-CD	-3.13	102.87	113.58
1	G	26	PCA	OE-CD-CG	-3.10	121.36	126.76
1	G	26	PCA	CB-CA-C	-2.99	108.59	112.70
1	C	26	PCA	CA-N-CD	-2.95	103.46	113.58
1	I	26	PCA	CA-N-CD	-2.95	103.46	113.58
1	A	26	PCA	CA-N-CD	-2.94	103.51	113.58
1	E	26	PCA	OE-CD-CG	-2.92	121.66	126.76
1	K	26	PCA	CB-CA-N	2.91	111.65	103.30
1	E	26	PCA	CA-N-CD	-2.90	103.64	113.58
1	G	26	PCA	CA-N-CD	-2.86	103.77	113.58
1	C	26	PCA	OE-CD-CG	-2.79	121.89	126.76
1	E	26	PCA	CB-CA-C	-2.75	108.92	112.70
1	C	26	PCA	CB-CA-N	2.75	111.19	103.30
1	I	26	PCA	CB-CA-N	2.71	111.07	103.30
1	E	26	PCA	CB-CA-N	2.68	110.98	103.30
1	A	26	PCA	CG-CD-N	2.63	115.19	108.39
1	K	26	PCA	O-C-CA	-2.57	118.04	124.78
1	K	26	PCA	CG-CD-N	2.54	114.96	108.39
1	G	26	PCA	CB-CA-N	2.52	110.54	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PCA	CB-CA-N	2.52	110.53	103.30
1	I	26	PCA	O-C-CA	-2.43	118.41	124.78
1	G	26	PCA	CG-CD-N	2.40	114.61	108.39
1	I	26	PCA	CG-CD-N	2.38	114.56	108.39
1	C	26	PCA	CG-CD-N	2.37	114.53	108.39
1	E	26	PCA	CG-CD-N	2.31	114.38	108.39
1	C	26	PCA	CB-CA-C	-2.20	109.67	112.70
1	I	26	PCA	CB-CA-C	-2.06	109.87	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	26	PCA	1	0
1	I	26	PCA	1	0

## 5.5 Carbohydrates [i](#)

24 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
5	NAG	Y	1	5,1	14,14,15	0.72	0	17,19,21	0.51	0
5	NAG	Y	2	5	14,14,15	0.27	0	17,19,21	0.49	0
5	BMA	Y	3	5	11,11,12	1.29	1 (9%)	15,15,17	0.95	0
5	MAN	Y	4	5	11,11,12	1.32	2 (18%)	15,15,17	1.41	2 (13%)
5	NAG	Z	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.51	0
5	NAG	Z	2	5	14,14,15	0.25	0	17,19,21	0.54	0
5	BMA	Z	3	5	11,11,12	1.11	1 (9%)	15,15,17	0.91	0
5	MAN	Z	4	5	11,11,12	1.03	0	15,15,17	1.25	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	a	1	5,1	14,14,15	0.78	1 (7%)	17,19,21	0.45	0
5	NAG	a	2	5	14,14,15	0.31	0	17,19,21	0.59	0
5	BMA	a	3	5	11,11,12	1.03	1 (9%)	15,15,17	0.91	0
5	MAN	a	4	5	11,11,12	1.18	2 (18%)	15,15,17	1.54	2 (13%)
5	NAG	b	1	5,1	14,14,15	0.58	0	17,19,21	0.42	0
5	NAG	b	2	5	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
5	BMA	b	3	5	11,11,12	1.51	2 (18%)	15,15,17	1.27	2 (13%)
5	MAN	b	4	5	11,11,12	1.20	2 (18%)	15,15,17	1.44	2 (13%)
5	NAG	c	1	5,1	14,14,15	0.83	1 (7%)	17,19,21	0.62	0
5	NAG	c	2	5	14,14,15	0.42	0	17,19,21	0.46	0
5	BMA	c	3	5	11,11,12	1.06	1 (9%)	15,15,17	0.85	0
5	MAN	c	4	5	11,11,12	1.12	1 (9%)	15,15,17	1.40	2 (13%)
5	NAG	d	1	5,1	14,14,15	0.97	2 (14%)	17,19,21	0.63	0
5	NAG	d	2	5	14,14,15	0.38	0	17,19,21	0.51	0
5	BMA	d	3	5	11,11,12	1.28	2 (18%)	15,15,17	0.96	0
5	MAN	d	4	5	11,11,12	1.40	2 (18%)	15,15,17	1.43	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	1/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Z	4	5	-	1/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	1/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
5	MAN	a	4	5	-	1/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
5	MAN	b	4	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	c	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	c	2	5	-	1/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
5	MAN	c	4	5	-	1/2/19/22	0/1/1/1
5	NAG	d	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	BMA	d	3	5	-	1/2/19/22	0/1/1/1
5	MAN	d	4	5	-	1/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	b	3	BMA	C1-C2	3.95	1.61	1.52
5	d	3	BMA	C1-C2	3.19	1.59	1.52
5	d	4	MAN	C1-C2	3.11	1.59	1.52
5	Y	3	BMA	C1-C2	3.09	1.59	1.52
5	c	3	BMA	C1-C2	2.78	1.58	1.52
5	b	4	MAN	C1-C2	2.76	1.58	1.52
5	d	4	MAN	C2-C3	2.74	1.56	1.52
5	c	4	MAN	C1-C2	2.72	1.58	1.52
5	a	4	MAN	C2-C3	2.69	1.56	1.52
5	Y	4	MAN	C1-C2	2.69	1.58	1.52
5	Y	4	MAN	C2-C3	2.64	1.56	1.52
5	d	1	NAG	O5-C1	-2.57	1.39	1.43
5	Z	3	BMA	C1-C2	2.55	1.58	1.52
5	b	3	BMA	C2-C3	2.38	1.56	1.52
5	a	3	BMA	C1-C2	2.30	1.57	1.52
5	d	3	BMA	C2-C3	2.26	1.55	1.52
5	d	1	NAG	C1-C2	2.17	1.55	1.52
5	a	4	MAN	C1-C2	2.16	1.57	1.52
5	Z	1	NAG	O5-C1	-2.06	1.40	1.43
5	c	1	NAG	C1-C2	2.06	1.55	1.52
5	b	4	MAN	C2-C3	2.04	1.55	1.52
5	a	1	NAG	O5-C1	-2.00	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	4	MAN	C1-O5-C5	3.87	117.43	112.19
5	c	4	MAN	C1-O5-C5	3.51	116.95	112.19
5	Y	4	MAN	C1-O5-C5	3.43	116.84	112.19
5	d	4	MAN	C1-O5-C5	3.43	116.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	4	MAN	C1-O5-C5	3.42	116.83	112.19
5	Z	4	MAN	C1-O5-C5	3.38	116.77	112.19
5	b	3	BMA	C1-O5-C5	3.26	116.60	112.19
5	b	2	NAG	O4-C4-C3	-2.89	103.67	110.35
5	c	4	MAN	O2-C2-C3	-2.37	105.39	110.14
5	b	3	BMA	O3-C3-C2	2.20	114.20	109.99
5	b	4	MAN	O2-C2-C3	-2.12	105.90	110.14
5	a	4	MAN	C1-C2-C3	2.11	112.25	109.67
5	Y	4	MAN	C1-C2-C3	2.07	112.21	109.67

