Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 08:12 PM EDT

PDB ID	:	8F8W
Title	:	Crystal structure of Nb.X0 bound to the afucosylated human IgG1 fragment crystal form I
Authors	:	Goldgur, Y.; Ravetch, J.; Gupta, A.; Kao, K.; Oren, D.
Deposited on	:	2022-11-22
Resolution	:	2.71 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:

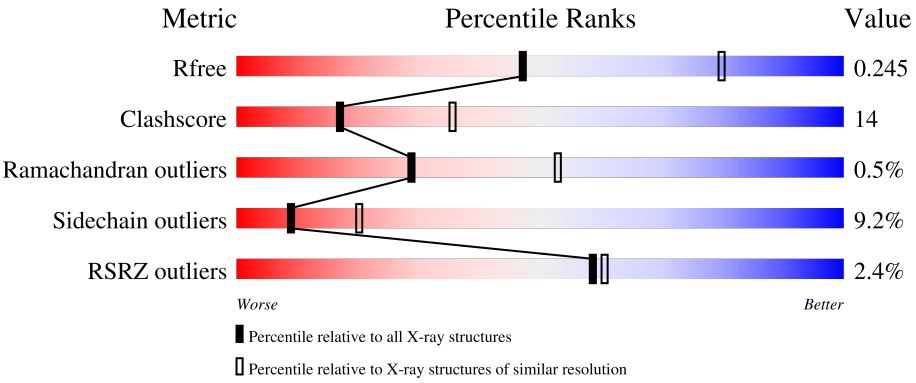
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 <=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	224	68% 20% • • 8%
1	B	224	2% 67% 21% • • 8%
1	E	224	% 61% 28% • 8%
1	F	224	3% 55% 29% 6% • 7%
2	C	120	% 67% 29% • •

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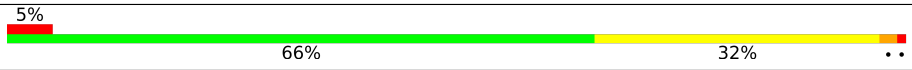
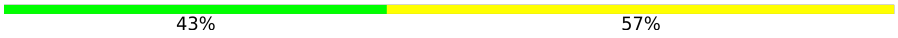
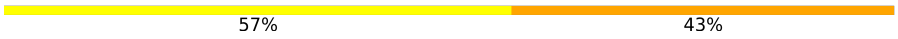
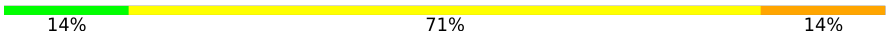
Mol	Chain	Length	Quality of chain
2	D	120	
2	G	120	
2	H	120	
3	I	7	
3	J	7	
3	K	7	
3	L	7	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10703 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 afucosylated IgG1 fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1661	1057	282	315	7			
1	B	207	Total	C	N	O	S	0	0	0
			1661	1057	282	315	7			
1	E	206	Total	C	N	O	S	0	0	0
			1657	1055	281	314	7			
1	F	208	Total	C	N	O	S	0	0	0
			1657	1055	283	312	7			

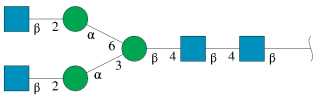
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	GLU	conflict	UNP Q6MZV7
B	382	ARG	GLU	conflict	UNP Q6MZV7
E	382	ARG	GLU	conflict	UNP Q6MZV7
F	382	ARG	GLU	conflict	UNP Q6MZV7

- Molecule 2 is a protein called Nb.X0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			923	578	162	179	4			
2	D	120	Total	C	N	O	S	0	0	0
			923	578	162	179	4			
2	G	120	Total	C	N	O	S	0	0	0
			923	578	162	179	4			
2	H	120	Total	C	N	O	S	0	0	0
			923	578	162	179	4			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
3	I	7	Total C N O 89 50 4 35	0	0	0
3	J	7	Total C N O 89 50 4 35	0	0	0
3	K	7	Total C N O 89 50 4 35	0	0	0
3	L	7	Total C N O 89 50 4 35	0	0	0

- Molecule 4 is water.

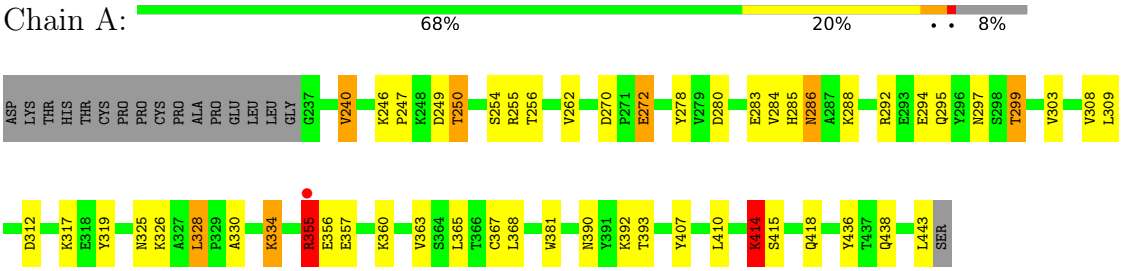
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	5	Total O 5 5	0	0
4	C	1	Total O 1 1	0	0
4	E	5	Total O 5 5	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

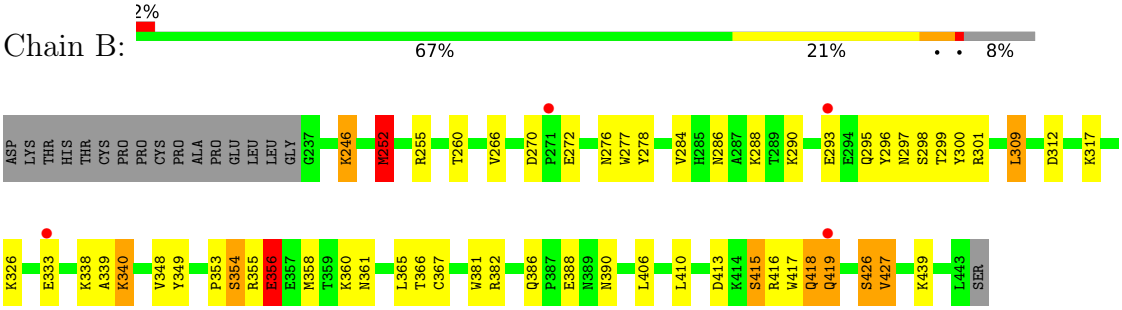
• Molecule 1: afucosylated IgG1 fragment

Chain A:



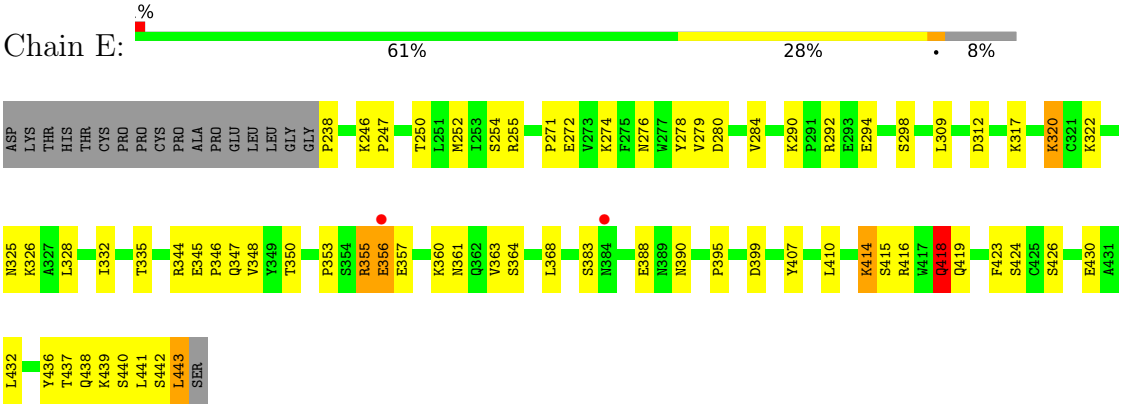
• Molecule 1: afucosylated IgG1 fragment

Chain B:



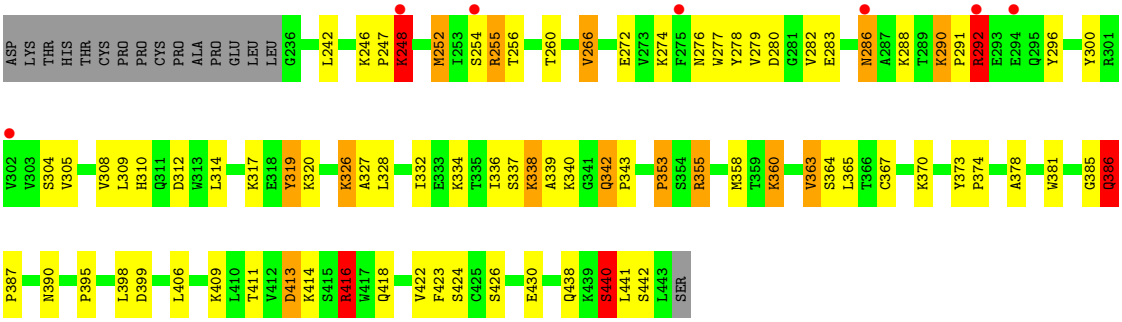
• Molecule 1: afucosylated IgG1 fragment

Chain E:



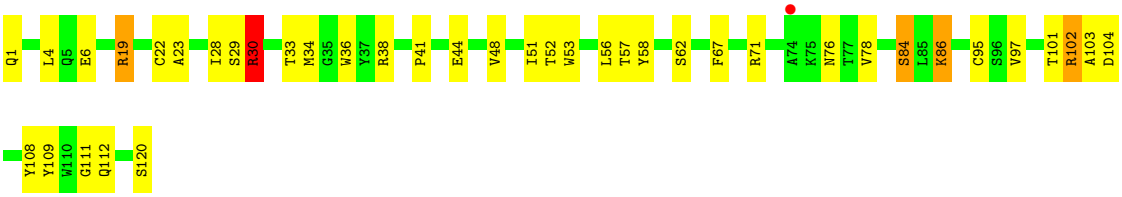
• Molecule 1: afucosylated IgG1 fragment

Chain F:



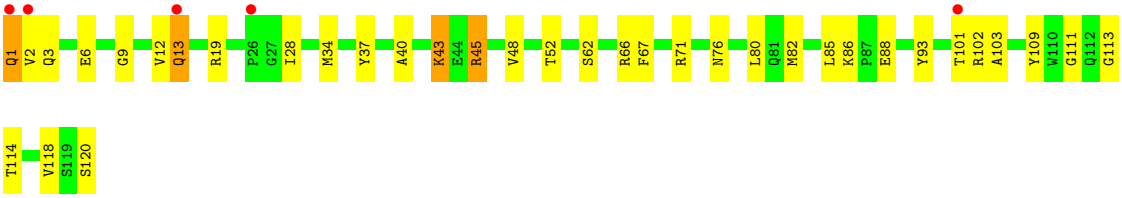
• Molecule 2: Nb.X0

Chain C:



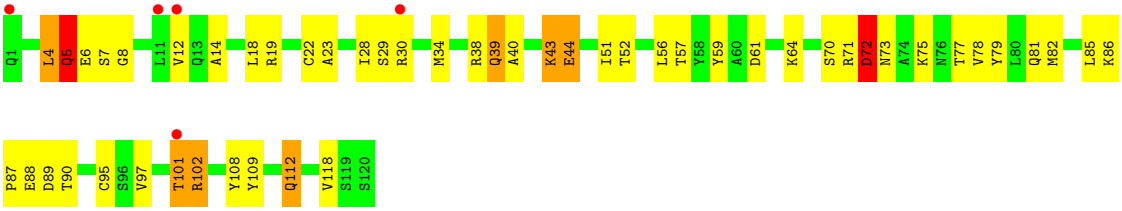
• Molecule 2: Nb.X0

Chain D:



