



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 01:25 AM UTC

PDB ID : 3NGB / pdb_00003ngb
Title : Crystal structure of broadly and potently neutralizing antibody VRC01 in complex with HIV-1 gp120
Authors : Zhou, T.; Kwong, P.D.
Deposited on : 2010-06-11
Resolution : 2.68 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

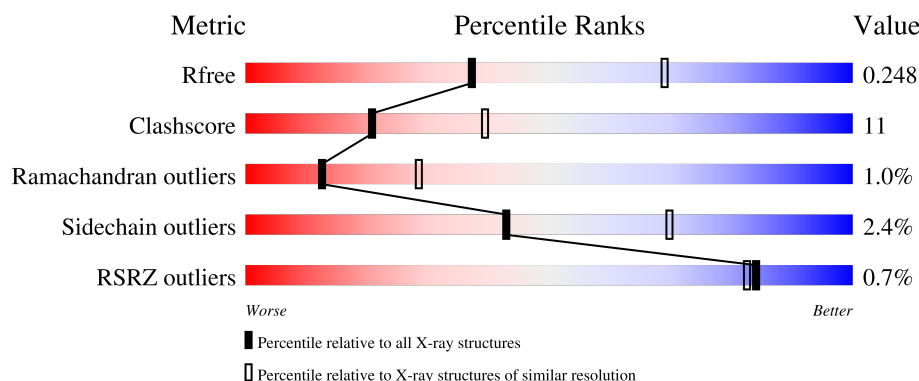
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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.



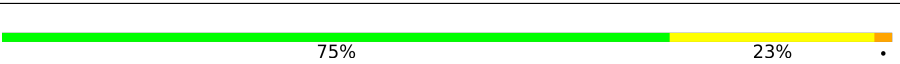
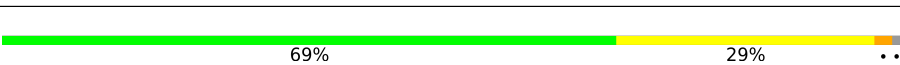
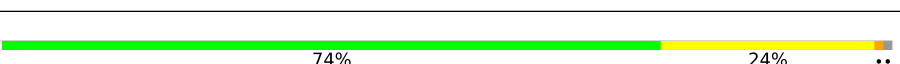
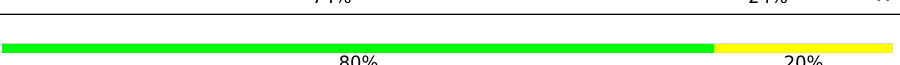
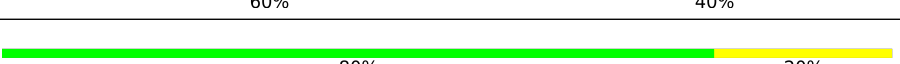
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	353	% 73% 24% ..
1	D	353	% 73% 24% ..
1	G	353	% 75% 22% ..
1	I	353	% 76% 22% ..
2	B	224	74% 26%

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Mol	Chain	Length	Quality of chain
2	E	224	
2	H	224	
2	J	224	
3	C	210	
3	F	210	
3	K	210	
3	L	210	
4	M	5	
4	N	5	
4	P	5	
5	O	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25808 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	347	Total	C	N	O	S	0	0	0
			2713	1700	472	518	23			
1	A	349	Total	C	N	O	S	0	0	0
			2723	1705	474	521	23			
1	D	350	Total	C	N	O	S	0	0	0
			2727	1707	475	522	23			
1	I	349	Total	C	N	O	S	0	0	0
			2721	1704	474	520	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
A	124	GLY	-	linker	UNP Q0ED31
A	198	GLY	-	linker	UNP Q0ED31
A	318	GLY	-	linker	UNP Q0ED31
A	319	GLY	-	linker	UNP Q0ED31
A	320	SER	-	linker	UNP Q0ED31
A	321	GLY	-	linker	UNP Q0ED31
A	322	SER	-	linker	UNP Q0ED31
A	323	GLY	-	linker	UNP Q0ED31
D	124	GLY	-	linker	UNP Q0ED31
D	198	GLY	-	linker	UNP Q0ED31
D	318	GLY	-	linker	UNP Q0ED31
D	319	GLY	-	linker	UNP Q0ED31
D	320	SER	-	linker	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	321	GLY	-	linker	UNP Q0ED31
D	322	SER	-	linker	UNP Q0ED31
D	323	GLY	-	linker	UNP Q0ED31
I	124	GLY	-	linker	UNP Q0ED31
I	198	GLY	-	linker	UNP Q0ED31
I	302	GLY	-	linker	UNP Q0ED31
I	319	GLY	-	linker	UNP Q0ED31
I	320	SER	-	linker	UNP Q0ED31
I	321	GLY	-	linker	UNP Q0ED31
I	322	SER	-	linker	UNP Q0ED31
I	323	GLY	-	linker	UNP Q0ED31

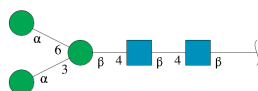
- Molecule 2 is a protein called Antigen binding fragment of heavy chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	B	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	E	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	J	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			

- Molecule 3 is a protein called Antigen binding fragment of light chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1615	1011	277	322	5			
3	C	210	Total	C	N	O	S	0	0	0
			1632	1022	279	326	5			
3	F	208	Total	C	N	O	S	0	0	0
			1615	1011	277	322	5			
3	K	210	Total	C	N	O	S	0	0	0
			1632	1022	279	326	5			

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



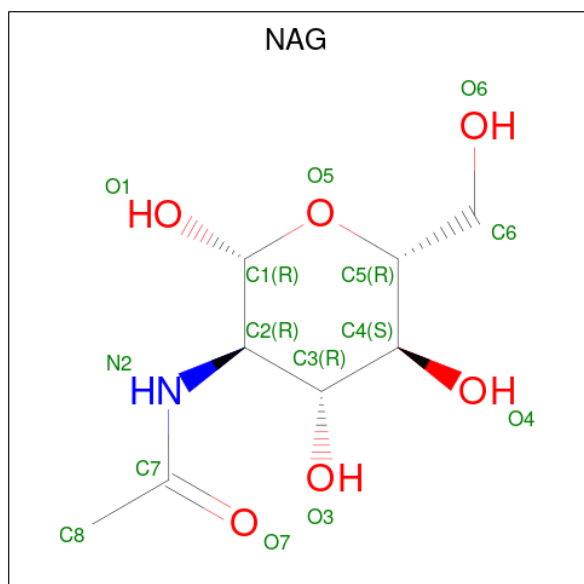
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

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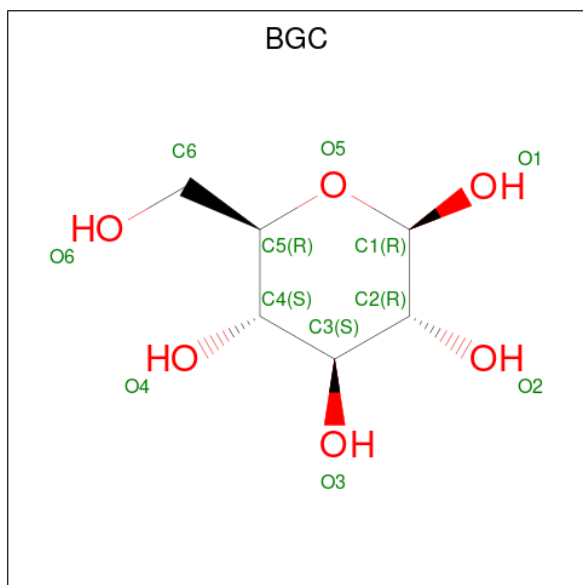
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1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

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

- Molecule 7 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



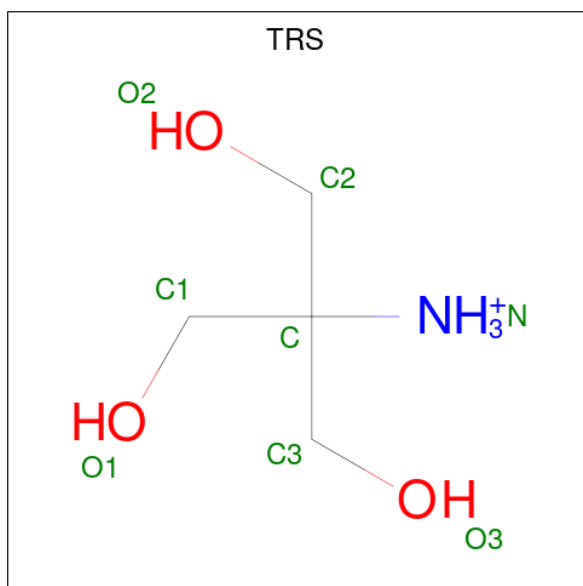
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			12	6	6		
7	A	1	Total	C	O	0	0
			12	6	6		
7	A	1	Total	C	O	0	0
			12	6	6		
7	A	1	Total	C	O	0	0
			12	6	6		
7	A	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		
7	C	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			12	6	6		
7	E	1	Total	C	O	0	0
			12	6	6		
7	I	1	Total	C	O	0	0
			12	6	6		
7	I	1	Total	C	O	0	0
			12	6	6		
7	J	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			8	4	1	3		
8	A	1	Total	C	N	O	0	0
			8	4	1	3		
8	D	1	Total	C	N	O	0	0
			8	4	1	3		
8	D	1	Total	C	N	O	0	0
			8	4	1	3		
8	I	1	Total	C	N	O	0	0
			8	4	1	3		
8	J	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	K	1	Total	C	N	O	0	0
			8	4	1	3		

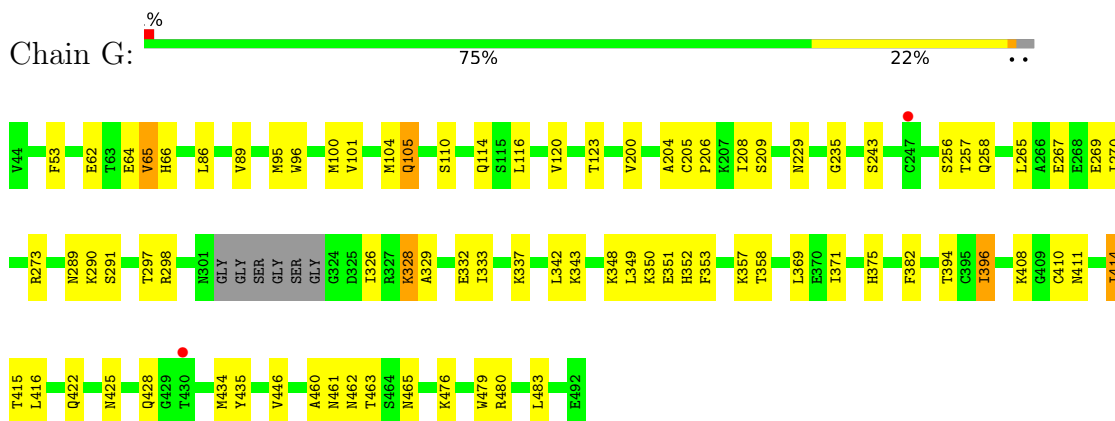
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	66	Total	O	0	0
			66	66		
9	H	53	Total	O	0	0
			53	53		
9	L	43	Total	O	0	0
			43	43		
9	A	89	Total	O	0	0
			89	89		
9	B	45	Total	O	0	0
			45	45		
9	C	33	Total	O	0	0
			33	33		
9	D	55	Total	O	0	0
			55	55		
9	E	32	Total	O	0	0
			32	32		
9	F	8	Total	O	0	0
			8	8		
9	I	44	Total	O	0	0
			44	44		
9	J	24	Total	O	0	0
			24	24		
9	K	31	Total	O	0	0
			31	31		

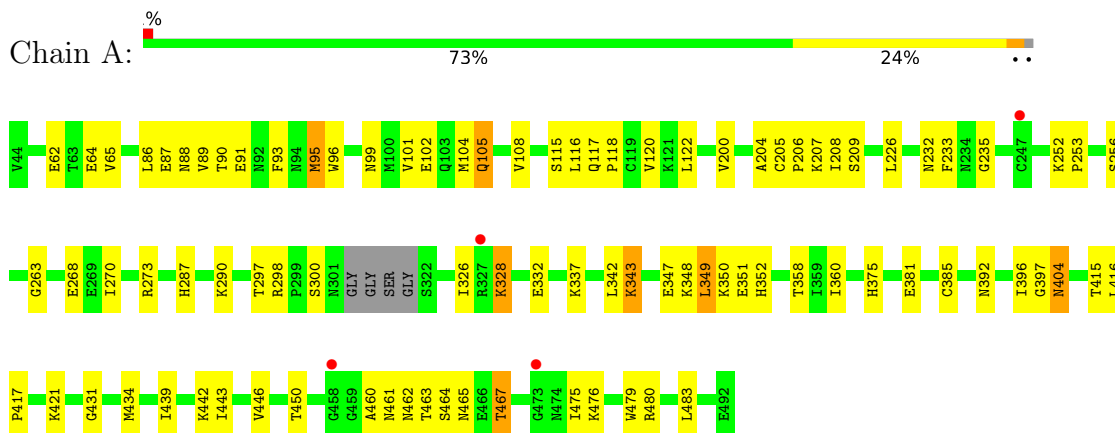
3 Residue-property plots

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.

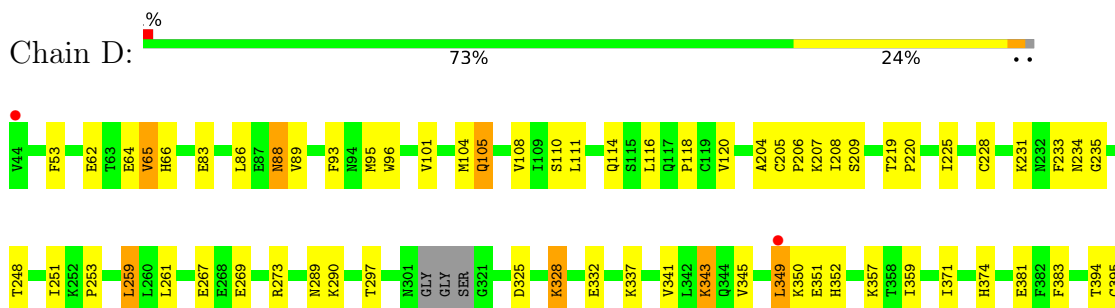
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

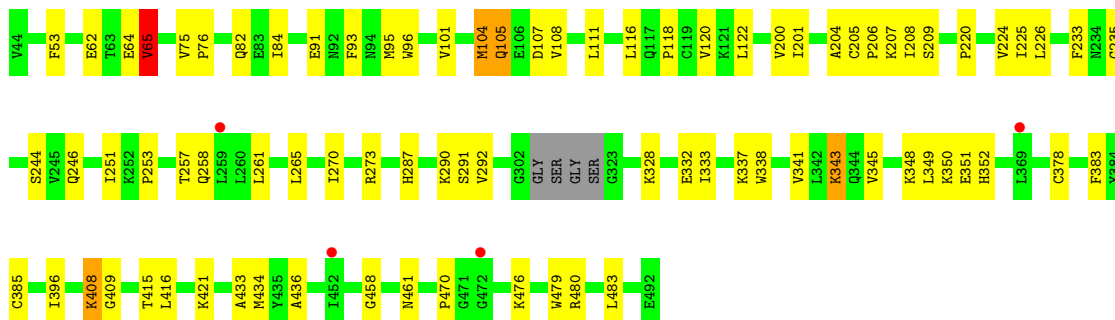
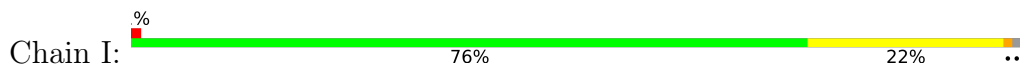