There are no chirality outliers.

All (22) torsion outliers are listed below:

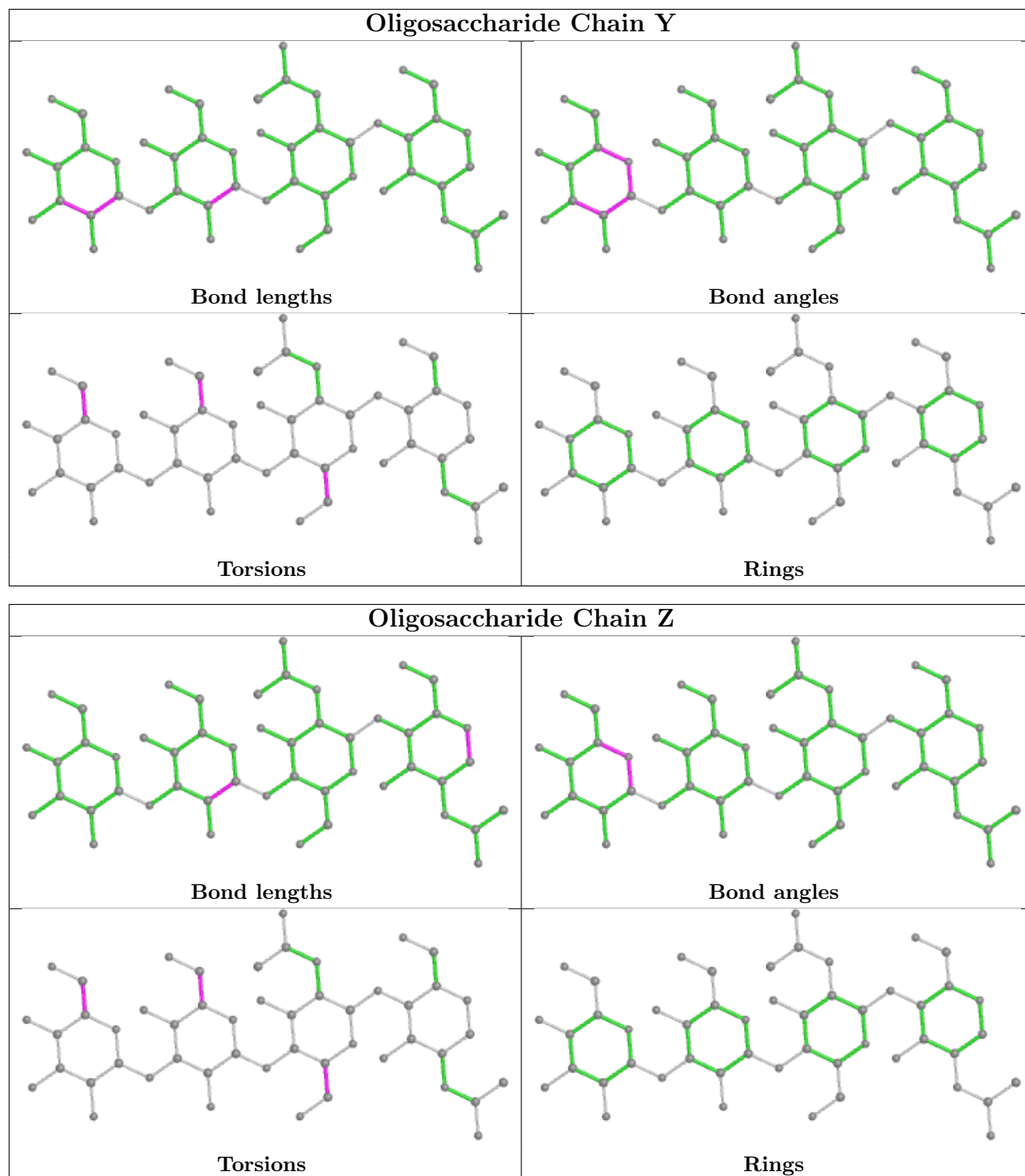
Mol	Chain	Res	Type	Atoms
5	c	1	NAG	C4-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	a	4	MAN	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	Y	4	MAN	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
5	d	4	MAN	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
5	Z	4	MAN	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
5	c	4	MAN	O5-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6
5	c	1	NAG	C1-C2-N2-C7

