



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:17 AM UTC

PDB ID : 4JU0 / pdb_00004ju0
Title : Crystal structure of 2009 pandemic influenza virus hemagglutinin mutant D225E complexed with human receptor analogue LSTc
Authors : Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.
Deposited on : 2013-03-24
Resolution : 2.91 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

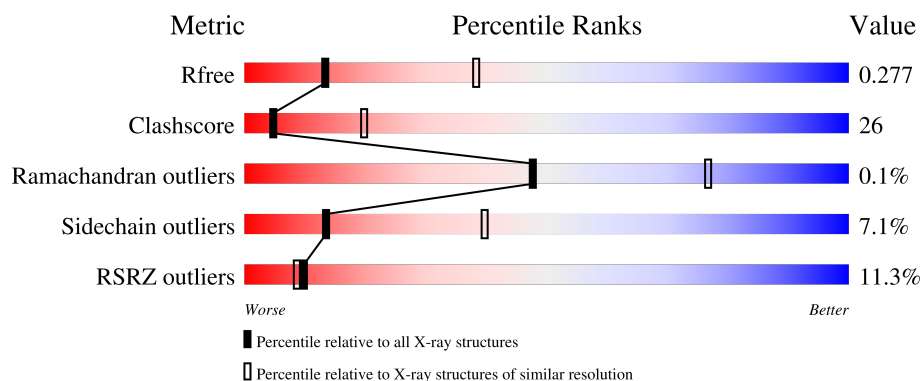
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	322	10% 63% 32% 5%
1	C	322	9% 57% 37% . .
1	E	322	6% 61% 35% .
1	G	322	11% 62% 34% .
1	I	322	9% 59% 37% .

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Mol	Chain	Length	Quality of chain
1	K	322	
2	B	164	
2	D	164	
2	F	164	
2	H	164	
2	J	164	
2	L	164	
3	M	4	
3	N	4	
3	P	4	
3	Q	4	
3	R	4	
4	O	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23507 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	322	Total	C	N	O	S	0	0	0
			2513	1590	434	478	11			
1	C	321	Total	C	N	O	S	0	0	0
			2510	1587	433	479	11			
1	E	321	Total	C	N	O	S	0	0	0
			2510	1587	433	479	11			
1	G	322	Total	C	N	O	S	0	0	0
			2513	1590	434	478	11			
1	I	321	Total	C	N	O	S	0	0	0
			2510	1587	433	479	11			
1	K	321	Total	C	N	O	S	0	0	0
			2510	1587	433	479	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	GLU	ASP	engineered mutation	UNP C3W5S1
C	228	GLU	ASP	engineered mutation	UNP C3W5S1
E	228	GLU	ASP	engineered mutation	UNP C3W5S1
G	228	GLU	ASP	engineered mutation	UNP C3W5S1
I	228	GLU	ASP	engineered mutation	UNP C3W5S1
K	228	GLU	ASP	engineered mutation	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	D	164	Total	C	N	O	S	0	0	0
			1315	826	221	262	6			
2	F	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	J	164	Total	C	N	O	S	0	0	0
			1315	826	221	262	6			
2	L	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	4	Total	C	N	O	0	0	0
			56	31	2	23			
3	N	4	Total	C	N	O	0	0	0
			56	31	2	23			
3	P	4	Total	C	N	O	0	0	0
			56	31	2	23			
3	Q	4	Total	C	N	O	0	0	0
			56	31	2	23			
3	R	4	Total	C	N	O	0	0	0
			56	31	2	23			

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



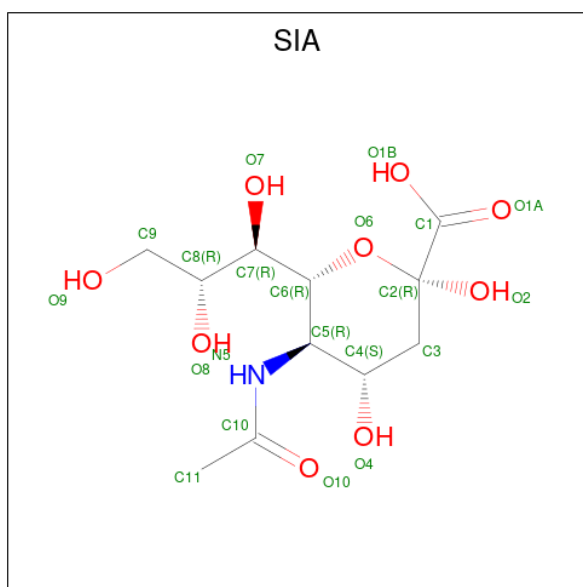
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	22	Total	O	0	0
			22	22		
7	B	6	Total	O	0	0
			6	6		
7	C	20	Total	O	0	0
			20	20		
7	D	5	Total	O	0	0
			5	5		
7	E	18	Total	O	0	0
			18	18		
7	F	11	Total	O	0	0
			11	11		
7	G	16	Total	O	0	0
			16	16		
7	H	6	Total	O	0	0
			6	6		
7	I	25	Total	O	0	0
			25	25		
7	J	22	Total	O	0	0
			22	22		
7	K	26	Total	O	0	0
			26	26		

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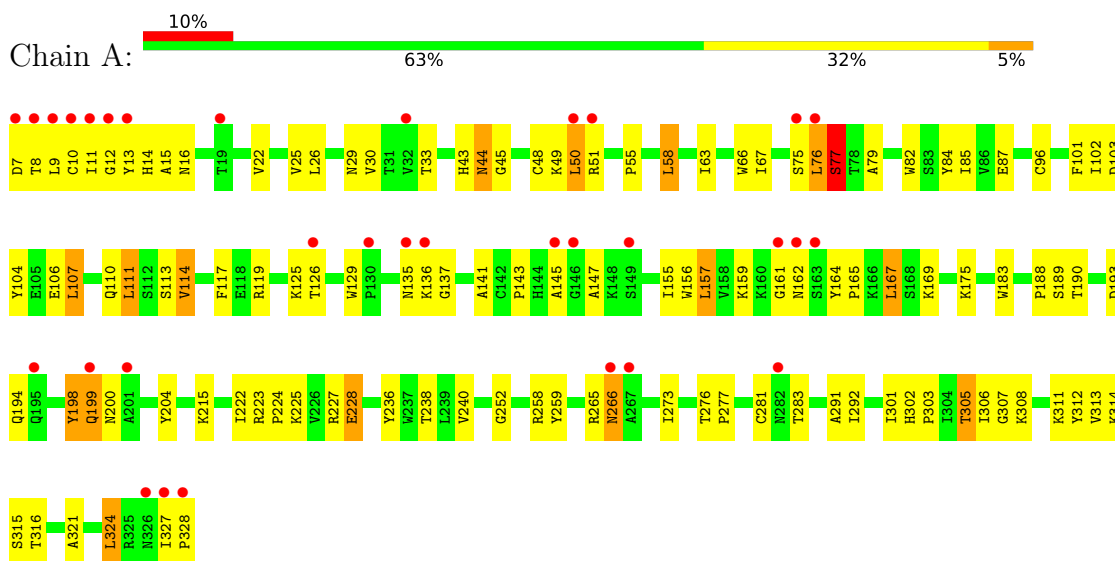
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	8	Total	O	0	0
			8	8		

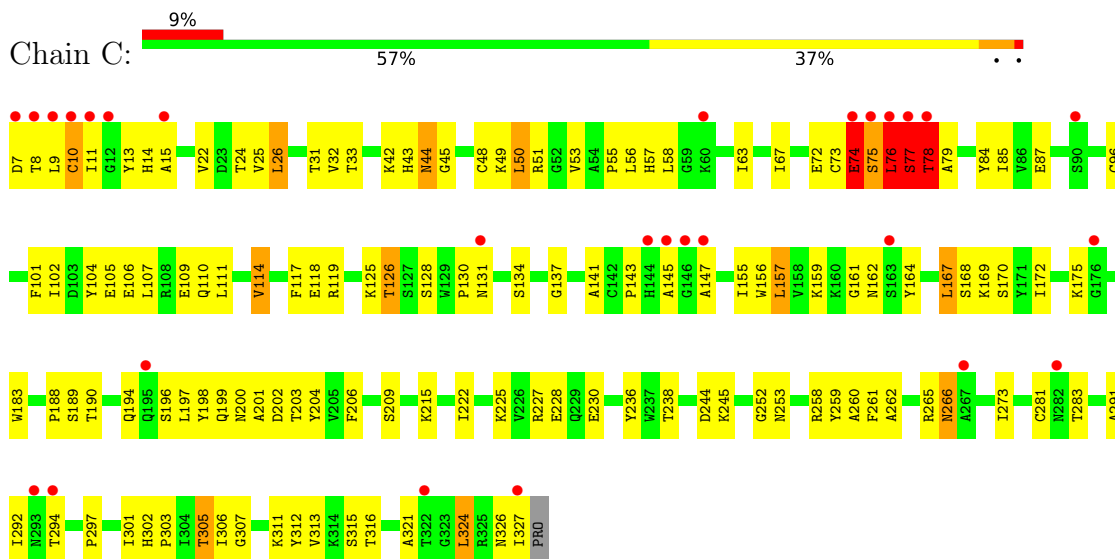
3 Residue-property plots

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.