- Molecule 1: Envelope glycoprotein gp160

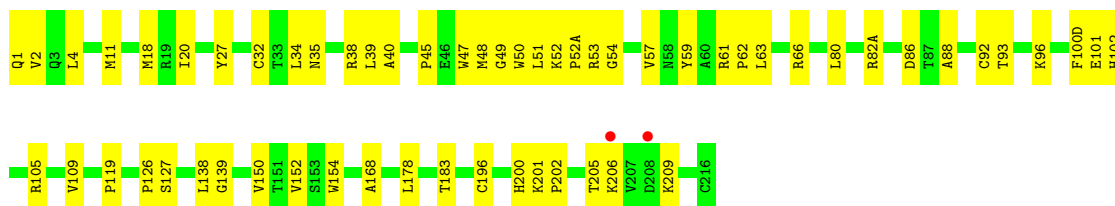
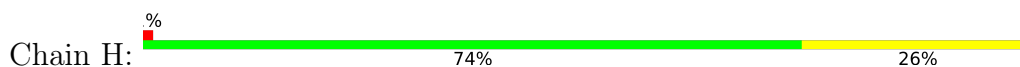




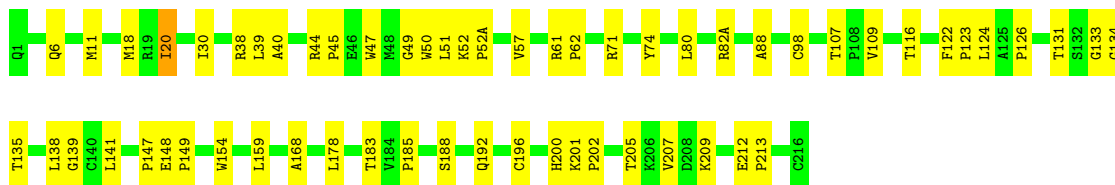
- Molecule 1: Envelope glycoprotein gp160



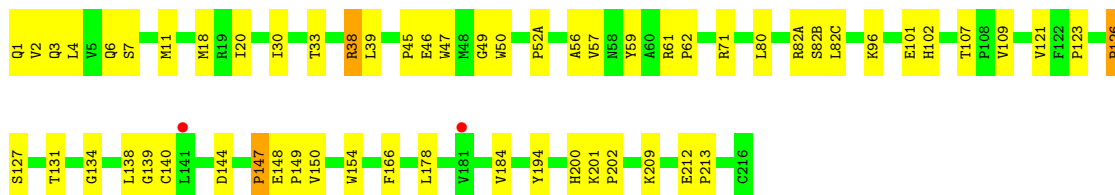
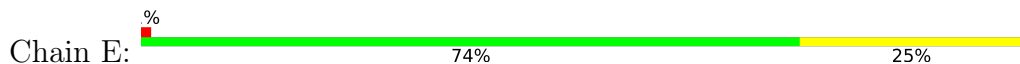
- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01



- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

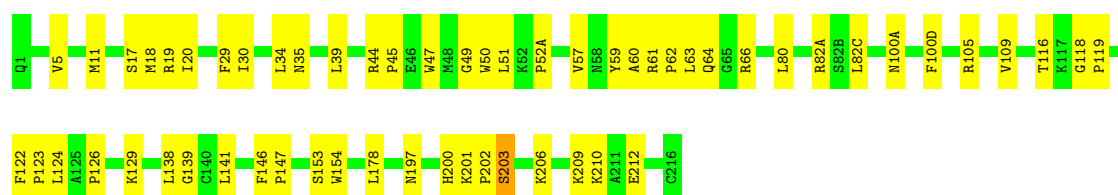


- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01



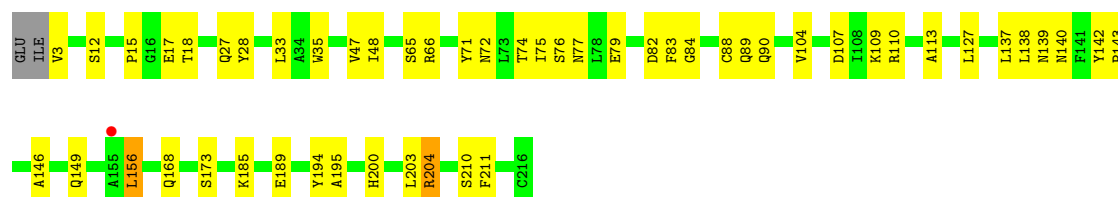
- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

Chain J:  74% 25%



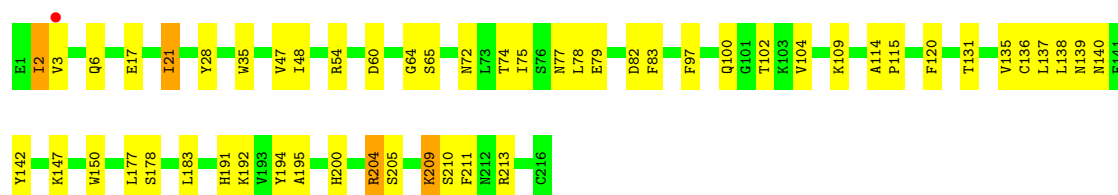
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01

Chain L:  74% 24% ..



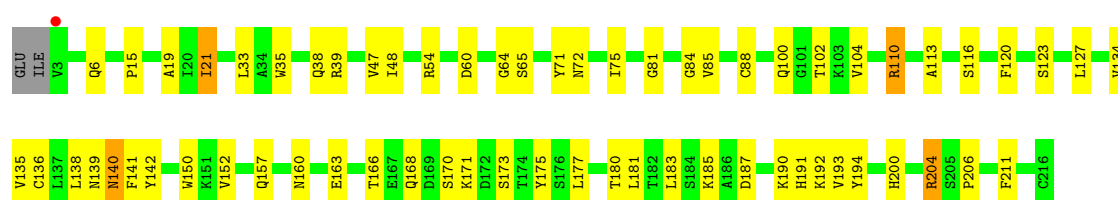
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01

Chain C:  75% 23% .



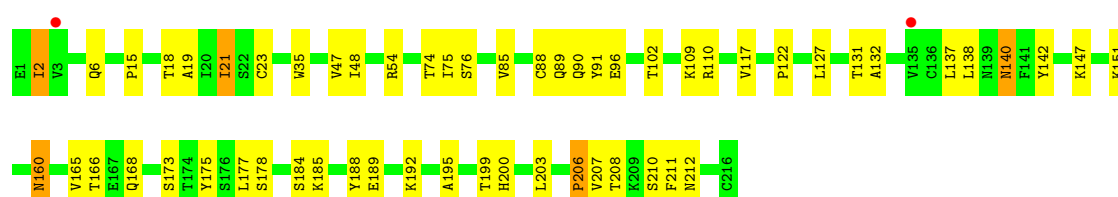
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01

Chain F:  69% 29% ..



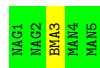
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01

Chain K:  73% 25% .



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

Chain M:  80% 20%



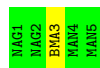
• Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain N:  60% 40%



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

Chain P:  80% 20%



• Molecule 5: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain O:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.63Å 98.28Å 205.26Å 90.00° 99.68° 90.00°	Depositor
Resolution (Å)	49.73 – 2.68 49.73 – 2.68	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.73-2.68) 81.3 (49.73-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.197 , 0.256 0.189 , 0.248	Depositor DCC
R_{free} test set	4868 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.2	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25808	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

