



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:43 AM UTC

PDB ID : 4F23 / pdb_00004f23
Title : Influenza A virus hemagglutinin H16 HA0 structure with an alpha-helix con-
formation in the cleavage site: a potential drug target
Authors : Lu, X.; Shi, Y.; Gao, F.; Xiao, H.; Qi, J.; Gao, G.F.
Deposited on : 2012-05-07
Resolution : 1.70 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

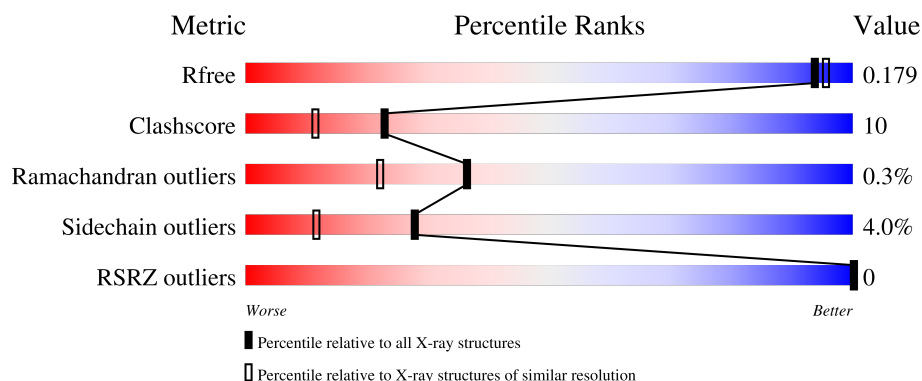
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

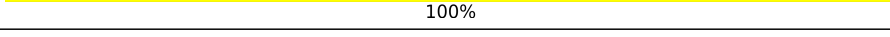
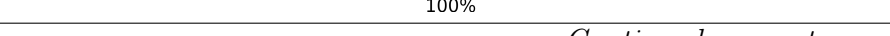
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	515	
1	B	515	
1	C	515	
2	D	2	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14190 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	3	0
			4040	2522	719	781	18			
1	B	509	Total	C	N	O	S	0	1	0
			4025	2513	716	778	18			
1	C	509	Total	C	N	O	S	0	0	0
			4019	2510	715	776	18			

There are 48 discrepancies between the modelled and reference sequences:

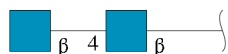
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q5DL24
A	-4	HIS	-	expression tag	UNP Q5DL24
A	-3	HIS	-	expression tag	UNP Q5DL24
A	-2	HIS	-	expression tag	UNP Q5DL24
A	-1	HIS	-	expression tag	UNP Q5DL24
A	0	HIS	-	expression tag	UNP Q5DL24
A	1	ALA	-	SEE REMARK 999	UNP Q5DL24
A	2	ASP	-	SEE REMARK 999	UNP Q5DL24
A	3	GLY	-	SEE REMARK 999	UNP Q5DL24
A	4	ILE	-	SEE REMARK 999	UNP Q5DL24
A	5	GLN	-	SEE REMARK 999	UNP Q5DL24
A	505	ARG	-	SEE REMARK 999	UNP Q5DL24
A	506	LEU	-	SEE REMARK 999	UNP Q5DL24
A	507	VAL	-	SEE REMARK 999	UNP Q5DL24
A	508	PRO	-	SEE REMARK 999	UNP Q5DL24
A	509	ARG	-	SEE REMARK 999	UNP Q5DL24
B	-5	HIS	-	expression tag	UNP Q5DL24
B	-4	HIS	-	expression tag	UNP Q5DL24
B	-3	HIS	-	expression tag	UNP Q5DL24
B	-2	HIS	-	expression tag	UNP Q5DL24
B	-1	HIS	-	expression tag	UNP Q5DL24
B	0	HIS	-	expression tag	UNP Q5DL24
B	1	ALA	-	SEE REMARK 999	UNP Q5DL24

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ASP	-	SEE REMARK 999	UNP Q5DL24
B	3	GLY	-	SEE REMARK 999	UNP Q5DL24
B	4	ILE	-	SEE REMARK 999	UNP Q5DL24
B	5	GLN	-	SEE REMARK 999	UNP Q5DL24
B	505	ARG	-	SEE REMARK 999	UNP Q5DL24
B	506	LEU	-	SEE REMARK 999	UNP Q5DL24
B	507	VAL	-	SEE REMARK 999	UNP Q5DL24
B	508	PRO	-	SEE REMARK 999	UNP Q5DL24
B	509	ARG	-	SEE REMARK 999	UNP Q5DL24
C	-5	HIS	-	expression tag	UNP Q5DL24
C	-4	HIS	-	expression tag	UNP Q5DL24
C	-3	HIS	-	expression tag	UNP Q5DL24
C	-2	HIS	-	expression tag	UNP Q5DL24
C	-1	HIS	-	expression tag	UNP Q5DL24
C	0	HIS	-	expression tag	UNP Q5DL24
C	1	ALA	-	SEE REMARK 999	UNP Q5DL24
C	2	ASP	-	SEE REMARK 999	UNP Q5DL24
C	3	GLY	-	SEE REMARK 999	UNP Q5DL24
C	4	ILE	-	SEE REMARK 999	UNP Q5DL24
C	5	GLN	-	SEE REMARK 999	UNP Q5DL24
C	505	ARG	-	SEE REMARK 999	UNP Q5DL24
C	506	LEU	-	SEE REMARK 999	UNP Q5DL24
C	507	VAL	-	SEE REMARK 999	UNP Q5DL24
C	508	PRO	-	SEE REMARK 999	UNP Q5DL24
C	509	ARG	-	SEE REMARK 999	UNP Q5DL24

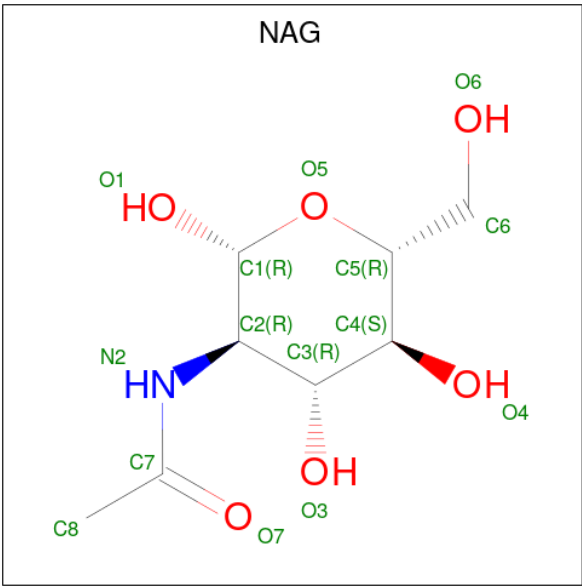
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

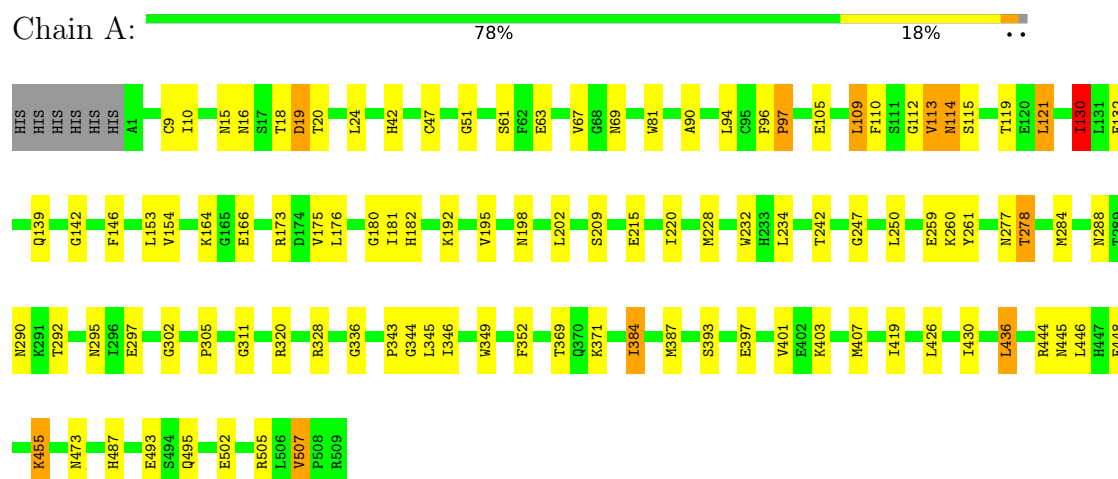
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	676	Total	O	0	0
			676	676		
4	B	650	Total	O	0	0
			650	650		
4	C	654	Total	O	0	0
			654	654		