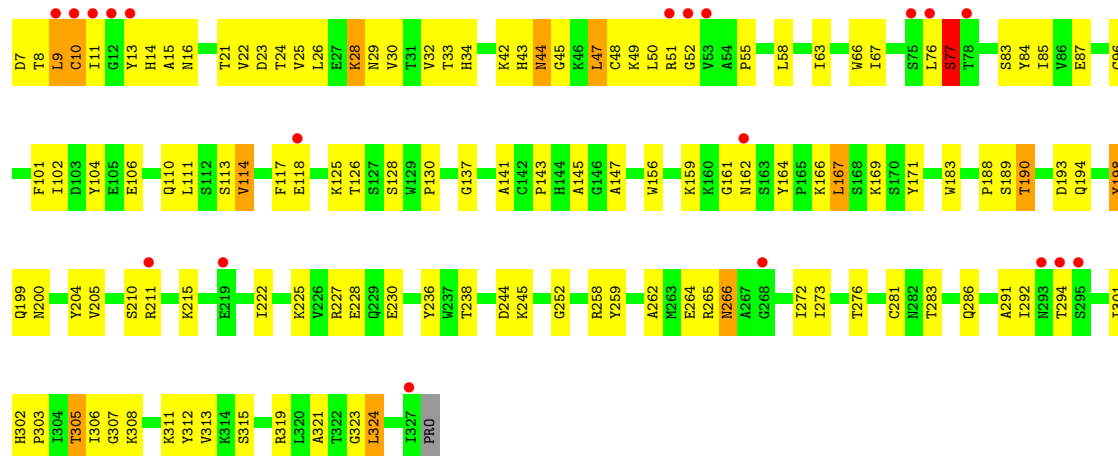
• Molecule 1: Hemagglutinin



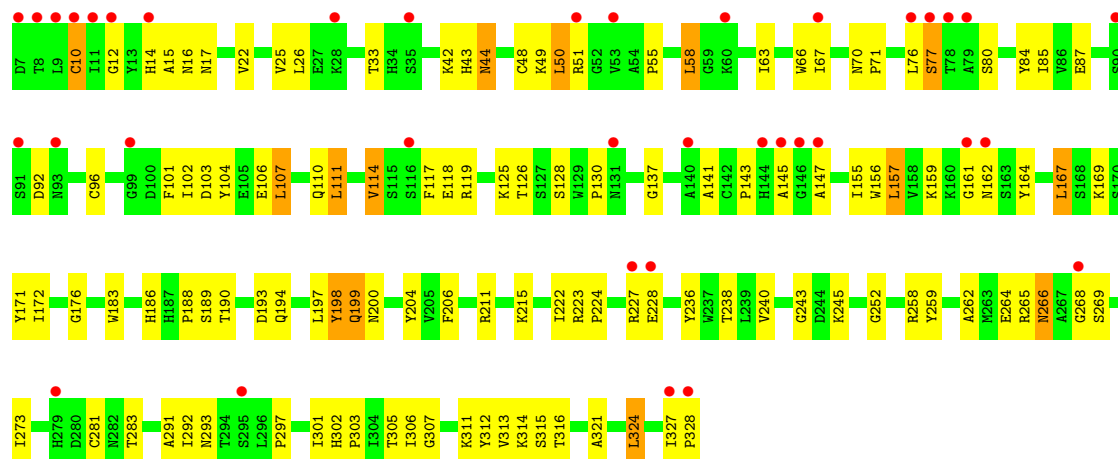
• Molecule 1: Hemagglutinin



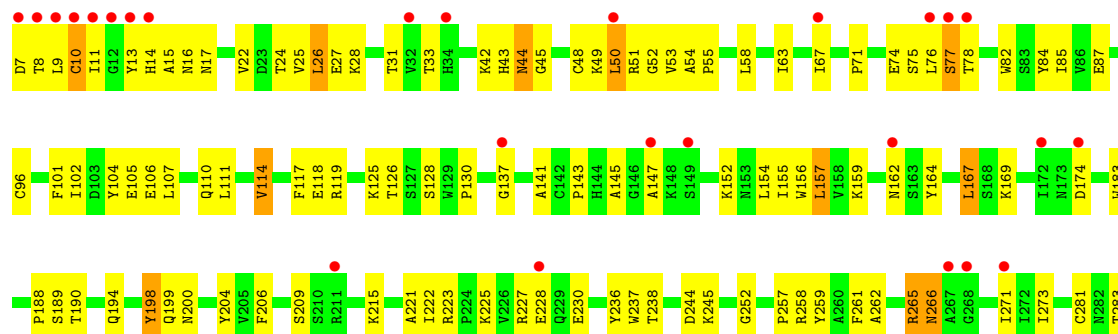
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

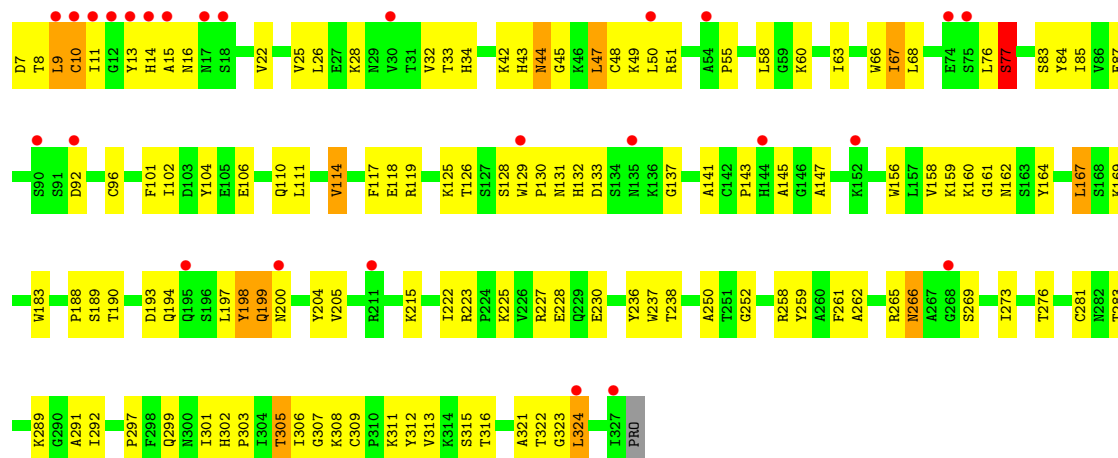


• Molecule 1: Hemagglutinin

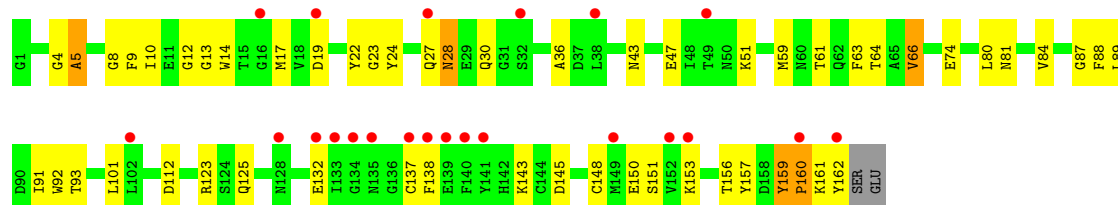




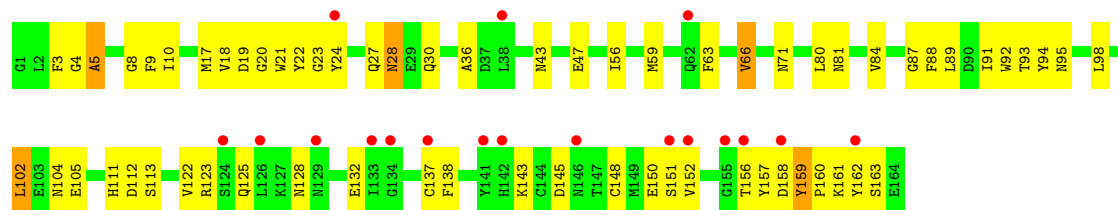
• Molecule 1: Hemagglutinin



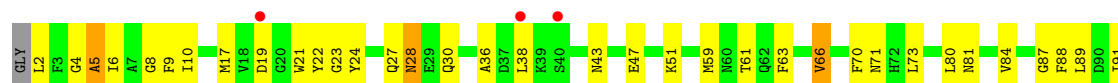
• Molecule 2: Hemagglutinin

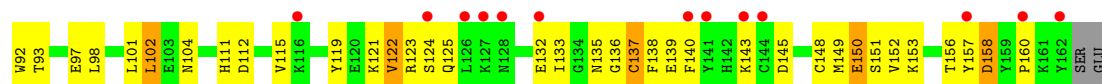


• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin

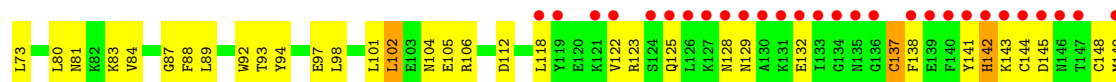
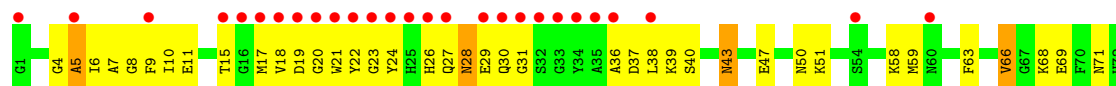
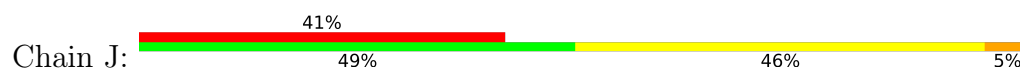




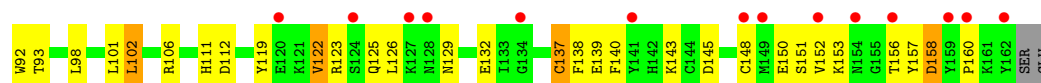
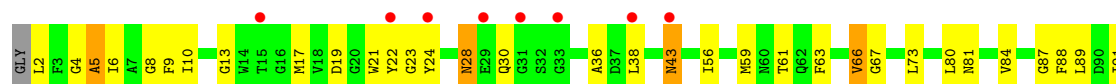
• Molecule 2: Hemagglutinin



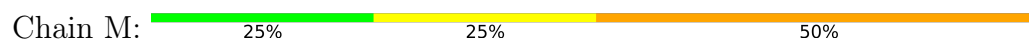
• Molecule 2: Hemagglutinin



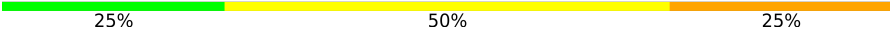
• Molecule 2: Hemagglutinin



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain N:  25% 50% 25%

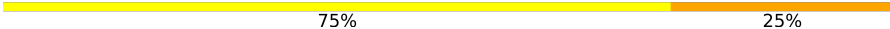


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain P:  50% 25% 25%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain Q:  75% 25%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain R:  25% 25% 50%



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

Chain O:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.87Å 116.81Å 116.50Å 62.06° 77.76° 81.54°	Depositor
Resolution (Å)	40.22 – 2.91 40.22 – 2.91	Depositor EDS
% Data completeness (in resolution range)	88.2 (40.22-2.91) 94.2 (40.22-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.240 , 0.283 0.238 , 0.277	Depositor DCC
R_{free} test set	3175 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23507	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/2577	0.97	13/3501 (0.4%)
1	C	0.35	1/2573 (0.0%)	1.02	12/3494 (0.3%)
1	E	0.30	0/2573	0.84	6/3494 (0.2%)
1	G	0.33	0/2577	0.90	11/3501 (0.3%)
1	I	0.30	0/2573	0.85	6/3494 (0.2%)
1	K	0.30	0/2573	0.88	5/3494 (0.1%)
2	B	0.29	0/1333	0.76	3/1797 (0.2%)
2	D	0.31	0/1343	0.75	2/1811 (0.1%)
2	F	0.31	0/1330	0.72	2/1794 (0.1%)
2	H	0.29	0/1333	0.73	2/1797 (0.1%)
2	J	0.30	0/1343	0.75	2/1811 (0.1%)
2	L	0.31	0/1330	0.71	2/1794 (0.1%)
All	All	0.31	1/23458 (0.0%)	0.86	66/31782 (0.2%)