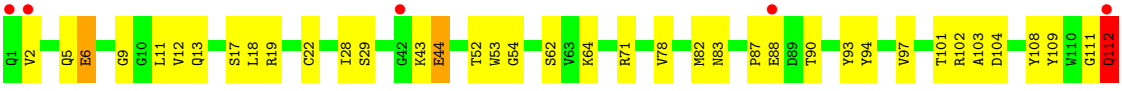
• Molecule 2: Nb.X0

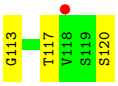
Chain G:



• Molecule 2: Nb.X0

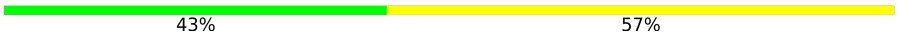
Chain H:





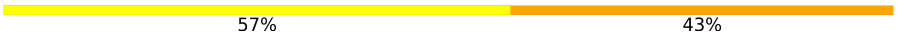
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



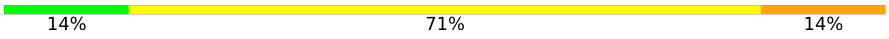
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:



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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	170.64Å 170.64Å 126.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.90 – 2.71 45.90 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.90-2.71) 99.7 (45.90-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.241 0.211 , 0.245	Depositor DCC
R_{free} test set	2013 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.63	3/1707 (0.2%)	0.83	3/2324 (0.1%)
1	B	0.73	3/1707 (0.2%)	1.02	10/2324 (0.4%)
1	E	0.81	7/1703 (0.4%)	1.00	16/2318 (0.7%)
1	F	0.75	6/1703 (0.4%)	1.38	27/2319 (1.2%)
2	C	0.58	0/945	1.01	6/1280 (0.5%)
2	D	0.62	2/945 (0.2%)	1.06	7/1280 (0.5%)
2	G	0.89	6/945 (0.6%)	1.30	16/1280 (1.2%)
2	H	0.59	0/945	1.55	5/1280 (0.4%)
All	All	0.72	27/10600 (0.3%)	1.14	90/14405 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	3
1	F	0	6
2	C	0	1
2	D	0	1
2	G	0	4
2	H	0	1
All	All	0	17

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	356	GLU	CD-OE2	14.44	1.41	1.25
1	E	272	GLU	CD-OE2	11.29	1.38	1.25
1	B	356	GLU	CG-CD	10.00	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	GLU	CD-OE2	9.76	1.36	1.25
2	G	5	GLN	CG-CD	-9.55	1.29	1.51
2	G	5	GLN	CB-CG	-8.91	1.28	1.52
1	E	356	GLU	CG-CD	8.86	1.65	1.51
2	G	44	GLU	CG-CD	8.65	1.65	1.51
1	A	414	LYS	CE-NZ	-8.63	1.27	1.49
1	F	290	LYS	CE-NZ	8.26	1.69	1.49
1	F	360	LYS	CE-NZ	8.18	1.69	1.49
1	E	272	GLU	CD-OE1	7.88	1.34	1.25
2	G	44	GLU	CB-CG	7.60	1.66	1.52
1	F	290	LYS	CD-CE	7.08	1.69	1.51
1	E	356	GLU	CB-CG	6.90	1.65	1.52
2	G	30	ARG	CB-CG	-6.69	1.34	1.52
1	A	288	LYS	CB-CG	6.53	1.70	1.52
2	G	112	GLN	CD-NE2	6.45	1.49	1.32
2	D	13	GLN	CB-CG	-6.06	1.36	1.52
1	F	363	VAL	CB-CG1	-5.96	1.40	1.52
1	F	416	ARG	CB-CG	-5.94	1.36	1.52
1	E	357	GLU	CB-CG	5.85	1.63	1.52
1	B	417	TRP	CB-CG	-5.78	1.39	1.50
1	E	272	GLU	CG-CD	5.41	1.60	1.51
2	D	13	GLN	CA-CB	-5.21	1.42	1.53
1	F	326	LYS	CD-CE	5.07	1.64	1.51
1	A	288	LYS	CD-CE	5.05	1.63	1.51

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	44	GLU	OE1-CD-OE2	-37.08	78.80	123.30
2	H	44	GLU	CG-CD-OE1	20.90	160.09	118.30
2	H	44	GLU	CG-CD-OE2	-18.40	81.50	118.30
1	F	416	ARG	CG-CD-NE	-16.84	76.44	111.80
1	F	292	ARG	CA-CB-CG	15.83	148.23	113.40
1	B	356	GLU	OE1-CD-OE2	-15.04	105.25	123.30
1	F	309	LEU	CA-CB-CG	14.07	147.66	115.30
1	F	363	VAL	CG1-CB-CG2	-13.96	88.57	110.90
2	C	112	GLN	CA-CB-CG	-13.76	83.14	113.40
1	B	356	GLU	CG-CD-OE1	13.74	145.78	118.30
1	F	266	VAL	CG1-CB-CG2	-13.05	90.02	110.90
2	D	13	GLN	CA-CB-CG	12.47	140.83	113.40
1	B	356	GLU	CG-CD-OE2	-12.38	93.55	118.30
2	G	5	GLN	N-CA-C	12.21	143.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	292	ARG	CD-NE-CZ	11.69	139.96	123.60
1	E	356	GLU	N-CA-C	-11.52	79.90	111.00
1	A	328	LEU	CA-CB-CG	11.36	141.44	115.30
1	F	360	LYS	CD-CE-NZ	-11.03	86.33	111.70
2	G	44	GLU	CA-CB-CG	11.03	137.66	113.40
1	E	272	GLU	CA-CB-CG	10.53	136.55	113.40
1	F	290	LYS	CD-CE-NZ	-10.43	87.71	111.70
2	D	43	LYS	CD-CE-NZ	-9.76	89.26	111.70
2	G	4	LEU	CA-CB-CG	9.55	137.27	115.30
1	B	309	LEU	CA-CB-CG	9.53	137.22	115.30
1	E	290	LYS	CD-CE-NZ	9.26	133.01	111.70
2	G	30	ARG	CG-CD-NE	-9.19	92.51	111.80
1	B	356	GLU	CB-CA-C	-9.14	92.11	110.40
2	D	45	ARG	CB-CG-CD	9.10	135.26	111.60
2	G	5	GLN	CA-CB-CG	9.02	133.25	113.40
1	E	355	ARG	C-N-CA	-8.56	100.31	121.70
1	F	326	LYS	CB-CG-CD	8.46	133.59	111.60
1	E	356	GLU	CG-CD-OE2	-8.33	101.64	118.30
1	B	419	GLN	N-CA-CB	-8.26	95.73	110.60
1	F	326	LYS	CD-CE-NZ	8.14	130.41	111.70
2	G	5	GLN	CB-CG-CD	-7.92	91.02	111.60
1	F	247	PRO	C-N-CA	-7.79	102.23	121.70
2	G	44	GLU	CG-CD-OE2	7.75	133.81	118.30
1	F	292	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	E	414	LYS	CA-CB-CG	7.58	130.08	113.40
1	F	360	LYS	N-CA-CB	-7.49	97.12	110.60
2	D	45	ARG	CG-CD-NE	7.48	127.50	111.80
1	F	360	LYS	CG-CD-CE	7.44	134.21	111.90
1	E	272	GLU	N-CA-CB	7.43	123.98	110.60
2	D	45	ARG	CA-CB-CG	-7.29	97.36	113.40
2	G	5	GLN	CB-CA-C	-7.20	96.00	110.40
2	G	72	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	B	356	GLU	N-CA-CB	6.97	123.16	110.60
1	F	248	LYS	CA-CB-CG	6.97	128.73	113.40
1	B	355	ARG	C-N-CA	-6.93	104.39	121.70
2	H	112	GLN	N-CA-CB	6.78	122.80	110.60
2	D	43	LYS	CB-CG-CD	6.75	129.16	111.60
1	F	342	GLN	CA-CB-CG	6.67	128.07	113.40
2	G	44	GLU	CG-CD-OE1	-6.63	105.04	118.30
1	B	252	MET	CG-SD-CE	-6.62	89.60	100.20
1	E	356	GLU	N-CA-CB	6.61	122.49	110.60
1	F	248	LYS	N-CA-CB	6.57	122.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	356	GLU	CB-CA-C	-6.57	97.26	110.40
1	F	248	LYS	CD-CE-NZ	-6.57	96.60	111.70
2	C	86	LYS	CB-CG-CD	-6.54	94.59	111.60
1	E	356	GLU	CG-CD-OE1	6.50	131.29	118.30
1	E	272	GLU	CB-CA-C	-6.49	97.42	110.40
1	E	441	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	F	326	LYS	CG-CD-CE	-6.46	92.52	111.90
1	A	414	LYS	CB-CA-C	6.33	123.07	110.40
1	F	248	LYS	CB-CA-C	-6.28	97.84	110.40
1	E	418	GLN	CA-CB-CG	6.13	126.88	113.40
1	F	248	LYS	CB-CG-CD	-6.03	95.93	111.60
1	E	344	ARG	CB-CG-CD	5.94	127.05	111.60
1	E	272	GLU	N-CA-C	-5.90	95.06	111.00
1	F	292	ARG	CB-CA-C	5.89	122.19	110.40
2	D	13	GLN	CB-CA-C	-5.78	98.83	110.40
2	G	72	ASP	CB-CA-C	5.73	121.86	110.40
2	G	112	GLN	CB-CA-C	5.73	121.87	110.40
2	C	112	GLN	CB-CA-C	5.72	121.83	110.40
2	C	30	ARG	CG-CD-NE	5.71	123.79	111.80
1	F	440	SER	CB-CA-C	5.69	120.91	110.10
1	F	360	LYS	CB-CA-C	5.66	121.73	110.40
2	C	112	GLN	N-CA-CB	-5.66	100.42	110.60
2	G	112	GLN	N-CA-CB	-5.51	100.68	110.60
2	G	39	GLN	C-N-CA	5.50	135.44	121.70
1	A	355	ARG	N-CA-CB	-5.44	100.81	110.60
1	E	344	ARG	CG-CD-NE	5.25	122.83	111.80
2	C	19	ARG	CB-CA-C	-5.25	99.90	110.40
1	F	386	GLN	CB-CG-CD	-5.24	97.99	111.60
1	F	338	LYS	CG-CD-CE	-5.16	96.43	111.90
2	G	72	ASP	N-CA-C	-5.14	97.11	111.00
1	F	385	GLY	C-N-CA	5.10	134.44	121.70
2	H	111	GLY	C-N-CA	-5.03	109.12	121.70
2	G	5	GLN	C-N-CA	5.02	134.25	121.70
1	B	418	GLN	C-N-CA	5.01	134.24	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	356	GLU	Sidechain
2	C	30	ARG	Sidechain
2	D	45	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	271	PRO	Peptide
1	E	355	ARG	Peptide
1	E	418	GLN	Peptide
1	F	252	MET	Peptide
1	F	291	PRO	Peptide
1	F	292	ARG	Sidechain
1	F	386	GLN	Peptide
1	F	416	ARG	Sidechain
1	F	440	SER	Peptide
2	G	112	GLN	Sidechain
2	G	4	LEU	Peptide
2	G	5	GLN	Peptide,Mainchain
2	H	112	GLN	Sidechain

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	1661	0	1632	31	1
1	B	1661	0	1632	38	1
1	E	1657	0	1630	40	1
1	F	1657	0	1627	68	1
2	C	923	0	884	26	0
2	D	923	0	884	22	0
2	G	923	0	884	51	0
2	H	923	0	884	28	0
3	I	89	0	76	1	0
3	J	89	0	76	4	0
3	K	89	0	76	2	0
3	L	89	0	76	0	0
4	A	7	0	0	1	0
4	B	5	0	0	0	0
4	C	1	0	0	0	0
4	E	5	0	0	1	0
4	F	1	0	0	0	0
All	All	10703	0	10361	295	2

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 14.