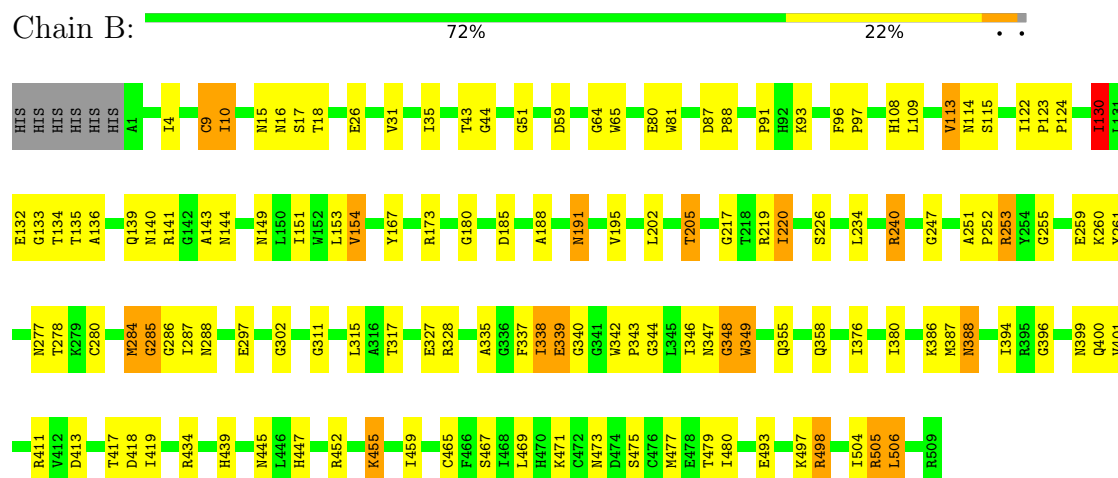
3 Residue-property plots

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.

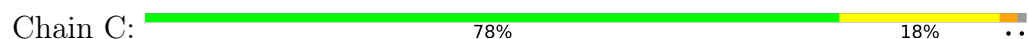
• Molecule 1: Hemagglutinin

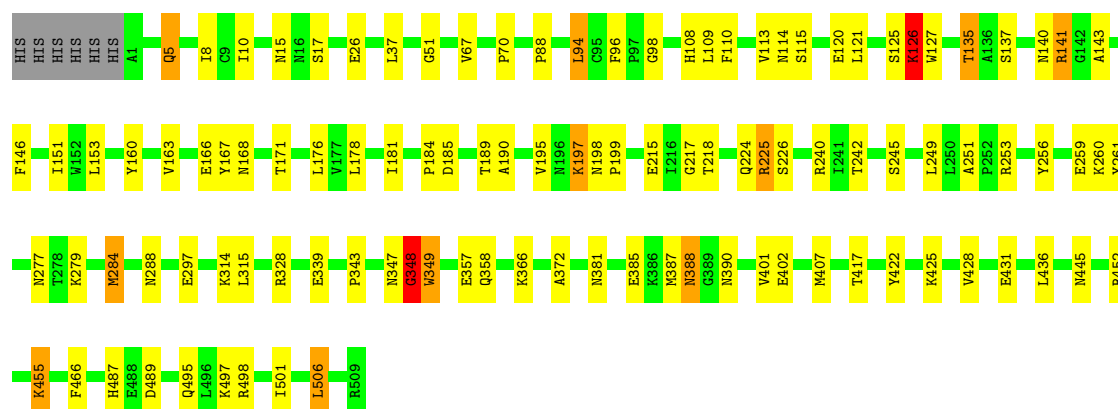


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





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

Chain D: 100%

NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

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

Chain F: 100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.33Å 240.94Å 69.67Å 90.00° 119.79° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70 25.00 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.00-1.70) 97.6 (25.00-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.160 , 0.192 0.153 , 0.179	Depositor DCC
R_{free} test set	10596 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.217 for -h-l,k,h 0.217 for l,k,-h-l 0.097 for h,-k,-h-l 0.095 for -h-l,-k,l 0.090 for l,-k,h	Xtriage
Reported twinning fraction	0.659 for H, K, L 0.209 for -H-L, K, H 0.132 for L, K, -H-L	Depositor
Outliers	0 of 210913 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14190	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	1.57	24/4123 (0.6%)	1.18	6/5583 (0.1%)
1	B	1.60	36/4108 (0.9%)	1.21	11/5565 (0.2%)
1	C	1.59	33/4102 (0.8%)	1.19	4/5556 (0.1%)
All	All	1.59	93/12333 (0.8%)	1.20	21/16704 (0.1%)