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	E	0	1
1	K	0	1
2	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	CYS	CA-C	-5.35	1.47	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	THR	N-CA-C	23.65	143.70	111.54
1	C	76	LEU	CB-CA-C	-17.64	89.24	111.82
1	K	199	GLN	CB-CA-C	-15.78	81.24	111.06
1	A	76	LEU	N-CA-C	14.97	128.08	110.41
1	A	77	SER	N-CA-C	14.90	130.02	111.69
1	A	76	LEU	N-CA-CB	-13.81	95.22	111.79
1	G	200	ASN	N-CA-C	-12.03	89.15	109.24
1	K	200	ASN	N-CA-C	-11.00	90.86	109.24
2	J	142	HIS	N-CA-C	10.48	124.61	110.35
1	A	119	ARG	NE-CZ-NH2	10.16	128.34	119.20
1	G	119	ARG	NE-CZ-NH2	10.01	128.21	119.20
1	C	75	SER	CB-CA-C	-9.83	95.00	110.14
1	I	77	SER	CB-CA-C	-9.61	91.80	109.29
1	C	78	THR	CB-CA-C	-9.50	97.92	111.80
1	G	119	ARG	NE-CZ-NH1	-9.36	112.14	121.50
1	A	119	ARG	NE-CZ-NH1	-9.30	112.20	121.50
1	A	200	ASN	N-CA-C	-9.14	93.97	109.24
1	C	200	ASN	N-CA-C	-8.90	94.89	109.40
1	C	77	SER	N-CA-CB	-8.63	95.13	109.28
1	C	75	SER	N-CA-C	8.46	122.30	108.26
1	I	200	ASN	N-CA-C	-8.30	95.87	109.40
1	A	30	VAL	N-CA-C	8.06	119.47	108.84
1	E	200	ASN	N-CA-C	-7.93	96.48	109.40
1	I	78	THR	N-CA-CB	-7.71	97.44	109.69
2	B	5	ALA	N-CA-C	7.48	119.33	111.03
1	A	119	ARG	CD-NE-CZ	7.46	134.85	124.40
1	G	119	ARG	CD-NE-CZ	7.40	134.76	124.40
1	A	75	SER	N-CA-C	7.39	122.40	113.23
1	G	76	LEU	N-CA-C	7.39	123.04	114.62
2	F	5	ALA	N-CA-C	7.38	119.22	111.03
2	D	163	SER	N-CA-C	7.23	124.59	110.56
2	H	5	ALA	N-CA-C	7.01	119.95	111.40
2	L	157	TYR	N-CA-C	-6.74	102.32	111.55
1	E	77	SER	N-CA-C	6.67	119.70	108.02
1	E	198	TYR	CB-CA-C	6.57	120.85	109.15
1	G	199	GLN	CB-CA-C	-6.46	98.86	111.06
2	D	5	ALA	N-CA-C	6.35	118.08	111.03
1	C	76	LEU	N-CA-C	-6.22	102.67	111.56
2	L	5	ALA	N-CA-C	6.20	119.24	111.24
1	K	77	SER	N-CA-C	6.19	119.82	107.62
2	B	66	VAL	CB-CA-C	-6.17	101.17	111.29
1	G	200	ASN	N-CA-CB	6.11	122.06	111.00
1	I	198	TYR	CB-CA-C	6.10	120.00	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	VAL	CB-CA-C	-6.09	101.31	111.29
1	G	77	SER	N-CA-C	6.07	119.66	107.41
1	I	75	SER	N-CA-C	-6.04	102.53	110.33
1	A	198	TYR	CB-CA-C	5.85	119.56	109.15
2	F	157	TYR	N-CA-C	-5.85	102.81	111.81
2	J	5	ALA	N-CA-C	5.80	118.72	111.24
1	K	198	TYR	CB-CA-C	5.76	118.12	109.13
1	A	77	SER	CB-CA-C	-5.72	100.23	110.70
2	B	159	TYR	N-CA-CB	-5.68	102.78	110.74
1	G	76	LEU	N-CA-CB	-5.64	102.27	111.18
1	A	29	ASN	N-CA-C	5.59	122.70	110.80
1	C	74	GLU	N-CA-C	-5.56	97.15	107.71
1	C	77	SER	N-CA-C	-5.54	101.99	110.30
1	G	198	TYR	CB-CA-C	5.42	118.14	109.02
1	C	78	THR	N-CA-CB	-5.32	103.91	111.84
1	E	30	VAL	N-CA-C	5.30	116.38	108.54
1	G	16	ASN	N-CA-C	5.19	114.68	107.73
1	I	16	ASN	N-CA-C	5.18	114.68	107.73
1	C	79	ALA	N-CA-C	5.14	117.80	110.24
1	E	28	LYS	CB-CA-C	-5.12	100.16	109.38
1	K	16	ASN	N-CA-C	5.09	114.55	107.73
1	A	16	ASN	N-CA-C	5.05	114.50	107.73
1	E	16	ASN	N-CA-C	5.03	114.47	107.73

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	77	SER	Peptide
2	J	141	TYR	Peptide
1	K	77	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2513	0	2457	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2510	0	2452	164	0
1	E	2510	0	2453	133	0
1	G	2513	0	2455	121	0
1	I	2510	0	2452	167	0
1	K	2510	0	2452	155	0
2	B	1305	0	1228	57	0
2	D	1315	0	1227	74	0
2	F	1302	0	1226	87	0
2	H	1305	0	1228	61	0
2	J	1315	0	1227	156	0
2	L	1302	0	1226	84	0
3	M	56	0	47	3	0
3	N	56	0	47	4	0
3	P	56	0	47	3	0
3	Q	56	0	47	5	0
3	R	56	0	47	2	0
4	O	28	0	25	1	0
5	C	28	0	26	5	0
5	G	14	0	13	0	0
5	I	14	0	13	0	0
5	K	28	0	26	9	0
6	K	20	0	17	1	0
7	A	22	0	0	31	0
7	B	6	0	0	3	0
7	C	20	0	0	40	0
7	D	5	0	0	14	0
7	E	18	0	0	31	0
7	F	11	0	0	24	0
7	G	16	0	0	15	0
7	H	6	0	0	12	0
7	I	25	0	0	51	0
7	J	22	0	0	53	0
7	K	26	0	0	52	0
7	L	8	0	0	17	0
All	All	23507	0	22438	1169	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 26.