All (295) 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:F:360:LYS:CE	1:F:360:LYS:NZ	1.69	1.56
1:F:290:LYS:CE	1:F:290:LYS:NZ	1.69	1.52
2:G:5:GLN:HE22	2:G:23:ALA:N	1.51	1.06
1:F:360:LYS:NZ	1:F:360:LYS:CD	2.19	1.05
2:G:57:THR:HG1	2:G:59:TYR:HE1	1.08	1.01
2:G:5:GLN:NE2	2:G:22:CYS:SG	2.34	1.00
1:F:373:TYR:HD1	1:F:374:PRO:HA	1.27	0.98
2:G:40:ALA:H	2:G:43:LYS:HE3	1.27	0.95
1:B:360:LYS:HE3	1:B:361:ASN:H	1.30	0.94
1:B:252:MET:SD	1:B:255:ARG:HG3	2.07	0.93
1:F:290:LYS:NZ	1:F:290:LYS:CD	2.34	0.90
2:C:101:THR:O	2:C:103:ALA:N	2.07	0.87
1:B:388:GLU:OE2	1:B:416:ARG:NH2	2.07	0.86
1:F:353:PRO:HG3	1:F:363:VAL:HG11	1.57	0.86
2:H:112:GLN:HE21	2:H:112:GLN:H	1.23	0.85
2:H:5:GLN:HB2	2:H:112:GLN:HE22	1.42	0.84
2:C:33:THR:HG22	2:C:52:THR:HA	1.58	0.83
1:F:373:TYR:CD1	1:F:374:PRO:HA	2.15	0.82
2:G:86:LYS:HG3	2:G:87:PRO:HD2	1.61	0.82
2:D:2:VAL:HG13	2:D:28:ILE:HG21	1.61	0.81
2:H:2:VAL:HG13	2:H:28:ILE:HG21	1.62	0.80
1:B:295:GLN:HG2	3:J:1:NAG:H62	1.63	0.79
1:F:353:PRO:CG	1:F:363:VAL:HG11	2.12	0.79
2:D:101:THR:O	2:D:103:ALA:N	2.16	0.79
1:F:312:ASP:OD2	1:F:317:LYS:NZ	2.14	0.79
1:F:353:PRO:HB3	1:F:363:VAL:CG1	2.14	0.78
2:G:5:GLN:NE2	2:G:23:ALA:N	2.30	0.76
1:B:272:GLU:OE2	1:B:272:GLU:N	2.17	0.76
1:B:297:ASN:OD1	1:B:299:THR:OG1	2.02	0.75
1:B:353:PRO:HD3	1:B:365:LEU:HD23	1.70	0.74
2:H:112:GLN:HE21	2:H:112:GLN:N	1.86	0.73
1:A:284:VAL:HG12	1:A:286:ASN:HB3	1.71	0.72
1:F:360:LYS:NZ	1:F:360:LYS:HD3	2.00	0.72
1:A:312:ASP:OD1	1:A:317:LYS:NZ	2.20	0.72
2:G:38:ARG:HG3	2:G:43:LYS:NZ	2.06	0.71
1:F:319:TYR:HB2	1:F:336:ILE:HG22	1.71	0.71
2:D:6:GLU:N	2:D:6:GLU:OE1	2.22	0.70
2:C:51:ILE:HD13	2:C:57:THR:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:VAL:O	2:D:118:VAL:HA	1.93	0.69
2:H:97:VAL:HG23	2:H:108:TYR:HB2	1.74	0.69
2:G:5:GLN:OE1	2:G:22:CYS:HA	1.93	0.68
2:D:1:GLN:OE1	2:D:3:GLN:NE2	2.26	0.68
1:F:386:GLN:HB3	1:F:387:PRO:HD3	1.76	0.68
2:C:6:GLU:OE2	2:C:111:GLY:HA3	1.93	0.67
1:F:353:PRO:HG3	1:F:363:VAL:CG1	2.23	0.67
1:F:373:TYR:HD1	1:F:374:PRO:CA	2.05	0.67
1:E:247:PRO:O	1:E:250:THR:HG22	1.95	0.66
1:B:415:SER:O	1:B:419:GLN:HG3	1.95	0.66
1:E:246:LYS:NZ	3:K:7:NAG:O4	2.29	0.66
2:H:87:PRO:O	2:H:90:THR:HG23	1.95	0.66
2:H:112:GLN:H	2:H:112:GLN:NE2	1.92	0.66
1:B:312:ASP:HB3	1:B:317:LYS:HD2	1.78	0.65
1:B:266:VAL:HG22	1:B:300:TYR:HB2	1.78	0.65
2:H:5:GLN:CB	2:H:112:GLN:HE22	2.10	0.64
1:F:286:ASN:OD1	1:F:286:ASN:O	2.15	0.64
1:E:432:LEU:HD13	1:E:437:THR:HG22	1.80	0.64
1:A:246:LYS:NZ	4:A:501:HOH:O	2.29	0.64
2:G:86:LYS:HG3	2:G:87:PRO:CD	2.28	0.64
2:C:97:VAL:HG13	2:C:108:TYR:HB2	1.78	0.63
2:D:2:VAL:HG11	2:D:109:TYR:CE1	2.32	0.63
1:B:360:LYS:HE3	1:B:361:ASN:N	2.10	0.63
1:F:353:PRO:CB	1:F:363:VAL:CG1	2.76	0.62
2:G:23:ALA:HA	2:G:77:THR:HG22	1.80	0.62
2:C:38:ARG:HD3	2:C:48:VAL:HG22	1.82	0.62
1:F:390:ASN:ND2	1:F:411:THR:OG1	2.32	0.62
2:D:88:GLU:HG3	2:D:88:GLU:O	1.99	0.62
1:F:290:LYS:CD	1:F:290:LYS:HZ2	2.11	0.62
1:E:418:GLN:HA	1:E:443:LEU:HD23	1.82	0.61
1:E:347:GLN:N	1:E:347:GLN:OE1	2.33	0.61
2:H:101:THR:O	2:H:104:ASP:N	2.27	0.61
1:A:280:ASP:OD2	1:A:317:LYS:HD2	2.00	0.60
2:G:40:ALA:O	2:G:43:LYS:HB3	2.01	0.60
2:G:43:LYS:HG3	2:G:44:GLU:N	2.15	0.60
1:F:365:LEU:HD12	1:F:441:LEU:HD21	1.82	0.60
1:B:296:TYR:HD1	2:C:58:TYR:HE2	1.50	0.60
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.37	0.59
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.84	0.59
1:A:418:GLN:HA	1:A:443:LEU:HD12	1.84	0.59
2:H:101:THR:O	2:H:103:ALA:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:TYR:HD1	2:C:58:TYR:CE2	2.20	0.59
2:G:82:MET:HB3	2:G:85:LEU:HD21	1.84	0.59
1:A:283:GLU:HG2	1:A:285:HIS:NE2	2.17	0.59
1:B:296:TYR:O	2:C:33:THR:HG21	2.02	0.59
1:F:278:TYR:HB2	1:F:320:LYS:HB3	1.84	0.58
1:F:360:LYS:HD3	1:F:360:LYS:HZ3	1.67	0.58
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.86	0.58
2:D:86:LYS:O	2:D:118:VAL:HG21	2.04	0.58
1:A:262:VAL:HG13	1:A:303:VAL:HG12	1.85	0.57
3:J:4:MAN:H4	3:J:5:NAG:H83	1.86	0.57
1:A:325:ASN:O	1:A:328:LEU:HB3	2.04	0.57
1:E:280:ASP:OD2	1:E:317:LYS:HD2	2.05	0.57
1:F:310:HIS:O	1:F:314:LEU:HD23	2.05	0.57
1:F:360:LYS:O	1:F:414:LYS:HE3	2.04	0.57
1:F:355:ARG:HA	1:F:358:MET:HG2	1.86	0.57
1:F:424:SER:HA	1:F:440:SER:HB3	1.86	0.57
1:A:328:LEU:HD13	1:A:330:ALA:O	2.04	0.57
1:F:312:ASP:HB3	1:F:317:LYS:HG3	1.87	0.56
2:G:5:GLN:HE22	2:G:22:CYS:C	2.07	0.56
1:E:312:ASP:HB3	1:E:317:LYS:HG3	1.88	0.56
1:B:277:TRP:C	1:B:278:TYR:HD1	2.08	0.56
1:A:247:PRO:O	1:A:250:THR:HG22	2.05	0.56
1:F:278:TYR:HE1	1:F:283:GLU:HG2	1.70	0.56
2:G:12:VAL:O	2:G:118:VAL:HA	2.05	0.56
1:A:240:VAL:HG22	1:A:334:LYS:HD3	1.86	0.56
1:A:363:VAL:HG22	1:A:414:LYS:HB2	1.87	0.55
2:C:4:LEU:HD22	2:C:22:CYS:SG	2.47	0.55
2:C:97:VAL:HG11	2:C:109:TYR:HD2	1.71	0.55
1:F:363:VAL:HG12	1:F:364:SER:H	1.72	0.55
1:F:292:ARG:HG3	1:F:292:ARG:HH11	1.71	0.55
1:F:363:VAL:HG12	1:F:364:SER:N	2.21	0.55
2:D:67:PHE:CE1	2:D:82:MET:HG2	2.41	0.54
1:F:340:LYS:HA	1:F:340:LYS:CE	2.37	0.54
1:F:278:TYR:CE1	1:F:283:GLU:HG2	2.43	0.54
1:A:295:GLN:HG3	3:I:1:NAG:H62	1.88	0.54
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.42	0.54
1:B:284:VAL:HG22	1:B:286:ASN:HB3	1.89	0.54
2:G:22:CYS:O	2:G:77:THR:HA	2.07	0.54
2:H:97:VAL:CG2	2:H:108:TYR:HB2	2.37	0.54
1:B:413:ASP:O	1:B:416:ARG:N	2.40	0.54
1:B:266:VAL:HG13	1:B:300:TYR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:51:ILE:HG21	2:G:71:ARG:HB2	1.89	0.53
2:G:5:GLN:HG3	2:G:6:GLU:N	2.23	0.53
1:F:353:PRO:HB3	1:F:363:VAL:HG12	1.90	0.53
2:G:5:GLN:CD	2:G:22:CYS:HA	2.28	0.53
2:H:112:GLN:N	2:H:112:GLN:NE2	2.54	0.53
2:G:19:ARG:HB2	2:G:81:GLN:NE2	2.23	0.53
1:E:312:ASP:OD1	4:E:501:HOH:O	2.19	0.53
2:C:101:THR:O	2:C:102:ARG:C	2.47	0.53
2:D:9:GLY:H	2:D:114:THR:HG21	1.74	0.53
1:E:278:TYR:HB2	1:E:320:LYS:HB3	1.92	0.52
1:E:238:PRO:HG2	1:E:328:LEU:HD13	1.90	0.52
1:F:353:PRO:CG	1:F:363:VAL:CG1	2.82	0.52
2:H:52:THR:OG1	2:H:53:TRP:N	2.42	0.52
2:G:34:MET:CE	2:G:78:VAL:HB	2.40	0.52
1:B:312:ASP:CB	1:B:317:LYS:HD2	2.39	0.52
1:E:309:LEU:HB2	1:E:312:ASP:OD1	2.10	0.52
2:C:101:THR:O	2:C:104:ASP:N	2.41	0.52
2:C:6:GLU:HG3	2:C:95:CYS:SG	2.50	0.51
1:F:255:ARG:NE	1:F:256:THR:H	2.08	0.51
2:G:38:ARG:NH1	2:G:89:ASP:HA	2.25	0.51
2:G:61:ASP:HA	2:G:64:LYS:HG3	1.93	0.51
2:G:90:THR:CG2	2:G:118:VAL:H	2.23	0.51
2:G:97:VAL:HG11	2:G:109:TYR:HD2	1.76	0.51
1:E:345:GLU:HG3	1:E:432:LEU:HD23	1.92	0.50
3:K:4:MAN:O2	3:K:5:NAG:H83	2.11	0.50
1:E:353:PRO:HB3	1:E:363:VAL:CG1	2.41	0.50
2:C:84:SER:O	2:C:84:SER:OG	2.22	0.50
1:E:294:GLU:OE1	1:E:298:SER:HA	2.11	0.50