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLY	N-CA	8.53	1.53	1.45
1	A	175	VAL	CA-CB	-7.75	1.44	1.54
1	A	181	ILE	CA-CB	7.38	1.64	1.54
1	C	143	ALA	CA-CB	-7.12	1.39	1.54
1	B	253	ARG	N-CA	7.07	1.54	1.46
1	C	151	ILE	C-O	7.07	1.31	1.24
1	A	232	TRP	N-CA	7.05	1.54	1.45
1	A	175	VAL	N-CA	7.04	1.55	1.46
1	B	504	ILE	N-CA	7.04	1.54	1.46
1	C	348	GLY	N-CA	-6.96	1.34	1.45
1	B	226	SER	N-CA	6.87	1.53	1.45
1	B	154	VAL	C-O	6.81	1.31	1.23
1	B	180	GLY	N-CA	6.80	1.52	1.45
1	B	349	TRP	N-CA	6.58	1.54	1.46
1	C	226	SER	N-CA	6.56	1.53	1.45
1	B	247	GLY	N-CA	6.53	1.54	1.45
1	C	189	THR	C-O	-6.51	1.16	1.24
1	A	182	HIS	C-O	-6.46	1.16	1.24
1	C	349	TRP	N-CA	6.46	1.54	1.46
1	B	220	ILE	N-CA	6.45	1.53	1.46
1	C	146	PHE	N-CA	6.39	1.53	1.46
1	B	10	ILE	C-O	6.37	1.30	1.24
1	C	181	ILE	CA-CB	6.34	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLY	N-CA	6.26	1.54	1.45
1	A	198	ASN	C-O	6.24	1.26	1.23
1	C	166	GLU	C-O	6.21	1.31	1.23
1	B	411	ARG	N-CA	-6.13	1.39	1.46
1	B	396	GLY	C-O	6.11	1.33	1.23
1	C	466	PHE	C-O	6.07	1.30	1.24
1	A	507	VAL	N-CA	-6.05	1.41	1.46
1	A	195	VAL	CA-CB	6.05	1.62	1.54
1	B	418	ASP	C-O	-6.01	1.17	1.24
1	B	188	ALA	CA-CB	5.99	1.62	1.53
1	B	143	ALA	C-O	-5.93	1.17	1.23
1	B	123	PRO	C-O	-5.92	1.19	1.24
1	B	123	PRO	CA-C	5.85	1.56	1.52
1	C	5	GLN	N-CA	5.83	1.53	1.46
1	C	225	ARG	N-CA	5.81	1.53	1.46
1	C	184	PRO	C-O	5.75	1.30	1.23
1	C	167	TYR	C-O	5.75	1.30	1.24
1	B	133	GLY	C-O	-5.74	1.17	1.23
1	B	439	HIS	C-O	-5.73	1.17	1.24
1	C	67	VAL	C-O	-5.71	1.17	1.24
1	C	195	VAL	N-CA	5.68	1.53	1.46
1	B	284	MET	C-O	5.66	1.31	1.24
1	C	498	ARG	N-CA	5.64	1.53	1.46
1	C	431	GLU	C-O	-5.62	1.17	1.24
1	B	505	ARG	CD-NE	5.59	1.54	1.46
1	B	149	ASN	N-CA	5.59	1.53	1.46
1	C	70	PRO	N-CA	5.58	1.54	1.47
1	A	42	HIS	C-O	5.54	1.30	1.23
1	A	192	LYS	N-CA	5.50	1.52	1.46
1	C	347	ASN	CA-C	5.48	1.60	1.53
1	B	311	GLY	C-O	5.46	1.28	1.23
1	B	255	GLY	C-O	5.45	1.30	1.23
1	B	349	TRP	C-O	-5.44	1.17	1.24
1	C	171	THR	CA-CB	5.42	1.62	1.53
1	C	137	SER	N-CA	-5.39	1.39	1.46
1	A	132	GLU	C-O	5.37	1.30	1.24
1	C	431	GLU	CB-CG	5.37	1.68	1.52
1	A	139	GLN	N-CA	5.37	1.52	1.45
1	A	507	VAL	CA-CB	5.36	1.60	1.54
1	C	217	GLY	N-CA	5.33	1.50	1.45
1	B	251	ALA	N-CA	5.30	1.53	1.45
1	A	295	ASN	N-CA	5.29	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	HIS	N-CA	-5.29	1.40	1.46
1	B	302	GLY	C-O	5.28	1.27	1.24
1	C	402	GLU	CA-CB	5.27	1.60	1.53
1	C	178	LEU	N-CA	5.26	1.52	1.46
1	A	250	LEU	C-O	5.25	1.30	1.23
1	A	112	GLY	CA-C	-5.24	1.46	1.51
1	A	397	GLU	C-O	-5.22	1.17	1.24
1	B	167	TYR	C-O	5.22	1.29	1.24
1	C	390	ASN	N-CA	5.20	1.52	1.46
1	A	209	SER	N-CA	-5.19	1.40	1.46
1	A	446	LEU	C-O	-5.18	1.18	1.24
1	A	311	GLY	C-O	5.16	1.28	1.23
1	C	8	ILE	C-O	5.13	1.29	1.24
1	B	205	THR	CA-CB	-5.13	1.46	1.53
1	B	219	ARG	CZ-NH2	5.12	1.40	1.33
1	A	146	PHE	N-CA	5.12	1.52	1.46
1	B	191	ASN	N-CA	5.11	1.52	1.46
1	C	190	ALA	C-O	5.10	1.30	1.24
1	B	130	ILE	CG1-CD1	-5.10	1.31	1.51
1	A	493	GLU	N-CA	5.08	1.52	1.46
1	B	493	GLU	N-CA	5.07	1.52	1.46
1	B	9	CYS	C-O	5.07	1.30	1.24
1	C	506	LEU	N-CA	5.07	1.52	1.46
1	B	180	GLY	C-O	5.06	1.28	1.23
1	C	372	ALA	C-O	-5.04	1.18	1.24
1	C	417	THR	CA-CB	5.03	1.61	1.53
1	B	285	GLY	N-CA	5.03	1.50	1.45
1	B	65	TRP	C-N	-5.03	1.27	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	SER	N-CA-C	9.02	121.05	111.03
1	B	498	ARG	N-CA-C	-8.45	102.15	111.36
1	B	349	TRP	N-CA-C	7.52	121.16	108.90
1	A	69	ASN	O-C-N	6.15	126.27	121.47
1	B	340	GLY	N-CA-C	-6.05	107.31	115.36
1	A	336	GLY	N-CA-C	-6.04	107.41	115.32
1	B	130	ILE	CG1-CB-CG2	6.02	128.75	110.70
1	B	327	GLU	N-CA-C	-5.90	105.35	112.54
1	C	347	ASN	N-CA-C	5.83	119.28	111.24
1	A	130	ILE	N-CA-CB	-5.70	105.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	PRO	CB-CA-C	-5.62	104.66	111.46
1	B	344	GLY	N-CA-C	5.60	119.42	112.64
1	B	130	ILE	N-CA-CB	-5.53	104.77	112.52
1	B	347	ASN	N-CA-C	5.53	119.02	111.39
1	C	347	ASN	O-C-N	-5.49	116.11	122.86
1	B	96	PHE	N-CA-C	-5.47	102.06	110.32
1	B	311	GLY	N-CA-C	-5.27	104.50	112.41
1	C	126	LYS	N-CA-C	5.11	117.51	111.33
1	A	142	GLY	N-CA-C	5.09	122.11	115.40
1	A	302	GLY	N-CA-C	5.03	116.64	111.56
1	A	384	ILE	N-CA-C	5.01	115.30	110.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4040	0	3923	72	0
1	B	4025	0	3908	109	0
1	C	4019	0	3903	86	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
4	A	676	0	0	30	0
4	B	650	0	0	49	0
4	C	654	0	0	40	0
All	All	14190	0	11848	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (250) 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:B:480:ILE:HD12	4:B:1261:HOH:O	1.25	1.27
1:A:90:ALA:HB3	4:A:1086:HOH:O	1.42	1.20
1:B:467:SER:HB2	4:B:872:HOH:O	1.58	1.04
1:B:459:ILE:HB	4:B:872:HOH:O	1.58	1.03
1:A:202:LEU:HB3	4:A:1211:HOH:O	1.60	1.00
1:C:501:ILE:HD11	4:C:1338:HOH:O	1.63	0.98
1:B:253:ARG:HG3	4:B:1271:HOH:O	1.65	0.96
1:A:130:ILE:HA	4:A:1017:HOH:O	1.70	0.91
1:B:80:GLU:HA	4:B:1330:HOH:O	1.71	0.91
1:A:328:ARG:HA	1:C:445:ASN:HD21	1.35	0.90
1:C:253:ARG:HG2	4:C:1076:HOH:O	1.71	0.89
1:A:228:MET:HB2	4:A:1292:HOH:O	1.70	0.89
1:B:278:THR:HG22	1:B:280:CYS:H	1.35	0.88
1:B:445:ASN:HD21	1:C:328:ARG:HA	1.40	0.85
1:A:352:PHE:HD1	4:A:1175:HOH:O	1.58	0.85
1:B:317:THR:O	4:B:1101:HOH:O	1.94	0.85
1:C:51:GLY:H	1:C:277:ASN:HD21	1.24	0.84