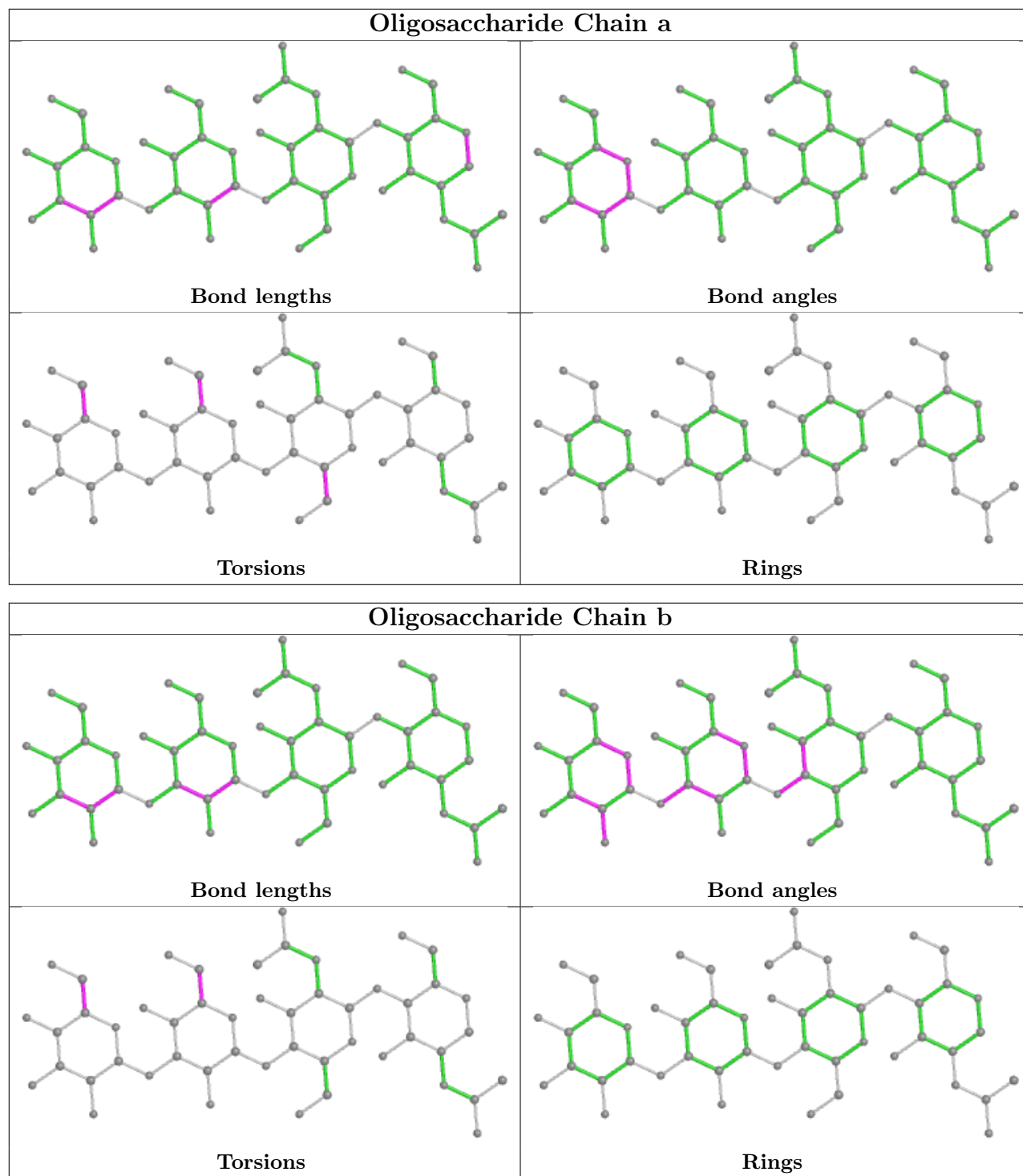
There are no ring outliers.