1:F:326:LYS:O	1:F:327:ALA:HB3	2.12	0.50
2:H:71:ARG:HB2	2:H:78:VAL:HG23	1.93	0.50
1:E:415:SER:O	1:E:419:GLN:N	2.43	0.49
1:E:395:PRO:HG2	1:F:395:PRO:HG2	1.93	0.49
1:F:338:LYS:NZ	1:F:430:GLU:OE2	2.40	0.49
2:G:71:ARG:HG3	2:G:72:ASP:N	2.27	0.49
1:A:249:ASP:OD1	1:A:255:ARG:NH1	2.45	0.49
1:F:355:ARG:HA	1:F:358:MET:CG	2.42	0.49
2:G:5:GLN:NE2	2:G:23:ALA:O	2.46	0.49
1:A:309:LEU:HD12	1:A:312:ASP:OD2	2.13	0.49
1:E:309:LEU:HD12	1:E:312:ASP:OD1	2.13	0.49
2:G:40:ALA:N	2:G:43:LYS:HE3	2.11	0.49
1:F:328:LEU:HD11	1:F:332:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:ASP:OD2	1:F:409:LYS:NZ	2.26	0.49
2:H:28:ILE:HG13	2:H:29:SER:N	2.28	0.49
2:H:11:LEU:HD23	2:H:117:THR:OG1	2.13	0.49
1:B:416:ARG:HA	1:B:419:GLN:CG	2.43	0.48
1:E:424:SER:HB2	1:E:438:GLN:OE1	2.13	0.48
1:E:361:ASN:HA	1:E:414:LYS:NZ	2.28	0.48
1:F:255:ARG:O	1:F:310:HIS:NE2	2.45	0.48
1:A:272:GLU:OE1	1:A:326:LYS:HG3	2.14	0.48
1:B:260:THR:HG21	3:J:7:NAG:H62	1.95	0.48
1:B:295:GLN:CG	3:J:1:NAG:H62	2.38	0.48
1:A:308:VAL:HG22	1:A:319:TYR:CE2	2.49	0.48
2:G:5:GLN:NE2	2:G:22:CYS:C	2.66	0.48
1:B:416:ARG:HA	1:B:419:GLN:CD	2.34	0.48
1:F:248:LYS:HB3	1:F:378:ALA:HB2	1.96	0.48
1:F:340:LYS:HA	1:F:340:LYS:HE3	1.95	0.48
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.49	0.47
1:E:274:LYS:HE3	1:E:276:ASN:HD21	1.78	0.47
1:E:388:GLU:OE2	1:E:416:ARG:NH2	2.35	0.47
1:F:288:LYS:HB3	1:F:288:LYS:HE2	1.58	0.47
1:F:255:ARG:HD2	1:F:255:ARG:HA	1.57	0.47
2:G:28:ILE:HB	2:G:109:TYR:CE2	2.50	0.47
2:G:5:GLN:HE22	2:G:23:ALA:CA	2.25	0.47
1:A:297:ASN:OD1	1:A:299:THR:HG22	2.15	0.47
1:B:296:TYR:CD1	2:C:58:TYR:HE2	2.29	0.47
1:B:416:ARG:O	1:B:419:GLN:HB2	2.13	0.47
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.96	0.47
2:H:9:GLY:HA2	2:H:18:LEU:HD21	1.97	0.47
2:D:66:ARG:NH1	2:D:86:LYS:HG2	2.30	0.47
2:D:2:VAL:HG11	2:D:109:TYR:CZ	2.50	0.47
1:E:279:VAL:HG12	1:E:284:VAL:CG2	2.45	0.46
2:H:2:VAL:HG11	2:H:109:TYR:CZ	2.50	0.46
2:G:86:LYS:NZ	2:G:88:GLU:OE1	2.48	0.46
2:G:90:THR:HG22	2:G:118:VAL:H	1.80	0.46
1:B:338:LYS:HG2	1:B:339:ALA:N	2.30	0.46
1:A:294:GLU:OE1	2:D:52:THR:OG1	2.28	0.46
1:F:367:CYS:HB2	1:F:381:TRP:CZ2	2.51	0.46
1:E:252:MET:HG2	1:E:255:ARG:HG2	1.97	0.45
1:F:338:LYS:HG3	1:F:339:ALA:N	2.31	0.45
2:G:14:ALA:HA	2:G:85:LEU:O	2.16	0.45
1:E:361:ASN:OD1	1:E:361:ASN:N	2.46	0.45
1:F:423:PHE:O	1:F:440:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LYS:O	1:A:414:LYS:HE3	2.17	0.45
1:B:293:GLU:HB2	1:B:301:ARG:O	2.16	0.45
1:F:312:ASP:HB2	1:F:319:TYR:OH	2.17	0.45
1:A:278:TYR:HD1	1:A:283:GLU:HA	1.82	0.45
2:G:5:GLN:HG3	2:G:6:GLU:HG3	1.98	0.45
2:G:39:GLN:HA	2:G:43:LYS:HG2	1.99	0.45
1:B:296:TYR:CD1	2:C:58:TYR:CE2	3.04	0.45
2:D:6:GLU:OE2	2:D:111:GLY:HA3	2.17	0.45
1:F:386:GLN:CB	1:F:387:PRO:CD	2.94	0.45
1:F:422:VAL:HG12	1:F:442:SER:HB3	1.99	0.45
2:G:52:THR:CG2	2:G:56:LEU:HB2	2.47	0.45
2:G:82:MET:HB3	2:G:85:LEU:HD11	1.99	0.45
1:A:355:ARG:HD3	1:A:356:GLU:HG2	1.99	0.44
2:C:28:ILE:HD12	2:C:109:TYR:CD2	2.52	0.44
2:D:67:PHE:CZ	2:D:82:MET:HG2	2.52	0.44
2:G:43:LYS:HG3	2:G:44:GLU:O	2.17	0.44
1:F:319:TYR:HB2	1:F:336:ILE:CG2	2.44	0.44
1:E:328:LEU:HD21	1:E:332:ILE:HG13	1.99	0.44
1:A:363:VAL:HG13	1:A:414:LYS:HB2	2.00	0.44
1:B:293:GLU:OE1	1:B:301:ARG:HD3	2.18	0.44
1:A:360:LYS:N	1:A:360:LYS:HE2	2.33	0.44
1:A:390:ASN:O	1:A:410:LEU:HD12	2.18	0.44
1:F:279:VAL:O	1:F:282:VAL:HG22	2.18	0.43
2:C:67:PHE:N	2:C:67:PHE:CD2	2.85	0.43
1:E:383:SER:HB2	1:E:423:PHE:CD1	2.53	0.43
1:E:443:LEU:H	1:E:443:LEU:HG	1.55	0.43
1:F:343:PRO:HA	1:F:373:TYR:O	2.19	0.43
2:G:38:ARG:HG3	2:G:43:LYS:HZ2	1.83	0.43
1:B:348:VAL:HG21	1:B:427:VAL:HG11	2.00	0.43
1:E:346:PRO:HD2	1:E:432:LEU:HD21	2.01	0.43
1:A:312:ASP:OD1	1:A:317:LYS:HG3	2.19	0.43
2:C:57:THR:C	2:C:58:TYR:CD1	2.92	0.43
1:E:294:GLU:OE2	2:H:54:GLY:HA3	2.18	0.43
1:E:361:ASN:C	1:E:414:LYS:HG3	2.39	0.43
2:G:19:ARG:HD3	2:G:79:TYR:HD2	1.83	0.43
2:G:71:ARG:HG3	2:G:72:ASP:H	1.84	0.43
1:B:246:LYS:HD3	1:B:246:LYS:N	2.34	0.43
1:B:415:SER:C	1:B:419:GLN:HG3	2.39	0.43
2:C:34:MET:HG3	2:C:71:ARG:NH1	2.33	0.43
2:D:9:GLY:HA3	2:D:114:THR:HG22	2.01	0.43
1:F:246:LYS:HD3	1:F:246:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:ALA:HB3	2:D:43:LYS:HG3	2.01	0.42
2:G:86:LYS:NZ	2:G:88:GLU:CD	2.71	0.42
2:G:101:THR:O	2:G:102:ARG:C	2.58	0.42
1:F:266:VAL:HG23	1:F:300:TYR:O	2.18	0.42
2:G:5:GLN:OE1	2:G:6:GLU:HA	2.19	0.42
2:D:37:TYR:HA	2:D:48:VAL:HG23	2.00	0.42
1:E:432:LEU:CD1	1:E:437:THR:HG22	2.46	0.42
1:F:272:GLU:OE2	1:F:326:LYS:HG3	2.20	0.42
1:F:363:VAL:O	1:F:411:THR:HA	2.19	0.42
2:G:8:GLY:O	2:G:18:LEU:HD11	2.18	0.42
2:C:4:LEU:O	2:C:23:ALA:O	2.38	0.42
2:D:34:MET:HG3	2:D:71:ARG:NH2	2.34	0.42
2:H:6:GLU:OE1	2:H:94:TYR:HA	2.20	0.42
1:E:353:PRO:HB3	1:E:363:VAL:HG12	2.00	0.42
1:F:398:LEU:HD13	1:F:399:ASP:O	2.19	0.42
2:G:23:ALA:CA	2:G:77:THR:HG22	2.49	0.42
1:B:340:LYS:HD3	1:B:340:LYS:HA	1.77	0.42
1:F:308:VAL:HG13	1:F:319:TYR:OH	2.20	0.42
2:H:5:GLN:HG3	2:H:5:GLN:O	2.18	0.42
1:B:284:VAL:CG2	1:B:286:ASN:HB3	2.50	0.42
2:C:56:LEU:HB3	2:C:58:TYR:HE1	1.84	0.42
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.54	0.42
2:C:30:ARG:HD2	2:C:53:TRP:CH2	2.54	0.42
2:D:93:TYR:O	2:D:113:GLY:HA2	2.19	0.42
1:F:242:LEU:HD12	1:F:260:THR:O	2.20	0.42
1:F:274:LYS:HE3	1:F:276:ASN:OD1	2.19	0.42
2:H:82:MET:C	2:H:83:ASN:HD22	2.24	0.42
1:F:340:LYS:HE3	1:F:340:LYS:CA	2.47	0.41
1:E:325:ASN:O	1:E:328:LEU:HB2	2.20	0.41
1:F:277:TRP:O	1:F:278:TYR:HD1	2.02	0.41
1:E:363:VAL:HG12	1:E:364:SER:N	2.35	0.41
2:H:2:VAL:HG11	2:H:109:TYR:CE1	2.55	0.41
2:C:57:THR:C	2:C:58:TYR:HD1	2.24	0.41
2:D:80:LEU:HA	2:D:80:LEU:HD12	1.82	0.41
2:H:93:TYR:N	2:H:93:TYR:CD2	2.88	0.41
1:A:256:THR:O	1:A:256:THR:HG23	2.21	0.41
1:E:276:ASN:HB2	1:E:322:LYS:HB3	2.02	0.41
1:F:413:ASP:OD1	1:F:413:ASP:N	2.54	0.41
2:G:97:VAL:HG13	2:G:108:TYR:HB2	2.03	0.41
2:H:6:GLU:CD	2:H:113:GLY:H	2.24	0.41
1:E:348:VAL:HG12	1:E:439:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:ASN:O	1:E:410:LEU:HD12	2.21	0.41
1:F:296:TYR:CD1	2:G:102:ARG:HG2	2.56	0.40
2:G:5:GLN:CD	2:G:22:CYS:SG	2.97	0.40
2:G:75:LYS:O	2:G:77:THR:HG23	2.21	0.40
2:H:12:VAL:CG1	2:H:13:GLN:N	2.84	0.40
1:B:354:SER:C	1:B:356:GLU:N	2.71	0.40
2:C:36:TRP:HE1	2:C:78:VAL:HG22	1.85	0.40
1:E:368:LEU:HD13	1:E:407:TYR:CZ	2.57	0.40
2:H:2:VAL:HG13	2:H:28:ILE:HD13	2.04	0.40
1:E:350:THR:HG21	1:E:440:SER:O	2.21	0.40
2:H:93:TYR:N	2:H:93:TYR:HD2	2.19	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TYR:OH	1:B:426:SER:OG[5_554]	1.93	0.27
1:E:436:TYR:OH	1:F:426:SER:OG[5_554]	1.99	0.21