1:B:15:ASN:HD22	1:B:16:ASN:H	1.20	0.84
1:C:113:VAL:HA	4:C:1278:HOH:O	1.77	0.84
1:B:64:GLY:HA3	4:B:1113:HOH:O	1.78	0.83
1:B:286:GLY:N	4:B:1062:HOH:O	2.10	0.82
1:C:260:LYS:O	4:C:1278:HOH:O	1.97	0.82
1:C:218:THR:HG21	1:C:225:ARG:NH2	1.94	0.82
1:B:144:ASN:HB3	4:B:992:HOH:O	1.80	0.82
1:C:261:TYR:HA	4:C:1278:HOH:O	1.78	0.81
4:A:972:HOH:O	1:B:220:ILE:HG12	1.79	0.81
1:B:346:ILE:HG13	1:B:348:GLY:HA2	1.62	0.81
1:C:160:TYR:HE2	4:C:1056:HOH:O	1.64	0.80
1:B:51:GLY:H	1:B:277:ASN:HD21	1.29	0.79
1:C:343:PRO:HD2	1:C:348:GLY:CA	2.13	0.79
1:B:477:MET:SD	4:B:1261:HOH:O	2.40	0.79
1:A:352:PHE:CD1	4:A:1175:HOH:O	2.31	0.79
4:A:920:HOH:O	1:B:506:LEU:HD12	1.82	0.78
1:B:447:HIS:HB2	4:B:1069:HOH:O	1.84	0.77
1:C:163:VAL:HG22	4:C:1056:HOH:O	1.84	0.77
1:A:51:GLY:H	1:A:277:ASN:HD21	1.33	0.76
1:C:452:ARG:O	1:C:455:LYS:HD2	1.86	0.74
1:C:489:ASP:OD2	4:C:1299:HOH:O	2.06	0.73
1:C:245:SER:O	4:C:1056:HOH:O	2.06	0.73
1:C:5:GLN:NE2	4:C:1338:HOH:O	2.20	0.73
1:A:110:PHE:CE2	1:A:176:LEU:HD22	2.24	0.72
1:C:135:THR:OG1	4:C:1268:HOH:O	1.85	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:TYR:CE2	4:C:1056:HOH:O	2.40	0.72
1:A:9:CYS:O	4:A:1175:HOH:O	2.06	0.71
1:C:199:PRO:HA	4:C:1295:HOH:O	1.89	0.71
1:C:197:LYS:HG3	4:C:1267:HOH:O	1.91	0.71
1:B:343:PRO:HD2	1:B:348:GLY:HA3	1.71	0.71
1:A:114:ASN:HB3	1:A:260[B]:LYS:HB2	1.72	0.70
1:C:120:GLU:HG3	4:C:1076:HOH:O	1.91	0.70
1:B:413:ASP:HA	4:B:1122:HOH:O	1.91	0.70
1:A:445:ASN:HD21	1:B:328:ARG:HA	1.57	0.70
1:B:130:ILE:HG21	1:B:153:LEU:HD22	1.75	0.69
1:B:376:ILE:HG13	4:B:1101:HOH:O	1.91	0.69
1:B:15:ASN:ND2	1:B:16:ASN:H	1.90	0.68
1:C:218:THR:CG2	1:C:225:ARG:NH2	2.56	0.68
1:B:497:LYS:HG2	4:B:1234:HOH:O	1.94	0.68
1:B:388:ASN:H	1:B:388:ASN:HD22	1.41	0.68
1:C:489:ASP:HB3	4:C:1243:HOH:O	1.93	0.67
1:A:284:MET:HG3	1:A:297:GLU:HB2	1.76	0.67
1:C:51:GLY:H	1:C:277:ASN:ND2	1.92	0.66
1:C:15:ASN:OD1	4:C:995:HOH:O	2.14	0.65
1:C:153:LEU:HD12	4:C:1280:HOH:O	1.96	0.65
1:B:417:THR:HG22	4:B:966:HOH:O	1.96	0.65
1:B:15:ASN:HD22	1:B:16:ASN:N	1.93	0.64
1:B:122:ILE:O	4:B:1271:HOH:O	2.15	0.64
1:C:115:SER:HB3	1:C:259:GLU:HB3	1.80	0.63
1:A:164:LYS:HE3	4:A:1310:HOH:O	1.99	0.62
1:B:477:MET:HA	4:B:1261:HOH:O	1.98	0.62
1:B:394:ILE:HD12	4:B:1122:HOH:O	2.00	0.62
1:B:285:GLY:CA	4:B:1062:HOH:O	2.47	0.62
1:B:285:GLY:HA3	4:B:1062:HOH:O	2.00	0.62
1:C:163:VAL:HG13	4:C:1056:HOH:O	2.01	0.61
1:B:278:THR:HG22	1:B:280:CYS:N	2.14	0.61
1:C:114:ASN:HB2	1:C:260:LYS:HD2	1.82	0.61
1:B:115:SER:HB3	1:B:259:GLU:HB3	1.83	0.60
1:C:224:GLN:NE2	4:C:1268:HOH:O	2.35	0.60
1:B:337:PHE:CZ	1:B:339:GLU:HG2	2.36	0.60
1:B:387:MET:HG3	1:C:422:TYR:CE1	2.36	0.60
1:C:168:ASN:OD1	1:C:240:ARG:HG3	2.00	0.60
1:C:343:PRO:HD2	1:C:348:GLY:HA2	1.83	0.60
1:B:51:GLY:H	1:B:277:ASN:ND2	2.00	0.59
1:B:15:ASN:HB2	4:B:1151:HOH:O	2.01	0.59
1:A:344:GLY:O	4:A:1371:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:GLN:HG3	4:C:1260:HOH:O	2.03	0.59
1:B:43:THR:OG1	4:B:1062:HOH:O	2.16	0.59
1:A:292:THR:HG21	4:A:1169:HOH:O	2.01	0.59
1:B:342:TRP:NE1	4:B:1151:HOH:O	2.29	0.59
1:A:444:ARG:HG2	4:A:1120:HOH:O	2.02	0.58
1:C:245:SER:HB3	4:C:1280:HOH:O	2.02	0.58
1:A:10:ILE:HD12	4:A:1175:HOH:O	2.02	0.58
1:A:110:PHE:CZ	1:A:176:LEU:HD22	2.37	0.58
1:A:401:VAL:HG12	1:A:401:VAL:O	2.03	0.58
1:B:284:MET:HG3	1:B:297:GLU:HB2	1.84	0.58
1:B:337:PHE:CE2	1:B:338:ILE:O	2.57	0.58
1:A:47:CYS:HB2	1:A:278:THR:HG22	1.84	0.58
1:A:18:THR:O	1:A:19:ASP:HB2	2.03	0.57
1:B:467:SER:CB	4:B:872:HOH:O	2.31	0.57
1:C:388:ASN:H	1:C:388:ASN:HD22	1.52	0.57
1:A:130:ILE:HG21	1:A:153:LEU:HD22	1.86	0.57
1:A:130:ILE:HG12	1:A:153:LEU:HB3	1.86	0.57
1:B:355:GLN:NE2	4:B:1034:HOH:O	2.36	0.57
1:C:185:ASP:OD1	1:C:225:ARG:NH1	2.37	0.57
1:A:202:LEU:HD22	1:B:217:GLY:HA3	1.88	0.56
1:A:130:ILE:HG13	1:A:154:VAL:O	2.05	0.56
1:C:343:PRO:HD2	1:C:348:GLY:HA3	1.86	0.56
1:A:290:ASN:HA	4:A:1294:HOH:O	2.05	0.56
1:A:215:GLU:CD	4:A:1100:HOH:O	2.49	0.56
1:B:467:SER:O	4:B:872:HOH:O	2.17	0.56
1:B:132:GLU:HG2	1:B:151:ILE:CG2	2.36	0.55
1:C:88:PRO:HG2	4:C:1285:HOH:O	2.06	0.55
1:C:215:GLU:HA	4:C:1273:HOH:O	2.05	0.55
1:B:434:ARG:HD2	4:B:883:HOH:O	2.05	0.55
1:C:37:LEU:HD12	1:C:428:VAL:HG21	1.88	0.55
1:B:114:ASN:C	4:B:1330:HOH:O	2.49	0.55
1:A:345:LEU:N	4:A:921:HOH:O	2.39	0.54
1:B:338:ILE:HG23	1:B:339:GLU:H	1.71	0.54
1:B:144:ASN:ND2	4:B:992:HOH:O	2.37	0.54
1:B:93:LYS:HA	4:B:1113:HOH:O	2.08	0.54
1:B:387:MET:HG3	1:C:422:TYR:CD1	2.42	0.54
1:C:357:GLU:HB2	4:C:1288:HOH:O	2.07	0.53
1:C:455:LYS:HD3	1:C:487:HIS:CD2	2.43	0.53
1:A:202:LEU:HD23	4:A:1211:HOH:O	2.09	0.53
1:B:278:THR:HG23	1:B:287:ILE:O	2.09	0.53
1:C:197:LYS:HD2	4:C:1178:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:SER:CA	4:B:872:HOH:O	2.56	0.52
1:B:140:ASN:OD1	1:B:141:ARG:HD2	2.09	0.52
1:B:386:LYS:HD3	1:C:425:LYS:HD3	1.91	0.52
1:A:115:SER:HB3	1:A:259:GLU:HB3	1.91	0.52
1:A:166:GLU:HB2	4:A:1012:HOH:O	2.09	0.52
1:A:403:LYS:O	1:A:407:MET:HG3	2.10	0.51
1:B:278:THR:CG2	1:B:280:CYS:H	2.16	0.51
1:A:242:THR:OG1	4:A:972:HOH:O	2.19	0.51
1:A:61:SER:N	4:A:1086:HOH:O	2.42	0.51
1:C:366:LYS:HD2	4:C:1261:HOH:O	2.11	0.51
1:A:119:THR:HG23	1:A:121:LEU:HD13	1.91	0.51
1:A:114:ASN:HB3	1:A:260[A]:LYS:HB3	1.93	0.51
1:C:126:LYS:O	1:C:126:LYS:HD3	2.11	0.51