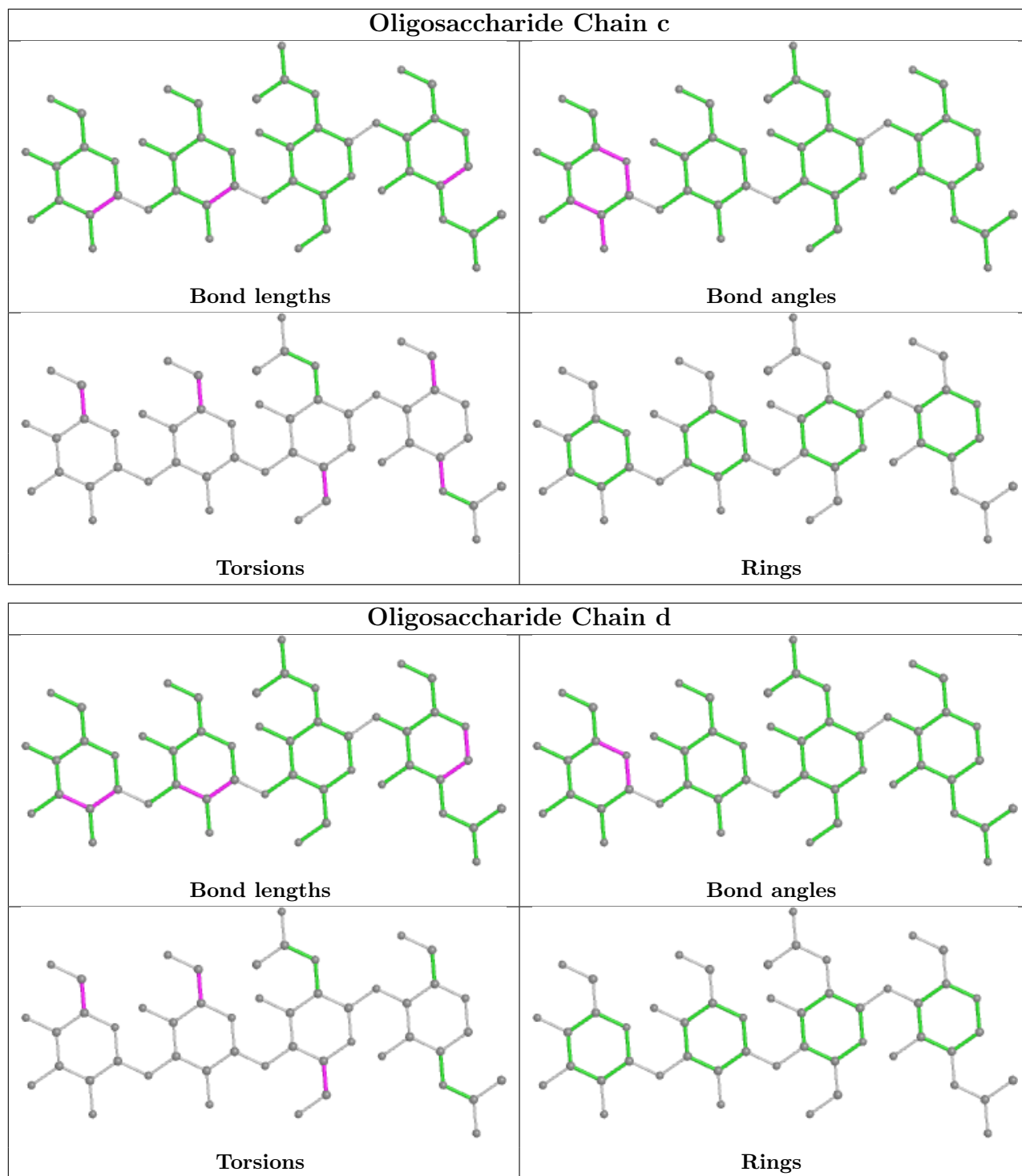
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Z	1	NAG	1	0
5	Z	2	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](#)