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	205/224 (92%)	200 (98%)	5 (2%)	0	100	100
1	B	205/224 (92%)	199 (97%)	6 (3%)	0	100	100
1	E	204/224 (91%)	200 (98%)	4 (2%)	0	100	100
1	F	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	29	53
2	C	118/120 (98%)	114 (97%)	3 (2%)	1 (1%)	19	41
2	D	118/120 (98%)	114 (97%)	3 (2%)	1 (1%)	19	41
2	G	118/120 (98%)	114 (97%)	2 (2%)	2 (2%)	9	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	118/120 (98%)	117 (99%)	0	1 (1%)	19 41
All	All	1292/1376 (94%)	1256 (97%)	30 (2%)	6 (0%)	29 53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	102	ARG
2	D	102	ARG
2	G	5	GLN
2	H	102	ARG
1	F	292	ARG
2	G	102	ARG

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	193/208 (93%)	178 (92%)	15 (8%)	12 28
1	B	193/208 (93%)	170 (88%)	23 (12%)	5 11
1	E	193/208 (93%)	181 (94%)	12 (6%)	18 39
1	F	191/208 (92%)	170 (89%)	21 (11%)	6 14
2	C	95/95 (100%)	85 (90%)	10 (10%)	7 15
2	D	95/95 (100%)	89 (94%)	6 (6%)	18 38
2	G	95/95 (100%)	87 (92%)	8 (8%)	11 24
2	H	95/95 (100%)	84 (88%)	11 (12%)	5 12
All	All	1150/1212 (95%)	1044 (91%)	106 (9%)	9 20

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	VAL
1	A	250	THR

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Mol	Chain	Res	Type
1	A	254	SER
1	A	270	ASP
1	A	272	GLU
1	A	286	ASN
1	A	292	ARG
1	A	299	THR
1	A	334	LYS
1	A	355	ARG
1	A	392	LYS
1	A	393	THR
1	A	414	LYS
1	A	415	SER
1	A	438	GLN
1	B	246	LYS
1	B	252	MET
1	B	270	ASP
1	B	276	ASN
1	B	288	LYS
1	B	290	LYS
1	B	298	SER
1	B	309	LEU
1	B	326	LYS
1	B	333	GLU
1	B	340	LYS
1	B	354	SER
1	B	358	MET
1	B	366	THR
1	B	382	ARG
1	B	386	GLN
1	B	390	ASN
1	B	406	LEU
1	B	415	SER
1	B	418	GLN
1	B	426	SER
1	B	427	VAL
1	B	439	LYS
2	C	1	GLN
2	C	19	ARG
2	C	29	SER
2	C	41	PRO
2	C	44	GLU
2	C	62	SER

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Mol	Chain	Res	Type
2	C	76	ASN
2	C	84	SER
2	C	86	LYS
2	C	120	SER
2	D	1	GLN
2	D	13	GLN
2	D	19	ARG
2	D	62	SER
2	D	76	ASN
2	D	120	SER
1	E	254	SER
1	E	292	ARG
1	E	320	LYS
1	E	326	LYS
1	E	335	THR
1	E	356	GLU
1	E	360	LYS
1	E	418	GLN
1	E	426	SER
1	E	430	GLU
1	E	442	SER
1	E	443	LEU
1	F	248	LYS
1	F	252	MET
1	F	254	SER
1	F	255	ARG
1	F	280	ASP
1	F	286	ASN
1	F	292	ARG
1	F	304	SER
1	F	305	VAL
1	F	319	TYR
1	F	334	LYS
1	F	337	SER
1	F	342	GLN
1	F	353	PRO
1	F	355	ARG
1	F	370	LYS
1	F	406	LEU
1	F	413	ASP
1	F	416	ARG
1	F	418	GLN

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Mol	Chain	Res	Type
1	F	438	GLN
2	G	7	SER
2	G	29	SER
2	G	43	LYS
2	G	70	SER
2	G	72	ASP
2	G	73	ASN
2	G	95	CYS
2	G	101	THR
2	H	6	GLU
2	H	17	SER
2	H	19	ARG
2	H	22	CYS
2	H	43	LYS
2	H	44	GLU
2	H	62	SER
2	H	64	LYS
2	H	88	GLU
2	H	112	GLN
2	H	120	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	389	ASN
2	D	39	GLN
1	F	286	ASN
1	F	390	ASN
1	F	435	HIS
1	F	438	GLN
2	G	5	GLN
2	G	76	ASN
2	G	81	GLN
2	H	39	GLN
2	H	83	ASN
2	H	112	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

28 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	$\#\|Z\| > 2$
3	NAG	I	1	3,1	14,14,15	0.33	0	17,19,21	0.56	0
3	NAG	I	2	3	14,14,15	0.55	0	17,19,21	0.66	0
3	BMA	I	3	3	11,11,12	1.77	3 (27%)	15,15,17	1.52	3 (20%)
3	MAN	I	4	3	11,11,12	1.42	3 (27%)	15,15,17	1.45	2 (13%)
3	NAG	I	5	3	14,14,15	0.47	0	17,19,21	0.57	0
3	MAN	I	6	3	11,11,12	0.93	0	15,15,17	1.43	2 (13%)
3	NAG	I	7	3	14,14,15	0.42	0	17,19,21	0.57	0
3	NAG	J	1	3,1	14,14,15	0.71	0	17,19,21	0.78	1 (5%)
3	NAG	J	2	3	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
3	BMA	J	3	3	11,11,12	1.00	0	15,15,17	1.30	1 (6%)
3	MAN	J	4	3	11,11,12	0.99	0	15,15,17	1.46	2 (13%)
3	NAG	J	5	3	14,14,15	0.65	1 (7%)	17,19,21	0.76	1 (5%)
3	MAN	J	6	3	11,11,12	0.94	0	15,15,17	1.30	3 (20%)
3	NAG	J	7	3	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	K	1	3,1	14,14,15	0.49	0	17,19,21	0.58	0
3	NAG	K	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.73	1 (5%)
3	BMA	K	3	3	11,11,12	1.15	2 (18%)	15,15,17	1.44	1 (6%)
3	MAN	K	4	3	11,11,12	1.31	1 (9%)	15,15,17	1.22	1 (6%)
3	NAG	K	5	3	14,14,15	0.45	0	17,19,21	0.59	0
3	MAN	K	6	3	11,11,12	1.20	1 (9%)	15,15,17	1.57	2 (13%)
3	NAG	K	7	3	14,14,15	0.46	0	17,19,21	0.56	0
3	NAG	L	1	3,1	14,14,15	0.38	0	17,19,21	0.79	0
3	NAG	L	2	3	14,14,15	0.35	0	17,19,21	0.74	0
3	BMA	L	3	3	11,11,12	1.33	1 (9%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	L	4	3	11,11,12	1.69	2 (18%)	15,15,17	1.40	2 (13%)
3	NAG	L	5	3	14,14,15	0.67	0	17,19,21	0.50	0
3	MAN	L	6	3	11,11,12	1.61	2 (18%)	15,15,17	1.52	2 (13%)
3	NAG	L	7	3	14,14,15	0.43	0	17,19,21	0.52	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
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	NAG	I	5	3	-	4/6/23/26	0/1/1/1
3	MAN	I	6	3	-	0/2/19/22	0/1/1/1
3	NAG	I	7	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	NAG	J	5	3	-	3/6/23/26	0/1/1/1
3	MAN	J	6	3	-	0/2/19/22	0/1/1/1
3	NAG	J	7	3	-	4/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	MAN	K	4	3	-	2/2/19/22	0/1/1/1
3	NAG	K	5	3	-	2/6/23/26	0/1/1/1
3	MAN	K	6	3	-	0/2/19/22	0/1/1/1
3	NAG	K	7	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	2/2/19/22	0/1/1/1
3	NAG	L	5	3	-	4/6/23/26	0/1/1/1
3	MAN	L	6	3	-	0/2/19/22	0/1/1/1
3	NAG	L	7	3	-	4/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	4	MAN	O5-C1	-4.75	1.36	1.43
3	L	6	MAN	O5-C1	-4.45	1.36	1.43
3	K	4	MAN	O5-C1	-3.50	1.38	1.43
3	I	4	MAN	O5-C1	-3.18	1.38	1.43
3	I	3	BMA	C4-C5	2.90	1.59	1.53
3	I	3	BMA	C4-C3	2.77	1.59	1.52
3	I	3	BMA	C1-C2	2.57	1.58	1.52
3	L	3	BMA	C4-C3	2.57	1.58	1.52
3	K	2	NAG	O5-C1	-2.48	1.39	1.43
3	K	3	BMA	C4-C3	2.29	1.58	1.52
3	L	6	MAN	O2-C2	2.28	1.48	1.43
3	I	4	MAN	O5-C5	2.24	1.48	1.43
3	K	6	MAN	O4-C4	-2.23	1.37	1.43
3	I	4	MAN	C4-C5	2.22	1.57	1.53
3	K	3	BMA	C2-C3	-2.09	1.49	1.52
3	L	4	MAN	C1-C2	2.06	1.56	1.52
3	J	5	NAG	O5-C1	-2.03	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	3	BMA	O2-C2-C3	-4.40	101.32	110.14
3	I	6	MAN	O2-C2-C3	-4.16	101.81	110.14
3	J	4	MAN	O2-C2-C3	-4.08	101.95	110.14
3	I	3	BMA	O2-C2-C3	-3.91	102.30	110.14
3	K	6	MAN	C1-C2-C3	-3.66	105.17	109.67
3	I	4	MAN	O2-C2-C3	-3.58	102.97	110.14
3	L	4	MAN	O2-C2-C3	-3.48	103.16	110.14
3	L	6	MAN	O2-C2-C1	3.36	116.02	109.15
3	K	6	MAN	O2-C2-C3	-3.22	103.68	110.14
3	K	4	MAN	O2-C2-C3	-3.19	103.75	110.14
3	J	3	BMA	O2-C2-C3	-2.98	104.16	110.14
3	J	2	NAG	C1-O5-C5	2.93	116.16	112.19
3	L	6	MAN	O2-C2-C3	-2.89	104.34	110.14
3	L	3	BMA	C1-C2-C3	2.68	112.97	109.67
3	J	6	MAN	O2-C2-C1	2.50	114.27	109.15
3	J	6	MAN	C1-C2-C3	-2.30	106.84	109.67
3	L	4	MAN	O2-C2-C1	2.20	113.64	109.15
3	J	6	MAN	O2-C2-C3	-2.19	105.75	110.14
3	I	4	MAN	C6-C5-C4	2.19	118.14	113.00
3	I	3	BMA	C1-C2-C3	2.18	112.34	109.67
3	J	5	NAG	C1-O5-C5	2.15	115.11	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	BMA	C3-C4-C5	2.14	114.05	110.24
3	I	6	MAN	O2-C2-C1	2.13	113.50	109.15
3	K	2	NAG	C1-O5-C5	2.08	115.01	112.19
3	J	4	MAN	O5-C5-C6	2.02	110.37	107.20
3	J	1	NAG	O4-C4-C5	-2.00	104.32	109.30