¹Theoretical 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: BGC, BMA, TRS, 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	0.26	0/2780	0.70	0/3773
1	D	0.25	0/2784	0.68	1/3778 (0.0%)
1	G	0.26	0/2770	0.71	0/3760
1	I	0.26	0/2778	0.69	1/3770 (0.0%)
2	B	0.26	0/1755	0.70	0/2387
2	E	0.26	0/1755	0.69	0/2387
2	H	0.26	0/1755	0.70	0/2387
2	J	0.26	0/1755	0.69	0/2387
3	C	0.25	0/1669	0.66	0/2265
3	F	0.24	0/1652	0.68	0/2242
3	K	0.26	0/1669	0.68	0/2265
3	L	0.25	0/1652	0.68	0/2242
All	All	0.26	0/24774	0.69	2/33643 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	VAL	N-CA-C	5.28	115.90	110.36
1	D	65	VAL	N-CA-C	5.23	115.85	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2723	0	2649	60	0
1	D	2727	0	2652	63	0
1	G	2713	0	2642	56	0
1	I	2721	0	2648	64	0
2	B	1710	0	1680	49	0
2	E	1710	0	1680	37	0
2	H	1710	0	1680	40	0
2	J	1710	0	1680	45	0
3	C	1632	0	1573	40	0
3	F	1615	0	1553	44	0
3	K	1632	0	1573	41	0
3	L	1615	0	1553	37	0
4	M	61	0	52	0	0
4	N	61	0	52	1	0
4	P	61	0	52	0	0
5	O	28	0	25	1	0
6	A	168	0	156	2	0
6	D	168	0	156	1	0
6	G	154	0	143	1	0
6	I	154	0	142	1	0
7	A	48	0	48	6	0
7	B	24	0	24	1	0
7	C	12	0	12	0	0
7	D	12	0	12	0	0
7	E	12	0	12	0	0
7	G	12	0	12	1	0
7	I	24	0	24	1	0
7	J	12	0	12	1	0
8	A	16	0	24	0	0
8	D	16	0	24	1	0
8	I	8	0	12	2	0
8	J	8	0	12	0	0
8	K	8	0	12	1	0
9	A	89	0	0	1	0
9	B	45	0	0	1	0
9	C	33	0	0	2	0
9	D	55	0	0	0	0
9	E	32	0	0	1	0
9	F	8	0	0	0	0
9	G	66	0	0	2	0
9	H	53	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	44	0	0	2	0
9	J	24	0	0	2	0
9	K	31	0	0	0	0
9	L	43	0	0	1	0
All	All	25808	0	24581	553	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 (553) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:GLN:HG3	1:G:476:LYS:HG2	1.47	0.96
1:G:104:MET:HE3	1:G:479:TRP:HB3	1.51	0.91
1:A:342:LEU:HD23	1:A:396:ILE:HD11	1.54	0.88
1:I:105:GLN:HG3	1:I:476:LYS:HG2	1.56	0.87
1:G:95:MET:HE2	1:G:235:GLY:HA3	1.59	0.85
3:F:6:GLN:HE21	3:F:21:ILE:HD11	1.42	0.85
1:A:95:MET:HE2	1:A:235:GLY:HA3	1.60	0.84
2:H:11:MET:HE1	1:D:434:MET:HB2	1.60	0.83
1:A:104:MET:HE3	1:A:479:TRP:HB3	1.61	0.81
1:D:349:LEU:HB3	1:D:359:ILE:HG12	1.63	0.79
1:I:408:LYS:HG2	1:I:409:GLY:H	1.48	0.78
1:A:434:MET:HB2	2:J:11:MET:HE1	1.66	0.78
2:B:20:ILE:HD11	2:B:80:LEU:HD23	1.66	0.77
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.68	0.76
2:B:11:MET:HE1	1:I:434:MET:HB2	1.67	0.75
2:J:39:LEU:HD21	2:J:45:PRO:HG3	1.66	0.74
1:I:62:GLU:HG3	1:I:64:GLU:H	1.51	0.74
1:D:65:VAL:HG21	1:D:208:ILE:HD12	1.70	0.74
1:G:65:VAL:HG21	1:G:208:ILE:HD12	1.71	0.73
1:I:84:ILE:HB	1:I:244:SER:HB3	1.71	0.72
1:I:95:MET:HE2	1:I:235:GLY:HA3	1.70	0.72
2:J:126:PRO:HG3	2:J:138:LEU:HB3	1.73	0.70
2:H:39:LEU:HD21	2:H:45:PRO:HG3	1.71	0.70
3:F:204:ARG:H	3:F:204:ARG:HD3	1.54	0.70
7:A:517:BGC:H6C1	2:B:74:TYR:HB2	1.71	0.70
2:B:11:MET:HG2	1:I:122:LEU:HD12	1.74	0.69
2:B:126:PRO:HD2	2:B:213:PRO:HA	1.74	0.69
1:A:460:ALA:HB3	2:B:61:ARG:HD2	1.75	0.69
3:C:195:ALA:HB2	3:C:210:SER:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:GLU:HG3	1:G:64:GLU:H	1.58	0.68
1:A:95:MET:HE3	1:A:96:TRP:NE1	2.09	0.68
1:D:95:MET:HE2	1:D:235:GLY:HA3	1.76	0.68
1:A:62:GLU:HG3	1:A:64:GLU:H	1.59	0.67
3:F:163:GLU:HB3	3:F:177:LEU:HD11	1.77	0.67
1:D:95:MET:HE1	1:D:273:ARG:HB3	1.76	0.67
2:J:18:MET:HE3	2:J:82(C):LEU:HD21	1.77	0.67
2:E:126:PRO:HG3	2:E:138:LEU:HD23	1.76	0.67
1:A:350:LYS:O	1:A:351:GLU:HB3	1.96	0.66
1:A:332:GLU:HG2	1:A:415:THR:HG22	1.76	0.66
1:A:86:LEU:O	1:A:89:VAL:HG12	1.97	0.65
3:L:47:VAL:HG12	3:L:48:ILE:HG12	1.77	0.65
1:D:332:GLU:HG2	1:D:415:THR:HG22	1.77	0.65
1:G:265:LEU:HD21	1:G:291:SER:HB3	1.80	0.64
2:E:6:GLN:HE21	2:E:107:THR:HG23	1.62	0.64
1:I:204:ALA:C	1:I:206:PRO:HD3	2.21	0.64
1:I:104:MET:HE3	1:I:479:TRP:HB3	1.78	0.64
1:A:95:MET:HE3	1:A:96:TRP:CE2	2.33	0.64
2:J:35:ASN:OD1	2:J:50:TRP:HB3	1.98	0.64
1:G:204:ALA:C	1:G:206:PRO:HD3	2.23	0.64
1:D:120:VAL:HG12	1:D:434:MET:HB3	1.80	0.64
2:J:201:LYS:HB2	2:J:202:PRO:HD3	1.80	0.63
1:I:332:GLU:HG2	1:I:415:THR:HG22	1.81	0.62
1:G:332:GLU:HG2	1:G:415:THR:HG22	1.81	0.62
1:D:371:ILE:HD13	2:E:56:ALA:HB2	1.82	0.62
1:I:207:LYS:HE2	1:I:436:ALA:HB3	1.82	0.62
1:A:205:CYS:N	1:A:206:PRO:HD3	2.15	0.61
3:K:110:ARG:HD2	3:K:173:SER:HB2	1.81	0.61
3:F:187:ASP:HA	3:F:190:LYS:HE3	1.81	0.61
3:F:21:ILE:HD12	3:F:102:THR:HB	1.81	0.61
1:I:350:LYS:O	1:I:351:GLU:HB3	2.00	0.61
3:C:47:VAL:HG12	3:C:48:ILE:HG12	1.81	0.61
3:K:21:ILE:HD12	3:K:102:THR:HB	1.82	0.61
1:G:446:VAL:HG21	6:G:507:NAG:H82	1.82	0.61
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.82	0.61
1:G:105:GLN:CG	1:G:476:LYS:HG2	2.27	0.61
1:I:95:MET:HE3	1:I:96:TRP:CE2	2.36	0.61
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.36	0.60
2:J:30:ILE:HA	2:J:52(A):PRO:HB2	1.83	0.60
2:J:17:SER:OG	7:J:502:BGC:H5	2.02	0.60
1:G:105:GLN:HG3	1:G:476:LYS:CG	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:HA2	7:A:517:BGC:O4	2.02	0.60
1:I:265:LEU:HD21	1:I:291:SER:HB3	1.84	0.60
1:G:358:THR:O	1:G:465:ASN:HB2	2.02	0.60
3:F:152:VAL:HG23	3:F:157:GLN:HG3	1.83	0.59
1:D:405:GLU:O	1:D:408:LYS:HG3	2.03	0.59
2:E:61:ARG:HB2	2:E:62:PRO:HD3	1.84	0.59
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.84	0.59
1:G:342:LEU:HD23	1:G:396:ILE:HD11	1.84	0.59
1:I:246:GLN:HB2	9:I:625:HOH:O	2.02	0.58
6:A:505:NAG:H5	3:C:28:TYR:OH	2.03	0.58
1:D:350:LYS:O	1:D:351:GLU:HB3	2.03	0.58
1:G:290:LYS:HE2	1:G:337:LYS:HE3	1.85	0.58
1:I:105:GLN:HG2	1:I:479:TRP:HE1	1.67	0.57
3:C:192:LYS:HA	3:C:213:ARG:HB3	1.86	0.57
3:F:47:VAL:HG12	3:F:48:ILE:HG12	1.85	0.57
2:J:20:ILE:HD11	2:J:80:LEU:HD23	1.87	0.57
3:K:195:ALA:HA	3:K:210:SER:HB3	1.86	0.57
7:A:517:BGC:C6	2:B:74:TYR:HB2	2.34	0.57
3:F:192:LYS:HG3	3:F:193:VAL:HG23	1.86	0.57
3:K:203:LEU:HD13	3:K:207:VAL:HG23	1.87	0.57
1:A:65:VAL:HG21	1:A:208:ILE:HD12	1.85	0.57
1:D:95:MET:HE3	1:D:96:TRP:CE2	2.40	0.57
1:D:101:VAL:HG21	1:D:480:ARG:HG2	1.87	0.57
1:D:204:ALA:C	1:D:206:PRO:HD3	2.30	0.57
1:G:357:LYS:HB3	1:G:465:ASN:HA	1.86	0.57
1:A:290:LYS:HE2	1:A:337:LYS:HE3	1.86	0.57
2:E:82(A):ARG:HB3	2:E:82(A):ARG:NH1	2.20	0.57
3:K:137:LEU:C	3:K:138:LEU:HD12	2.31	0.56
2:J:63:LEU:HD23	2:J:66:ARG:HH12	1.71	0.56
3:K:117:VAL:HG22	3:K:138:LEU:HG	1.88	0.56
3:K:177:LEU:HD23	3:K:178:SER:N	2.21	0.56
1:D:207:LYS:HG2	1:D:439:ILE:HG23	1.86	0.56
2:E:148:GLU:HB3	2:E:149:PRO:HA	1.87	0.56
1:I:105:GLN:HG3	1:I:476:LYS:CG	2.33	0.56
1:G:350:LYS:O	1:G:351:GLU:HB3	2.06	0.56
2:J:18:MET:CE	2:J:109:VAL:HG11	2.36	0.56
2:J:5:VAL:HG13	2:J:105:ARG:HH22	1.69	0.56
1:I:65:VAL:HG21	1:I:208:ILE:HD12	1.86	0.56
1:G:350:LYS:C	1:G:352:HIS:H	2.14	0.55
1:I:101:VAL:HG21	1:I:480:ARG:HG2	1.87	0.55
2:E:30:ILE:HA	2:E:52(A):PRO:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82(A):ARG:HH11	2:H:82(A):ARG:HB3	1.71	0.55
2:J:47:TRP:CZ2	2:J:49:GLY:HA2	2.41	0.55
3:K:185:LYS:O	3:K:189:GLU:HG2	2.07	0.55
1:G:95:MET:HE3	1:G:96:TRP:NE1	2.21	0.55
3:L:146:ALA:HB2	3:L:200:HIS:HD2	1.72	0.55
2:J:18:MET:HE1	2:J:109:VAL:HG11	1.88	0.55
3:F:194:TYR:HB2	3:F:211:PHE:HE2	1.72	0.55
1:I:270:ILE:HB	1:I:348:LYS:HG3	1.89	0.55
1:A:463:THR:O	1:A:464:SER:HB3	2.07	0.55
1:D:207:LYS:HG2	1:D:439:ILE:CG2	2.36	0.55
2:E:47:TRP:CH2	2:E:49:GLY:HA2	2.42	0.55
1:G:205:CYS:N	1:G:206:PRO:HD3	2.22	0.54
3:C:21:ILE:HD11	3:C:35:TRP:HZ3	1.72	0.54
1:A:116:LEU:O	1:A:118:PRO:HD3	2.07	0.54
3:C:209:LYS:HB2	3:C:209:LYS:NZ	2.22	0.54
1:D:341:VAL:O	1:D:345:VAL:HG23	2.06	0.54
1:I:105:GLN:HG2	1:I:479:TRP:NE1	2.22	0.54
3:K:140:ASN:ND2	8:K:301:TRS:H21	2.23	0.54
2:H:105:ARG:HD2	9:E:418:HOH:O	2.06	0.54
1:G:64:GLU:HA	1:G:209:SER:HB3	1.88	0.54
1:A:95:MET:CE	1:A:235:GLY:HA3	2.34	0.54
1:A:350:LYS:C	1:A:352:HIS:H	2.16	0.54
5:O:1:NAG:O3	5:O:2:NAG:H2	2.07	0.54
2:B:51:LEU:HD21	2:B:71:ARG:HB3	1.89	0.54
1:I:53:PHE:HA	8:I:514:TRS:H21	1.89	0.54
1:D:53:PHE:HA	8:D:513:TRS:H31	1.89	0.54
3:L:195:ALA:HB2	3:L:210:SER:HB3	1.89	0.53
3:C:54:ARG:NE	3:C:60:ASP:HA	2.23	0.53
3:C:2:ILE:HG22	3:C:3:VAL:H	1.73	0.53
1:D:116:LEU:O	1:D:118:PRO:HD3	2.09	0.53
2:B:82(A):ARG:HB3	2:B:82(A):ARG:NH1	2.22	0.53
1:I:273:ARG:HH12	1:I:287:HIS:CG	2.27	0.53
2:J:200:HIS:CD2	2:J:202:PRO:HD2	2.44	0.53
1:A:463:THR:HG22	9:A:681:HOH:O	2.08	0.53
1:D:205:CYS:N	1:D:206:PRO:HD3	2.23	0.53
2:B:98:CYS:HB2	7:B:302:BGC:H6C2	1.91	0.53
3:F:194:TYR:HB2	3:F:211:PHE:CE2	2.44	0.53
3:L:168:GLN:HE21	3:L:173:SER:HB3	1.73	0.53
3:K:6:GLN:NE2	3:K:21:ILE:HD11	2.24	0.53
2:H:66:ARG:HD3	9:H:303:HOH:O	2.08	0.52
3:F:38:GLN:HB3	3:F:85:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:MET:HE1	1:I:251:ILE:HG21	1.91	0.52
3:C:137:LEU:C	3:C:138:LEU:HD12	2.34	0.52
2:E:18:MET:HE3	2:E:82(C):LEU:HD21	1.91	0.52
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.45	0.52
3:F:6:GLN:NE2	3:F:21:ILE:HD11	2.20	0.52
2:B:131:THR:HG23	2:B:133:GLY:H	1.74	0.52
1:D:408:LYS:HD2	1:D:408:LYS:C	2.34	0.52
1:D:261:LEU:HD21	1:D:374:HIS:CE1	2.45	0.52
2:J:82(A):ARG:HB3	2:J:82(A):ARG:NH1	2.25	0.52
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.92	0.52
2:H:82(A):ARG:HB3	2:H:82(A):ARG:NH1	2.24	0.52
1:A:105:GLN:HG3	1:A:476:LYS:HG2	1.90	0.52
2:H:178:LEU:HD12	2:H:178:LEU:C	2.34	0.52
3:L:79:GLU:H	3:L:82:ASP:HB2	1.75	0.52
1:D:62:GLU:HG3	1:D:64:GLU:H	1.75	0.52
2:E:20:ILE:HD11	2:E:80:LEU:HD23	1.91	0.52
1:G:86:LEU:HB2	1:G:89:VAL:HG11	1.92	0.51
2:H:35:ASN:HB2	2:H:93:THR:OG1	2.10	0.51
1:D:105:GLN:HG3	1:D:476:LYS:HG2	1.93	0.51
1:I:116:LEU:HD13	1:I:208:ILE:HD11	1.92	0.51
2:B:18:MET:CE	2:B:109:VAL:HG11	2.41	0.51
2:B:47:TRP:HZ2	2:B:50:TRP:CD1	2.28	0.51
1:I:104:MET:HE2	1:I:483:LEU:HD11	1.92	0.51
1:I:385:CYS:SG	1:I:416:LEU:HB2	2.51	0.51
3:L:77:ASN:HB2	9:L:312:HOH:O	2.10	0.51
3:L:204:ARG:H	3:L:204:ARG:HE	1.57	0.51
2:B:178:LEU:C	2:B:178:LEU:HD12	2.35	0.51
1:I:292:VAL:HG21	1:I:338:TRP:HE3	1.75	0.51
2:J:139:GLY:HA2	2:J:154:TRP:CH2	2.46	0.51
1:D:408:LYS:C	1:D:410:CYS:H	2.18	0.51
3:F:168:GLN:HB2	3:F:175:TYR:CE1	2.46	0.51
1:A:87:GLU:O	1:A:88:ASN:HB2	2.10	0.51
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.92	0.51
1:G:120:VAL:HG12	1:G:434:MET:HE2	1.92	0.51
3:C:109:LYS:HA	3:C:142:TYR:OH	2.11	0.51
3:L:27:GLN:HG3	3:L:28:TYR:N	2.27	0.50
1:A:105:GLN:CG	1:A:476:LYS:HG2	2.41	0.50
3:F:110:ARG:HH12	3:F:113:ALA:HB2	1.75	0.50
1:G:463:THR:HG21	2:H:61:ARG:NH2	2.25	0.50
3:C:79:GLU:H	3:C:82:ASP:HB2	1.77	0.50
1:I:350:LYS:C	1:I:352:HIS:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:142:TYR:O	3:K:200:HIS:HE1	1.94	0.50
2:B:44:ARG:HG2	3:C:100:GLN:HA	1.94	0.50
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.46	0.50
1:I:64:GLU:HA	1:I:209:SER:HB3	1.94	0.50
3:L:185:LYS:O	3:L:189:GLU:HG2	2.12	0.50
2:B:201:LYS:HE2	2:B:201:LYS:HA	1.93	0.50
3:K:35:TRP:CZ3	3:K:88:CYS:HB3	2.46	0.50
1:A:120:VAL:HG12	1:A:434:MET:HE2	1.93	0.50
3:F:191:HIS:HB2	3:F:194:TYR:OH	2.11	0.50
1:A:421:LYS:NZ	7:A:518:BGC:H3	2.26	0.50
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.46	0.50
1:D:231:LYS:HD2	1:D:267:GLU:HB3	1.94	0.50
2:E:3:GLN:C	2:E:4:LEU:HD12	2.37	0.50
2:E:18:MET:CE	2:E:109:VAL:HG11	2.42	0.50
3:C:21:ILE:HD12	3:C:102:THR:HB	1.93	0.49
3:L:110:ARG:HH12	3:L:113:ALA:HB2	1.76	0.49
2:B:134:GLY:HA3	9:B:437:HOH:O	2.13	0.49
1:D:95:MET:HE3	1:D:96:TRP:NE1	2.28	0.49
1:A:108:VAL:HG22	1:A:253:PRO:HB3	1.94	0.49
1:I:290:LYS:HD2	6:I:506:NAG:H82	1.95	0.49
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.48	0.49
3:F:65:SER:OG	3:F:72:ASN:HB2	2.13	0.49
1:G:371:ILE:HD11	2:H:54:GLY:HA3	1.94	0.49
1:A:104:MET:HE2	1:A:483:LEU:HD11	1.95	0.49
1:D:261:LEU:HD21	1:D:374:HIS:HE1	1.78	0.49
1:I:95:MET:SD	1:I:273:ARG:HD3	2.53	0.49
2:B:30:ILE:HA	2:B:52(A):PRO:HB2	1.94	0.48
2:B:124:LEU:HD11	2:B:141:LEU:HB2	1.95	0.48
2:E:7:SER:O	2:E:107:THR:HG22	2.12	0.48
1:D:328:LYS:O	1:D:328:LYS:HD3	2.13	0.48
2:J:124:LEU:HD11	2:J:141:LEU:HB2	1.95	0.48
2:B:135:THR:HG22	2:B:185:PRO:HA	1.95	0.48
2:J:210:LYS:NZ	2:J:212:GLU:HG2	2.28	0.48
2:H:205:THR:C	2:H:206:LYS:HD2	2.38	0.48
2:B:124:LEU:HB3	3:C:120:PHE:CD1	2.48	0.48
2:E:123:PRO:HG3	2:E:209:LYS:HD2	1.95	0.48
3:L:89:GLN:HG2	3:L:90:GLN:N	2.27	0.48
2:E:139:GLY:HA2	2:E:154:TRP:HH2	1.79	0.48
3:K:131:THR:HG22	3:K:184:SER:HA	1.96	0.48
1:G:434:MET:HB2	2:E:11:MET:HE1	1.94	0.48
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:LEU:HB2	1:D:89:VAL:HG11	1.96	0.48
3:K:48:ILE:HD13	3:K:54:ARG:HA	1.96	0.48
3:K:165:VAL:HG12	3:K:166:THR:O	2.14	0.48
3:L:127:LEU:O	3:L:185:LYS:HD2	2.14	0.48
2:H:50:TRP:CZ3	2:H:52:LYS:HG3	2.49	0.48
2:B:126:PRO:HG3	2:B:138:LEU:HD23	1.95	0.48
1:D:325:ASP:O	1:D:328:LYS:HG3	2.13	0.48
2:E:150:VAL:HG23	2:E:178:LEU:HD21	1.96	0.48
1:A:256:SER:HA	1:A:375:HIS:O	2.14	0.47
1:D:394:THR:HG23	1:D:407:MET:HE2	1.95	0.47
3:L:204:ARG:H	3:L:204:ARG:NE	2.12	0.47
3:C:77:ASN:HB2	9:C:408:HOH:O	2.14	0.47
3:C:191:HIS:O	3:C:213:ARG:HD3	2.13	0.47
1:A:273:ARG:HH12	1:A:287:HIS:CG	2.33	0.47
1:D:108:VAL:HG22	1:D:253:PRO:HB3	1.96	0.47
1:I:341:VAL:O	1:I:345:VAL:HG23	2.14	0.47
2:J:51:LEU:HD23	2:J:51:LEU:C	2.39	0.47
2:J:129:LYS:NZ	3:K:211:PHE:HA	2.29	0.47
3:K:147:LYS:HB3	3:K:199:THR:OG1	2.15	0.47
1:A:421:LYS:HZ2	7:A:518:BGC:H3	1.80	0.47
1:I:93:PHE:HB2	1:I:233:PHE:CZ	2.50	0.47
1:A:204:ALA:C	1:A:206:PRO:HD3	2.40	0.47
3:K:199:THR:HG22	3:K:206:PRO:HB3	1.95	0.47
1:A:263:GLY:O	1:A:450:THR:HG21	2.14	0.47
2:B:61:ARG:HB2	2:B:62:PRO:HD3	1.96	0.47
2:B:116:THR:HG22	2:B:147:PRO:HD3	1.96	0.47
3:C:131:THR:HB	3:C:183:LEU:O	2.14	0.47
3:C:177:LEU:HD23	3:C:178:SER:N	2.30	0.47
1:D:446:VAL:HG11	6:D:507:NAG:H82	1.97	0.47
2:E:96:LYS:HG3	2:E:101:GLU:OE1	2.14	0.47