1:A:51:GLY:H	1:A:277:ASN:ND2	2.05	0.51
1:B:195:VAL:HG12	4:B:1162:HOH:O	2.10	0.50
1:C:114:ASN:ND2	4:C:1323:HOH:O	2.44	0.50
1:C:366:LYS:HD3	4:C:1027:HOH:O	2.09	0.50
1:A:242:THR:HG21	1:B:220:ILE:HG21	1.94	0.50
1:B:401:VAL:HG12	1:B:401:VAL:O	2.10	0.50
1:C:197:LYS:HG2	1:C:197:LYS:O	2.12	0.50
1:C:96:PHE:CE1	4:C:1268:HOH:O	2.64	0.50
1:B:130:ILE:HG13	1:B:154:VAL:O	2.12	0.49
1:B:452:ARG:O	1:B:455:LYS:HE3	2.12	0.49
1:B:144:ASN:CB	4:B:992:HOH:O	2.52	0.49
1:B:455:LYS:HE2	4:B:1243:HOH:O	2.11	0.49
1:C:249:LEU:HB3	4:C:1280:HOH:O	2.12	0.49
1:A:220:ILE:HG21	1:C:242:THR:HG21	1.94	0.49
1:A:384:ILE:HA	4:A:1169:HOH:O	2.11	0.49
1:B:317:THR:CG2	1:B:380:ILE:HD11	2.43	0.49
1:B:445:ASN:ND2	1:C:328:ARG:HA	2.20	0.49
1:A:234:LEU:HB3	4:A:1355:HOH:O	2.12	0.49
1:A:328:ARG:HA	1:C:445:ASN:ND2	2.17	0.49
1:B:10:ILE:HB	4:B:1069:HOH:O	2.13	0.49
1:B:475:SER:O	1:B:479:THR:HG23	2.13	0.49
1:C:198:ASN:N	1:C:199:PRO:HD3	2.28	0.48
1:B:343:PRO:HD3	1:B:349:TRP:CE2	2.48	0.48
1:B:113:VAL:O	4:B:1330:HOH:O	2.20	0.48
1:B:44:GLY:N	4:B:1062:HOH:O	2.47	0.48
1:B:335:ALA:O	1:B:342:TRP:HZ2	1.97	0.48
1:A:455:LYS:HD3	1:A:487:HIS:NE2	2.29	0.48
1:C:163:VAL:HG21	4:C:1280:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PHE:CZ	1:C:176:LEU:HD22	2.49	0.47
1:C:497:LYS:HD2	4:C:1338:HOH:O	2.14	0.47
1:B:43:THR:N	4:B:1062:HOH:O	2.46	0.47
1:B:358:GLN:OE1	1:B:473:ASN:HB2	2.15	0.47
1:C:366:LYS:NZ	4:C:989:HOH:O	2.48	0.47
1:A:24:LEU:HD22	1:A:430:ILE:HG12	1.96	0.46
1:B:205:THR:HA	1:B:240:ARG:O	2.16	0.46
1:A:10:ILE:CD1	4:A:1175:HOH:O	2.62	0.46
1:A:320:ARG:HB2	1:A:436:LEU:HG	1.97	0.46
4:A:1316:HOH:O	1:C:455:LYS:HE3	2.16	0.46
1:C:284:MET:HG3	1:C:297:GLU:HB2	1.97	0.46
1:A:495:GLN:NE2	1:B:505:ARG:HH22	2.14	0.45
1:B:108:HIS:HE2	1:C:407:MET:CE	2.29	0.45
1:B:202:LEU:HD23	4:B:854:HOH:O	2.15	0.45
1:B:134:THR:C	4:B:992:HOH:O	2.59	0.45
1:B:185:ASP:HA	1:B:217:GLY:O	2.17	0.45
1:A:260[A]:LYS:O	1:A:260[A]:LYS:HG2	2.16	0.45
1:A:473:ASN:ND2	4:A:906:HOH:O	2.49	0.44
1:B:81:TRP:CZ2	1:B:113:VAL:HG13	2.52	0.44
1:B:35:ILE:HD13	1:B:380:ILE:HD13	1.99	0.44
1:A:10:ILE:HD12	1:A:10:ILE:N	2.33	0.44
4:B:1051:HOH:O	1:C:407:MET:SD	2.62	0.44
1:C:110:PHE:CE2	1:C:176:LEU:HD22	2.52	0.44
1:A:220:ILE:HD13	1:C:242:THR:HG23	1.99	0.44
1:A:81:TRP:CZ2	1:A:113:VAL:HG13	2.53	0.44
1:A:61:SER:HB3	4:A:1086:HOH:O	2.17	0.44
1:A:346:ILE:HD11	1:A:369:THR:HG23	1.99	0.44
1:A:401:VAL:HG13	4:C:1223:HOH:O	2.18	0.44
1:A:15:ASN:CG	1:A:16:ASN:H	2.26	0.43
1:A:97:PRO:O	4:A:1292:HOH:O	2.21	0.43
1:C:10:ILE:HD12	1:C:10:ILE:N	2.32	0.43
1:A:305:PRO:HD3	4:A:842:HOH:O	2.18	0.43
1:B:113:VAL:HB	1:B:261:TYR:HB3	2.00	0.43
1:A:455:LYS:HD3	1:A:487:HIS:CD2	2.53	0.43
1:B:240:ARG:NH2	4:B:1204:HOH:O	2.52	0.43
1:B:191:ASN:OD1	4:B:1209:HOH:O	2.21	0.43
1:B:343:PRO:HG2	1:B:348:GLY:O	2.19	0.43
1:B:278:THR:HG21	1:B:287:ILE:N	2.34	0.43
1:C:381:ASN:O	1:C:385:GLU:HB2	2.19	0.43
1:B:17:SER:HA	4:B:925:HOH:O	2.19	0.43
1:B:328:ARG:HD2	4:B:972:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LYS:HE2	1:B:473:ASN:HB3	2.00	0.43
1:C:314:LYS:NZ	4:C:1245:HOH:O	2.52	0.43
1:A:63:GLU:O	1:A:67:VAL:HG22	2.19	0.42
1:A:505:ARG:HH22	1:C:495:GLN:NE2	2.17	0.42
1:B:317:THR:HG22	1:B:380:ILE:HD11	2.02	0.42
1:A:96:PHE:O	1:A:97:PRO:C	2.61	0.42
1:B:220:ILE:HG23	4:B:1110:HOH:O	2.19	0.42
1:C:127:TRP:CZ2	1:C:251:ALA:HB1	2.55	0.42
1:B:260:LYS:HE2	1:B:260:LYS:HB3	1.86	0.42
1:C:94:LEU:HD23	1:C:98:GLY:C	2.44	0.42
1:C:388:ASN:ND2	4:C:1225:HOH:O	2.51	0.42
1:A:502:GLU:HG3	4:A:1303:HOH:O	2.19	0.42
1:B:87:ASP:HA	1:B:88:PRO:HD3	1.95	0.42
1:C:125:SER:HB3	4:C:1281:HOH:O	2.19	0.42
1:A:110:PHE:HE2	1:A:176:LEU:HD22	1.80	0.41
1:C:140:ASN:CG	1:C:141:ARG:HD2	2.45	0.41
1:C:497:LYS:HD3	1:C:497:LYS:HA	1.75	0.41
1:A:9:CYS:C	1:A:10:ILE:HD12	2.46	0.41
1:A:401:VAL:O	1:A:401:VAL:CG1	2.68	0.41
1:B:9:CYS:HA	1:B:465:CYS:HA	2.02	0.41
1:B:394:ILE:HB	4:B:1122:HOH:O	2.21	0.41
1:C:37:LEU:HD12	1:C:428:VAL:CG2	2.49	0.41
1:B:469:LEU:C	4:B:1234:HOH:O	2.62	0.41
1:B:328:ARG:HD2	1:B:328:ARG:HH11	1.71	0.41
1:B:17:SER:HB2	1:B:31:VAL:O	2.21	0.41
1:B:136:ALA:O	1:B:139:GLN:HG3	2.21	0.41
1:C:176:LEU:HD23	1:C:256:TYR:HD2	1.85	0.41
1:C:218:THR:HG22	1:C:225:ARG:CZ	2.51	0.41
1:A:343:PRO:HD3	1:A:349:TRP:CE2	2.56	0.41
1:B:59:ASP:O	1:B:91:PRO:HD2	2.20	0.41
1:C:96:PHE:CD1	4:C:1268:HOH:O	2.57	0.41
1:A:444:ARG:O	1:A:448:GLU:HG2	2.21	0.41
1:C:114:ASN:CB	1:C:260:LYS:HD2	2.49	0.40
1:C:343:PRO:HD3	1:C:349:TRP:CE2	2.57	0.40
1:A:419:ILE:HG21	1:B:419:ILE:HD13	2.04	0.40
1:B:337:PHE:HZ	1:B:339:GLU:HG2	1.82	0.40
1:B:399:ASN:OD1	1:B:399:ASN:C	2.62	0.40
1:C:215:GLU:HG2	4:C:1273:HOH:O	2.21	0.40
1:C:401:VAL:HG22	1:C:401:VAL:O	2.22	0.40
1:A:113:VAL:HB	1:A:261:TYR:HB3	2.03	0.40
1:A:105:GLU:O	1:A:109:LEU:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:HIS:HE2	1:C:407:MET:HE2	1.86	0.40
1:B:124:PRO:HD3	4:B:1271:HOH:O	2.21	0.40
1:B:469:LEU:HD13	1:B:498:ARG:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/515 (99%)	495 (97%)	14 (3%)	1 (0%)	43	28
1	B	508/515 (99%)	488 (96%)	17 (3%)	3 (1%)	21	9
1	C	507/515 (98%)	488 (96%)	18 (4%)	1 (0%)	43	28
All	All	1525/1545 (99%)	1471 (96%)	49 (3%)	5 (0%)	36	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	B	339	GLU
1	C	348	GLY
1	B	348	GLY
1	B	338	ILE