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	4	MAN	O5-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
3	L	4	MAN	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
3	L	7	NAG	O5-C5-C6-O6
3	I	5	NAG	O5-C5-C6-O6
3	J	7	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	5	NAG	O5-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	I	5	NAG	C4-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
3	L	4	MAN	C4-C5-C6-O6
3	K	4	MAN	C4-C5-C6-O6
3	K	7	NAG	O5-C5-C6-O6
3	I	5	NAG	C8-C7-N2-C2
3	I	5	NAG	O7-C7-N2-C2
3	J	5	NAG	C8-C7-N2-C2
3	J	5	NAG	O7-C7-N2-C2
3	J	7	NAG	C8-C7-N2-C2
3	J	7	NAG	O7-C7-N2-C2
3	K	5	NAG	C8-C7-N2-C2
3	K	5	NAG	O7-C7-N2-C2
3	L	5	NAG	C8-C7-N2-C2
3	L	5	NAG	O7-C7-N2-C2
3	L	7	NAG	C8-C7-N2-C2
3	L	7	NAG	O7-C7-N2-C2
3	J	7	NAG	C4-C5-C6-O6
3	L	7	NAG	C4-C5-C6-O6
3	K	7	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C4-C5-C6-O6
3	L	5	NAG	C4-C5-C6-O6
3	J	5	NAG	O5-C5-C6-O6

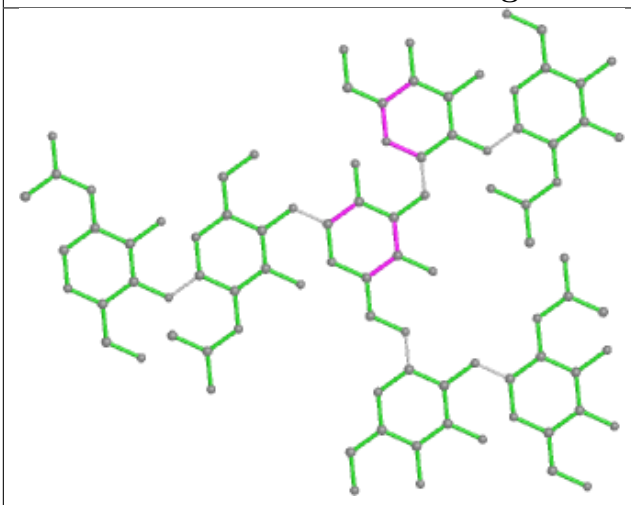
There are no ring outliers.

8 monomers are involved in 7 short contacts:

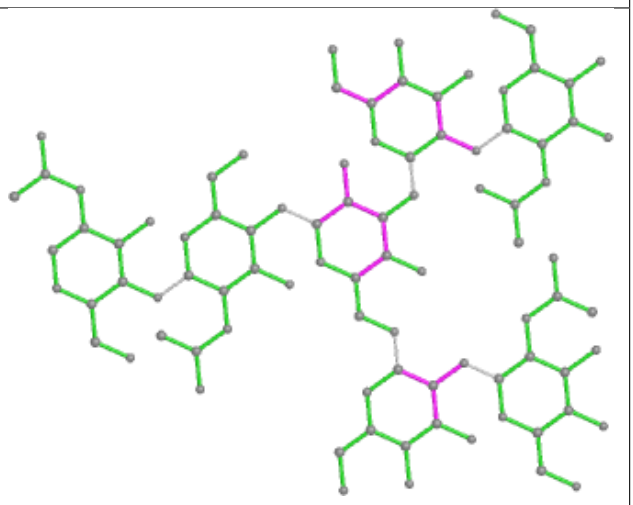
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
3	J	1	NAG	2	0
3	J	7	NAG	1	0
3	K	7	NAG	1	0
3	J	4	MAN	1	0
3	K	4	MAN	1	0
3	K	5	NAG	1	0
3	J	5	NAG	1	0