3:F:110:ARG:HD2	3:F:173:SER:HB2	1.96	0.47
3:F:160:ASN:HD22	3:F:183:LEU:HD21	1.80	0.47
3:K:89:GLN:HG2	3:K:90:GLN:N	2.29	0.47
1:G:256:SER:HA	1:G:375:HIS:O	2.15	0.47
3:C:2:ILE:HD13	3:C:97:PHE:HD2	1.79	0.47
1:I:104:MET:HG2	1:I:479:TRP:CG	2.49	0.47
2:J:63:LEU:HD23	2:J:66:ARG:NH1	2.29	0.47
3:L:18:THR:HG22	3:L:76:SER:O	2.14	0.47
1:A:207:LYS:HG2	1:A:439:ILE:CG2	2.45	0.47
2:J:123:PRO:HG3	2:J:209:LYS:HD2	1.96	0.47
3:C:17:GLU:O	3:C:78:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:75:ILE:HD12	3:F:75:ILE:N	2.30	0.47
3:L:33:LEU:HD13	3:L:71:TYR:CG	2.50	0.46
3:F:139:ASN:O	3:F:140:ASN:C	2.59	0.46
1:I:458:GLY:O	2:J:60:ALA:HA	2.15	0.46
1:G:394:THR:HB	9:G:601:HOH:O	2.15	0.46
1:D:95:MET:SD	1:D:273:ARG:HD3	2.55	0.46
2:E:201:LYS:N	2:E:202:PRO:CD	2.78	0.46
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.98	0.46
3:K:23:CYS:HB2	3:K:35:TRP:CH2	2.50	0.46
2:H:40:ALA:HB2	2:H:88:ALA:HB2	1.97	0.46
3:L:149:GLN:CD	3:L:156:LEU:HD21	2.40	0.46
1:D:259:LEU:HB2	1:D:374:HIS:CE1	2.51	0.46
1:I:116:LEU:O	1:I:118:PRO:HD3	2.15	0.46
1:I:333:ILE:N	1:I:333:ILE:HD12	2.30	0.46
1:G:414:ILE:HD11	1:G:416:LEU:HD21	1.98	0.46
2:H:20:ILE:HD11	2:H:80:LEU:HD23	1.97	0.46
1:A:298:ARG:HD2	1:A:326:ILE:O	2.14	0.46
2:B:38:ARG:C	2:B:39:LEU:HD23	2.41	0.46
1:D:343:LYS:NZ	1:D:343:LYS:HB3	2.30	0.46
1:I:95:MET:HE3	1:I:96:TRP:NE1	2.30	0.46
1:G:349:LEU:O	1:G:353:PHE:HD2	1.98	0.46
2:E:39:LEU:HD21	2:E:45:PRO:HG3	1.96	0.46
3:L:66:ARG:HG3	3:L:71:TYR:CZ	2.51	0.46
1:A:360:ILE:O	1:A:467:THR:HA	2.14	0.46
1:A:392:ASN:O	1:A:396:ILE:HD13	2.15	0.46
2:B:39:LEU:HD22	2:B:45:PRO:HB3	1.97	0.46
1:D:207:LYS:HE2	1:D:436:ALA:HB3	1.97	0.46
3:K:160:ASN:H	3:K:160:ASN:HD22	1.64	0.46
1:G:120:VAL:HG12	1:G:434:MET:HB3	1.98	0.46
3:L:12:SER:HB3	3:L:107:ASP:HB2	1.98	0.46
2:E:121:VAL:HG13	2:E:140:CYS:HB3	1.98	0.46
1:A:358:THR:HB	1:A:465:ASN:HB3	1.96	0.46
3:F:54:ARG:NE	3:F:60:ASP:HA	2.31	0.46
2:E:200:HIS:CE1	2:E:202:PRO:HB2	2.50	0.45
3:K:127:LEU:O	3:K:185:LYS:HD2	2.16	0.45
2:H:57:VAL:HG21	2:H:59:TYR:CE1	2.52	0.45
3:L:83:PHE:HA	3:L:104:VAL:HG23	1.98	0.45
3:L:110:ARG:HD2	3:L:173:SER:HB2	1.98	0.45
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.98	0.45
2:E:131:THR:HG23	2:E:134:GLY:H	1.81	0.45
3:F:116:SER:OG	3:F:139:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:MET:HE3	2:H:63:LEU:HD13	1.99	0.45
2:H:183:THR:HG21	3:L:139:ASN:ND2	2.32	0.45
3:L:194:TYR:HB2	3:L:211:PHE:CE2	2.51	0.45
1:A:351:GLU:OE2	7:A:516:BGC:H6C1	2.15	0.45
1:D:425:ASN:ND2	1:D:432:GLN:HG2	2.31	0.45
6:A:507:NAG:H82	6:A:507:NAG:H2	1.87	0.45
2:B:148:GLU:HB3	2:B:149:PRO:HA	1.98	0.45
1:D:248:THR:HA	1:D:486:TYR:CE1	2.51	0.45
3:F:204:ARG:H	3:F:204:ARG:CD	2.19	0.45
2:J:57:VAL:HG21	2:J:59:TYR:CE1	2.52	0.45
2:H:61:ARG:HB2	2:H:62:PRO:HD3	1.99	0.45
1:A:91:GLU:HG3	1:A:226:LEU:HD13	1.99	0.45
1:A:232:ASN:OD1	1:A:268:GLU:HB3	2.17	0.45
2:E:147:PRO:HB2	2:E:148:GLU:H	1.44	0.45
1:I:120:VAL:HG12	1:I:434:MET:HB3	1.99	0.45
3:L:168:GLN:NE2	3:L:173:SER:HB3	2.32	0.45
3:L:65:SER:OG	3:L:72:ASN:HB2	2.17	0.45
2:E:82(A):ARG:HB3	2:E:82(A):ARG:HH11	1.81	0.45
1:I:105:GLN:HG2	1:I:479:TRP:CD1	2.51	0.45
3:K:18:THR:HG22	3:K:76:SER:O	2.17	0.45
1:D:101:VAL:HG13	1:D:479:TRP:HB2	1.98	0.45
1:I:95:MET:HE1	1:I:273:ARG:HB3	1.99	0.45
1:I:108:VAL:HG22	1:I:253:PRO:HB3	1.97	0.45
3:C:209:LYS:HB2	3:C:209:LYS:HZ2	1.80	0.45
3:C:142:TYR:O	3:C:200:HIS:HE1	2.00	0.45
1:D:93:PHE:HB2	1:D:233:PHE:HZ	1.82	0.45
1:I:290:LYS:HE2	1:I:337:LYS:HE3	1.99	0.45
1:G:95:MET:SD	1:G:273:ARG:HD3	2.57	0.44
1:G:104:MET:HE2	1:G:483:LEU:HD11	1.99	0.44
2:B:154:TRP:HB2	2:B:159:LEU:HB3	1.98	0.44
3:F:33:LEU:HD13	3:F:71:TYR:CD1	2.52	0.44
2:J:178:LEU:HD12	2:J:178:LEU:C	2.42	0.44
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.52	0.44
2:J:44:ARG:NH1	3:K:2:ILE:HD11	2.31	0.44
3:K:21:ILE:HD12	3:K:102:THR:CB	2.47	0.44
2:H:53:ARG:HB3	9:H:308:HOH:O	2.16	0.44
1:D:381:GLU:HB2	1:D:383:PHE:HE2	1.82	0.44
3:F:120:PHE:HB2	3:F:135:VAL:HB	1.99	0.44
3:F:138:LEU:HB2	3:F:177:LEU:HB3	2.00	0.44
3:F:142:TYR:O	3:F:200:HIS:HE1	2.00	0.44
1:I:421:LYS:HE2	1:I:421:LYS:HB3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:VAL:HG12	1:G:66:HIS:N	2.32	0.44
2:B:40:ALA:HB2	2:B:88:ALA:HB2	2.00	0.44
3:C:177:LEU:HD23	3:C:177:LEU:C	2.42	0.44
3:F:139:ASN:O	3:F:141:PHE:HD1	2.01	0.44
3:K:47:VAL:HG12	3:K:48:ILE:HG12	2.00	0.44
2:H:18:MET:CE	2:H:109:VAL:HG11	2.48	0.44
1:D:290:LYS:HE2	1:D:337:LYS:HE3	2.00	0.44
1:I:111:LEU:C	1:I:111:LEU:HD23	2.43	0.44
3:K:6:GLN:HE21	3:K:21:ILE:HD11	1.82	0.44
3:C:147:LYS:HE3	9:C:405:HOH:O	2.18	0.44
2:E:47:TRP:HZ2	2:E:50:TRP:CD1	2.35	0.44
2:J:66:ARG:HD3	9:J:603:HOH:O	2.17	0.44
3:C:2:ILE:HD13	3:C:97:PHE:CD2	2.53	0.44
3:C:114:ALA:HA	3:C:115:PRO:HD3	1.76	0.44
1:D:357:LYS:HD3	1:D:466:GLU:HG2	1.98	0.44
1:I:461:ASN:OD1	3:K:2:ILE:HG22	2.17	0.44
1:G:269:GLU:HA	1:G:289:ASN:ND2	2.32	0.44
2:H:51:LEU:HD13	2:H:51:LEU:C	2.43	0.44
1:A:64:GLU:HA	1:A:209:SER:HB3	1.99	0.44
1:A:99:ASN:HA	1:A:102:GLU:HG2	2.00	0.44
1:I:120:VAL:HG12	1:I:434:MET:HE2	2.00	0.44
1:I:378:CYS:HB3	1:I:383:PHE:CE2	2.53	0.44
2:J:82(A):ARG:HB3	2:J:82(A):ARG:HH11	1.83	0.44
3:K:151:LYS:HB2	3:K:195:ALA:HB3	1.99	0.44
1:G:269:GLU:HA	1:G:289:ASN:HD22	1.83	0.43
3:L:75:ILE:N	3:L:75:ILE:HD12	2.33	0.43
3:L:203:LEU:HD22	3:L:204:ARG:HH21	1.82	0.43
1:A:270:ILE:O	1:A:348:LYS:HE2	2.17	0.43
2:B:82(A):ARG:HB3	2:B:82(A):ARG:HH11	1.83	0.43
1:G:53:PHE:HB2	9:G:626:HOH:O	2.17	0.43
3:L:137:LEU:C	3:L:138:LEU:HD12	2.43	0.43
3:F:39:ARG:HD3	3:F:81:GLY:O	2.17	0.43
2:J:47:TRP:CH2	2:J:49:GLY:HA2	2.53	0.43
1:G:229:ASN:HD21	1:G:243:SER:HB3	1.82	0.43
2:H:2:VAL:HB	2:H:102:HIS:CD2	2.53	0.43
2:H:11:MET:HE2	2:H:11:MET:HB3	1.93	0.43
1:I:118:PRO:HB3	1:I:433:ALA:HB1	1.99	0.43
1:G:408:LYS:HD2	1:G:408:LYS:N	2.34	0.43
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.53	0.43
1:D:93:PHE:CE2	1:D:228:CYS:HB2	2.54	0.43
1:I:408:LYS:HG2	1:I:409:GLY:N	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:460:ALA:HB3	2:H:61:ARG:HD3	2.00	0.43
2:B:138:LEU:C	2:B:138:LEU:HD12	2.43	0.43
2:E:38:ARG:HG3	2:E:46:GLU:HB3	2.00	0.43
3:F:6:GLN:H	3:F:100:GLN:HE22	1.67	0.43
3:K:109:LYS:HA	3:K:142:TYR:OH	2.18	0.43
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.54	0.43
1:A:252:LYS:HA	1:A:253:PRO:HD3	1.83	0.43
1:G:461:ASN:HD22	3:L:3:VAL:HG13	1.84	0.43
2:B:123:PRO:HG3	2:B:209:LYS:HD2	2.00	0.43
3:C:135:VAL:HG12	3:C:136:CYS:N	2.33	0.43
3:C:136:CYS:HB2	3:C:150:TRP:CZ2	2.54	0.43
3:K:207:VAL:HG12	3:K:208:THR:N	2.34	0.43
1:G:95:MET:HE3	1:G:96:TRP:CE2	2.54	0.43
1:G:110:SER:O	1:G:114:GLN:HG2	2.18	0.43
2:H:27:TYR:HE2	2:H:32:CYS:HB2	1.83	0.43
1:A:349:LEU:HD12	1:A:349:LEU:HA	1.82	0.43
1:G:422:GLN:HB3	1:G:435:TYR:O	2.19	0.43
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.01	0.43
1:A:122:LEU:HD12	2:J:11:MET:HG2	2.01	0.43
2:B:188:SER:O	2:B:192:GLN:HB2	2.18	0.43
2:B:196:CYS:SG	2:B:209:LYS:HB3	2.59	0.43
2:H:196:CYS:SG	2:H:209:LYS:HB3	2.58	0.43
2:B:168:ALA:HA	2:B:178:LEU:HB3	2.00	0.43
2:B:212:GLU:CD	2:B:213:PRO:HD2	2.43	0.43
1:D:64:GLU:HA	1:D:209:SER:HB3	2.00	0.43
2:E:184:VAL:HG21	2:E:194:TYR:CE1	2.54	0.43
2:J:116:THR:HG22	2:J:147:PRO:HD3	2.01	0.43
2:J:59:TYR:HB2	2:J:64:GLN:HG2	2.01	0.42
1:G:257:THR:O	1:G:258:GLN:HB2	2.19	0.42
3:C:78:LEU:HD23	3:C:83:PHE:CZ	2.54	0.42
1:G:333:ILE:HD12	1:G:333:ILE:N	2.35	0.42
3:C:65:SER:OG	3:C:72:ASN:HB2	2.18	0.42
2:E:2:VAL:HB	2:E:102:HIS:NE2	2.34	0.42
2:E:57:VAL:HG21	2:E:59:TYR:CE1	2.53	0.42
2:E:212:GLU:HA	2:E:213:PRO:HD3	1.92	0.42
3:F:136:CYS:HB2	3:F:150:TRP:CH2	2.54	0.42
1:I:201:ILE:N	1:I:201:ILE:HD12	2.34	0.42
2:J:19:ARG:HA	2:J:80:LEU:O	2.19	0.42
2:H:35:ASN:O	2:H:92:CYS:HA	2.19	0.42
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.27	0.42
1:I:205:CYS:N	1:I:206:PRO:HD3	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:3:BMA:H61	4:N:5:MAN:H2	1.68	0.42
2:H:96:LYS:HG3	2:H:101:GLU:OE1	2.20	0.42
2:H:206:LYS:HD2	2:H:206:LYS:N	2.34	0.42
1:A:65:VAL:HG13	1:A:115:SER:OG	2.20	0.42
1:I:107:ASP:OD2	8:I:514:TRS:H32	2.20	0.42
3:C:64:GLY:HA2	3:C:72:ASN:O	2.19	0.42
3:C:75:ILE:HD12	3:C:75:ILE:N	2.35	0.42
3:F:104:VAL:HG23	3:F:104:VAL:O	2.20	0.42
1:G:343:LYS:NZ	1:G:343:LYS:HB3	2.34	0.42
2:B:6:GLN:HE21	2:B:107:THR:HG23	1.84	0.42
3:F:139:ASN:CG	3:F:140:ASN:H	2.27	0.42
2:J:61:ARG:HB2	2:J:62:PRO:HD3	2.01	0.42
2:J:206:LYS:HD3	2:J:206:LYS:N	2.34	0.42
3:K:19:ALA:O	3:K:74:THR:HA	2.19	0.42
3:K:160:ASN:HD22	3:K:160:ASN:N	2.17	0.42
2:B:11:MET:HE1	1:I:434:MET:CB	2.44	0.42
3:C:195:ALA:HB2	3:C:210:SER:CB	2.46	0.42
2:E:178:LEU:C	2:E:178:LEU:HD12	2.45	0.42
3:F:35:TRP:CZ3	3:F:88:CYS:HB3	2.54	0.42
3:K:75:ILE:HD12	3:K:75:ILE:N	2.34	0.42
1:G:297:THR:O	1:G:329:ALA:HB1	2.20	0.42
3:C:83:PHE:HA	3:C:104:VAL:HG23	2.02	0.42
1:D:93:PHE:HB2	1:D:233:PHE:CZ	2.55	0.42
2:J:122:PHE:HA	2:J:123:PRO:HD3	1.82	0.42
3:K:192:LYS:O	3:K:212:ASN:HA	2.20	0.42
2:B:11:MET:CE	1:I:434:MET:HB2	2.43	0.42
1:D:88:ASN:OD1	1:D:88:ASN:N	2.52	0.42
3:K:127:LEU:HD23	3:K:132:ALA:HB2	2.02	0.42
2:H:11:MET:HE1	1:D:434:MET:CB	2.41	0.41
2:H:150:VAL:HG12	2:H:200:HIS:CD2	2.55	0.41
1:D:111:LEU:C	1:D:111:LEU:HD23	2.44	0.41
2:J:29:PHE:O	2:J:52(A):PRO:HG2	2.19	0.41
3:C:204:ARG:HG2	3:C:205:SER:N	2.35	0.41
3:F:170:SER:C	3:F:171:LYS:HD2	2.45	0.41
1:I:82:GLN:HB3	9:I:625:HOH:O	2.18	0.41
2:J:146:PHE:HA	2:J:147:PRO:HA	1.88	0.41
1:A:115:SER:O	1:A:117:GLN:HG3	2.19	0.41
1:A:343:LYS:NZ	1:A:343:LYS:HB3	2.34	0.41
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.84	0.41
2:B:50:TRP:CZ3	2:B:52:LYS:HG3	2.55	0.41
1:D:416:LEU:HA	1:D:417:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HB3	1:A:442:LYS:N	2.36	0.41
1:D:66:HIS:CD2	1:D:111:LEU:HD11	2.56	0.41
1:D:269:GLU:HA	1:D:289:ASN:ND2	2.35	0.41
3:F:64:GLY:HA2	3:F:72:ASN:O	2.20	0.41
3:F:100:GLN:H	3:F:100:GLN:CD	2.28	0.41
1:G:100:MET:HE2	1:G:483:LEU:HD22	2.02	0.41
3:L:27:GLN:HG3	3:L:28:TYR:H	1.84	0.41
3:L:66:ARG:HG3	3:L:71:TYR:CE2	2.55	0.41
3:L:84:GLY:H	3:L:104:VAL:HG23	1.85	0.41
3:L:149:GLN:OE1	3:L:156:LEU:HD21	2.20	0.41
1:A:328:LYS:HD3	1:A:328:LYS:O	2.21	0.41
2:J:35:ASN:HD21	2:J:100(A):ASN:ND2	2.18	0.41
1:G:298:ARG:HD2	1:G:326:ILE:O	2.20	0.41
1:G:342:LEU:HD12	1:G:342:LEU:HA	1.95	0.41
2:H:201:LYS:N	2:H:202:PRO:CD	2.83	0.41
2:B:122:PHE:HA	2:B:123:PRO:HD3	1.84	0.41
2:B:201:LYS:N	2:B:202:PRO:CD	2.83	0.41
3:C:6:GLN:H	3:C:100:GLN:NE2	2.18	0.41
1:D:349:LEU:HA	1:D:349:LEU:HD12	1.86	0.41
1:I:343:LYS:NZ	1:I:343:LYS:HB3	2.36	0.41
1:D:83:GLU:CD	1:D:83:GLU:H	2.29	0.41
1:I:480:ARG:NH1	7:I:513:BGC:H2	2.35	0.41
2:J:153:SER:OG	2:J:197:ASN:HB2	2.20	0.41
3:K:91:TYR:HB3	3:K:96:GLU:OE1	2.20	0.41
3:K:177:LEU:HD23	3:K:177:LEU:C	2.46	0.41
1:G:328:LYS:O	1:G:328:LYS:HD3	2.21	0.41
1:D:297:THR:HB	1:D:444:ASN:OD1	2.21	0.41
3:K:122:PRO:HG2	3:K:188:TYR:CZ	2.56	0.41
1:G:270:ILE:O	1:G:348:LYS:HE2	2.21	0.41
2:H:18:MET:HE2	2:H:109:VAL:HG11	2.02	0.41
1:A:86:LEU:HB2	1:A:89:VAL:HG11	2.02	0.41
1:D:350:LYS:C	1:D:352:HIS:H	2.28	0.41
2:E:166:PHE:HA	3:F:166:THR:HG22	2.02	0.41
3:F:190:LYS:NZ	3:F:190:LYS:HB2	2.35	0.41
1:I:91:GLU:HG3	1:I:226:LEU:HD13	2.01	0.41
1:I:257:THR:O	1:I:258:GLN:HB2	2.21	0.41
2:J:17:SER:HB3	9:J:613:HOH:O	2.19	0.41
2:J:118:GLY:HA2	2:J:119:PRO:HD3	1.81	0.41
3:L:33:LEU:C	3:L:33:LEU:HD23	2.45	0.41
1:A:421:LYS:HE2	1:A:421:LYS:HB3	1.87	0.41
1:A:461:ASN:HD21	3:C:2:ILE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:127:LEU:HB3	3:F:185:LYS:NZ	2.36	0.41
1:I:75:VAL:HB	1:I:76:PRO:HD2	2.03	0.41
3:L:142:TYR:CG	3:L:143:PRO:HA	2.56	0.40
2:B:183:THR:HG21	3:C:139:ASN:HD22	1.86	0.40
2:B:205:THR:HG22	2:B:207:VAL:HG23	2.02	0.40
3:F:19:ALA:HB3	3:F:75:ILE:HD13	2.04	0.40
2:J:17:SER:CB	2:J:82(A):ARG:HA	2.51	0.40
1:G:425:ASN:HD21	7:G:512:BGC:H1	1.85	0.40
2:H:52(A):PRO:O	2:H:53:ARG:C	2.63	0.40
3:L:142:TYR:O	3:L:200:HIS:HE1	2.04	0.40
3:C:78:LEU:HD23	3:C:83:PHE:CE1	2.56	0.40
1:D:219:THR:HA	1:D:220:PRO:HD3	1.87	0.40
1:D:234:ASN:O	1:D:273:ARG:HG2	2.21	0.40
1:D:448:ASN:O	1:D:450:THR:HG23	2.21	0.40
3:F:134:VAL:O	3:F:180:THR:HA	2.20	0.40
3:K:160:ASN:N	3:K:160:ASN:ND2	2.69	0.40
1:G:116:LEU:HD13	1:G:382:PHE:HZ	1.86	0.40
1:D:110:SER:O	1:D:114:GLN:HG2	2.21	0.40
2:J:201:LYS:C	2:J:203:SER:H	2.29	0.40
2:B:50:TRP:CH2	2:B:52:LYS:HE3	2.56	0.40
1:D:104:MET:HE1	1:D:251:ILE:HG22	2.03	0.40
1:D:225:ILE:HG21	1:D:486:TYR:HD1	1.86	0.40
2:E:123:PRO:O	3:F:123:SER:HB3	2.22	0.40
2:E:200:HIS:C	2:E:202:PRO:HD2	2.47	0.40
3:K:168:GLN:HB2	3:K:175:TYR:CE1	2.56	0.40
1:G:350:LYS:C	1:G:352:HIS:N	2.79	0.40
3:L:17:GLU:OE1	3:L:109:LYS:HE3	2.22	0.40
1:A:397:GLY:O	1:A:404:ASN:HB2	2.22	0.40
3:C:194:TYR:HB2	3:C:211:PHE:CE2	2.57	0.40
2:E:71:ARG:O	2:E:71:ARG:HD3	2.21	0.40
3:F:84:GLY:H	3:F:104:VAL:HG23	1.86	0.40
1:I:224:VAL:HG22	1:I:225:ILE:N	2.37	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	345/353 (98%)	312 (90%)	30 (9%)	3 (1%)	14	31
1	D	346/353 (98%)	314 (91%)	30 (9%)	2 (1%)	21	41
1	G	343/353 (97%)	315 (92%)	25 (7%)	3 (1%)	14	31
1	I	345/353 (98%)	311 (90%)	31 (9%)	3 (1%)	14	31
2	B	222/224 (99%)	203 (91%)	19 (9%)	0	100	100
2	E	222/224 (99%)	192 (86%)	25 (11%)	5 (2%)	5	11
2	H	222/224 (99%)	201 (90%)	19 (9%)	2 (1%)	14	31
2	J	222/224 (99%)	206 (93%)	14 (6%)	2 (1%)	14	31
3	C	208/210 (99%)	178 (86%)	28 (14%)	2 (1%)	12	28
3	F	206/210 (98%)	176 (85%)	26 (13%)	4 (2%)	6	15
3	K	208/210 (99%)	188 (90%)	16 (8%)	4 (2%)	6	15
3	L	206/210 (98%)	192 (93%)	12 (6%)	2 (1%)	12	28
All	All	3095/3148 (98%)	2788 (90%)	275 (9%)	32 (1%)	12	28