All (1169) 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:C:56:LEU:CD1	1:C:76:LEU:HD12	1.48	1.42
1:C:56:LEU:HD12	1:C:76:LEU:CD1	1.49	1.40
1:C:8:THR:HB	7:D:204:HOH:O	1.18	1.31
1:C:110:GLN:HB2	7:C:714:HOH:O	1.20	1.29
1:G:245:LYS:HA	7:G:516:HOH:O	1.14	1.28
2:J:152:VAL:HG13	7:J:210:HOH:O	1.34	1.26
1:A:113:SER:CA	7:A:913:HOH:O	1.84	1.23
2:J:7:ALA:CB	7:J:211:HOH:O	1.91	1.18
2:F:125:GLN:HB2	7:F:209:HOH:O	1.43	1.16
1:A:113:SER:HA	7:A:913:HOH:O	1.38	1.15
1:C:78:THR:HG21	1:K:289:LYS:HE3	1.27	1.15
1:K:309:CYS:SG	7:K:717:HOH:O	2.06	1.14
1:C:31:THR:HG22	7:C:717:HOH:O	1.43	1.13
1:C:74:GLU:O	1:C:74:GLU:HG2	1.42	1.12
1:K:68:LEU:N	7:K:725:HOH:O	1.81	1.11
1:A:114:VAL:N	7:A:913:HOH:O	1.81	1.10
1:A:307:GLY:N	7:A:917:HOH:O	1.82	1.10
2:D:3:PHE:CD1	7:D:202:HOH:O	2.03	1.10
1:A:114:VAL:CB	7:A:922:HOH:O	1.97	1.09
2:F:104:ASN:ND2	7:F:207:HOH:O	1.83	1.09
2:J:15:THR:N	7:J:216:HOH:O	1.85	1.09
2:J:162:TYR:CD1	7:J:212:HOH:O	2.06	1.09
1:I:10:CYS:SG	7:I:710:HOH:O	2.09	1.09
1:I:154:LEU:HA	7:I:709:HOH:O	1.51	1.08
1:A:114:VAL:HG12	7:A:922:HOH:O	1.55	1.06
1:K:131:ASN:C	7:K:719:HOH:O	1.97	1.06
2:D:113:SER:CA	7:D:202:HOH:O	2.02	1.05
2:J:6:ILE:HG22	7:J:211:HOH:O	1.55	1.05
1:E:11:ILE:HD12	2:F:119:TYR:HA	1.34	1.04
1:A:114:VAL:CG1	7:A:922:HOH:O	2.05	1.04
2:J:7:ALA:HB2	7:J:211:HOH:O	1.50	1.04
1:K:313:VAL:N	7:K:721:HOH:O	1.90	1.04
1:K:132:HIS:CA	7:K:722:HOH:O	2.06	1.03
2:D:160:PRO:CA	7:D:203:HOH:O	2.04	1.03
2:J:7:ALA:N	7:J:211:HOH:O	1.90	1.03
7:K:723:HOH:O	2:L:13:GLY:HA2	1.57	1.02
2:D:160:PRO:HA	7:D:203:HOH:O	1.59	1.02
2:J:163:SER:N	7:J:212:HOH:O	1.82	1.02
2:J:97:GLU:CD	7:J:221:HOH:O	2.01	1.01
2:D:113:SER:N	7:D:202:HOH:O	1.94	1.01
1:E:24:THR:CA	7:E:714:HOH:O	2.09	1.00
1:K:106:GLU:CD	7:K:718:HOH:O	2.05	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:HIS:N	7:K:719:HOH:O	1.95	0.99
1:K:167:LEU:HB3	7:K:715:HOH:O	1.60	0.99
1:C:106:GLU:HA	7:C:711:HOH:O	1.61	0.99
1:K:133:ASP:N	7:K:722:HOH:O	1.82	0.99
1:C:32:VAL:N	7:C:717:HOH:O	1.93	0.98
2:J:43:ASN:HB2	7:J:222:HOH:O	1.63	0.98
2:L:101:LEU:HB3	7:L:208:HOH:O	1.60	0.98
2:J:11:GLU:HA	7:J:217:HOH:O	1.61	0.98
1:K:132:HIS:HA	7:K:722:HOH:O	1.63	0.98
1:I:8:THR:OG1	2:J:27:GLN:HB3	1.63	0.98
1:C:196:SER:O	7:C:715:HOH:O	1.80	0.98
1:I:11:ILE:HG12	2:J:24:TYR:CD2	1.98	0.98
1:G:92:ASP:HA	7:G:512:HOH:O	1.65	0.97
2:J:162:TYR:CG	7:J:212:HOH:O	2.17	0.97
1:C:56:LEU:HD12	1:C:76:LEU:HD12	0.99	0.96
1:A:307:GLY:O	7:A:917:HOH:O	1.83	0.95
2:D:3:PHE:CG	7:D:202:HOH:O	2.14	0.95
1:K:11:ILE:HD12	2:L:119:TYR:HA	1.45	0.95
1:I:316:THR:N	7:I:724:HOH:O	1.81	0.95
1:A:114:VAL:HB	7:A:922:HOH:O	1.60	0.95
1:A:136:LYS:N	7:A:914:HOH:O	2.00	0.95
1:C:197:LEU:HA	7:C:715:HOH:O	1.67	0.95
1:I:10:CYS:CA	7:I:710:HOH:O	2.12	0.94
1:K:312:TYR:HA	7:K:721:HOH:O	1.66	0.94
2:L:101:LEU:C	7:L:208:HOH:O	2.09	0.94
1:E:21:THR:HB	1:E:29:ASN:OD1	1.68	0.94
2:J:84:VAL:C	7:J:213:HOH:O	2.09	0.94
1:E:24:THR:HA	7:E:714:HOH:O	1.65	0.94
2:L:129:ASN:N	7:L:207:HOH:O	2.01	0.94
1:C:75:SER:O	1:C:76:LEU:HB2	1.63	0.93
1:E:319:ARG:NH2	7:E:711:HOH:O	1.97	0.93
1:I:174:ASP:HA	7:I:703:HOH:O	1.67	0.93
1:A:164:TYR:CD2	7:A:919:HOH:O	2.20	0.93
1:K:312:TYR:CD1	7:K:721:HOH:O	2.22	0.93
1:A:162:ASN:ND2	1:A:199:GLN:HE21	1.65	0.93
1:C:56:LEU:HD11	1:C:76:LEU:HD12	1.46	0.93
1:I:10:CYS:CB	7:I:710:HOH:O	2.16	0.93
1:C:56:LEU:CD1	1:C:76:LEU:CD1	2.25	0.93
1:E:110:GLN:NE2	7:E:716:HOH:O	2.01	0.93
1:C:26:LEU:O	7:C:712:HOH:O	1.85	0.93
1:C:162:ASN:ND2	1:C:199:GLN:HE21	1.64	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:309:CYS:CB	7:K:717:HOH:O	2.14	0.93
1:G:171:TYR:O	7:G:516:HOH:O	1.86	0.92
1:K:312:TYR:CA	7:K:721:HOH:O	2.16	0.92
2:L:126:LEU:C	7:L:207:HOH:O	2.13	0.92
1:I:106:GLU:CB	7:I:713:HOH:O	2.18	0.92
1:K:299:GLN:O	7:K:721:HOH:O	1.85	0.92
1:E:159:LYS:HZ2	1:E:199:GLN:HG2	1.35	0.92
1:E:264:GLU:OE1	7:E:703:HOH:O	1.87	0.92
1:E:25:VAL:N	7:E:714:HOH:O	1.99	0.91
1:I:265:ARG:C	7:I:718:HOH:O	2.12	0.91
1:C:74:GLU:O	1:C:74:GLU:CG	2.19	0.91
2:J:11:GLU:CA	7:J:217:HOH:O	2.13	0.91
2:D:113:SER:HA	7:D:202:HOH:O	1.61	0.91
2:J:73:LEU:C	7:K:718:HOH:O	2.14	0.91
1:C:313:VAL:HG12	1:C:315:SER:H	1.36	0.91
1:K:60:LYS:HD2	5:K:602:NAG:H81	1.52	0.91
1:K:309:CYS:HB2	7:K:717:HOH:O	1.68	0.91
1:A:165:PRO:O	7:A:919:HOH:O	1.87	0.90
1:I:313:VAL:HG12	1:I:315:SER:H	1.36	0.90
1:E:24:THR:O	7:E:713:HOH:O	1.88	0.90
1:A:164:TYR:CE2	7:A:919:HOH:O	2.22	0.90
1:C:106:GLU:CA	7:C:711:HOH:O	2.14	0.90
1:C:175:LYS:O	7:C:706:HOH:O	1.89	0.90
1:E:11:ILE:CD1	2:F:119:TYR:HA	2.00	0.90
1:K:25:VAL:N	7:L:208:HOH:O	2.04	0.90
2:F:135:ASN:HB3	7:F:205:HOH:O	1.71	0.90
1:I:106:GLU:HB2	7:I:713:HOH:O	1.69	0.90
2:J:26:HIS:NE2	7:J:214:HOH:O	2.05	0.89
1:K:129:TRP:O	7:K:716:HOH:O	1.91	0.89
1:A:82:TRP:O	7:A:913:HOH:O	1.91	0.89
1:E:313:VAL:HG12	1:E:315:SER:H	1.36	0.89
1:G:313:VAL:HG12	1:G:315:SER:H	1.37	0.89
1:C:143:PRO:O	7:C:713:HOH:O	1.91	0.89
1:A:313:VAL:HG12	1:A:315:SER:H	1.36	0.88
1:I:318:LEU:CD2	7:J:221:HOH:O	2.19	0.88
1:C:57:HIS:CG	7:C:720:HOH:O	2.24	0.88
1:K:13:TYR:O	7:K:723:HOH:O	1.89	0.88
1:G:17:ASN:ND2	7:G:514:HOH:O	1.86	0.88
1:E:21:THR:CB	1:E:29:ASN:OD1	2.22	0.88
2:F:104:ASN:HB2	7:F:207:HOH:O	1.73	0.88
1:E:171:TYR:OH	7:E:715:HOH:O	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:CYS:HA	2:F:137:CYS:HA	1.56	0.87
1:C:106:GLU:C	7:C:711:HOH:O	2.16	0.87
2:J:26:HIS:CD2	7:J:214:HOH:O	2.25	0.87
2:J:84:VAL:CA	7:J:213:HOH:O	2.22	0.87
1:E:319:ARG:NH1	7:E:711:HOH:O	2.02	0.87
2:F:149:MET:HB2	7:F:204:HOH:O	1.74	0.87
1:K:313:VAL:HG12	1:K:315:SER:H	1.37	0.87
1:C:57:HIS:ND1	7:C:720:HOH:O	2.08	0.86
2:J:97:GLU:OE2	7:J:221:HOH:O	1.90	0.86
1:K:322:THR:OG1	7:K:720:HOH:O	1.93	0.86
1:A:114:VAL:C	7:A:922:HOH:O	2.18	0.86
1:A:159:LYS:HZ2	1:A:199:GLN:HG3	1.38	0.86
1:K:237:TRP:CD1	7:K:724:HOH:O	2.27	0.86
2:F:125:GLN:N	7:F:209:HOH:O	2.09	0.86
2:J:83:LYS:O	7:J:213:HOH:O	1.94	0.86
7:C:718:HOH:O	3:N:4:SIA:O4	1.93	0.86
1:E:23:ASP:O	7:F:207:HOH:O	1.92	0.85
2:F:149:MET:C	7:F:204:HOH:O	2.19	0.85
2:H:125:GLN:C	7:H:204:HOH:O	2.19	0.85
1:I:27:GLU:HA	7:I:719:HOH:O	1.78	0.84
1:K:106:GLU:OE1	7:K:718:HOH:O	1.95	0.84
1:I:17:ASN:O	7:I:722:HOH:O	1.94	0.84
2:J:125:GLN:OE1	7:J:210:HOH:O	1.94	0.84
1:C:159:LYS:HZ2	1:C:199:GLN:CG	1.90	0.84
7:A:917:HOH:O	2:B:64:THR:O	1.94	0.83
2:J:84:VAL:HA	7:J:213:HOH:O	1.78	0.83
2:J:39:LYS:O	7:J:222:HOH:O	1.96	0.83
1:C:25:VAL:HG21	2:D:102:LEU:HD12	1.60	0.83
1:C:57:HIS:CE1	7:C:720:HOH:O	2.31	0.83
1:E:171:TYR:CE1	7:E:715:HOH:O	2.30	0.83
2:B:74:GLU:OE2	7:B:205:HOH:O	1.94	0.83
1:G:114:VAL:HG11	1:G:117:PHE:HB2	1.61	0.83
1:A:114:VAL:O	7:A:922:HOH:O	1.95	0.82
1:I:159:LYS:HZ2	1:I:199:GLN:HG2	1.44	0.82
1:I:55:PRO:C	7:I:720:HOH:O	2.23	0.82
1:C:114:VAL:HG11	1:C:117:PHE:HB2	1.62	0.82
1:I:266:ASN:N	7:I:718:HOH:O	2.12	0.81
1:A:175:LYS:HE2	7:A:911:HOH:O	1.79	0.81