4 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
6	NAG	B	1001	2	14,14,15	0.38	0	17,19,21	0.51	0
6	NAG	L	1001	2	14,14,15	0.51	0	17,19,21	0.60	0
6	NAG	J	1001	2	14,14,15	0.52	0	17,19,21	0.41	0
6	NAG	F	1001	-	14,14,15	0.28	0	17,19,21	0.48	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
6	NAG	B	1001	2	-	3/6/23/26	0/1/1/1
6	NAG	L	1001	2	-	1/6/23/26	0/1/1/1
6	NAG	J	1001	2	-	2/6/23/26	0/1/1/1
6	NAG	F	1001	-	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1001	NAG	O5-C5-C6-O6
6	B	1001	NAG	C4-C5-C6-O6
6	F	1001	NAG	O5-C5-C6-O6
6	J	1001	NAG	O5-C5-C6-O6
6	B	1001	NAG	C3-C2-N2-C7
6	L	1001	NAG	C3-C2-N2-C7
6	J	1001	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	72/84 (85%)	-0.08	2 (2%) 53 51	57, 89, 118, 123	0
1	C	75/84 (89%)	-0.01	1 (1%) 77 76	61, 88, 124, 127	0
1	E	72/84 (85%)	-0.22	0 100 100	54, 96, 122, 124	0
1	G	75/84 (89%)	0.01	3 (4%) 38 37	59, 96, 126, 137	0
1	I	77/84 (91%)	-0.15	3 (3%) 39 38	60, 95, 125, 129	0
1	K	69/84 (82%)	-0.07	1 (1%) 75 74	67, 93, 122, 134	0
2	B	404/414 (97%)	-0.33	2 (0%) 91 90	55, 70, 109, 130	0
2	D	404/414 (97%)	-0.36	0 100 100	61, 75, 110, 131	0
2	F	401/414 (96%)	-0.40	0 100 100	52, 75, 109, 122	0
2	H	395/414 (95%)	-0.39	1 (0%) 94 93	55, 80, 120, 131	0
2	J	389/414 (93%)	-0.38	2 (0%) 91 90	60, 77, 118, 130	0
2	L	396/414 (95%)	-0.29	1 (0%) 94 93	64, 80, 123, 133	0
3	M	225/231 (97%)	-0.45	0 100 100	56, 70, 79, 100	0
3	O	224/231 (96%)	-0.42	0 100 100	65, 71, 79, 95	1 (0%)
3	Q	229/231 (99%)	-0.41	0 100 100	55, 78, 93, 96	0
3	S	224/231 (96%)	-0.46	0 100 100	53, 58, 69, 83	0
3	U	215/231 (93%)	0.23	9 (4%) 36 35	74, 115, 150, 152	0
3	W	225/231 (97%)	-0.49	1 (0%) 92 92	64, 71, 81, 103	1 (0%)
4	N	213/214 (99%)	-0.40	0 100 100	55, 69, 85, 96	0
4	P	213/214 (99%)	-0.36	0 100 100	71, 81, 90, 93	0
4	R	213/214 (99%)	-0.38	0 100 100	61, 79, 92, 95	0
4	T	213/214 (99%)	-0.49	0 100 100	56, 65, 72, 79	0
4	V	209/214 (97%)	0.14	5 (2%) 59 57	91, 124, 152, 156	0
4	X	213/214 (99%)	-0.41	0 100 100	64, 72, 88, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5445/5658 (96%)	-0.32	31 (0%) 89   89	52, 75, 123, 156	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	103	THR	4.8
1	C	103	THR	4.4
2	B	211	SER	3.8
1	G	102	ALA	3.6
4	V	161	GLU	3.5
4	V	175	LEU	3.5
3	U	127	SER	3.1
1	I	103	THR	3.1
3	U	207	THR	3.0
3	U	196	VAL	2.9
2	J	541	SER	2.8
1	I	101	PRO	2.8
1	I	102	ALA	2.8
2	L	210	GLN	2.7
3	W	230	CYS	2.6
3	U	149	THR	2.6
1	A	103	THR	2.6
1	G	101	PRO	2.5
2	B	509	SER	2.4
3	U	205	THR	2.4
3	U	87	SER	2.4
4	V	11	LEU	2.4
3	U	126	SER	2.4
3	U	150	ALA	2.3
2	J	215	SER	2.3
3	U	134	SER	2.3
4	V	165	GLU	2.3
4	V	193	ALA	2.3
1	K	65	LYS	2.2
2	H	207	LEU	2.1
1	A	71	GLY	2.1