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	SER
2	E	147	PRO
1	G	410	CYS
2	H	100(D)	PHE
3	L	140	ASN
1	A	404	ASN
3	C	140	ASN
1	D	397	GLY
1	D	411	ASN
3	K	2	ILE
3	K	140	ASN
1	G	267	GLU
1	G	411	ASN
2	E	127	SER
3	F	140	ASN
1	I	396	ILE
2	J	203	SER
1	A	467	THR

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Mol	Chain	Res	Type
3	F	110	ARG
2	J	100(D)	PHE
1	A	462	ASN
2	E	82(B)	SER
2	E	144	ASP
3	F	15	PRO
3	K	15	PRO
3	L	15	PRO
1	I	470	PRO
3	K	206	PRO
3	C	2	ILE
3	F	206	PRO
1	I	220	PRO
2	E	126	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	310/311 (100%)	298 (96%)	12 (4%)	28	54
1	D	310/311 (100%)	299 (96%)	11 (4%)	32	58
1	G	309/311 (99%)	299 (97%)	10 (3%)	34	61
1	I	309/311 (99%)	300 (97%)	9 (3%)	37	64
2	B	192/192 (100%)	190 (99%)	2 (1%)	68	84
2	E	192/192 (100%)	189 (98%)	3 (2%)	55	78
2	H	192/192 (100%)	187 (97%)	5 (3%)	40	68
2	J	192/192 (100%)	191 (100%)	1 (0%)	81	91
3	C	182/182 (100%)	178 (98%)	4 (2%)	45	72
3	F	180/182 (99%)	177 (98%)	3 (2%)	53	77
3	K	182/182 (100%)	179 (98%)	3 (2%)	55	78
3	L	180/182 (99%)	177 (98%)	3 (2%)	53	77
All	All	2730/2740 (100%)	2664 (98%)	66 (2%)	43	70

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	65	VAL
1	G	105	GLN
1	G	123	THR
1	G	200	VAL
1	G	328	LYS
1	G	369	LEU
1	G	396	ILE
1	G	414	ILE
1	G	428	GLN
1	G	462	ASN
2	H	1	GLN
2	H	4	LEU
2	H	34	LEU
2	H	38	ARG
2	H	152	VAL
3	L	74	THR
3	L	156	LEU
3	L	204	ARG
1	A	90	THR
1	A	95	MET
1	A	105	GLN
1	A	200	VAL
1	A	297	THR
1	A	328	LYS
1	A	343	LYS
1	A	347	GLU
1	A	349	LEU
1	A	385	CYS
1	A	446	VAL
1	A	475	ILE
2	B	20	ILE
2	B	57	VAL
3	C	21	ILE
3	C	74	THR
3	C	204	ARG
3	C	209	LYS
1	D	88	ASN
1	D	105	GLN
1	D	259	LEU
1	D	328	LYS
1	D	343	LYS
1	D	349	LEU

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Mol	Chain	Res	Type
1	D	395	CYS
1	D	396	ILE
1	D	428	GLN
1	D	446	VAL
1	D	475	ILE
2	E	1	GLN
2	E	33	THR
2	E	38	ARG
3	F	21	ILE
3	F	181	LEU
3	F	204	ARG
1	I	65	VAL
1	I	104	MET
1	I	105	GLN
1	I	200	VAL
1	I	261	LEU
1	I	328	LYS
1	I	343	LYS
1	I	349	LEU
1	I	408	LYS
2	J	34	LEU
3	K	21	ILE
3	K	85	VAL
3	K	160	ASN

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

Mol	Chain	Res	Type
1	G	66	HIS
1	G	389	GLN
1	G	444	ASN
1	A	362	GLN
1	D	114	GLN
1	D	339	ASN
1	D	374	HIS
1	D	432	GLN
2	E	155	ASN
3	F	6	GLN
1	I	85	HIS
1	I	99	ASN
1	I	114	GLN
1	I	444	ASN

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Mol	Chain	Res	Type
2	J	10	GLN
2	J	197	ASN
3	K	42	GLN
3	K	149	GLN

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 ⓘ

17 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	M	1	4,3	14,14,15	0.55	0	17,19,21	0.75	0
4	NAG	M	2	4	14,14,15	0.52	0	17,19,21	0.80	0
4	BMA	M	3	4	11,11,12	0.62	0	15,15,17	0.73	1 (6%)
4	MAN	M	4	4	11,11,12	0.66	0	15,15,17	0.52	0
4	MAN	M	5	4	11,11,12	0.62	0	15,15,17	0.53	0
4	NAG	N	1	4,3	14,14,15	0.58	0	17,19,21	0.72	0
4	NAG	N	2	4	14,14,15	0.58	0	17,19,21	0.69	0
4	BMA	N	3	4	11,11,12	0.61	0	15,15,17	0.70	0
4	MAN	N	4	4	11,11,12	0.63	0	15,15,17	0.46	0
4	MAN	N	5	4	11,11,12	0.66	0	15,15,17	0.54	0
5	NAG	O	1	5,3	14,14,15	0.47	0	17,19,21	0.86	1 (5%)
5	NAG	O	2	5	14,14,15	0.52	0	17,19,21	0.58	0
4	NAG	P	1	4,3	14,14,15	0.57	0	17,19,21	0.82	0
4	NAG	P	2	4	14,14,15	0.54	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	P	3	4	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
4	MAN	P	4	4	11,11,12	0.60	0	15,15,17	0.54	0
4	MAN	P	5	4	11,11,12	0.65	0	15,15,17	0.59	0

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	3	BMA	C1-C2-C3	2.66	113.51	109.64
5	O	1	NAG	O5-C5-C6	2.13	111.81	107.66
4	M	3	BMA	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

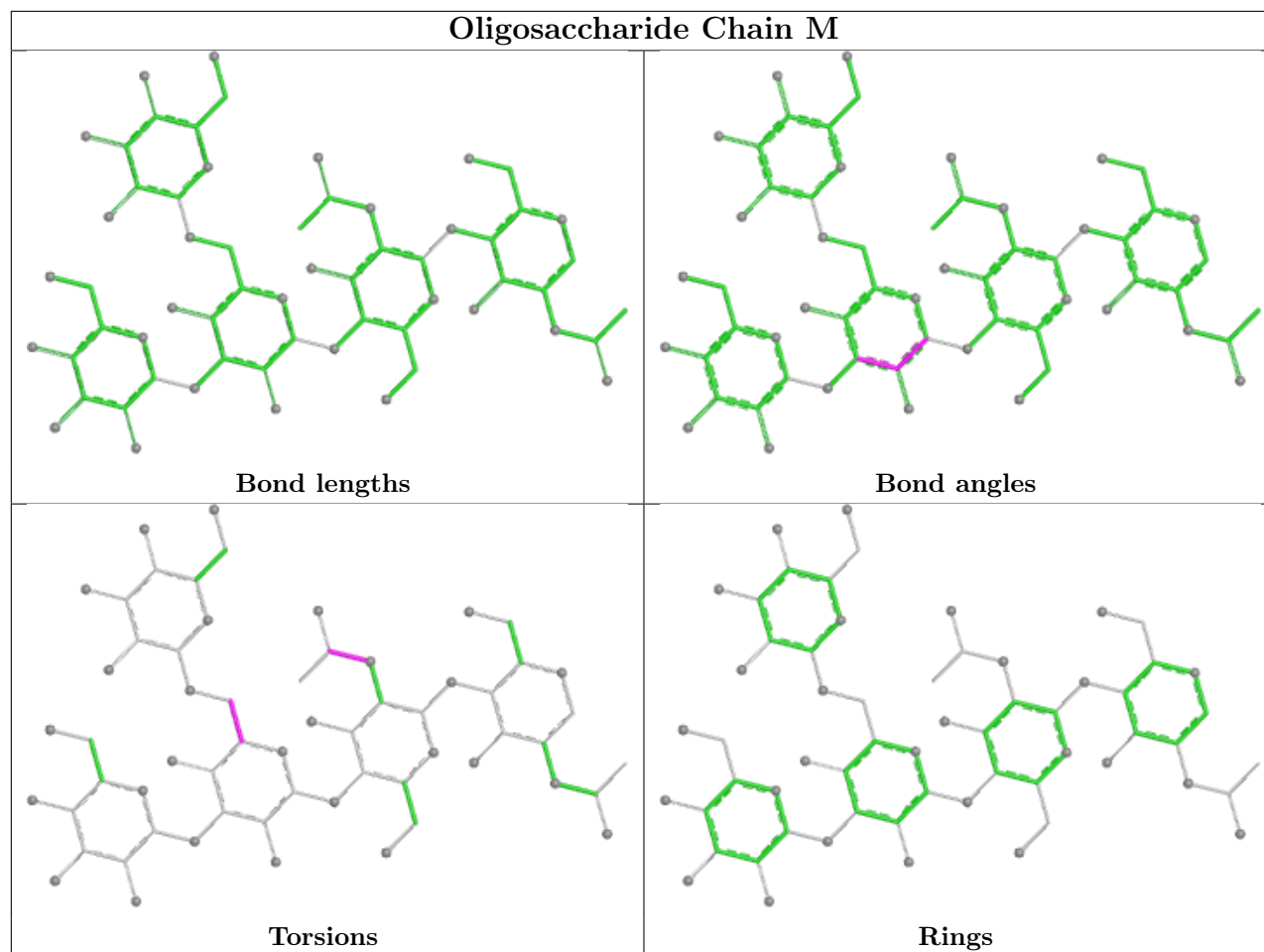
Mol	Chain	Res	Type	Atoms
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
4	N	3	BMA	O5-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
4	P	3	BMA	C4-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	P	1	NAG	C8-C7-N2-C2
4	M	3	BMA	O5-C5-C6-O6
4	N	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2