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	442/445 (99%)	424 (96%)	18 (4%)	27	11
1	B	440/445 (99%)	423 (96%)	17 (4%)	28	12
1	C	439/445 (99%)	421 (96%)	18 (4%)	27	11
All	All	1321/1335 (99%)	1268 (96%)	53 (4%)	28	12

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	94	LEU
1	A	97	PRO
1	A	109	LEU
1	A	113	VAL
1	A	114	ASN
1	A	121	LEU
1	A	130	ILE
1	A	173	ARG
1	A	278	THR
1	A	288	ASN
1	A	371	LYS
1	A	387	MET
1	A	393	SER
1	A	426	LEU
1	A	436	LEU
1	A	455	LYS
1	A	507	VAL
1	B	4	ILE
1	B	18	THR
1	B	26	GLU
1	B	97	PRO
1	B	109	LEU
1	B	113	VAL
1	B	130	ILE
1	B	135	THR
1	B	173	ARG
1	B	234	LEU
1	B	240	ARG
1	B	288	ASN
1	B	315	LEU
1	B	388	ASN
1	B	400	GLN
1	B	455	LYS

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Mol	Chain	Res	Type
1	B	506	LEU
1	C	26	GLU
1	C	94	LEU
1	C	109	LEU
1	C	121	LEU
1	C	126	LYS
1	C	135	THR
1	C	141	ARG
1	C	197	LYS
1	C	279	LYS
1	C	284	MET
1	C	288	ASN
1	C	315	LEU
1	C	339	GLU
1	C	387	MET
1	C	388	ASN
1	C	436	LEU
1	C	455	LYS
1	C	506	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	27	ASN
1	A	114	ASN
1	A	140	ASN
1	A	268	GLN
1	A	277	ASN
1	A	288	ASN
1	A	390	ASN
1	A	445	ASN
1	A	495	GLN
1	B	15	ASN
1	B	277	ASN
1	B	288	ASN
1	B	370	GLN
1	B	388	ASN
1	B	390	ASN
1	B	445	ASN
1	B	495	GLN
1	C	89	ASN

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Mol	Chain	Res	Type
1	C	92	HIS
1	C	114	ASN
1	C	139	GLN
1	C	277	ASN
1	C	288	ASN
1	C	290	ASN
1	C	347	ASN
1	C	388	ASN
1	C	445	ASN
1	C	495	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 ⓘ

6 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.78	0	17,19,21	0.76	1 (5%)
2	NAG	D	2	2	14,14,15	1.29	2 (14%)	17,19,21	1.52	4 (23%)
2	NAG	E	1	2,1	14,14,15	0.57	0	17,19,21	1.69	6 (35%)
2	NAG	E	2	2	14,14,15	0.61	0	17,19,21	1.45	3 (17%)
2	NAG	F	1	2,1	14,14,15	0.89	0	17,19,21	1.15	1 (5%)
2	NAG	F	2	2	14,14,15	0.64	0	17,19,21	1.50	4 (23%)

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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.71	1.56	1.52
2	D	2	NAG	O4-C4	2.05	1.48	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	4.11	128.41	122.90
2	D	2	NAG	C1-O5-C5	3.17	116.43	112.19
2	E	1	NAG	C1-C2-N2	-3.00	105.70	110.43
2	F	1	NAG	O5-C5-C4	-2.98	103.57	110.83
2	E	1	NAG	C1-O5-C5	2.82	115.96	112.19
2	D	2	NAG	C3-C4-C5	-2.77	105.20	110.23
2	D	2	NAG	C2-N2-C7	-2.70	119.28	122.90
2	E	1	NAG	O5-C1-C2	2.67	115.42	111.29
2	F	2	NAG	O5-C5-C6	2.49	112.52	107.66
2	E	1	NAG	C8-C7-N2	2.49	120.25	116.12
2	F	2	NAG	C2-N2-C7	2.43	126.16	122.90
2	E	1	NAG	O6-C6-C5	-2.41	103.11	111.33
2	E	1	NAG	O7-C7-C8	-2.39	117.79	122.05
2	E	2	NAG	C4-C3-C2	2.26	114.33	111.02
2	F	2	NAG	C1-C2-N2	2.24	113.96	110.43
2	E	2	NAG	C1-C2-N2	2.23	113.95	110.43
2	D	1	NAG	C3-C4-C5	-2.05	106.51	110.23
2	F	2	NAG	C1-O5-C5	-2.02	109.48	112.19
2	D	2	NAG	C6-C5-C4	-2.01	108.08	113.02

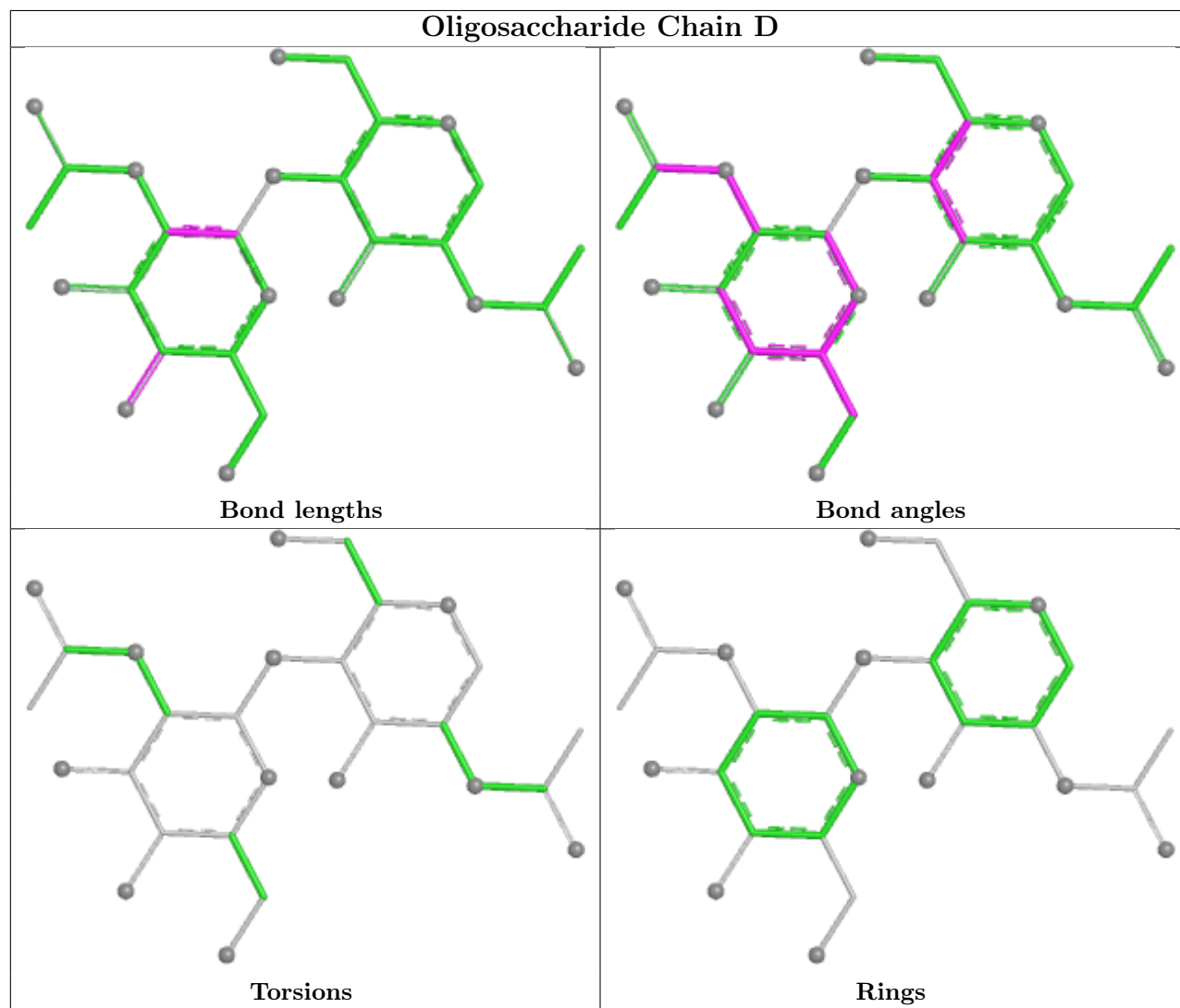
There are no chirality outliers.