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

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

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

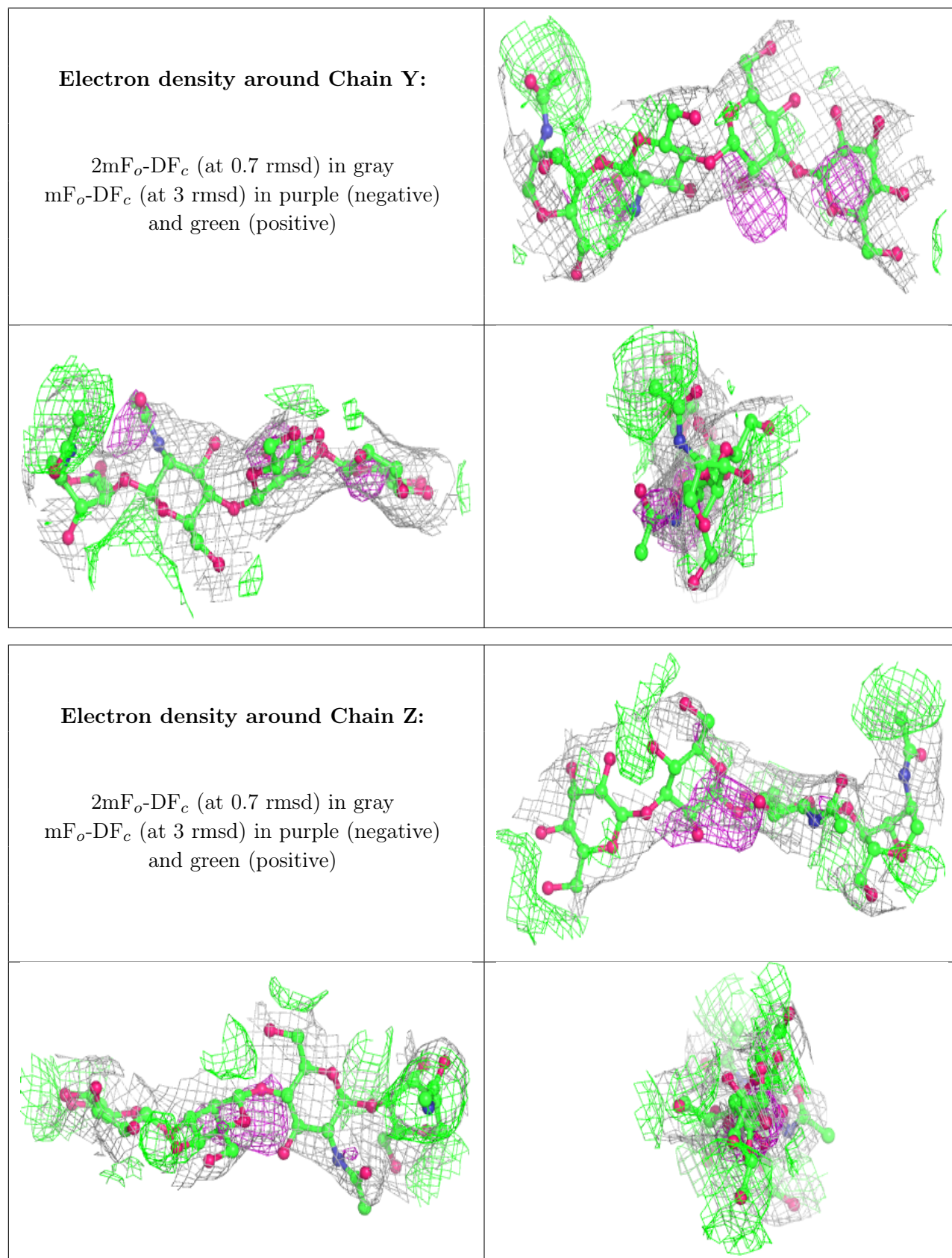
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	I	26	8/9	0.81	0.45	97,98,99,99	0
1	PCA	E	26	8/9	0.86	0.22	81,81,82,82	0
1	PCA	G	26	8/9	0.89	0.39	76,77,78,78	0
1	PCA	C	26	8/9	0.92	0.25	76,76,77,77	0
1	PCA	A	26	8/9	0.92	0.27	68,70,71,72	0
1	PCA	K	26	8/9	0.93	0.27	79,79,80,81	0