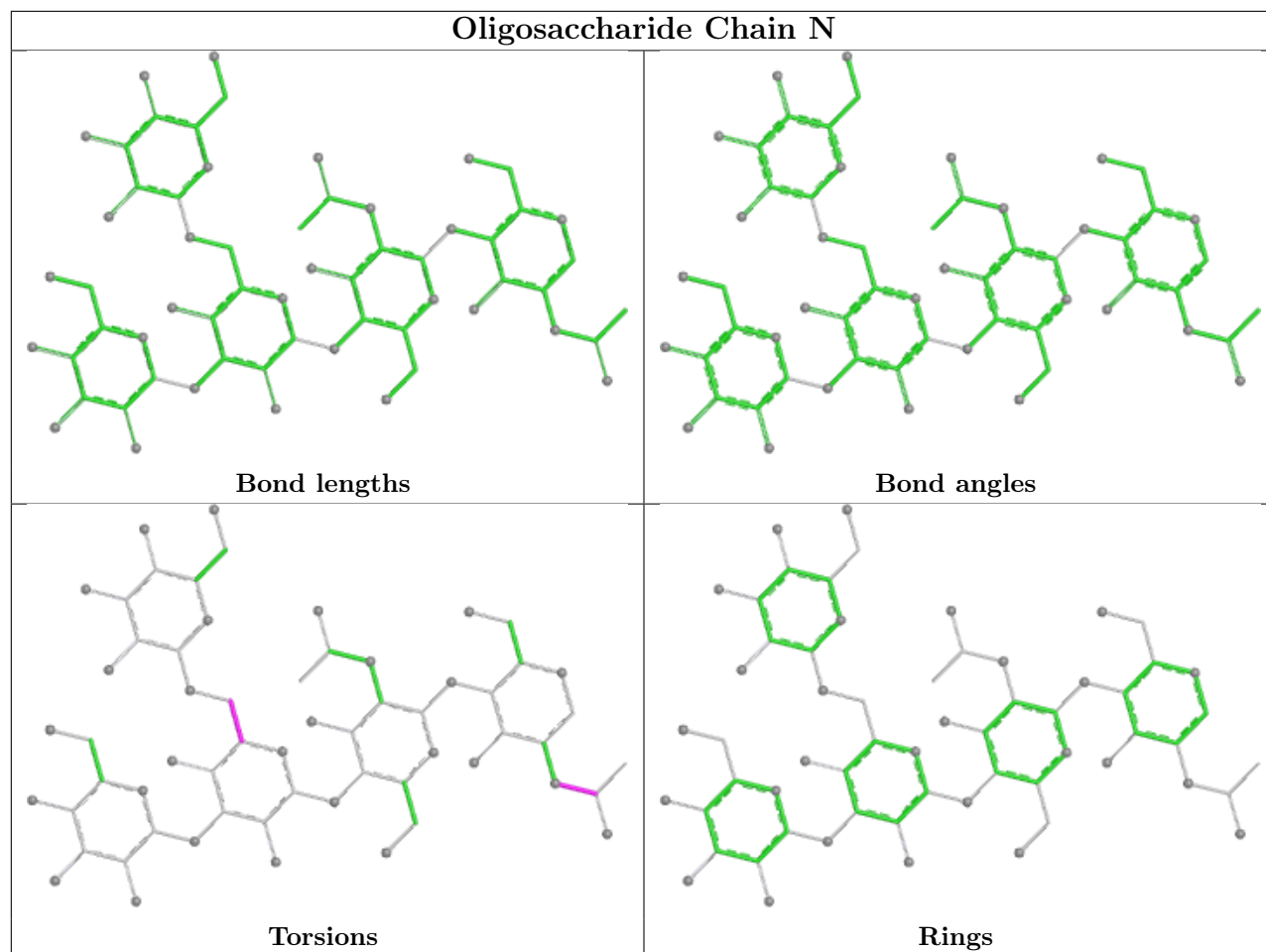
There are no ring outliers.

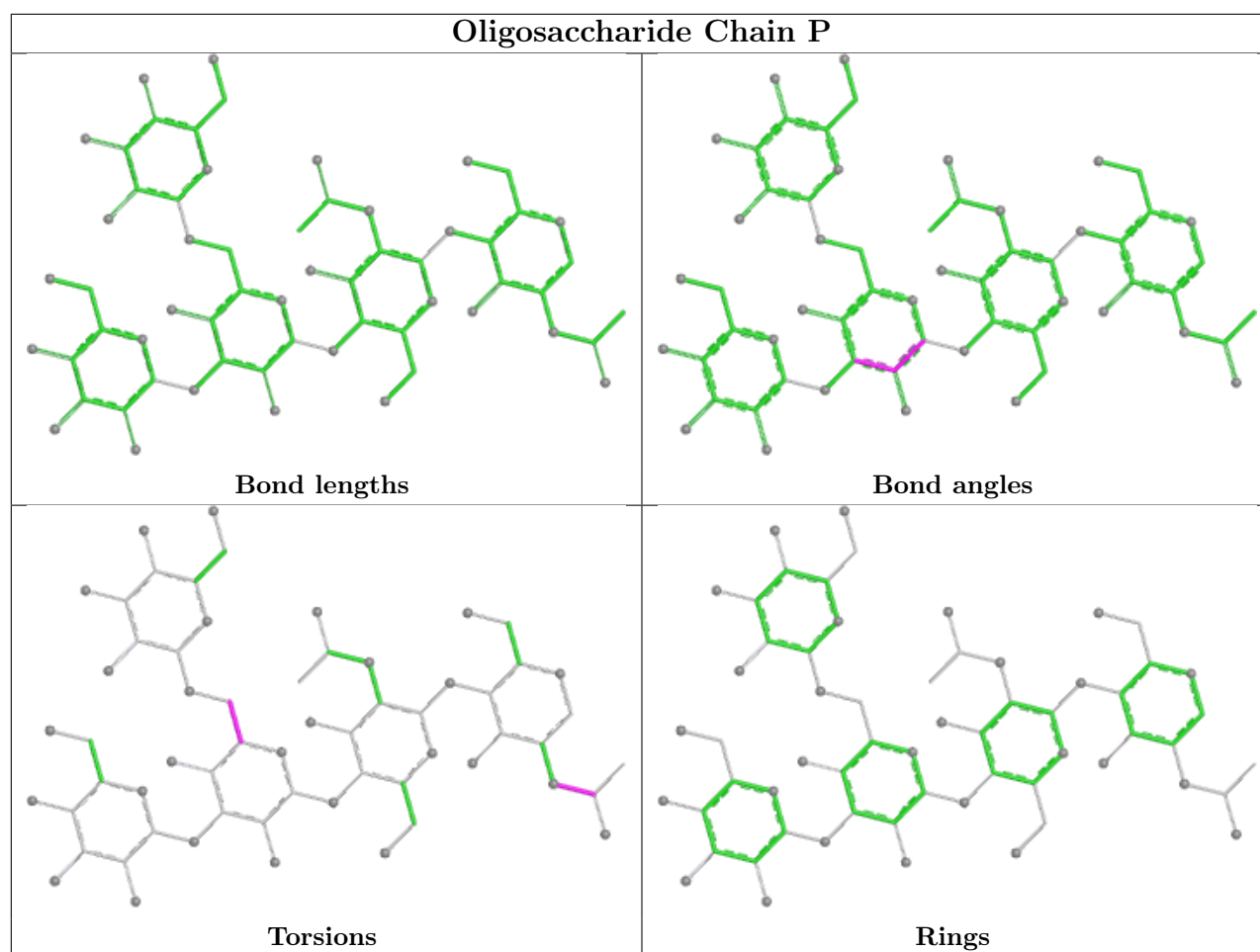
4 monomers are involved in 2 short contacts:

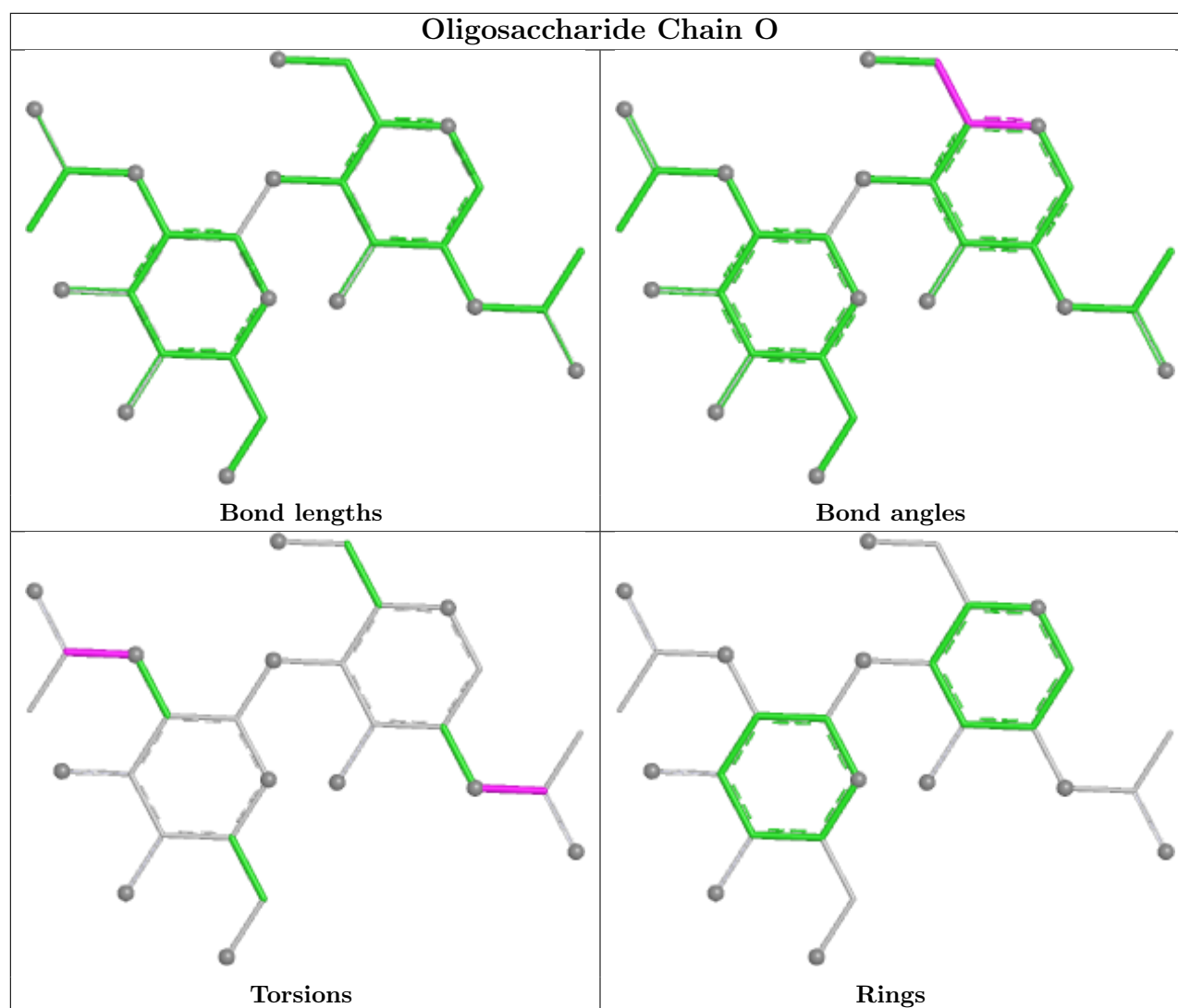
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	2	NAG	1	0
5	O	1	NAG	1	0
4	N	3	BMA	1	0
4	N	5	MAN	1	0

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](#)