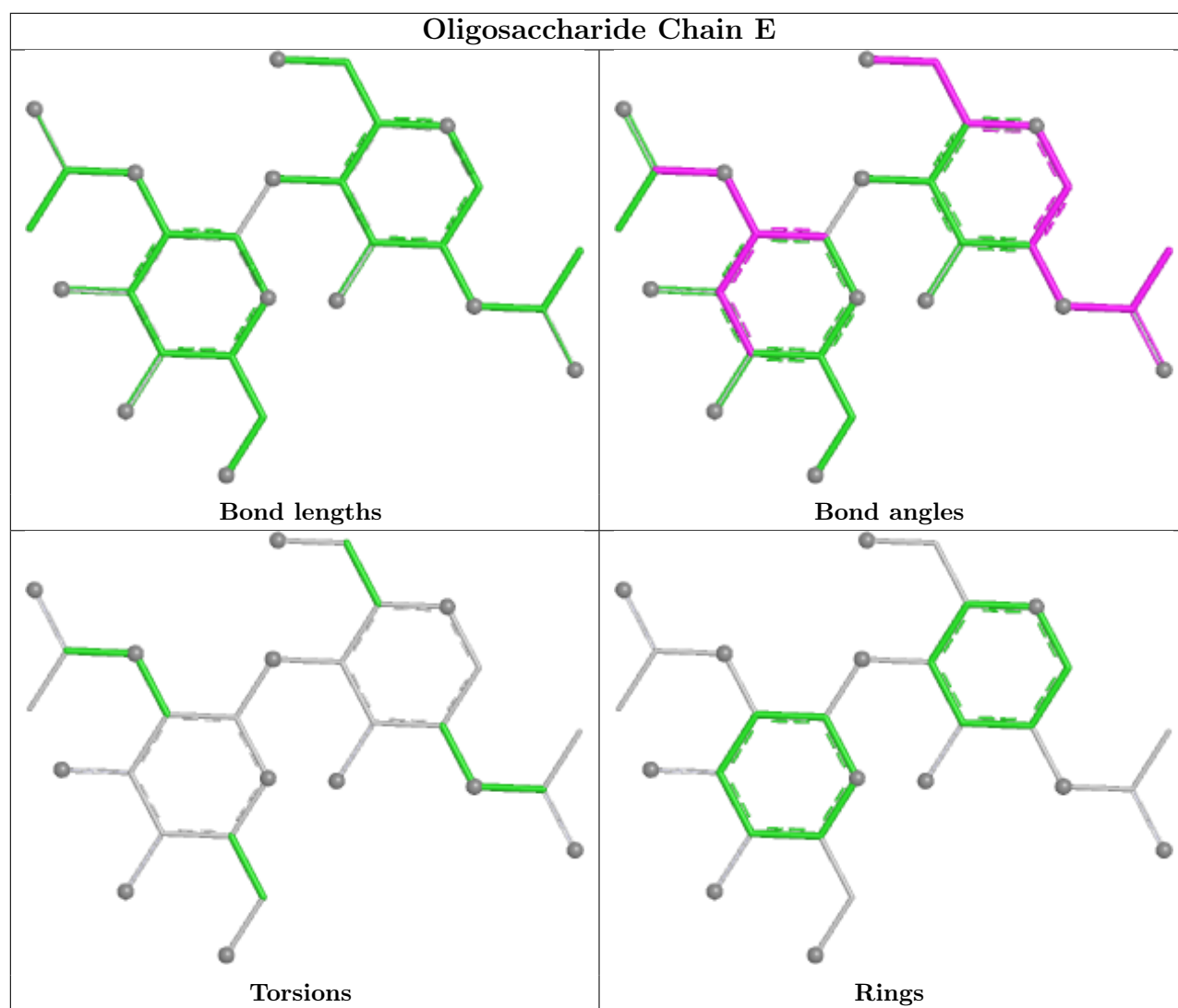
There are no torsion outliers.

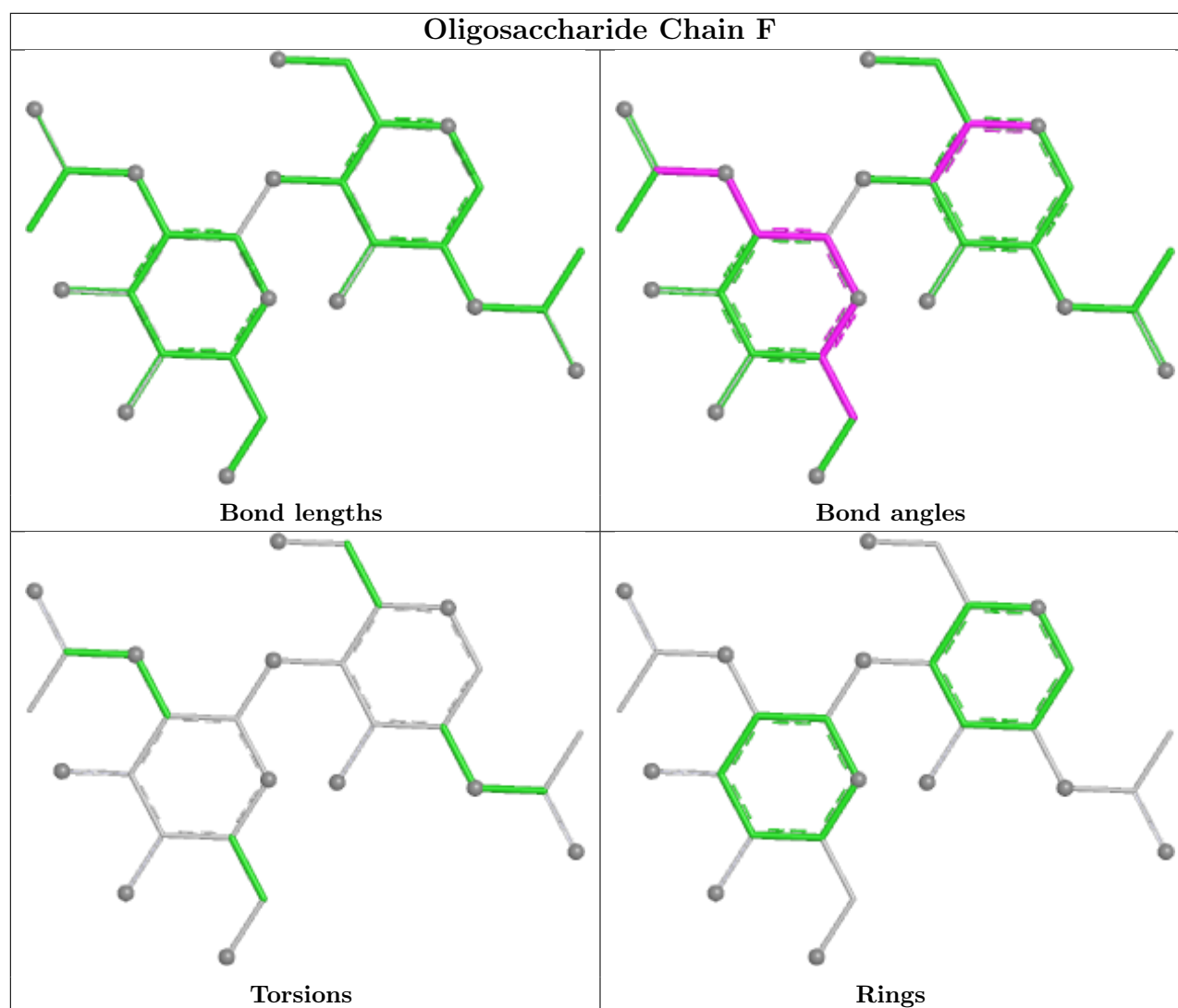
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

3 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	$\# Z > 2$
3	NAG	B	603	1	14,14,15	1.07	1 (7%)	17,19,21	1.13	2 (11%)
3	NAG	A	603	1	14,14,15	1.88	1 (7%)	17,19,21	1.27	2 (11%)
3	NAG	C	603	1	14,14,15	1.13	1 (7%)	17,19,21	1.55	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	C	603	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	NAG	C1-C2	6.21	1.60	1.52
3	B	603	NAG	C1-C2	3.19	1.56	1.52
3	C	603	NAG	C1-C2	2.84	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	NAG	C1-O5-C5	5.19	119.15	112.19
3	A	603	NAG	C4-C3-C2	-2.91	106.76	111.02
3	B	603	NAG	C2-N2-C7	-2.53	119.51	122.90
3	B	603	NAG	C1-O5-C5	2.45	115.47	112.19
3	C	603	NAG	O5-C1-C2	2.41	115.03	111.29
3	A	603	NAG	O3-C3-C4	2.31	115.83	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/515 (98%)	-1.17	0 100 100	7, 18, 28, 44	3 (0%)
1	B	509/515 (98%)	-1.19	0 100 100	9, 19, 30, 45	1 (0%)
1	C	509/515 (98%)	-1.19	0 100 100	9, 19, 29, 42	0
All	All	1527/1545 (98%)	-1.18	0 100 100	7, 19, 29, 45	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