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

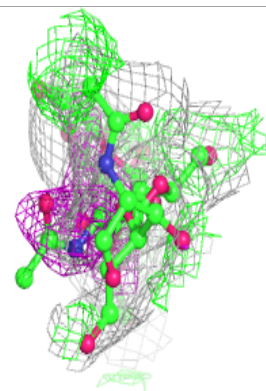
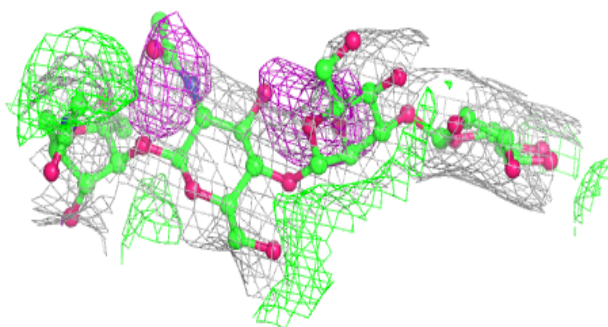
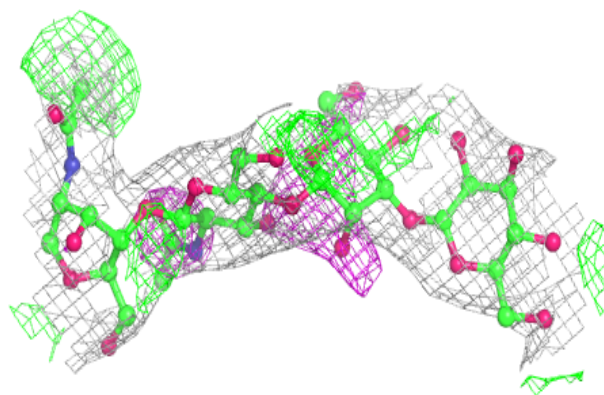
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BMA	Z	3	11/12	0.71	0.24	90,92,93,94	0
5	MAN	a	4	11/12	0.73	0.20	82,84,85,85	0
5	NAG	a	2	14/15	0.74	0.32	85,88,88,89	0
5	BMA	Y	3	11/12	0.74	0.21	84,85,86,86	0
5	BMA	b	3	11/12	0.74	0.25	77,80,82,82	0
5	MAN	Y	4	11/12	0.75	0.26	83,84,85,85	0
5	MAN	d	4	11/12	0.75	0.25	86,87,88,88	0
5	NAG	Z	2	14/15	0.76	0.30	92,93,94,94	0
5	MAN	c	4	11/12	0.77	0.28	117,118,119,119	0
5	NAG	Y	1	14/15	0.77	0.20	81,85,86,86	0
5	BMA	a	3	11/12	0.78	0.30	84,85,87,88	0
5	NAG	c	2	14/15	0.79	0.27	114,115,115,116	0
5	NAG	d	2	14/15	0.81	0.28	89,92,94,94	0
5	BMA	d	3	11/12	0.81	0.23	89,90,91,91	0
5	MAN	b	4	11/12	0.81	0.17	75,77,77,78	0
5	NAG	b	2	14/15	0.82	0.24	79,81,81,82	0
5	BMA	c	3	11/12	0.83	0.28	116,118,118,118	0
5	NAG	a	1	14/15	0.84	0.17	83,86,88,88	0
5	NAG	Z	1	14/15	0.84	0.16	85,88,90,90	0
5	NAG	b	1	14/15	0.84	0.17	76,79,80,80	0
5	NAG	d	1	14/15	0.85	0.15	87,91,93,93	0
5	NAG	Y	2	14/15	0.86	0.21	86,87,88,88	0
5	NAG	c	1	14/15	0.87	0.15	104,108,109,109	0
5	MAN	Z	4	11/12	0.87	0.14	88,90,90,91	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.

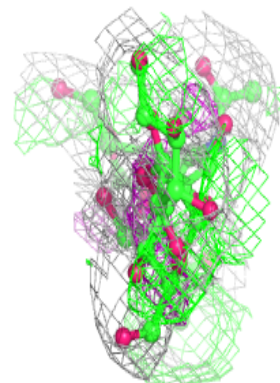
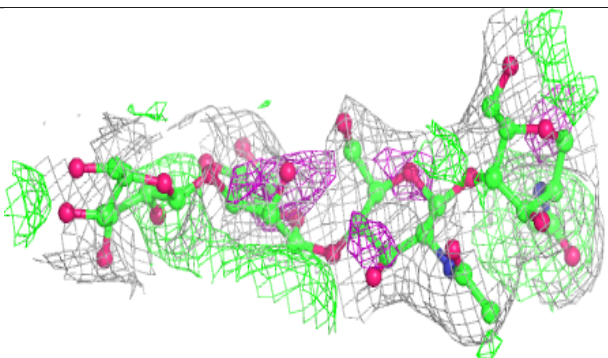
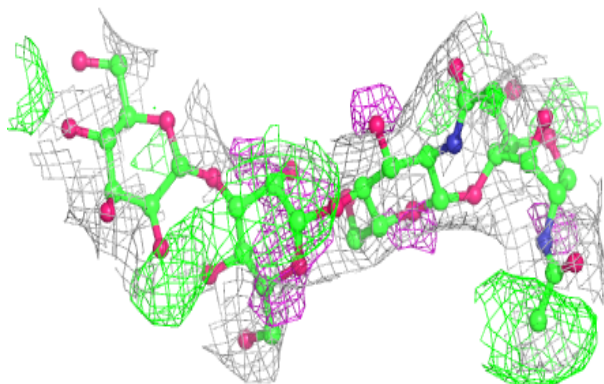