66 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	A	505	1	14,14,15	0.53	0	17,19,21	0.72	1 (5%)
6	NAG	G	505	1	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
6	NAG	A	509	1	14,14,15	0.54	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	509	1	14,14,15	0.54	0	17,19,21	0.64	0
6	NAG	I	510	1	14,14,15	0.52	0	17,19,21	0.81	1 (5%)
6	NAG	G	509	1	14,14,15	0.58	0	17,19,21	0.62	0
7	BGC	B	301	-	12,12,12	0.52	0	17,17,17	0.49	0
7	BGC	C	301	-	12,12,12	0.53	0	17,17,17	0.49	0
8	TRS	D	514	-	7,7,7	0.34	0	9,9,9	0.28	0
7	BGC	E	301	-	12,12,12	0.51	0	17,17,17	0.51	0
6	NAG	A	506	1	14,14,15	0.53	0	17,19,21	0.85	0
8	TRS	A	513	-	7,7,7	0.33	0	9,9,9	0.35	0
6	NAG	D	506	1	14,14,15	0.55	0	17,19,21	0.60	0
6	NAG	D	505	1	14,14,15	0.58	0	17,19,21	0.52	0
7	BGC	D	515	-	12,12,12	0.52	0	17,17,17	0.44	0
6	NAG	G	506	1	14,14,15	0.47	0	17,19,21	0.90	1 (5%)
6	NAG	D	511	1	14,14,15	0.54	0	17,19,21	0.69	0
6	NAG	I	501	1	14,14,15	0.53	0	17,19,21	0.99	2 (11%)
7	BGC	G	512	-	12,12,12	0.53	0	17,17,17	0.48	0
6	NAG	I	511	1	14,14,15	0.59	0	17,19,21	1.64	2 (11%)
8	TRS	J	501	-	7,7,7	0.33	0	9,9,9	0.31	0
6	NAG	G	503	1	14,14,15	0.53	0	17,19,21	0.66	0
7	BGC	A	515	-	12,12,12	0.52	0	17,17,17	0.51	0
6	NAG	I	508	1	14,14,15	0.56	0	17,19,21	0.55	0
6	NAG	G	502	1	14,14,15	0.53	0	17,19,21	0.67	0
6	NAG	A	502	1	14,14,15	0.52	0	17,19,21	0.76	0
6	NAG	D	507	1	14,14,15	0.56	0	17,19,21	0.64	0
7	BGC	A	517	-	12,12,12	0.52	0	17,17,17	0.45	0
6	NAG	I	504	1	14,14,15	0.54	0	17,19,21	0.73	0
6	NAG	A	512	1	14,14,15	0.53	0	17,19,21	0.59	0
6	NAG	D	512	1	14,14,15	0.54	0	17,19,21	0.54	0
6	NAG	I	503	1	14,14,15	0.54	0	17,19,21	0.52	0
7	BGC	A	518	-	12,12,12	0.53	0	17,17,17	0.57	0
7	BGC	B	302	-	12,12,12	0.52	0	17,17,17	0.48	0
6	NAG	I	506	1	14,14,15	0.49	0	17,19,21	0.93	1 (5%)
6	NAG	I	505	1	14,14,15	0.56	0	17,19,21	0.57	0
6	NAG	I	509	1	14,14,15	0.55	0	17,19,21	0.66	0
6	NAG	A	507	1	14,14,15	0.50	0	17,19,21	0.84	0
6	NAG	G	507	1	14,14,15	0.53	0	17,19,21	0.68	0
7	BGC	J	502	-	12,12,12	0.52	0	17,17,17	0.53	0
6	NAG	D	510	1	14,14,15	0.56	0	17,19,21	0.65	0
8	TRS	A	514	-	7,7,7	0.33	0	9,9,9	0.30	0
6	NAG	G	504	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
8	TRS	K	301	-	7,7,7	0.34	0	9,9,9	0.29	0
6	NAG	D	504	1	14,14,15	0.59	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BGC	I	512	-	12,12,12	0.53	0	17,17,17	0.50	0
6	NAG	I	502	1	14,14,15	0.50	0	17,19,21	0.76	0
6	NAG	A	510	1	14,14,15	0.56	0	17,19,21	0.68	0
6	NAG	G	510	1	14,14,15	0.54	0	17,19,21	0.64	0
6	NAG	A	503	1	14,14,15	0.51	0	17,19,21	0.81	0
7	BGC	I	513	-	12,12,12	0.54	0	17,17,17	0.55	0
6	NAG	D	503	1	14,14,15	0.53	0	17,19,21	0.58	0
8	TRS	D	513	-	7,7,7	0.33	0	9,9,9	0.34	0
6	NAG	A	501	1	14,14,15	0.54	0	17,19,21	0.74	0
6	NAG	D	501	1	14,14,15	0.53	0	17,19,21	0.63	0
7	BGC	A	516	-	12,12,12	0.52	0	17,17,17	0.54	0
6	NAG	G	501	1	14,14,15	0.51	0	17,19,21	0.55	0
6	NAG	D	502	1	14,14,15	0.53	0	17,19,21	0.60	0
6	NAG	A	508	1	14,14,15	0.53	0	17,19,21	0.59	0
6	NAG	D	508	1	14,14,15	0.53	0	17,19,21	0.72	1 (5%)
6	NAG	A	511	1	14,14,15	0.51	0	17,19,21	0.76	0
8	TRS	I	514	-	7,7,7	0.34	0	9,9,9	0.37	0
6	NAG	G	508	1	14,14,15	0.55	0	17,19,21	0.69	0
6	NAG	G	511	1	14,14,15	0.54	0	17,19,21	0.68	0
6	NAG	I	507	1	14,14,15	0.54	0	17,19,21	0.53	0
6	NAG	A	504	1	14,14,15	0.55	0	17,19,21	0.93	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	505	1	-	3/6/23/26	0/1/1/1
6	NAG	G	505	1	-	2/6/23/26	0/1/1/1
6	NAG	A	509	1	-	4/6/23/26	0/1/1/1
6	NAG	D	509	1	-	2/6/23/26	0/1/1/1
6	NAG	I	510	1	-	3/6/23/26	0/1/1/1
6	NAG	G	509	1	-	2/6/23/26	0/1/1/1
7	BGC	B	301	-	-	0/2/22/22	0/1/1/1
7	BGC	C	301	-	-	0/2/22/22	0/1/1/1
8	TRS	D	514	-	-	0/9/9/9	-
7	BGC	E	301	-	-	0/2/22/22	0/1/1/1
6	NAG	A	506	1	-	4/6/23/26	0/1/1/1
8	TRS	A	513	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	506	1	-	3/6/23/26	0/1/1/1
6	NAG	D	505	1	-	2/6/23/26	0/1/1/1
7	BGC	D	515	-	-	0/2/22/22	0/1/1/1
6	NAG	G	506	1	-	0/6/23/26	0/1/1/1
6	NAG	D	511	1	-	2/6/23/26	0/1/1/1
6	NAG	I	501	1	-	2/6/23/26	0/1/1/1
7	BGC	G	512	-	-	0/2/22/22	0/1/1/1
6	NAG	I	511	1	-	4/6/23/26	0/1/1/1
8	TRS	J	501	-	-	0/9/9/9	-
6	NAG	G	503	1	-	2/6/23/26	0/1/1/1
7	BGC	A	515	-	-	0/2/22/22	0/1/1/1
6	NAG	I	508	1	-	3/6/23/26	0/1/1/1
6	NAG	G	502	1	-	2/6/23/26	0/1/1/1
6	NAG	A	502	1	-	2/6/23/26	0/1/1/1
6	NAG	D	507	1	-	0/6/23/26	0/1/1/1
7	BGC	A	517	-	-	1/2/22/22	0/1/1/1
6	NAG	I	504	1	-	2/6/23/26	0/1/1/1
6	NAG	A	512	1	-	3/6/23/26	0/1/1/1
6	NAG	D	512	1	-	2/6/23/26	0/1/1/1
6	NAG	I	503	1	-	0/6/23/26	0/1/1/1
7	BGC	A	518	-	-	1/2/22/22	0/1/1/1
7	BGC	B	302	-	-	1/2/22/22	0/1/1/1
6	NAG	I	506	1	-	0/6/23/26	0/1/1/1
6	NAG	I	505	1	-	3/6/23/26	0/1/1/1
6	NAG	I	509	1	-	3/6/23/26	0/1/1/1
6	NAG	A	507	1	-	2/6/23/26	0/1/1/1
6	NAG	G	507	1	-	0/6/23/26	0/1/1/1
7	BGC	J	502	-	-	2/2/22/22	0/1/1/1
6	NAG	D	510	1	-	0/6/23/26	0/1/1/1
8	TRS	A	514	-	-	0/9/9/9	-
6	NAG	G	504	1	-	4/6/23/26	0/1/1/1
8	TRS	K	301	-	-	0/9/9/9	-
6	NAG	D	504	1	-	0/6/23/26	0/1/1/1
7	BGC	I	512	-	-	1/2/22/22	0/1/1/1
6	NAG	I	502	1	-	3/6/23/26	0/1/1/1
6	NAG	A	510	1	-	0/6/23/26	0/1/1/1
6	NAG	G	510	1	-	2/6/23/26	0/1/1/1
6	NAG	A	503	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BGC	I	513	-	-	0/2/22/22	0/1/1/1
6	NAG	D	503	1	-	2/6/23/26	0/1/1/1
8	TRS	D	513	-	-	0/9/9/9	-
6	NAG	A	501	1	-	2/6/23/26	0/1/1/1
6	NAG	D	501	1	-	0/6/23/26	0/1/1/1
7	BGC	A	516	-	-	0/2/22/22	0/1/1/1
6	NAG	G	501	1	-	2/6/23/26	0/1/1/1
6	NAG	D	502	1	-	0/6/23/26	0/1/1/1
6	NAG	A	508	1	-	2/6/23/26	0/1/1/1
6	NAG	D	508	1	-	2/6/23/26	0/1/1/1
6	NAG	A	511	1	-	2/6/23/26	0/1/1/1
8	TRS	I	514	-	-	2/9/9/9	-
6	NAG	G	508	1	-	3/6/23/26	0/1/1/1
6	NAG	G	511	1	-	2/6/23/26	0/1/1/1
6	NAG	I	507	1	-	3/6/23/26	0/1/1/1
6	NAG	A	504	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	511	NAG	O5-C1-C2	4.61	118.42	111.29
6	I	511	NAG	C1-O5-C5	4.43	118.13	112.19
6	I	506	NAG	C1-O5-C5	3.11	116.35	112.19
6	G	504	NAG	C1-O5-C5	2.97	116.16	112.19
6	I	501	NAG	C1-O5-C5	2.84	115.99	112.19
6	G	506	NAG	C1-O5-C5	2.58	115.64	112.19
6	I	510	NAG	C1-O5-C5	2.50	115.53	112.19
6	A	504	NAG	C1-O5-C5	2.35	115.33	112.19
6	G	505	NAG	C1-O5-C5	2.32	115.29	112.19
6	A	505	NAG	C1-O5-C5	2.25	115.20	112.19
6	I	501	NAG	O5-C1-C2	2.18	114.67	111.29
6	D	508	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	501	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	G	501	NAG	O7-C7-N2-C2
6	G	502	NAG	C8-C7-N2-C2
6	G	502	NAG	O7-C7-N2-C2
6	G	504	NAG	C8-C7-N2-C2
6	G	504	NAG	O7-C7-N2-C2
6	G	509	NAG	C8-C7-N2-C2
6	G	509	NAG	O7-C7-N2-C2
6	G	511	NAG	C8-C7-N2-C2
6	G	511	NAG	O7-C7-N2-C2
6	A	503	NAG	C8-C7-N2-C2
6	A	503	NAG	O7-C7-N2-C2
6	A	504	NAG	C8-C7-N2-C2
6	A	504	NAG	O7-C7-N2-C2
6	A	506	NAG	C8-C7-N2-C2
6	A	506	NAG	O7-C7-N2-C2
6	A	507	NAG	C8-C7-N2-C2
6	A	507	NAG	O7-C7-N2-C2
6	A	509	NAG	C3-C2-N2-C7
6	A	509	NAG	C8-C7-N2-C2
6	A	509	NAG	O7-C7-N2-C2
6	A	511	NAG	C8-C7-N2-C2
6	A	511	NAG	O7-C7-N2-C2
6	D	503	NAG	C8-C7-N2-C2
6	D	503	NAG	O7-C7-N2-C2
6	D	506	NAG	C3-C2-N2-C7
6	D	506	NAG	C8-C7-N2-C2
6	D	506	NAG	O7-C7-N2-C2
6	D	508	NAG	C8-C7-N2-C2
6	D	508	NAG	O7-C7-N2-C2
6	D	509	NAG	O7-C7-N2-C2
6	I	502	NAG	C8-C7-N2-C2
6	I	502	NAG	O7-C7-N2-C2
6	I	505	NAG	C3-C2-N2-C7
6	I	505	NAG	C8-C7-N2-C2
6	I	505	NAG	O7-C7-N2-C2
6	I	507	NAG	C8-C7-N2-C2
6	I	507	NAG	O7-C7-N2-C2
6	I	510	NAG	C8-C7-N2-C2
6	I	510	NAG	O7-C7-N2-C2
8	A	513	TRS	N-C-C2-O2
8	I	514	TRS	N-C-C1-O1
6	D	509	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	I	508	NAG	C8-C7-N2-C2
6	I	508	NAG	O7-C7-N2-C2
6	G	504	NAG	O5-C5-C6-O6
6	D	512	NAG	C8-C7-N2-C2
6	G	505	NAG	C8-C7-N2-C2
6	A	502	NAG	C8-C7-N2-C2
6	A	512	NAG	C8-C7-N2-C2
6	D	511	NAG	C8-C7-N2-C2
6	A	506	NAG	O5-C5-C6-O6
6	G	505	NAG	O7-C7-N2-C2
6	G	510	NAG	C8-C7-N2-C2
6	G	510	NAG	O7-C7-N2-C2
6	A	501	NAG	C8-C7-N2-C2
6	A	501	NAG	O7-C7-N2-C2
6	A	502	NAG	O7-C7-N2-C2
6	A	505	NAG	C8-C7-N2-C2
6	A	505	NAG	O7-C7-N2-C2
6	A	512	NAG	O7-C7-N2-C2
6	D	505	NAG	C8-C7-N2-C2
6	D	505	NAG	O7-C7-N2-C2
6	D	511	NAG	O7-C7-N2-C2
6	D	512	NAG	O7-C7-N2-C2
6	I	511	NAG	C8-C7-N2-C2
6	G	504	NAG	C4-C5-C6-O6
7	J	502	BGC	O5-C5-C6-O6
6	I	504	NAG	C8-C7-N2-C2
6	I	511	NAG	O7-C7-N2-C2
6	A	508	NAG	C8-C7-N2-C2
6	I	507	NAG	O5-C5-C6-O6
6	I	509	NAG	C8-C7-N2-C2
6	I	504	NAG	O7-C7-N2-C2
6	I	508	NAG	O5-C5-C6-O6
7	A	518	BGC	O5-C5-C6-O6
6	I	509	NAG	O5-C5-C6-O6
7	B	302	BGC	O5-C5-C6-O6
7	A	517	BGC	O5-C5-C6-O6
6	G	508	NAG	O5-C5-C6-O6
6	I	511	NAG	C3-C2-N2-C7
7	I	512	BGC	O5-C5-C6-O6
6	A	509	NAG	O5-C5-C6-O6
6	A	512	NAG	O5-C5-C6-O6
6	I	502	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	I	510	NAG	O5-C5-C6-O6
8	A	513	TRS	C3-C-C2-O2
6	G	508	NAG	C8-C7-N2-C2
6	A	508	NAG	O7-C7-N2-C2
6	I	509	NAG	O7-C7-N2-C2
6	I	511	NAG	C1-C2-N2-C7
6	A	506	NAG	C4-C5-C6-O6
6	G	503	NAG	C8-C7-N2-C2
6	G	508	NAG	O7-C7-N2-C2
6	G	503	NAG	O7-C7-N2-C2
6	I	501	NAG	C8-C7-N2-C2
6	I	501	NAG	O7-C7-N2-C2
7	J	502	BGC	C4-C5-C6-O6
8	A	513	TRS	C1-C-C2-O2
8	I	514	TRS	C2-C-C1-O1
6	A	505	NAG	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	505	NAG	1	0
7	G	512	BGC	1	0
6	D	507	NAG	1	0
7	A	517	BGC	3	0
7	A	518	BGC	2	0
7	B	302	BGC	1	0
6	I	506	NAG	1	0
6	A	507	NAG	1	0
6	G	507	NAG	1	0
7	J	502	BGC	1	0
8	K	301	TRS	1	0
7	I	513	BGC	1	0
8	D	513	TRS	1	0
7	A	516	BGC	1	0
8	I	514	TRS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	349/353 (98%)	-0.33	4 (1%) 78 76	55, 89, 141, 225	0
1	D	350/353 (99%)	-0.24	4 (1%) 78 76	64, 97, 168, 273	0
1	G	347/353 (98%)	-0.25	2 (0%) 85 84	68, 103, 160, 241	0
1	I	349/353 (98%)	-0.13	4 (1%) 78 76	74, 118, 181, 249	0
2	B	224/224 (100%)	-0.24	0 100 100	59, 102, 172, 208	0
2	E	224/224 (100%)	-0.04	2 (0%) 81 79	70, 118, 264, 292	0
2	H	224/224 (100%)	-0.41	2 (0%) 81 79	59, 85, 117, 165	0
2	J	224/224 (100%)	-0.33	0 100 100	66, 101, 134, 202	0
3	C	210/210 (100%)	-0.17	1 (0%) 87 86	61, 116, 173, 216	0
3	F	208/210 (99%)	-0.02	1 (0%) 87 86	88, 181, 245, 270	0
3	K	210/210 (100%)	-0.25	2 (0%) 79 77	78, 114, 163, 210	0
3	L	208/210 (99%)	-0.26	1 (0%) 87 86	71, 112, 154, 228	0
All	All	3127/3148 (99%)	-0.23	23 (0%) 84 82	55, 105, 206, 292	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	GLY	4.1
2	E	181	VAL	4.0
1	I	259	LEU	3.7
3	F	3	VAL	3.5
1	A	327	ARG	3.2
1	D	349	LEU	3.2
3	C	3	VAL	3.2
1	D	459	GLY	3.0
1	A	247	CYS	2.8
1	I	452	ILE	2.8
3	K	3	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	247	CYS	2.6
3	L	155	ALA	2.5
1	A	458	GLY	2.4
3	K	135	VAL	2.4
1	D	472	GLY	2.3
2	H	208	ASP	2.3
2	E	141	LEU	2.2
1	I	369	LEU	2.1
1	G	430	THR	2.1
1	I	472	GLY	2.0
1	D	44	VAL	2.0
2	H	206	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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