1:C:107:LEU:O	7:C:714:HOH:O	1.98	0.81
2:J:40:SER:N	7:J:202:HOH:O	2.12	0.81
1:K:158:VAL:O	7:K:722:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:TYR:O	7:C:710:HOH:O	1.99	0.81
1:E:210:SER:O	7:E:705:HOH:O	1.99	0.81
1:I:11:ILE:N	7:I:710:HOH:O	2.01	0.81
1:I:223:ARG:HD2	7:I:721:HOH:O	1.79	0.81
1:C:159:LYS:NZ	1:C:199:GLN:HG2	1.95	0.81
2:H:127:LYS:N	7:H:204:HOH:O	2.02	0.81
2:J:123:ARG:HH12	2:L:123:ARG:NH2	1.77	0.81
2:L:158:ASP:O	2:L:160:PRO:HD3	1.80	0.81
1:I:258:ARG:N	7:I:709:HOH:O	2.13	0.81
2:F:149:MET:CB	7:F:204:HOH:O	2.26	0.80
1:I:31:THR:OG1	7:I:717:HOH:O	1.97	0.80
1:I:114:VAL:HG11	1:I:117:PHE:HB2	1.62	0.80
2:J:148:CYS:O	7:J:208:HOH:O	1.99	0.80
2:L:101:LEU:O	7:L:208:HOH:O	1.97	0.80
2:L:66:VAL:HA	7:L:206:HOH:O	1.81	0.80
2:F:104:ASN:CB	7:F:207:HOH:O	2.27	0.80
1:K:67:ILE:HG13	7:K:725:HOH:O	1.80	0.80
7:K:723:HOH:O	2:L:13:GLY:CA	2.21	0.80
1:I:315:SER:CA	7:I:724:HOH:O	2.29	0.80
1:K:102:ILE:O	7:K:724:HOH:O	2.00	0.80
1:A:159:LYS:HZ2	1:A:199:GLN:CG	1.96	0.79
1:C:159:LYS:HZ2	1:C:199:GLN:HG2	1.47	0.79
1:C:9:LEU:O	7:C:708:HOH:O	2.00	0.79
1:C:78:THR:CG2	1:K:289:LYS:HE3	2.12	0.79
1:I:223:ARG:CD	7:I:721:HOH:O	2.28	0.79
1:A:114:VAL:HG11	1:A:117:PHE:HB2	1.64	0.79
1:I:25:VAL:HG21	2:J:102:LEU:HD12	1.65	0.79
5:K:602:NAG:O6	7:K:726:HOH:O	2.00	0.78
2:J:142:HIS:N	7:J:209:HOH:O	2.14	0.78
3:Q:2:NAG:H83	3:Q:4:SIA:H112	1.65	0.78
2:D:138:PHE:O	7:D:204:HOH:O	2.01	0.78
2:F:150:GLU:N	7:F:204:HOH:O	2.17	0.78
2:J:31:GLY:O	7:J:214:HOH:O	2.01	0.78
1:C:105:GLU:O	7:C:711:HOH:O	2.02	0.78
1:E:114:VAL:HG21	1:E:117:PHE:HB2	1.65	0.77
1:I:106:GLU:HB3	7:I:704:HOH:O	1.82	0.77
1:E:13:TYR:CE2	2:F:6:ILE:HA	2.19	0.77
2:J:142:HIS:CD2	7:J:209:HOH:O	2.36	0.77
1:E:113:SER:O	7:E:717:HOH:O	2.01	0.77
1:E:272:ILE:O	7:E:710:HOH:O	2.02	0.77
2:F:97:GLU:OE2	7:F:208:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:SER:OG	7:C:719:HOH:O	2.01	0.77
2:F:71:ASN:O	7:F:211:HOH:O	2.03	0.77
2:H:126:LEU:N	7:H:204:HOH:O	2.18	0.77
1:K:13:TYR:CD1	7:K:723:HOH:O	2.37	0.77
1:I:318:LEU:HD21	7:J:221:HOH:O	1.84	0.77
1:K:114:VAL:HG21	1:K:117:PHE:HB2	1.66	0.77
1:G:66:TRP:HE1	1:G:77:SER:CB	1.98	0.77
1:K:11:ILE:CD1	2:L:119:TYR:HA	2.14	0.77
5:C:602:NAG:H83	7:C:713:HOH:O	1.84	0.76
1:G:172:ILE:HA	7:G:516:HOH:O	1.84	0.76
2:F:104:ASN:CG	7:F:207:HOH:O	2.23	0.76
2:H:126:LEU:CA	7:H:204:HOH:O	2.32	0.76
1:K:250:ALA:O	7:K:715:HOH:O	2.02	0.76
1:C:78:THR:HG21	1:K:289:LYS:CE	2.13	0.75
1:I:318:LEU:HD23	7:J:221:HOH:O	1.82	0.75
1:C:198:TYR:O	1:C:199:GLN:HB2	1.85	0.75
1:I:159:LYS:NZ	1:I:199:GLN:HG2	2.01	0.75
1:E:9:LEU:HA	7:F:206:HOH:O	1.85	0.75
1:I:24:THR:HG22	2:J:104:ASN:HB3	1.67	0.75
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.52	0.74
7:E:714:HOH:O	2:F:101:LEU:O	2.05	0.74
1:I:221:ALA:O	7:I:721:HOH:O	2.03	0.74
1:I:9:LEU:HB2	2:J:149:MET:SD	2.28	0.74
1:K:305:THR:CG2	7:K:717:HOH:O	2.35	0.74
2:L:67:GLY:N	7:L:206:HOH:O	2.00	0.74
2:J:31:GLY:C	7:J:214:HOH:O	2.30	0.74
2:L:30:GLN:HE22	2:L:145:ASP:HB2	1.53	0.74
2:J:6:ILE:C	7:J:211:HOH:O	2.23	0.74
2:J:157:TYR:CE2	7:J:219:HOH:O	2.40	0.74
1:I:26:LEU:HD22	2:J:105:GLU:CD	2.12	0.74
1:K:66:TRP:HE1	1:K:77:SER:HB2	1.52	0.74
1:C:56:LEU:HD12	1:C:76:LEU:HD11	1.62	0.74
2:F:30:GLN:HE22	2:F:145:ASP:HB2	1.53	0.73
1:K:25:VAL:CG2	7:L:208:HOH:O	2.34	0.73
1:E:85:ILE:O	7:E:710:HOH:O	2.06	0.73
1:C:11:ILE:HD11	2:D:122:VAL:HG21	1.69	0.73
2:B:13:GLY:HA2	7:B:204:HOH:O	1.87	0.73
2:H:127:LYS:HD2	7:H:204:HOH:O	1.88	0.73
1:I:7:ASP:OD2	7:I:715:HOH:O	2.05	0.73
1:K:198:TYR:O	1:K:199:GLN:HB2	1.88	0.73
1:I:105:GLU:OE2	2:J:71:ASN:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:LYS:HZ2	1:K:199:GLN:HE21	1.37	0.72
1:K:25:VAL:HG21	2:L:102:LEU:HD12	1.71	0.72
1:E:102:ILE:HG13	1:E:236:TYR:CE2	2.25	0.72
1:E:159:LYS:NZ	1:E:199:GLN:HG2	2.04	0.72
2:B:12:GLY:O	7:B:204:HOH:O	2.07	0.72
2:D:30:GLN:HE22	2:D:145:ASP:HB2	1.54	0.72
1:C:102:ILE:HG13	1:C:236:TYR:CE2	2.25	0.72
2:J:123:ARG:NH1	2:L:123:ARG:NH2	2.38	0.72
2:J:30:GLN:HE22	2:J:145:ASP:HB2	1.53	0.72
2:J:73:LEU:O	7:K:718:HOH:O	2.08	0.72
1:C:162:ASN:ND2	1:C:199:GLN:NE2	2.36	0.71
1:I:7:ASP:HA	2:J:27:GLN:O	1.91	0.71
1:K:102:ILE:HG13	1:K:236:TYR:CE2	2.26	0.71
1:K:312:TYR:CG	7:K:721:HOH:O	2.37	0.71
2:H:123:ARG:HD2	2:H:132:GLU:OE1	1.90	0.71
1:I:14:HIS:HB2	2:J:20:GLY:O	1.90	0.71
1:K:67:ILE:C	7:K:725:HOH:O	2.22	0.71
1:G:223:ARG:HG3	1:I:206:PHE:HZ	1.56	0.71
1:G:224:PRO:HG2	1:I:209:SER:HA	1.72	0.71
1:A:12:GLY:N	2:B:14:TRP:CH2	2.59	0.71
2:H:30:GLN:HE22	2:H:145:ASP:HB2	1.53	0.71
1:I:102:ILE:HG13	1:I:236:TYR:CE2	2.26	0.71
2:L:123:ARG:HD2	2:L:132:GLU:OE1	1.91	0.71
1:A:12:GLY:O	7:A:915:HOH:O	2.09	0.71
1:C:159:LYS:HD2	1:C:199:GLN:HG3	1.71	0.70
1:K:167:LEU:CB	7:K:715:HOH:O	2.29	0.70
1:C:110:GLN:CB	7:C:714:HOH:O	2.00	0.70
1:G:311:LYS:HG2	2:H:92:TRP:CE2	2.26	0.70
1:I:11:ILE:HG12	2:J:24:TYR:HD2	1.54	0.70
2:F:123:ARG:HD2	2:F:132:GLU:OE1	1.90	0.70
1:I:10:CYS:O	2:J:24:TYR:HA	1.90	0.70
1:I:7:ASP:HA	2:J:28:ASN:HA	1.72	0.70
1:E:66:TRP:HE1	1:E:77:SER:HB3	1.57	0.70
2:J:123:ARG:HD2	2:J:132:GLU:OE1	1.91	0.70
1:A:102:ILE:HG13	1:A:236:TYR:CE2	2.26	0.70
1:C:106:GLU:O	7:C:711:HOH:O	2.10	0.70
2:B:123:ARG:HD2	2:B:132:GLU:OE1	1.91	0.70
1:E:8:THR:O	7:E:709:HOH:O	2.10	0.70
1:G:327:ILE:HG23	1:G:328:PRO:HD2	1.73	0.70
1:I:266:ASN:CA	7:I:718:HOH:O	2.40	0.69
2:D:123:ARG:HD2	2:D:132:GLU:OE1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:VAL:HG21	2:F:102:LEU:HD12	1.74	0.69
1:E:21:THR:CG2	1:E:29:ASN:OD1	2.40	0.69
1:I:10:CYS:HA	7:I:712:HOH:O	1.91	0.69
1:I:223:ARG:N	7:I:721:HOH:O	2.19	0.69
2:J:11:GLU:O	7:J:217:HOH:O	2.10	0.69
1:K:311:LYS:HG2	2:L:92:TRP:CE2	2.27	0.69
1:E:166:LYS:O	7:E:718:HOH:O	2.11	0.69
1:I:324:LEU:HD21	2:J:21:TRP:CD1	2.27	0.69
1:C:143:PRO:HD2	5:C:602:NAG:H83	1.73	0.69
1:E:66:TRP:HE1	1:E:77:SER:CB	2.05	0.69
1:A:228:GLU:OE2	7:A:921:HOH:O	2.09	0.69
7:A:915:HOH:O	2:B:23:GLY:O	2.10	0.69
1:C:109:GLU:HB3	7:C:711:HOH:O	1.92	0.69
1:I:28:LYS:N	7:I:719:HOH:O	1.86	0.69
1:G:327:ILE:CG2	1:G:328:PRO:HD2	2.23	0.69
1:K:67:ILE:CB	7:K:725:HOH:O	2.41	0.69
2:L:66:VAL:CA	7:L:206:HOH:O	2.38	0.68
1:G:269:SER:C	7:G:515:HOH:O	2.35	0.68
1:E:171:TYR:HE1	7:E:715:HOH:O	1.73	0.68
1:G:102:ILE:HG13	1:G:236:TYR:CE2	2.28	0.68
1:A:7:ASP:N	7:A:907:HOH:O	2.26	0.68
1:C:9:LEU:C	7:C:708:HOH:O	2.37	0.68
1:I:58:LEU:HD11	1:I:63:ILE:HD13	1.76	0.68
2:J:129:ASN:HB2	7:J:219:HOH:O	1.93	0.67
1:K:58:LEU:HD11	1:K:63:ILE:HD13	1.76	0.67
1:C:305:THR:H	2:D:66:VAL:HG13	1.59	0.67
1:I:74:GLU:OE2	1:I:152:LYS:HE3	1.94	0.67
1:E:24:THR:HB	7:E:714:HOH:O	1.95	0.67
1:C:110:GLN:CA	7:C:714:HOH:O	2.37	0.67
2:J:4:GLY:N	7:J:215:HOH:O	2.27	0.67
1:C:10:CYS:HA	7:C:708:HOH:O	1.93	0.67
2:F:135:ASN:CB	7:F:205:HOH:O	2.33	0.67
1:I:13:TYR:HA	2:J:21:TRP:O	1.94	0.67
1:G:269:SER:N	7:G:515:HOH:O	2.11	0.67
2:B:51:LYS:HG3	1:E:25:VAL:HG12	1.75	0.67