**Electron density around Chain a:**

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

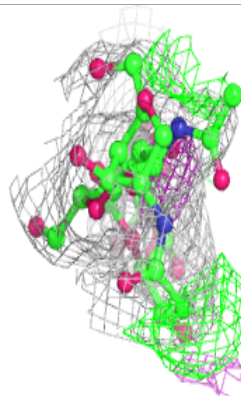
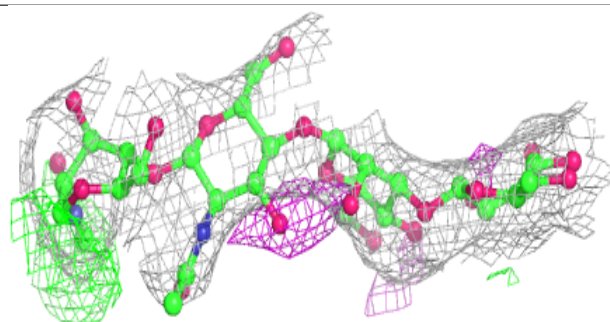
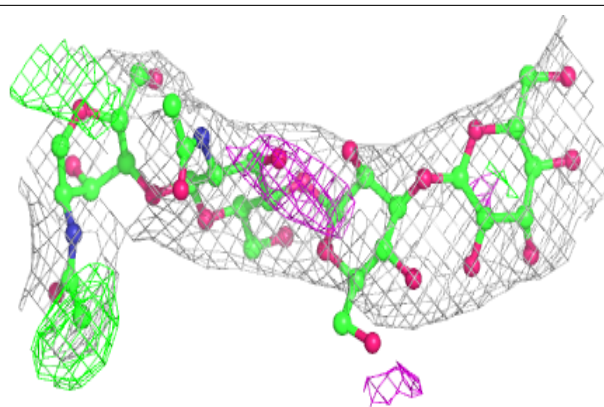
**Electron density around Chain b:**

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

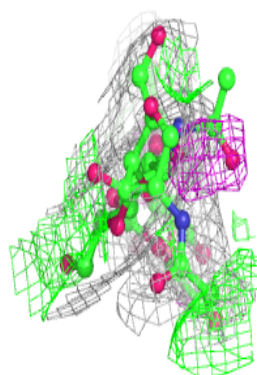
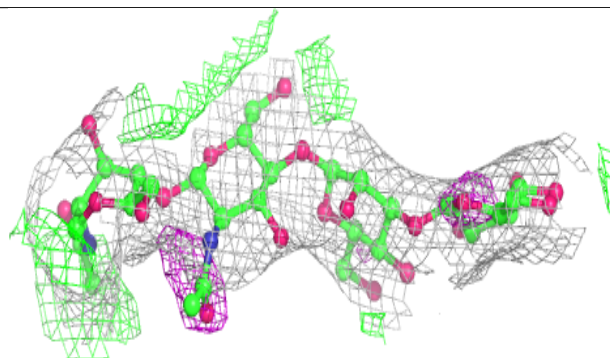
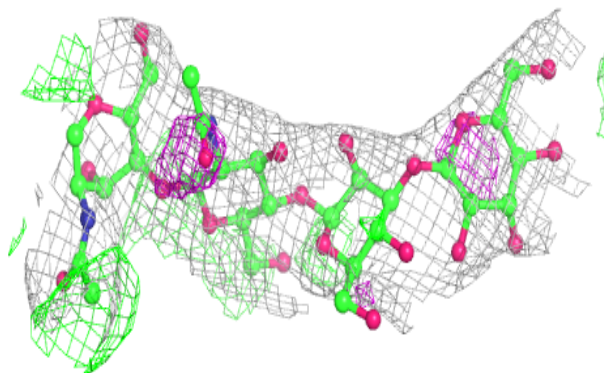


**Electron density around Chain c:**

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

**Electron density around Chain d:**

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



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	F	1001	14/15	0.78	0.27	100,102,103,103	0
6	NAG	L	1001	14/15	0.81	0.30	105,107,107,107	0
6	NAG	J	1001	14/15	0.82	0.23	92,94,95,95	0
6	NAG	B	1001	14/15	0.85	0.22	100,101,101,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.