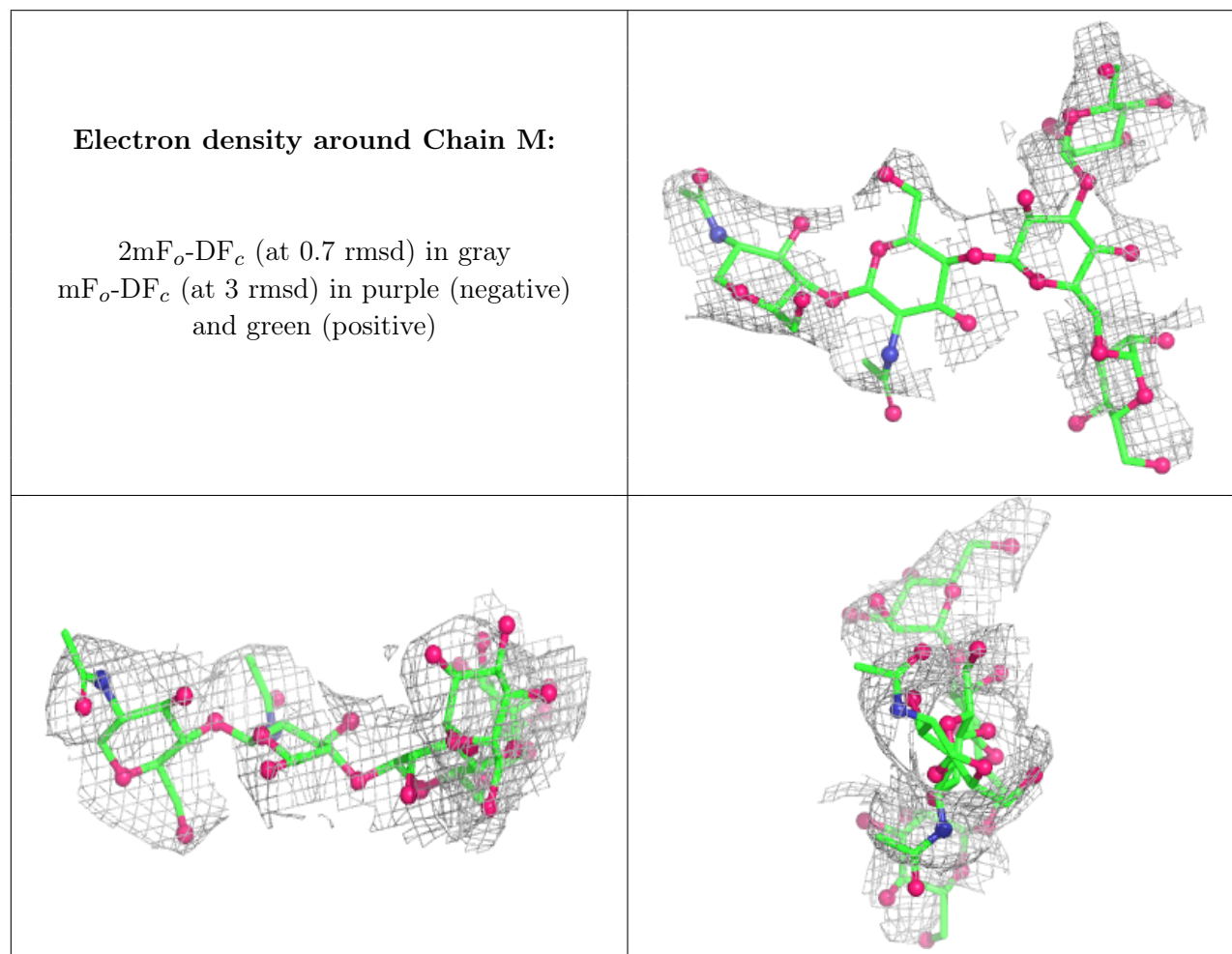
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	P	3	11/12	0.12	0.12	230,237,239,242	0
4	MAN	M	4	11/12	0.13	0.10	159,191,200,207	0
4	MAN	N	4	11/12	0.16	0.08	188,198,216,216	0
4	MAN	P	4	11/12	0.33	0.10	217,221,232,232	0
4	MAN	N	5	11/12	0.35	0.08	202,209,216,216	0
4	MAN	P	5	11/12	0.43	0.10	216,236,238,239	0
4	MAN	M	5	11/12	0.48	0.09	209,235,239,239	0
4	BMA	N	3	11/12	0.50	0.09	211,218,224,225	0
4	BMA	M	3	11/12	0.62	0.07	211,219,224,230	0
4	NAG	P	2	14/15	0.63	0.12	118,182,200,219	0
4	NAG	M	2	14/15	0.63	0.08	158,179,191,206	0
5	NAG	O	2	14/15	0.63	0.07	190,206,214,217	0
5	NAG	O	1	14/15	0.83	0.08	144,174,187,199	0
4	NAG	N	2	14/15	0.86	0.08	125,168,183,204	0
4	NAG	M	1	14/15	0.88	0.07	125,143,162,176	0
4	NAG	P	1	14/15	0.88	0.11	116,142,167,186	0

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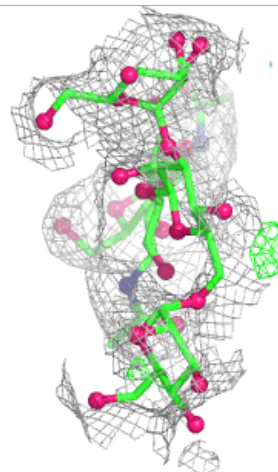
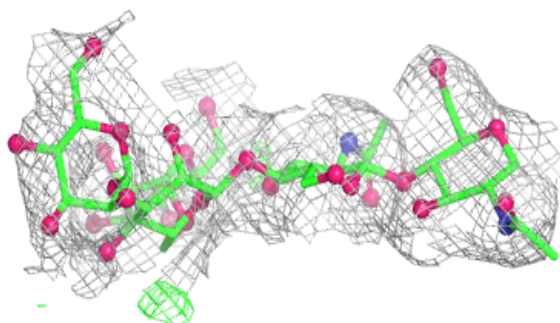
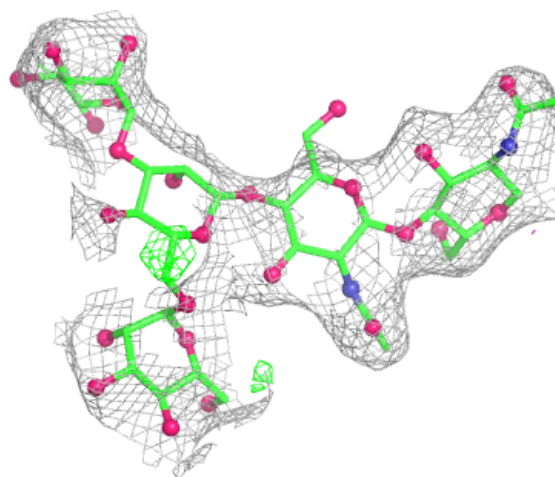
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	N	1	14/15	0.92	0.08	102,112,125,146	0

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.



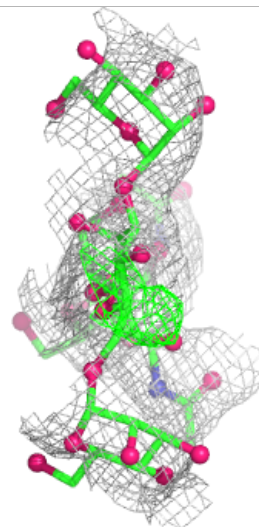
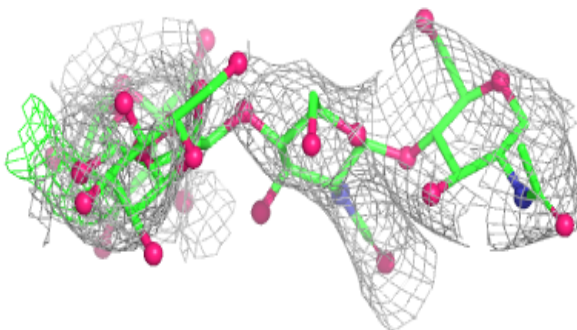
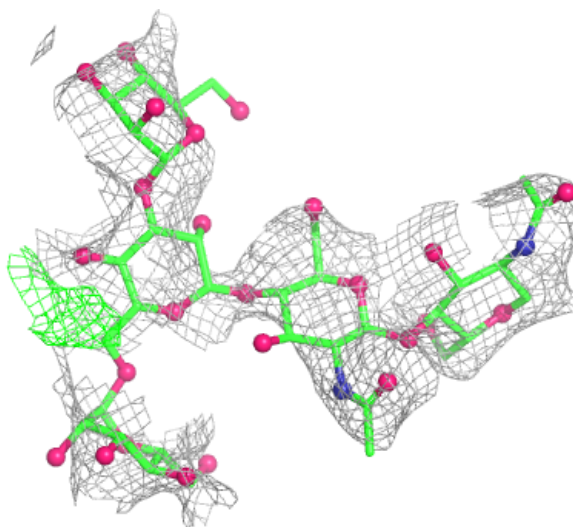
Electron density around Chain N:

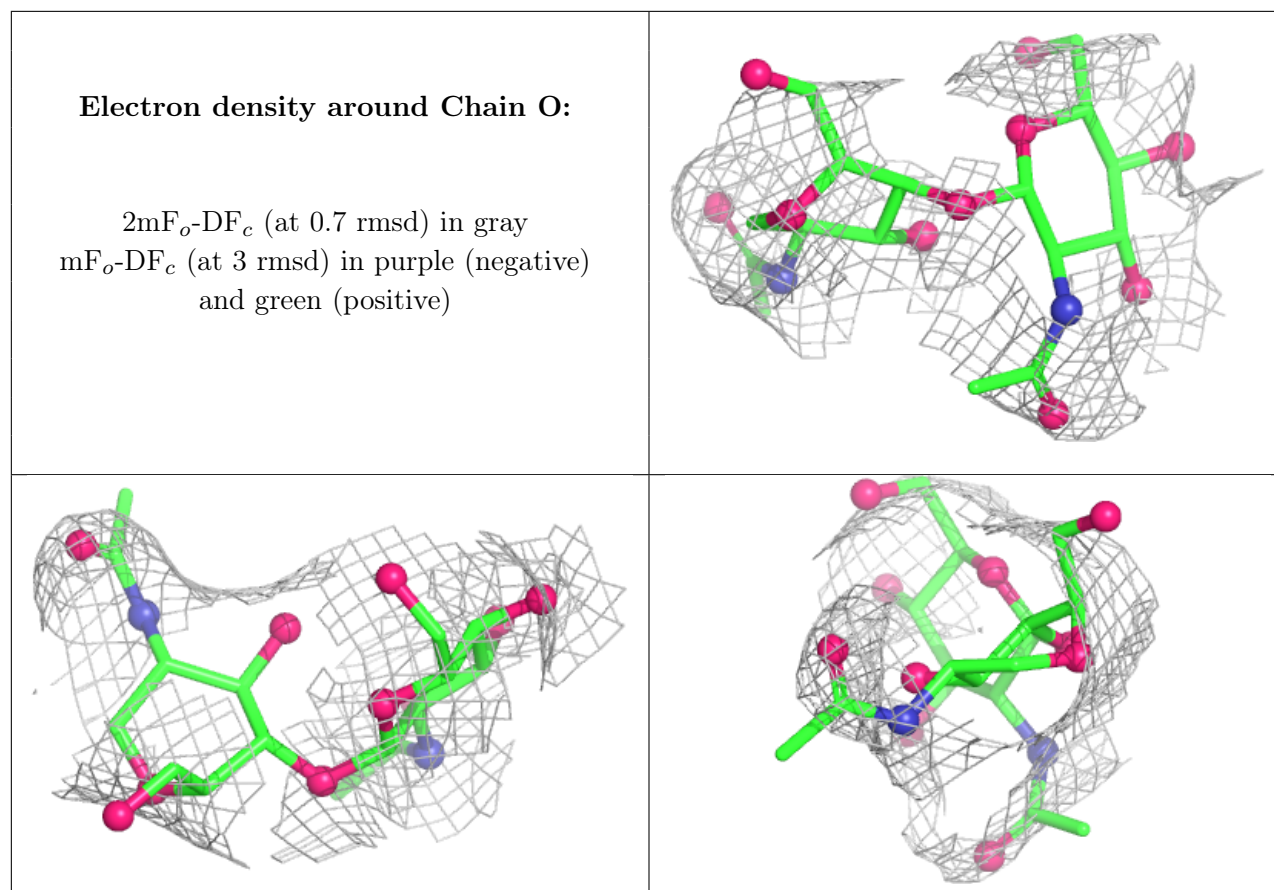
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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, 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
6	NAG	A	509	14/15	0.17	0.12	191,212,221,221	0
6	NAG	D	503	14/15	0.29	0.13	176,190,202,207	0
6	NAG	D	501	14/15	0.31	0.11	193,207,215,219	0
6	NAG	G	503	14/15	0.33	0.12	143,160,167,171	0
6	NAG	G	501	14/15	0.43	0.09	159,171,176,177	0
7	BGC	E	301	12/12	0.48	0.09	162,194,197,198	0
7	BGC	J	502	12/12	0.50	0.10	197,218,223,223	0
7	BGC	C	301	12/12	0.51	0.11	197,212,216,216	0
6	NAG	I	501	14/15	0.52	0.10	167,178,186,187	0
8	TRS	K	301	8/8	0.53	0.11	164,183,188,188	0
6	NAG	I	505	14/15	0.60	0.13	146,173,183,184	0
6	NAG	D	509	14/15	0.61	0.09	170,185,192,193	0
7	BGC	I	512	12/12	0.65	0.09	208,216,220,220	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	D	508	14/15	0.67	0.09	116,132,139,144	0
7	BGC	A	516	12/12	0.68	0.09	113,153,160,160	0
6	NAG	I	503	14/15	0.69	0.09	149,180,190,191	0
6	NAG	A	503	14/15	0.69	0.10	105,126,137,138	0
6	NAG	D	505	14/15	0.70	0.11	126,154,166,168	0
8	TRS	A	514	8/8	0.70	0.09	156,167,171,172	0
7	BGC	A	515	12/12	0.70	0.10	161,182,188,188	0
6	NAG	I	510	14/15	0.72	0.08	149,165,177,179	0
6	NAG	I	508	14/15	0.73	0.08	124,151,159,166	0
6	NAG	A	512	14/15	0.74	0.09	152,166,176,182	0
7	BGC	I	513	12/12	0.76	0.11	136,156,176,178	0
6	NAG	G	508	14/15	0.76	0.10	136,145,179,186	0
6	NAG	A	505	14/15	0.78	0.13	98,128,144,144	0
7	BGC	B	302	12/12	0.78	0.10	114,145,150,152	0
6	NAG	A	511	14/15	0.78	0.09	123,151,163,164	0
6	NAG	G	505	14/15	0.79	0.11	120,140,150,156	0
6	NAG	I	502	14/15	0.79	0.10	116,136,144,147	0
7	BGC	D	515	12/12	0.79	0.13	162,179,185,185	0
6	NAG	D	512	14/15	0.80	0.09	129,149,163,168	0
6	NAG	I	511	14/15	0.81	0.11	152,171,176,185	0
6	NAG	I	506	14/15	0.81	0.08	120,132,137,142	0
6	NAG	A	508	14/15	0.81	0.10	122,135,148,151	0
6	NAG	G	511	14/15	0.81	0.10	153,173,179,179	0
8	TRS	I	514	8/8	0.82	0.10	113,126,128,130	0
6	NAG	A	507	14/15	0.84	0.10	109,120,136,142	0
7	BGC	A	517	12/12	0.84	0.18	179,199,203,205	0
7	BGC	G	512	12/12	0.85	0.12	92,146,155,156	0
6	NAG	I	507	14/15	0.85	0.08	98,133,154,155	0
6	NAG	G	507	14/15	0.86	0.10	97,123,136,139	0
6	NAG	A	506	14/15	0.86	0.09	79,90,111,126	0
6	NAG	G	506	14/15	0.86	0.08	110,116,129,134	0
6	NAG	D	511	14/15	0.87	0.08	134,145,164,165	0
7	BGC	B	301	12/12	0.88	0.09	140,182,188,189	0
6	NAG	G	510	14/15	0.89	0.07	71,107,123,133	0
7	BGC	A	518	12/12	0.90	0.12	141,162,172,177	0
8	TRS	D	513	8/8	0.90	0.08	84,102,120,123	0
8	TRS	D	514	8/8	0.90	0.12	108,137,143,151	0
6	NAG	D	506	14/15	0.90	0.08	105,121,137,138	0
8	TRS	J	501	8/8	0.90	0.12	125,145,154,155	0
6	NAG	I	509	14/15	0.90	0.07	102,127,140,149	0
6	NAG	D	507	14/15	0.91	0.06	86,107,115,121	0
6	NAG	G	509	14/15	0.91	0.11	94,111,128,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	G	502	14/15	0.92	0.08	91,106,120,120	0
6	NAG	A	504	14/15	0.93	0.07	80,90,107,107	0
6	NAG	A	501	14/15	0.93	0.07	63,79,89,90	0
8	TRS	A	513	8/8	0.93	0.07	98,108,120,124	0
6	NAG	D	510	14/15	0.94	0.06	82,103,121,122	0
6	NAG	D	502	14/15	0.94	0.06	108,119,137,140	0
6	NAG	I	504	14/15	0.94	0.10	98,113,118,123	0
6	NAG	D	504	14/15	0.95	0.08	79,88,99,100	0
6	NAG	A	510	14/15	0.95	0.05	72,86,111,112	0
6	NAG	A	502	14/15	0.95	0.07	79,103,109,113	0
6	NAG	G	504	14/15	0.95	0.08	80,91,111,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.