1:C:58:LEU:HD11	1:C:63:ILE:HD13	1.76	0.67
1:E:58:LEU:HD11	1:E:63:ILE:HD13	1.76	0.67
1:A:44:ASN:HD21	1:A:291:ALA:H	1.43	0.66
1:A:162:ASN:ND2	1:A:199:GLN:NE2	2.42	0.66
1:G:66:TRP:HE1	1:G:77:SER:HB2	1.59	0.66
1:K:305:THR:HG23	7:K:717:HOH:O	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ILE:O	2:F:10:ILE:HD13	1.94	0.66
1:G:92:ASP:CA	7:G:512:HOH:O	2.31	0.66
1:K:34:HIS:HB3	7:K:720:HOH:O	1.94	0.66
1:C:201:ALA:O	7:C:709:HOH:O	2.13	0.66
2:J:37:ASP:C	7:J:202:HOH:O	2.37	0.66
1:E:24:THR:CB	7:E:714:HOH:O	2.40	0.66
1:K:10:CYS:HA	2:L:137:CYS:HA	1.78	0.66
1:K:25:VAL:HG23	7:L:208:HOH:O	1.95	0.66
2:J:123:ARG:HH12	2:L:123:ARG:HH22	1.43	0.66
1:G:26:LEU:HB3	2:J:47:GLU:HB3	1.76	0.66
1:C:260:ALA:HA	7:C:710:HOH:O	1.96	0.66
1:A:159:LYS:CD	1:A:199:GLN:HG3	2.25	0.65
1:E:44:ASN:HD21	1:E:291:ALA:H	1.44	0.65
5:C:602:NAG:C8	7:C:713:HOH:O	2.40	0.65
2:F:121:LYS:O	7:F:209:HOH:O	2.14	0.65
1:A:223:ARG:HG3	1:C:206:PHE:HZ	1.62	0.65
2:D:159:TYR:CG	2:D:159:TYR:O	2.49	0.65
1:I:315:SER:HA	7:I:724:HOH:O	1.92	0.65
2:J:28:ASN:H	2:J:28:ASN:HD22	1.44	0.65
1:A:224:PRO:HG2	1:C:209:SER:HA	1.79	0.65
1:G:269:SER:CA	7:G:515:HOH:O	2.42	0.65
1:C:170:SER:OG	1:G:264:GLU:OE1	2.09	0.65
1:I:305:THR:H	2:J:66:VAL:HG13	1.60	0.65
1:G:44:ASN:HD21	1:G:291:ALA:H	1.43	0.65
1:G:313:VAL:HG13	2:H:93:THR:HA	1.79	0.65
2:H:18:VAL:O	7:H:206:HOH:O	2.15	0.65
1:I:49:LYS:O	7:I:714:HOH:O	2.14	0.65
2:F:28:ASN:HD22	2:F:28:ASN:H	1.45	0.65
2:D:28:ASN:HD22	2:D:28:ASN:H	1.45	0.64
1:G:312:TYR:CD2	2:H:89:LEU:HD13	2.31	0.64
1:K:188:PRO:HG2	1:K:194:GLN:NE2	2.12	0.64
1:A:159:LYS:NZ	1:A:199:GLN:HG3	2.12	0.64
1:C:32:VAL:O	7:C:717:HOH:O	2.15	0.64
2:D:81:ASN:O	2:D:84:VAL:HG12	1.97	0.64
1:I:230:GLU:O	7:I:721:HOH:O	2.15	0.64
2:F:158:ASP:O	2:F:160:PRO:HD3	1.98	0.64
2:H:28:ASN:H	2:H:28:ASN:HD22	1.45	0.64
7:I:715:HOH:O	2:J:29:GLU:HG3	1.96	0.64
1:C:202:ASP:HA	7:C:709:HOH:O	1.97	0.64
1:E:21:THR:HG21	1:E:29:ASN:OD1	1.97	0.64
1:E:311:LYS:HG2	2:F:92:TRP:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:ASN:HD21	1:I:291:ALA:H	1.45	0.64
1:K:8:THR:HG22	2:L:139:GLU:HA	1.79	0.64
1:E:13:TYR:CD2	2:F:6:ILE:HG12	2.33	0.64
2:B:28:ASN:HD22	2:B:28:ASN:H	1.45	0.64
1:C:31:THR:CG2	7:C:717:HOH:O	2.18	0.64
2:B:81:ASN:O	2:B:84:VAL:HG12	1.98	0.64
2:H:159:TYR:N	2:H:160:PRO:HD3	2.13	0.63
1:G:269:SER:O	7:G:515:HOH:O	2.15	0.63
1:K:44:ASN:HD21	1:K:291:ALA:H	1.46	0.63
1:G:188:PRO:HG2	1:G:194:GLN:NE2	2.13	0.63
1:I:11:ILE:HD11	2:J:122:VAL:HG21	1.79	0.63
1:C:44:ASN:HD21	1:C:291:ALA:H	1.46	0.63
2:H:81:ASN:O	2:H:84:VAL:HG12	1.99	0.63
1:C:188:PRO:HG2	1:C:194:GLN:NE2	2.12	0.63
2:L:28:ASN:H	2:L:28:ASN:HD22	1.45	0.63
1:C:51:ARG:HH22	5:K:601:NAG:H62	1.64	0.63
1:G:92:ASP:O	7:G:512:HOH:O	2.16	0.63
1:G:198:TYR:O	1:G:199:GLN:HB2	1.99	0.63
2:J:11:GLU:C	7:J:217:HOH:O	2.39	0.63
2:L:81:ASN:O	2:L:84:VAL:HG12	1.99	0.63
1:E:159:LYS:HZ2	1:E:199:GLN:CG	2.11	0.62
1:E:188:PRO:HG2	1:E:194:GLN:NE2	2.14	0.62
1:I:27:GLU:CA	7:I:719:HOH:O	2.38	0.62
1:I:305:THR:HG22	2:J:66:VAL:CG1	2.29	0.62
2:F:81:ASN:O	2:F:84:VAL:HG12	1.98	0.62
1:G:10:CYS:HA	2:H:137:CYS:HA	1.81	0.62
1:K:305:THR:H	2:L:66:VAL:HG13	1.62	0.62
2:J:81:ASN:O	2:J:84:VAL:HG12	1.98	0.62
2:L:101:LEU:CA	7:L:208:HOH:O	2.41	0.62
1:A:188:PRO:HG2	1:A:194:GLN:NE2	2.14	0.62
2:B:161:LYS:HG2	2:B:162:TYR:H	1.65	0.62
1:I:188:PRO:HG2	1:I:194:GLN:NE2	2.14	0.62
2:H:18:VAL:CA	7:H:206:HOH:O	2.48	0.62
1:I:105:GLU:CD	2:J:71:ASN:HB3	2.25	0.62
1:I:10:CYS:HA	7:I:710:HOH:O	1.82	0.61
1:I:106:GLU:CG	7:I:713:HOH:O	2.46	0.61
1:I:159:LYS:HZ2	1:I:199:GLN:CG	2.13	0.61
1:K:132:HIS:HB3	7:K:722:HOH:O	2.00	0.61
1:K:13:TYR:CE2	2:L:6:ILE:HA	2.35	0.61
1:C:51:ARG:HH22	5:K:601:NAG:C6	2.12	0.61
1:C:245:LYS:NZ	1:G:264:GLU:OE2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:TRP:HE1	1:K:77:SER:CB	2.12	0.61
1:K:9:LEU:CD1	2:L:152:VAL:HG11	2.30	0.61
1:A:159:LYS:HD2	1:A:199:GLN:HG3	1.81	0.61
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.81	0.61
2:L:43:ASN:ND2	7:L:203:HOH:O	2.33	0.61
1:G:25:VAL:HG12	2:J:51:LYS:HA	1.81	0.61
1:G:50:LEU:HD11	1:G:306:ILE:HG22	1.83	0.61
2:H:40:SER:HA	7:H:205:HOH:O	2.01	0.61
1:C:72:GLU:HG2	5:C:602:NAG:H82	1.82	0.60
2:F:133:ILE:HB	7:F:205:HOH:O	2.01	0.60
1:I:266:ASN:CB	7:I:718:HOH:O	2.48	0.60
1:A:327:ILE:HG23	1:A:328:PRO:HD2	1.83	0.60
1:C:50:LEU:HD11	1:C:306:ILE:HG22	1.84	0.60
1:C:78:THR:HG22	1:C:78:THR:O	1.99	0.60
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.83	0.60
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.83	0.60
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.83	0.60
1:A:135:ASN:N	7:A:914:HOH:O	2.34	0.60
1:C:225:LYS:HE2	1:C:230:GLU:HG3	1.83	0.60
2:J:84:VAL:O	7:J:213:HOH:O	2.13	0.60
2:J:157:TYR:HE2	7:J:219:HOH:O	1.79	0.60
2:L:126:LEU:O	7:L:207:HOH:O	2.16	0.60
2:H:18:VAL:HA	7:H:206:HOH:O	2.02	0.60
2:F:158:ASP:C	2:F:160:PRO:HD3	2.27	0.60
1:C:109:GLU:CB	7:C:711:HOH:O	2.48	0.60
1:K:313:VAL:HG13	2:L:93:THR:HA	1.84	0.60
1:C:51:ARG:NH2	5:K:601:NAG:C6	2.65	0.59
2:H:18:VAL:C	7:H:206:HOH:O	2.44	0.59
1:I:312:TYR:CD2	2:J:89:LEU:HD13	2.36	0.59
7:I:715:HOH:O	2:J:29:GLU:CG	2.50	0.59
2:H:51:LYS:HG3	1:K:25:VAL:HG12	1.82	0.59
1:I:10:CYS:O	2:J:24:TYR:CA	2.50	0.59
1:I:266:ASN:HB3	7:I:718:HOH:O	2.01	0.59
1:K:167:LEU:N	7:K:715:HOH:O	2.05	0.59
1:E:198:TYR:O	1:E:199:GLN:HB2	2.01	0.59
1:G:159:LYS:HZ2	1:G:199:GLN:HG2	1.68	0.59
2:J:123:ARG:NH1	2:L:123:ARG:HH22	1.99	0.59
1:I:71:PRO:O	1:I:74:GLU:HG3	2.03	0.59
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.83	0.59
1:I:106:GLU:N	7:I:713:HOH:O	2.04	0.59
1:I:295:SER:N	7:I:716:HOH:O	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:ASN:ND2	7:D:205:HOH:O	2.28	0.59
7:E:712:HOH:O	4:O:2:NAG:O4	2.15	0.58
2:F:19:ASP:HB2	2:F:36:ALA:HB3	1.85	0.58
1:A:311:LYS:HG2	2:B:92:TRP:CE2	2.38	0.58
1:A:7:ASP:HA	2:B:27:GLN:O	2.03	0.58
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.85	0.58
1:C:172:ILE:HD13	1:G:266:ASN:HB3	1.85	0.58
2:H:160:PRO:HD2	2:H:161:LYS:HG3	1.84	0.58
2:D:19:ASP:HB2	2:D:36:ALA:HB3	1.85	0.58
1:G:206:PHE:HZ	1:K:223:ARG:HG3	1.67	0.58
1:C:14:HIS:N	2:D:21:TRP:O	2.37	0.58
1:A:50:LEU:HD11	1:A:306:ILE:HG22	1.85	0.58
1:G:58:LEU:HD21	1:G:63:ILE:HD13	1.85	0.58
1:I:13:TYR:CA	2:J:21:TRP:O	2.52	0.58
1:A:164:TYR:HD2	7:A:919:HOH:O	1.73	0.58
1:C:11:ILE:HG12	2:D:24:TYR:CD2	2.38	0.58
1:E:87:GLU:O	1:E:273:ILE:HA	2.04	0.58
2:F:70:PHE:C	7:F:211:HOH:O	2.47	0.58
2:J:5:ALA:N	7:J:215:HOH:O	2.35	0.58
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.84	0.58
2:F:70:PHE:O	7:F:211:HOH:O	2.17	0.58
1:I:10:CYS:O	2:J:24:TYR:HB3	2.04	0.57
2:L:19:ASP:HB2	2:L:36:ALA:HB3	1.85	0.57
1:A:58:LEU:HD21	1:A:63:ILE:HD13	1.85	0.57
1:K:87:GLU:O	1:K:273:ILE:HA	2.04	0.57
1:C:24:THR:HG22	2:D:104:ASN:HB3	1.84	0.57
1:E:9:LEU:N	2:F:138:PHE:O	2.35	0.57