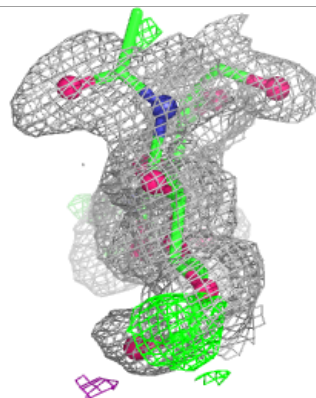
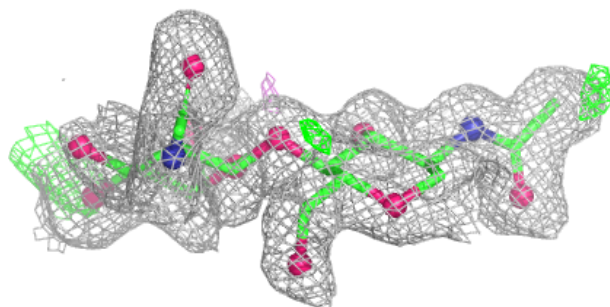
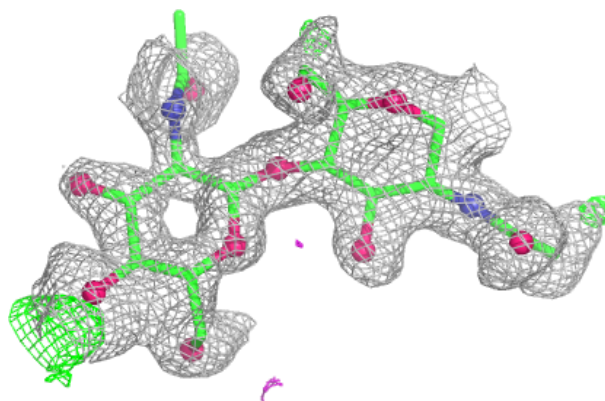
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.98	0.06	27,31,37,39	0
2	NAG	E	2	14/15	0.98	0.05	34,37,40,40	0
2	NAG	F	1	14/15	0.98	0.04	22,32,35,35	0
2	NAG	F	2	14/15	0.98	0.04	31,35,41,44	0
2	NAG	E	1	14/15	0.99	0.03	26,29,33,36	0
2	NAG	D	1	14/15	0.99	0.03	19,22,27,31	0

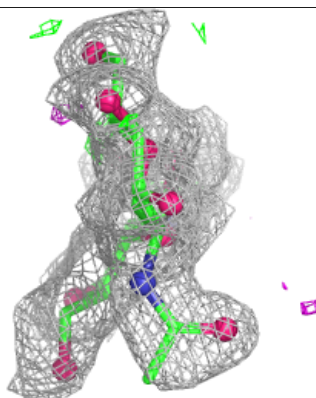
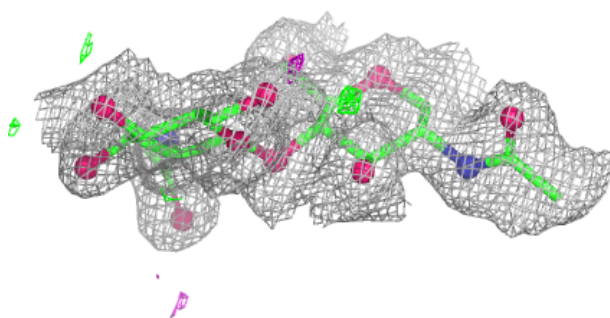
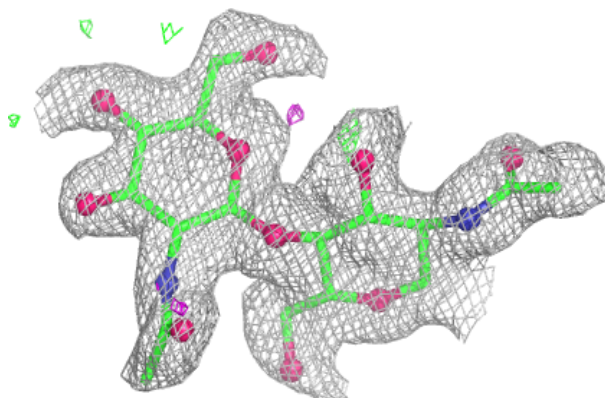
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

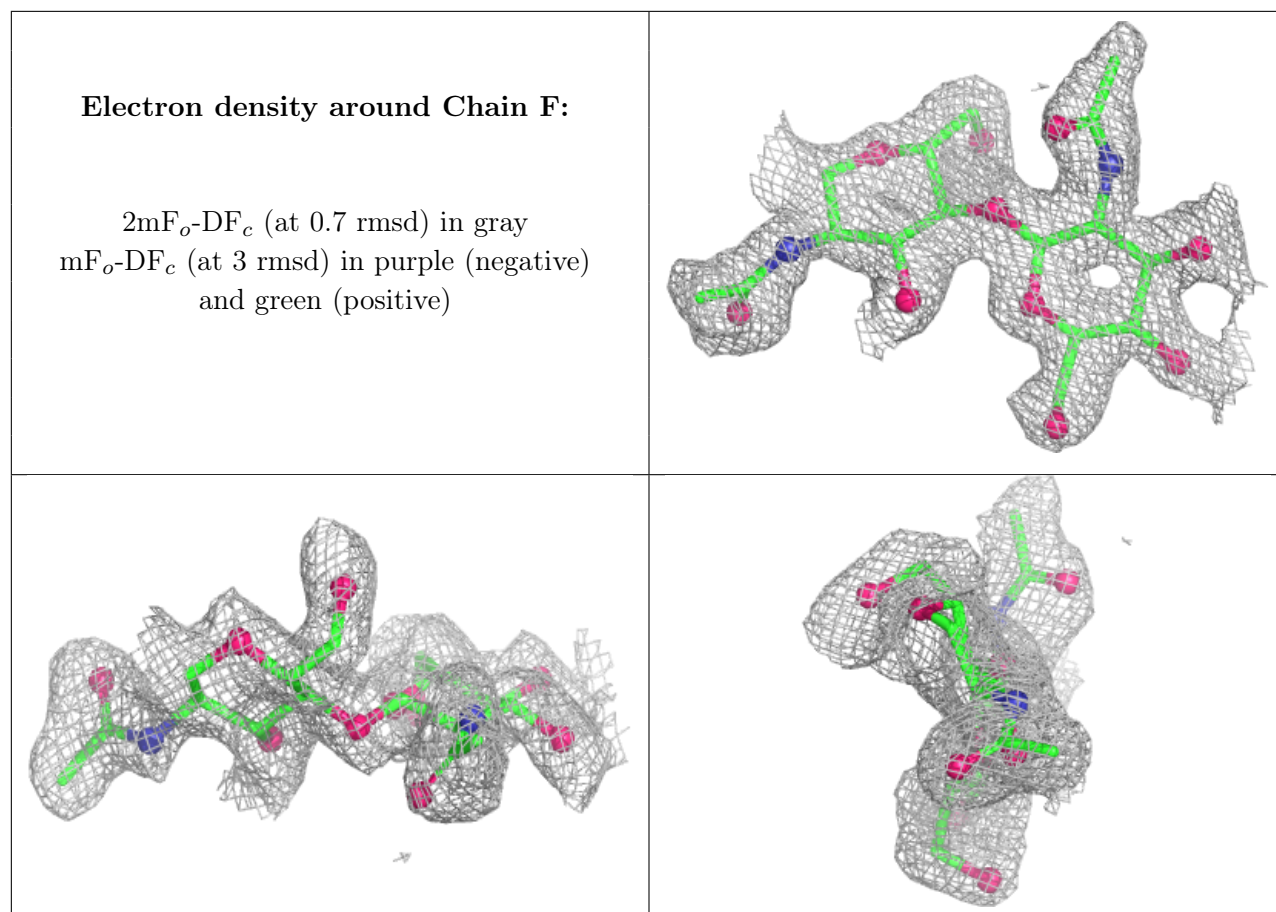
Electron density around Chain D:

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

**Electron density around Chain E:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
3	NAG	A	603	14/15	0.98	0.04	26,29,33,37	0
3	NAG	B	603	14/15	0.98	0.05	30,34,36,38	0
3	NAG	C	603	14/15	0.98	0.05	32,36,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.