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

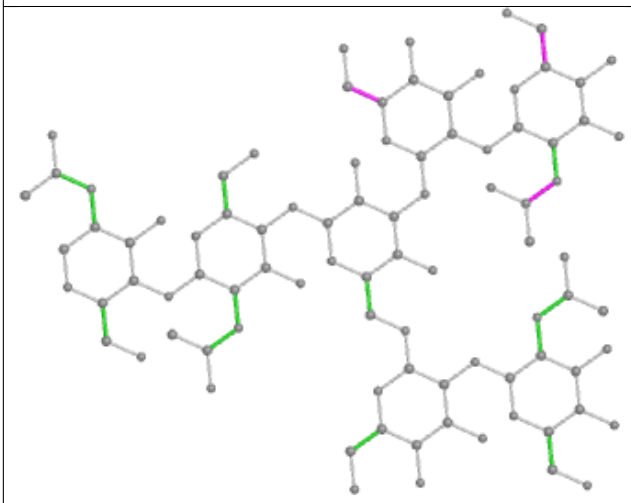
Oligosaccharide Chain I



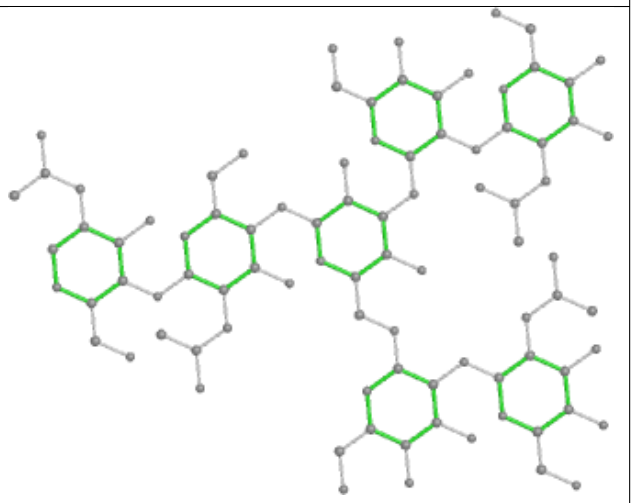
Bond lengths



Bond angles

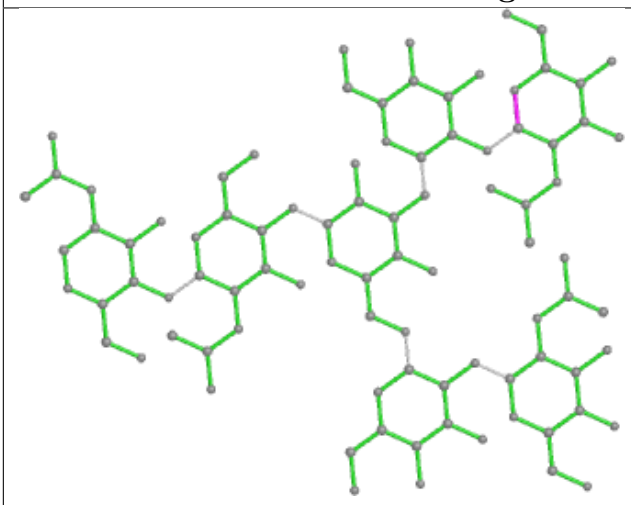


Torsions

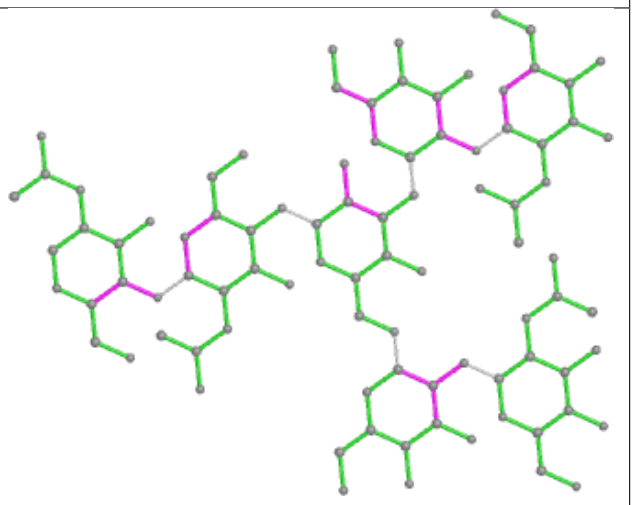


Rings

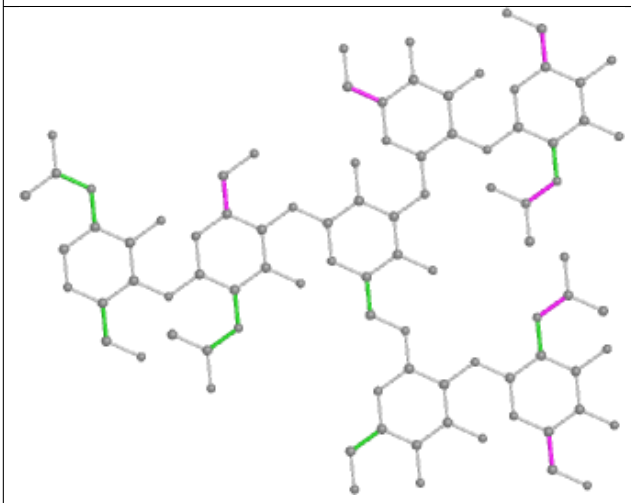
Oligosaccharide Chain J



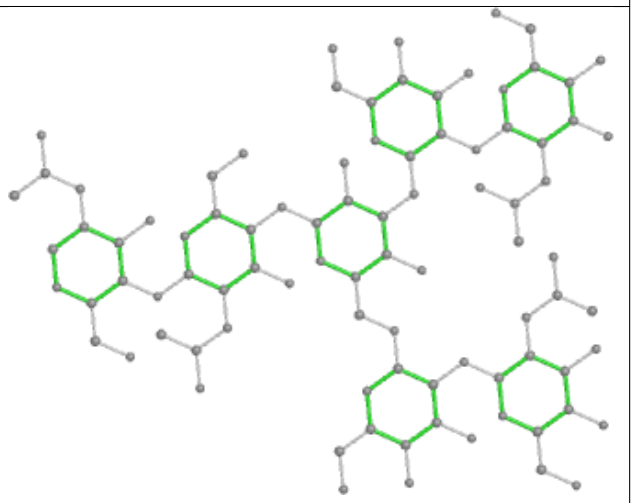
Bond lengths



Bond angles

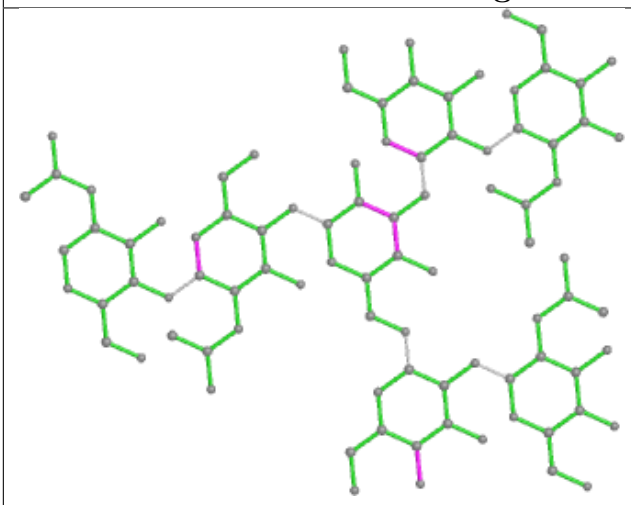


Torsions

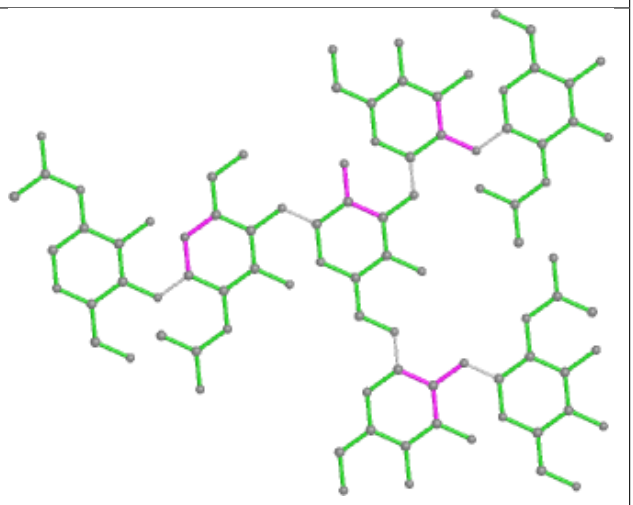


Rings

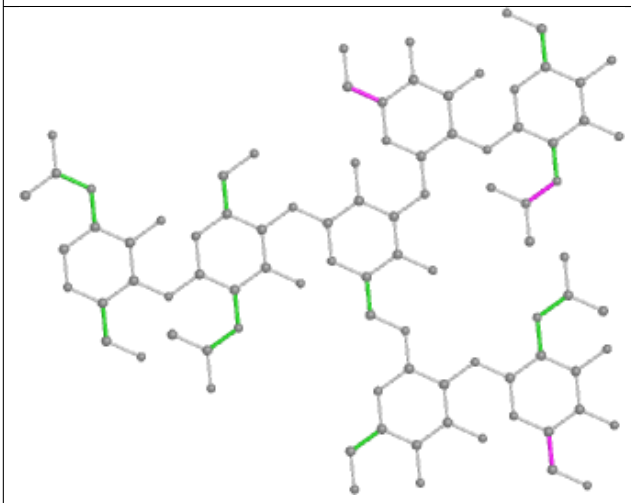
Oligosaccharide Chain K



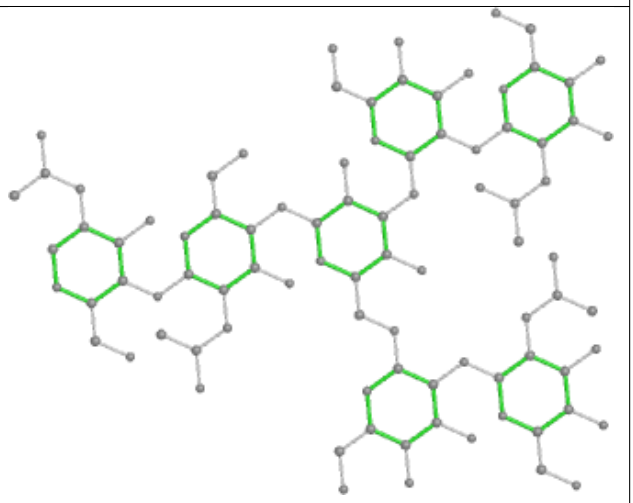
Bond lengths



Bond angles

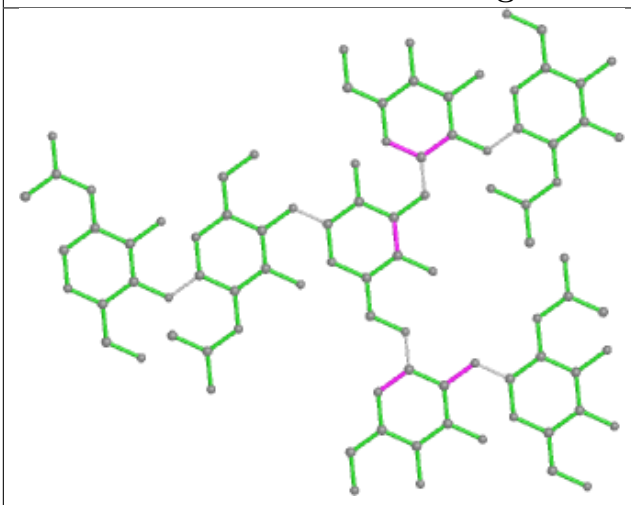


Torsions

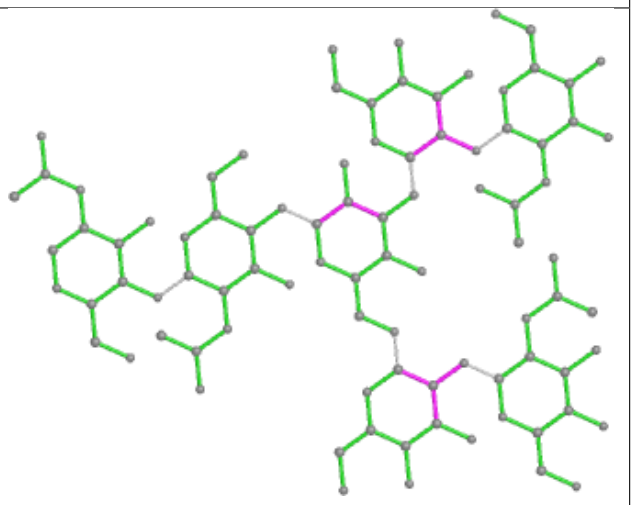


Rings

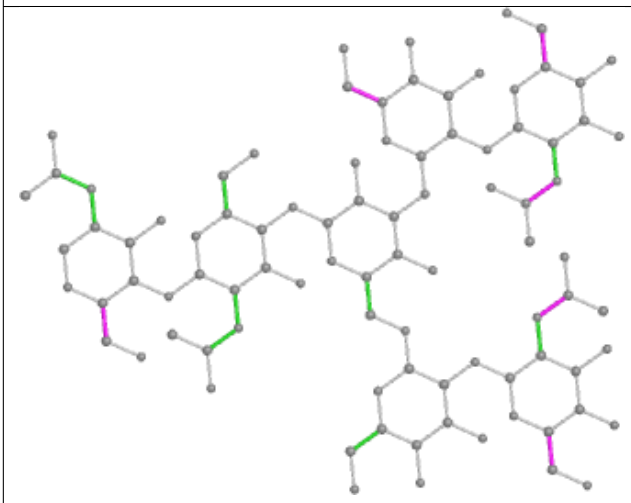
Oligosaccharide Chain L



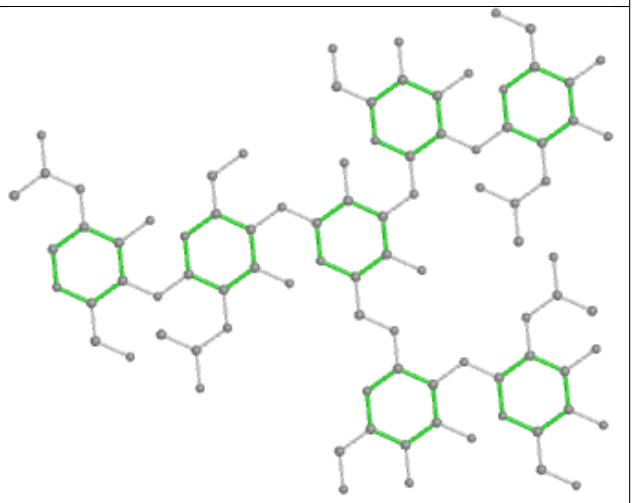
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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, 95^{th} 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	207/224 (92%)	0.04	1 (0%)	91	92	59, 77, 107, 124	0
1	B	207/224 (92%)	0.05	4 (1%)	66	69	61, 85, 112, 129	0
1	E	206/224 (91%)	0.01	2 (0%)	82	83	61, 84, 128, 146	0
1	F	208/224 (92%)	0.31	7 (3%)	45	45	68, 103, 135, 146	0
2	C	120/120 (100%)	0.02	1 (0%)	86	87	78, 94, 122, 139	0
2	D	120/120 (100%)	0.24	5 (4%)	36	35	69, 95, 131, 144	0
2	G	120/120 (100%)	0.23	5 (4%)	36	35	81, 104, 130, 171	0
2	H	120/120 (100%)	0.35	6 (5%)	28	28	80, 102, 132, 152	0
All	All	1308/1376 (95%)	0.14	31 (2%)	59	60	59, 92, 128, 171	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	GLN	11.2
2	H	2	VAL	7.2
2	D	2	VAL	5.5
2	G	1	GLN	5.0
1	F	286	ASN	3.9
2	D	1	GLN	3.6
1	A	355	ARG	3.3
1	B	293	GLU	3.2
1	F	254	SER	3.2
1	B	271	PRO	3.1
1	F	292	ARG	2.8
1	E	384	ASN	2.7
2	D	13	GLN	2.7
2	H	118	VAL	2.7
2	H	112	GLN	2.6
1	B	419	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	333	GLU	2.6
2	G	11	LEU	2.6
2	G	101	THR	2.5
2	H	42	GLY	2.5
1	F	275	PHE	2.3
2	C	74	ALA	2.2
1	F	248	LYS	2.2
1	F	302	VAL	2.2
1	E	356	GLU	2.2
1	F	294	GLU	2.2
2	D	26	PRO	2.1
2	D	101	THR	2.1
2	H	88	GLU	2.1
2	G	30	ARG	2.0
2	G	12	VAL	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	L	5	14/15	0.84	0.22	96,103,109,114	0
3	NAG	J	5	14/15	0.88	0.15	97,107,110,112	0
3	NAG	K	5	14/15	0.88	0.22	80,91,104,104	0
3	NAG	I	5	14/15	0.88	0.20	89,99,107,107	0
3	NAG	J	7	14/15	0.91	0.17	67,75,80,87	0
3	MAN	J	4	11/12	0.93	0.16	95,98,101,105	0
3	NAG	L	7	14/15	0.93	0.14	69,77,81,89	0
3	NAG	I	1	14/15	0.94	0.17	73,77,81,83	0
3	NAG	J	1	14/15	0.94	0.13	90,92,95,96	0
3	MAN	L	4	11/12	0.95	0.16	73,87,92,92	0
3	NAG	I	7	14/15	0.95	0.16	59,66,70,75	0
3	MAN	I	4	11/12	0.95	0.21	81,83,85,88	0
3	BMA	J	3	11/12	0.96	0.15	74,87,90,95	0