1:G:44:ASN:ND2	1:G:291:ALA:H	2.02	0.57
2:H:19:ASP:HB2	2:H:36:ALA:HB3	1.86	0.57
1:C:87:GLU:O	1:C:273:ILE:HA	2.04	0.57
2:J:19:ASP:HB2	2:J:36:ALA:HB3	1.86	0.57
1:K:132:HIS:CB	7:K:722:HOH:O	2.44	0.57
2:D:3:PHE:HB2	7:D:202:HOH:O	2.04	0.57
1:I:50:LEU:HD11	1:I:306:ILE:HG22	1.84	0.57
1:A:327:ILE:HG22	1:A:328:PRO:N	2.19	0.57
1:A:11:ILE:C	2:B:14:TRP:CH2	2.82	0.57
1:A:51:ARG:HB3	1:A:51:ARG:NH1	2.20	0.57
1:I:315:SER:HB3	7:I:724:HOH:O	2.04	0.57
2:H:40:SER:O	7:H:205:HOH:O	2.18	0.57
2:F:24:TYR:CD1	2:F:153:LYS:HE3	2.40	0.56
1:K:67:ILE:CG1	7:K:725:HOH:O	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:CD2	2:B:89:LEU:HD13	2.40	0.56
1:K:188:PRO:HG2	1:K:194:GLN:HE21	1.70	0.56
1:A:44:ASN:ND2	1:A:291:ALA:H	2.03	0.56
1:A:162:ASN:CG	1:A:199:GLN:NE2	2.63	0.56
1:E:164:TYR:CZ	1:E:252:GLY:HA2	2.40	0.56
1:G:87:GLU:O	1:G:273:ILE:HA	2.04	0.56
1:I:54:ALA:O	7:I:720:HOH:O	2.17	0.56
2:L:66:VAL:HG23	7:L:206:HOH:O	2.04	0.56
1:A:87:GLU:O	1:A:273:ILE:HA	2.04	0.56
1:A:137:GLY:HA3	1:A:156:TRP:HB3	1.88	0.56
1:A:327:ILE:CG2	1:A:328:PRO:HD2	2.36	0.56
1:E:225:LYS:HE2	1:E:230:GLU:HG3	1.86	0.56
2:H:24:TYR:CD1	2:H:153:LYS:HE3	2.40	0.56
1:I:8:THR:HG1	2:J:27:GLN:HB3	1.68	0.56
1:I:11:ILE:HD11	2:J:24:TYR:HE2	1.70	0.56
2:L:24:TYR:CD1	2:L:153:LYS:HE3	2.40	0.56
3:N:4:SIA:O1A	3:N:4:SIA:H6	2.05	0.56
2:B:24:TYR:CD1	2:B:153:LYS:HE3	2.41	0.56
1:C:162:ASN:HD22	1:C:199:GLN:HE21	1.51	0.56
3:M:4:SIA:H113	3:M:4:SIA:O7	2.06	0.56
1:C:14:HIS:HB2	2:D:21:TRP:HA	1.88	0.56
1:G:137:GLY:HA3	1:G:156:TRP:HB3	1.88	0.56
1:I:11:ILE:CG1	2:J:24:TYR:CD2	2.84	0.56
1:I:87:GLU:O	1:I:273:ILE:HA	2.05	0.56
1:K:25:VAL:HG22	7:L:208:HOH:O	2.01	0.56
1:I:324:LEU:CD2	2:J:21:TRP:CD1	2.89	0.56
3:Q:2:NAG:H83	3:Q:4:SIA:C11	2.34	0.56
2:D:159:TYR:N	2:D:160:PRO:CD	2.69	0.56
1:I:315:SER:CB	7:I:724:HOH:O	2.54	0.56
1:C:311:LYS:HG2	2:D:92:TRP:CE2	2.41	0.56
1:I:225:LYS:HE2	1:I:230:GLU:HG3	1.87	0.56
1:K:11:ILE:HD11	2:L:122:VAL:CG1	2.36	0.56
1:C:25:VAL:CG2	2:D:102:LEU:HD12	2.34	0.55
1:I:11:ILE:HA	2:J:23:GLY:O	2.07	0.55
1:K:34:HIS:CE1	2:L:21:TRP:HE1	2.24	0.55
1:E:161:GLY:O	1:E:162:ASN:HB2	2.05	0.55
2:J:94:TYR:CE1	2:L:59:MET:HB2	2.41	0.55
1:K:312:TYR:CD2	2:L:89:LEU:HD13	2.41	0.55
1:A:164:TYR:CZ	1:A:252:GLY:HA2	2.42	0.55
7:I:712:HOH:O	2:J:137:CYS:HA	2.06	0.55
1:A:159:LYS:NZ	1:A:199:GLN:CG	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LYS:CD	1:C:199:GLN:CG	2.84	0.55
1:G:49:LYS:HB3	7:G:508:HOH:O	2.07	0.55
2:H:97:GLU:HB3	2:J:58:LYS:HD2	1.88	0.55
2:J:40:SER:HA	7:J:222:HOH:O	2.05	0.55
1:C:110:GLN:C	7:C:714:HOH:O	2.50	0.55
1:C:164:TYR:CZ	1:C:252:GLY:HA2	2.42	0.55
2:F:135:ASN:N	7:F:205:HOH:O	2.30	0.55
1:I:44:ASN:ND2	1:I:291:ALA:H	2.05	0.55
1:A:266:ASN:H	1:A:266:ASN:ND2	2.05	0.55
1:C:188:PRO:HG2	1:C:194:GLN:HE21	1.71	0.55
1:E:137:GLY:HA3	1:E:156:TRP:HB3	1.89	0.55
1:I:225:LYS:NZ	3:R:3:GAL:O3	2.40	0.55
2:L:158:ASP:C	2:L:160:PRO:HD3	2.31	0.55
2:B:51:LYS:HG3	1:E:25:VAL:CG1	2.36	0.54
1:C:159:LYS:CD	1:C:199:GLN:HG3	2.36	0.54
2:D:3:PHE:CB	7:D:202:HOH:O	2.43	0.54
1:K:13:TYR:CD2	2:L:6:ILE:HG12	2.42	0.54
1:A:114:VAL:CA	7:A:922:HOH:O	2.35	0.54
1:E:8:THR:HG22	2:F:139:GLU:HA	1.88	0.54
1:G:188:PRO:HG2	1:G:194:GLN:HE21	1.71	0.54
1:C:14:HIS:HB2	2:D:20:GLY:O	2.08	0.54
1:C:25:VAL:HG12	2:F:51:LYS:HG3	1.89	0.54
1:C:168:SER:HB3	1:G:176:GLY:HA2	1.88	0.54
2:F:9:PHE:CD1	2:F:10:ILE:HG13	2.42	0.54
1:I:25:VAL:CG2	2:J:102:LEU:HD12	2.37	0.54
1:K:164:TYR:CZ	1:K:252:GLY:HA2	2.42	0.54
1:C:266:ASN:ND2	1:C:266:ASN:H	2.05	0.54
1:C:312:TYR:CD2	2:D:89:LEU:HD13	2.42	0.54
7:E:709:HOH:O	2:F:27:GLN:HB3	2.08	0.54
2:J:159:TYR:N	2:J:160:PRO:CD	2.70	0.54
1:I:189:SER:HB2	1:I:222:ILE:HD13	1.90	0.54
1:C:8:THR:OG1	2:D:27:GLN:HB3	2.06	0.54
1:G:164:TYR:CZ	1:G:252:GLY:HA2	2.43	0.54
1:A:9:LEU:HD11	2:B:24:TYR:HB3	1.90	0.54
1:E:44:ASN:ND2	1:E:291:ALA:H	2.04	0.54
1:G:266:ASN:H	1:G:266:ASN:ND2	2.06	0.54
1:I:26:LEU:HD22	2:J:105:GLU:OE2	2.07	0.54
1:K:137:GLY:HA3	1:K:156:TRP:HB3	1.89	0.54
1:K:297:PRO:HG3	2:L:56:ILE:HA	1.89	0.54
1:A:167:LEU:HD12	1:A:167:LEU:C	2.33	0.54
1:C:57:HIS:CD2	7:C:720:HOH:O	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:SER:HB2	1:G:222:ILE:HD13	1.90	0.54
1:I:266:ASN:H	1:I:266:ASN:ND2	2.06	0.54
1:A:188:PRO:HG2	1:A:194:GLN:HE21	1.72	0.54
1:E:266:ASN:ND2	1:E:266:ASN:H	2.05	0.54
1:K:141:ALA:C	1:K:143:PRO:HD3	2.33	0.54
2:B:91:ILE:HG21	2:F:91:ILE:HD13	1.89	0.54
7:C:718:HOH:O	3:N:2:NAG:C8	2.55	0.54
1:G:92:ASP:C	7:G:512:HOH:O	2.48	0.54
1:I:137:GLY:HA3	1:I:156:TRP:HB3	1.88	0.54
3:Q:4:SIA:O1A	3:Q:4:SIA:H6	2.06	0.54
1:I:14:HIS:N	2:J:21:TRP:O	2.42	0.53
2:D:59:MET:HE1	2:D:92:TRP:CH2	2.43	0.53
1:K:323:GLY:O	2:L:111:HIS:CD2	2.62	0.53
1:C:305:THR:HG22	2:D:66:VAL:CG1	2.38	0.53
1:E:7:ASP:O	2:F:140:PHE:N	2.38	0.53
1:K:60:LYS:HD2	5:K:602:NAG:C8	2.33	0.53
1:K:189:SER:HB2	1:K:222:ILE:HD13	1.89	0.53
1:K:160:LYS:HD2	7:K:719:HOH:O	2.08	0.53
2:L:9:PHE:CD1	2:L:10:ILE:HG13	2.44	0.53
1:C:137:GLY:HA3	1:C:156:TRP:HB3	1.90	0.53
1:C:167:LEU:C	1:C:167:LEU:HD12	2.33	0.53
1:E:313:VAL:HG13	2:F:93:THR:HA	1.91	0.53
1:G:141:ALA:C	1:G:143:PRO:HD3	2.34	0.53
1:G:167:LEU:C	1:G:167:LEU:HD12	2.33	0.53
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.44	0.53
1:E:50:LEU:HD21	1:E:306:ILE:HG22	1.91	0.53
1:I:11:ILE:HD13	2:J:118:LEU:HG	1.91	0.53
1:K:266:ASN:H	1:K:266:ASN:ND2	2.07	0.53
1:K:305:THR:HG21	7:K:717:HOH:O	2.01	0.53
1:C:203:THR:N	7:C:709:HOH:O	2.35	0.53
1:G:293:ASN:OD1	1:G:293:ASN:C	2.50	0.53
1:G:307:GLY:HA2	2:H:63:PHE:CE1	2.44	0.53
2:H:59:MET:HE1	2:H:92:TRP:CH2	2.43	0.53
1:K:44:ASN:ND2	1:K:291:ALA:H	2.06	0.53
1:A:141:ALA:C	1:A:143:PRO:HD3	2.34	0.53
1:E:188:PRO:HG2	1:E:194:GLN:HE21	1.71	0.53
1:K:60:LYS:CG	5:K:602:NAG:O7	2.57	0.53
1:C:26:LEU:HD22	2:D:105:GLU:CD	2.34	0.53
1:I:106:GLU:HG2	7:I:713:HOH:O	2.09	0.53
1:A:189:SER:HB2	1:A:222:ILE:HD13	1.90	0.52
2:B:59:MET:HE1	2:B:92:TRP:CH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:TYR:CZ	1:I:252:GLY:HA2	2.43	0.52
2:B:47:GLU:HB3	1:E:26:LEU:HB3	1.90	0.52
1:C:51:ARG:NH1	1:C:51:ARG:HB3	2.25	0.52
1:I:167:LEU:HD12	1:I:167:LEU:C	2.34	0.52
2:J:4:GLY:C	7:J:215:HOH:O	2.52	0.52
1:C:44:ASN:ND2	1:C:291:ALA:H	2.06	0.52
2:H:79:ASN:CB	2:J:68:LYS:HE3	2.39	0.52
1:I:198:TYR:O	1:I:199:GLN:HB2	2.10	0.52
2:J:59:MET:HE1	2:J:92:TRP:CH2	2.44	0.52
2:J:112:ASP:OD1	7:J:215:HOH:O	2.19	0.52
1:K:11:ILE:HD11	2:L:122:VAL:HG13	1.91	0.52
1:K:14:HIS:HB2	2:L:21:TRP:HA	1.91	0.52
1:K:66:TRP:NE1	1:K:77:SER:HB2	2.22	0.52
1:K:67:ILE:HB	7:K:725:HOH:O	2.08	0.52
1:A:77:SER:O	1:A:79:ALA:N	2.39	0.52
1:G:223:ARG:HG3	1:I:206:PHE:CZ	2.41	0.52
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.45	0.52
1:G:107:LEU:HD22	1:G:111:LEU:HD22	1.91	0.52
1:I:311:LYS:HG2	2:J:92:TRP:CE2	2.44	0.52
1:K:51:ARG:HB3	1:K:51:ARG:NH1	2.25	0.52
2:L:59:MET:HE1	2:L:92:TRP:CH2	2.44	0.52