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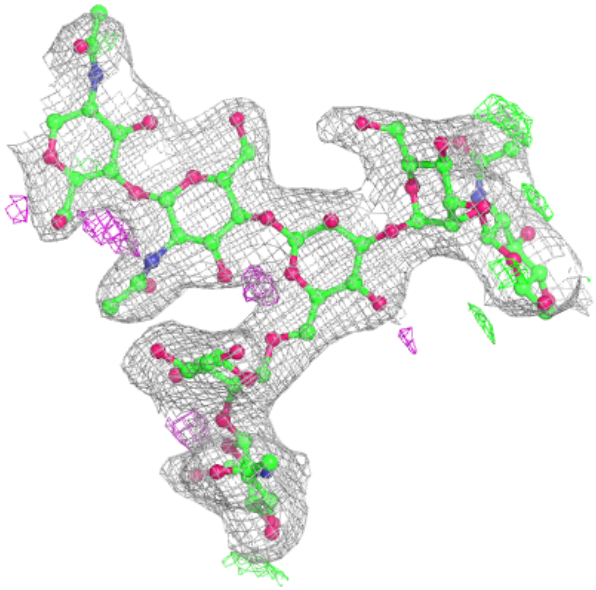
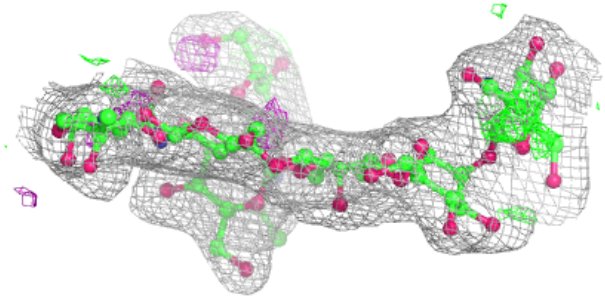
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	K	7	14/15	0.96	0.20	65,70,73,73	0
3	NAG	L	1	14/15	0.96	0.16	72,81,85,86	0
3	NAG	L	2	14/15	0.96	0.15	67,73,75,76	0
3	BMA	L	3	11/12	0.96	0.18	72,75,82,82	0
3	NAG	I	2	14/15	0.96	0.17	57,68,74,76	0
3	BMA	I	3	11/12	0.96	0.19	63,72,77,78	0
3	NAG	J	2	14/15	0.96	0.13	79,86,89,90	0
3	NAG	K	2	14/15	0.97	0.17	57,67,72,72	0
3	MAN	K	4	11/12	0.97	0.21	65,75,80,83	0
3	MAN	J	6	11/12	0.97	0.20	70,74,80,84	0
3	MAN	I	6	11/12	0.97	0.18	62,67,71,71	0
3	MAN	L	6	11/12	0.97	0.17	68,71,74,79	0
3	NAG	K	1	14/15	0.97	0.14	68,72,76,78	0
3	BMA	K	3	11/12	0.98	0.20	59,64,69,70	0
3	MAN	K	6	11/12	0.98	0.21	63,67,71,72	0

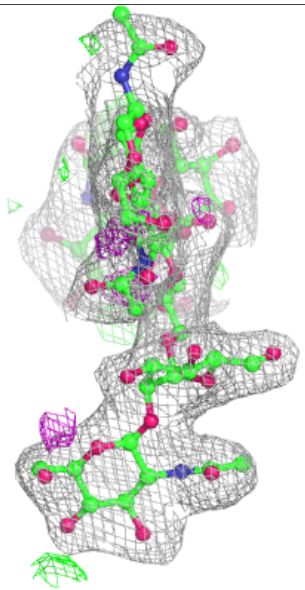
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

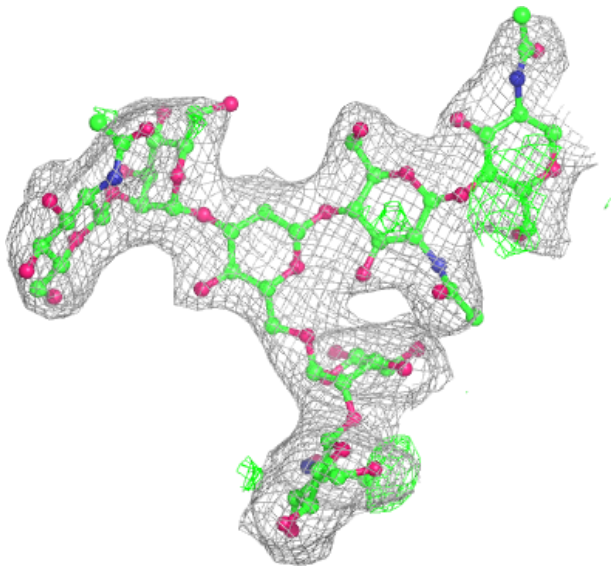


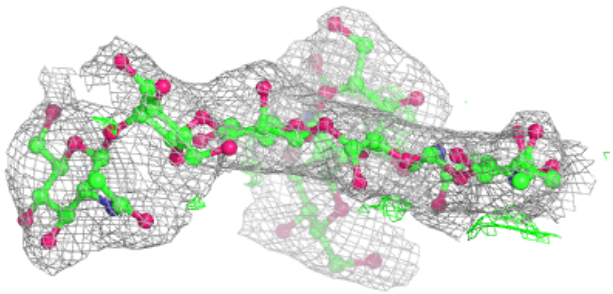


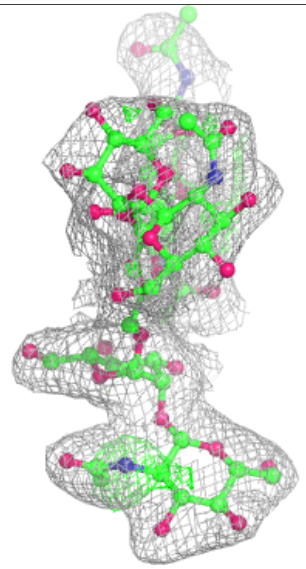


Electron density around Chain J:

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

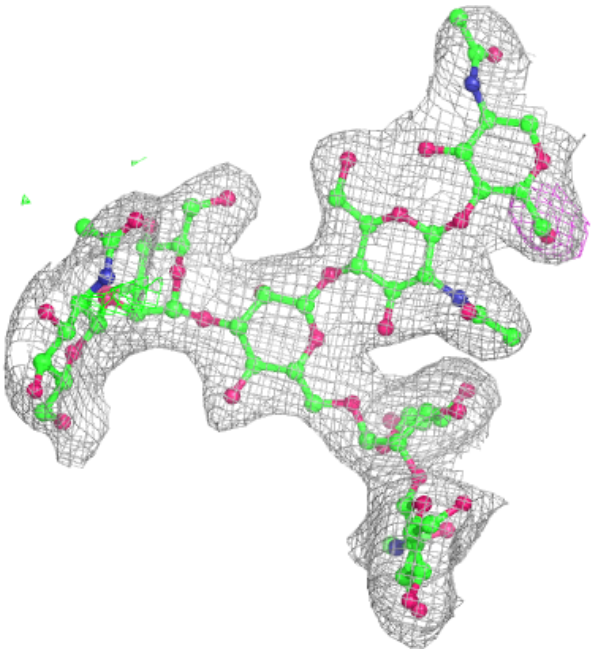


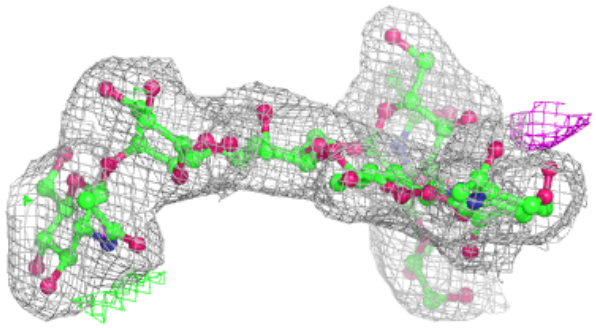


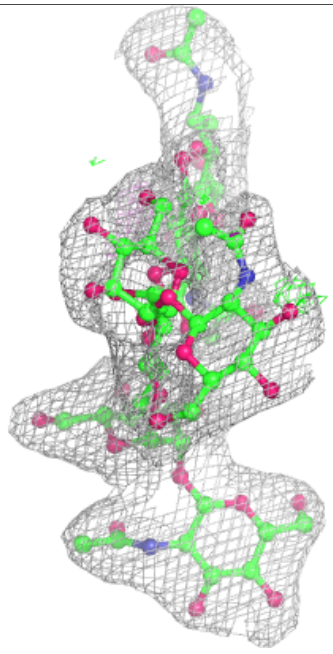


Electron density around Chain K:

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

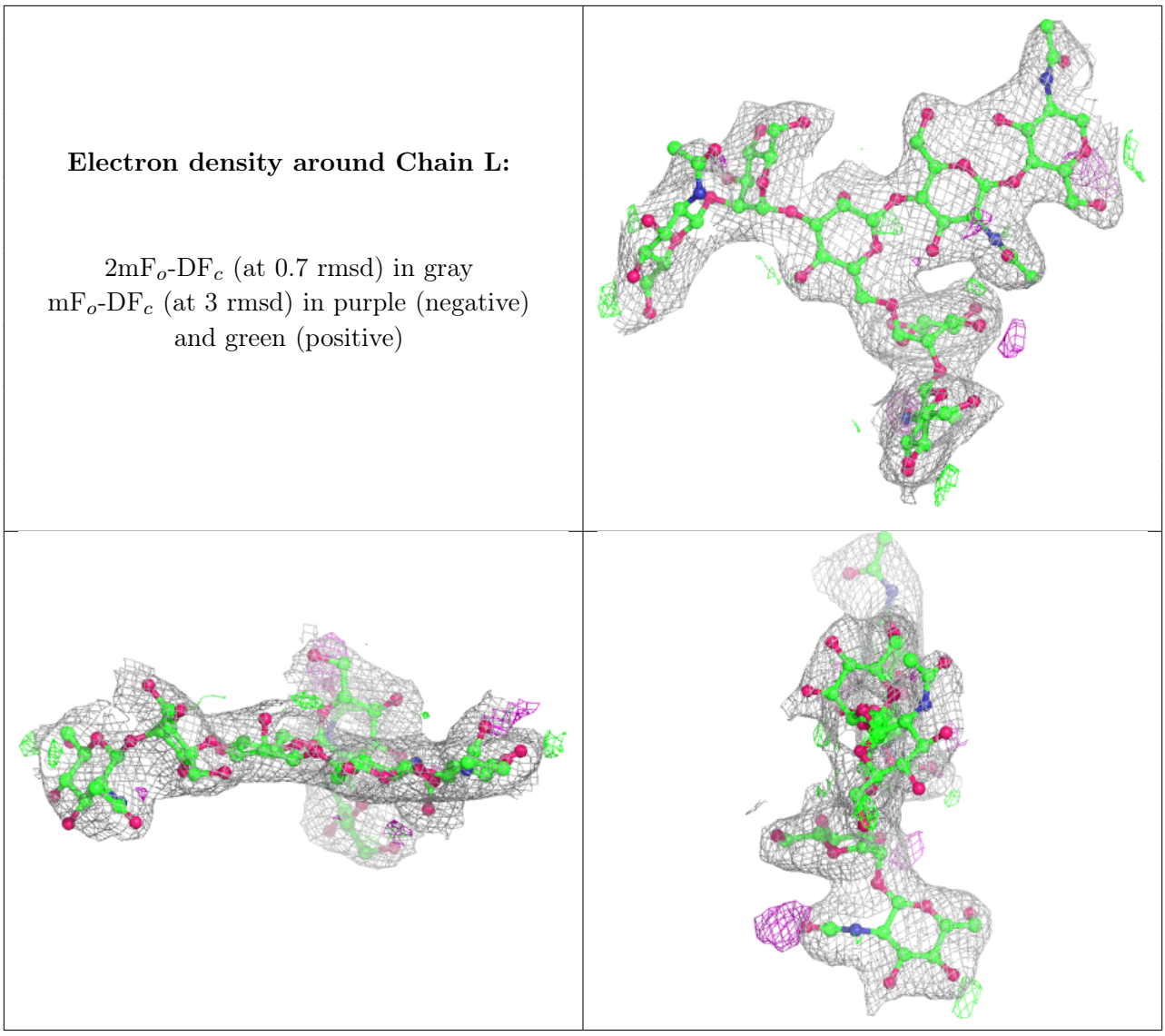






Electron density around Chain L:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.