1:E:43:HIS:HB3	1:E:301:ILE:HD13	1.92	0.52
1:I:51:ARG:HB3	1:I:51:ARG:NH1	2.24	0.52
1:I:141:ALA:C	1:I:143:PRO:HD3	2.35	0.52
1:C:189:SER:HB2	1:C:222:ILE:HD13	1.91	0.52
1:C:307:GLY:HA2	2:D:63:PHE:CE1	2.45	0.52
1:A:129:TRP:O	7:A:903:HOH:O	2.19	0.52
1:E:8:THR:HA	2:F:138:PHE:O	2.09	0.52
1:E:47:LEU:HD22	1:E:276:THR:O	2.10	0.52
2:F:59:MET:HE1	2:F:92:TRP:CH2	2.45	0.52
1:I:25:VAL:HG23	2:J:101:LEU:O	2.10	0.52
1:C:126:THR:CB	1:K:92:ASP:OD1	2.58	0.51
1:E:141:ALA:C	1:E:143:PRO:HD3	2.35	0.51
1:G:51:ARG:NH1	1:G:51:ARG:HB3	2.24	0.51
2:H:9:PHE:CD1	2:H:10:ILE:HG13	2.45	0.51
1:A:107:LEU:HD22	1:A:111:LEU:HD22	1.92	0.51
1:E:13:TYR:CZ	2:F:6:ILE:HG23	2.45	0.51
1:G:12:GLY:HA2	2:H:10:ILE:HG21	1.91	0.51
1:I:312:TYR:HD2	2:J:89:LEU:HD13	1.75	0.51
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.45	0.51
1:K:225:LYS:HE2	1:K:230:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:ARG:HD3	7:I:721:HOH:O	1.99	0.51
1:C:313:VAL:HG13	2:D:93:THR:HA	1.93	0.51
1:I:27:GLU:HG3	7:I:719:HOH:O	2.10	0.51
1:C:43:HIS:HB3	1:C:301:ILE:HD13	1.93	0.51
1:K:47:LEU:HD22	1:K:276:THR:O	2.11	0.51
1:E:312:TYR:CD2	2:F:89:LEU:HD13	2.46	0.51
1:G:25:VAL:CG1	2:J:51:LYS:HG3	2.41	0.51
1:A:129:TRP:HB2	7:A:903:HOH:O	2.09	0.51
1:E:189:SER:HB2	1:E:222:ILE:HD13	1.92	0.51
1:G:327:ILE:HG22	1:G:328:PRO:N	2.26	0.51
1:I:10:CYS:O	2:J:24:TYR:CB	2.59	0.51
1:I:43:HIS:HB3	1:I:301:ILE:HD13	1.93	0.51
1:I:188:PRO:HG2	1:I:194:GLN:HE21	1.73	0.51
3:M:4:SIA:H6	3:M:4:SIA:O1A	2.11	0.51
1:A:198:TYR:O	1:A:199:GLN:HB2	2.09	0.51
7:I:715:HOH:O	2:J:29:GLU:CB	2.59	0.51
1:E:113:SER:HB3	7:E:717:HOH:O	2.09	0.51
1:E:305:THR:H	2:F:66:VAL:HG13	1.75	0.51
1:G:159:LYS:CD	1:G:199:GLN:HG2	2.40	0.51
1:G:167:LEU:HD12	1:G:167:LEU:O	2.11	0.51
2:H:91:ILE:HG21	2:L:91:ILE:HD13	1.93	0.51
2:B:87:GLY:HA3	2:D:88:PHE:CZ	2.46	0.50
1:C:141:ALA:C	1:C:143:PRO:HD3	2.35	0.50
7:C:712:HOH:O	2:F:47:GLU:HA	2.10	0.50
1:A:175:LYS:HB3	7:A:902:HOH:O	2.11	0.50
1:E:51:ARG:NH1	1:E:51:ARG:HB3	2.25	0.50
1:G:312:TYR:HD2	2:H:89:LEU:HD13	1.75	0.50
2:J:159:TYR:O	2:J:161:LYS:N	2.44	0.50
1:C:198:TYR:CZ	1:C:253:ASN:HA	2.46	0.50
1:K:50:LEU:HD21	1:K:306:ILE:HG22	1.92	0.50
1:K:312:TYR:C	7:K:721:HOH:O	2.28	0.50
1:K:324:LEU:HB3	2:L:111:HIS:CB	2.41	0.50
1:A:161:GLY:O	1:A:162:ASN:HB2	2.10	0.50
1:C:7:ASP:HA	2:D:27:GLN:O	2.11	0.50
2:D:4:GLY:O	2:D:8:GLY:HA3	2.12	0.50
2:J:11:GLU:CB	7:J:217:HOH:O	2.52	0.50
2:J:128:ASN:O	7:J:220:HOH:O	2.19	0.50
3:P:4:SIA:H6	3:P:4:SIA:O1A	2.11	0.50
2:B:91:ILE:HD13	2:D:91:ILE:HG21	1.94	0.49
2:F:135:ASN:CA	7:F:205:HOH:O	2.60	0.49
1:A:190:THR:HG23	1:A:193:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:THR:HG22	2:J:104:ASN:CB	2.41	0.49
1:K:312:TYR:HD2	2:L:89:LEU:HD13	1.77	0.49
1:G:43:HIS:HB3	1:G:301:ILE:HD13	1.94	0.49
1:G:103:ASP:OD2	2:L:73:LEU:HD13	2.11	0.49
2:D:87:GLY:HA3	2:F:88:PHE:CZ	2.48	0.49
1:A:307:GLY:HA2	2:B:63:PHE:CE1	2.47	0.49
7:A:908:HOH:O	3:M:2:NAG:H2	2.12	0.49
2:D:159:TYR:H	2:D:160:PRO:CD	2.26	0.49
1:G:96:CYS:O	1:G:227:ARG:HD3	2.13	0.49
1:I:125:LYS:HD3	1:I:258:ARG:NH1	2.28	0.49
1:K:25:VAL:CG2	2:L:102:LEU:HD12	2.40	0.49
1:G:268:GLY:O	2:H:63:PHE:HE2	1.95	0.49
1:K:43:HIS:HB3	1:K:301:ILE:HD13	1.95	0.49
2:L:123:ARG:HG3	2:L:138:PHE:CZ	2.47	0.49
1:C:125:LYS:HD3	1:C:258:ARG:NH1	2.28	0.49
2:F:123:ARG:HG3	2:F:138:PHE:CZ	2.48	0.49
1:I:96:CYS:O	1:I:227:ARG:HD3	2.13	0.49
2:L:17:MET:SD	2:L:23:GLY:HA3	2.51	0.49
2:D:123:ARG:HG3	2:D:138:PHE:CZ	2.48	0.49
1:K:11:ILE:O	2:L:10:ILE:HD13	2.13	0.49
1:K:132:HIS:O	7:K:716:HOH:O	2.20	0.49
2:D:17:MET:SD	2:D:23:GLY:HA3	2.53	0.49
2:H:123:ARG:HG3	2:H:138:PHE:CZ	2.48	0.49
1:K:96:CYS:O	1:K:227:ARG:HD3	2.13	0.49
1:A:43:HIS:HB3	1:A:301:ILE:HD13	1.94	0.49
1:A:96:CYS:O	1:A:227:ARG:HD3	2.13	0.49
1:C:131:ASN:ND2	1:G:243:GLY:HA3	2.28	0.49
2:H:17:MET:SD	2:H:23:GLY:HA3	2.53	0.49
1:A:103:ASP:OD2	2:F:73:LEU:HD13	2.13	0.48
2:B:59:MET:HE1	2:B:92:TRP:CZ3	2.48	0.48
2:F:17:MET:SD	2:F:23:GLY:HA3	2.53	0.48
1:G:211:ARG:NH2	7:G:505:HOH:O	2.17	0.48
1:A:66:TRP:HE1	1:A:77:SER:HB3	1.78	0.48
1:G:49:LYS:CB	7:G:508:HOH:O	2.61	0.48
1:K:125:LYS:HD3	1:K:258:ARG:NH1	2.28	0.48
1:E:190:THR:HG23	1:E:193:ASP:H	1.78	0.48
1:I:51:ARG:N	7:I:711:HOH:O	1.82	0.48
1:K:28:LYS:HB2	5:K:601:NAG:H82	1.95	0.48
1:K:190:THR:HG23	1:K:193:ASP:H	1.79	0.48
1:K:307:GLY:HA2	2:L:63:PHE:CE1	2.47	0.48
1:C:258:ARG:HE	1:C:259:TYR:HE1	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:MET:HE1	2:H:92:TRP:CZ3	2.48	0.48
2:J:123:ARG:HG3	2:J:138:PHE:CZ	2.48	0.48
3:P:2:NAG:H83	3:P:4:SIA:H112	1.94	0.48
2:B:161:LYS:CG	2:B:162:TYR:H	2.27	0.48
2:B:123:ARG:HG3	2:B:138:PHE:CZ	2.49	0.48
1:E:96:CYS:O	1:E:227:ARG:HD3	2.14	0.48
1:I:167:LEU:HD12	1:I:167:LEU:O	2.13	0.48
1:I:265:ARG:O	7:I:718:HOH:O	2.20	0.48
2:J:17:MET:SD	2:J:23:GLY:HA3	2.53	0.48
1:C:76:LEU:O	1:C:77:SER:C	2.56	0.48
1:G:25:VAL:HG12	2:J:51:LYS:HG3	1.96	0.48
1:I:8:THR:O	2:J:26:HIS:HA	2.14	0.48
1:K:7:ASP:O	2:L:140:PHE:N	2.42	0.48
1:C:96:CYS:O	1:C:227:ARG:HD3	2.14	0.48
7:C:718:HOH:O	3:N:2:NAG:H81	2.13	0.48
1:E:171:TYR:CZ	7:E:715:HOH:O	2.42	0.48
1:G:125:LYS:HD3	1:G:258:ARG:NH1	2.29	0.48
1:I:82:TRP:HB3	7:I:720:HOH:O	2.13	0.48
1:I:258:ARG:HE	1:I:259:TYR:HE1	1.62	0.48
1:E:211:ARG:O	7:E:701:HOH:O	2.20	0.48
2:J:106:ARG:HH11	2:L:106:ARG:NH1	2.12	0.48
1:A:11:ILE:CA	2:B:14:TRP:HH2	2.26	0.48
1:A:258:ARG:HE	1:A:259:TYR:HE1	1.61	0.48
2:B:17:MET:SD	2:B:23:GLY:HA3	2.54	0.48
1:E:125:LYS:HD3	1:E:258:ARG:NH1	2.29	0.48
2:F:124:SER:C	7:F:209:HOH:O	2.54	0.48
1:G:26:LEU:O	2:J:50:ASN:HB3	2.14	0.48
2:J:4:GLY:CA	7:J:215:HOH:O	2.60	0.48
1:E:8:THR:CA	2:F:138:PHE:O	2.62	0.47
2:F:59:MET:HE1	2:F:92:TRP:CZ3	2.49	0.47
2:J:4:GLY:O	2:J:8:GLY:HA3	2.14	0.47
1:A:51:ARG:HB3	1:A:51:ARG:HH11	1.79	0.47
2:B:159:TYR:N	2:B:160:PRO:HD3	2.29	0.47
2:D:59:MET:HE1	2:D:92:TRP:CZ3	2.49	0.47
1:I:313:VAL:HG13	2:J:93:THR:HA	1.95	0.47
1:C:51:ARG:NH2	5:K:601:NAG:H62	2.28	0.47
1:A:167:LEU:HD12	1:A:167:LEU:O	2.13	0.47
1:A:313:VAL:HG13	2:B:93:THR:HA	1.97	0.47
1:C:101:PHE:HB3	1:C:104:TYR:HB2	1.96	0.47
1:C:106:GLU:O	1:C:110:GLN:HG3	2.14	0.47
1:G:155:ILE:HG22	1:G:157:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:THR:HG23	1:G:193:ASP:H	1.78	0.47
1:G:327:ILE:HG22	1:G:328:PRO:CD	2.44	0.47
2:J:59:MET:HE1	2:J:92:TRP:CZ3	2.49	0.47
1:K:14:HIS:N	2:L:21:TRP:O	2.47	0.47
2:L:28:ASN:HD22	2:L:28:ASN:N	2.09	0.47
3:R:4:SIA:H6	3:R:4:SIA:O1A	2.14	0.47
1:E:113:SER:N	7:E:717:HOH:O	2.47	0.47
1:G:258:ARG:HE	1:G:259:TYR:HE1	1.61	0.47
1:C:9:LEU:HD23	2:D:152:VAL:HG11	1.97	0.47
1:C:44:ASN:C	1:C:44:ASN:HD22	2.22	0.47
1:C:131:ASN:HD21	1:G:243:GLY:HA3	1.80	0.47
1:C:167:LEU:HD12	1:C:167:LEU:O	2.14	0.47
1:G:106:GLU:O	1:G:110:GLN:HG3	2.15	0.47
1:I:14:HIS:CE1	2:J:18:VAL:HA	2.50	0.47
1:I:324:LEU:HD21	2:J:21:TRP:CG	2.50	0.47
1:K:106:GLU:O	1:K:110:GLN:HG3	2.15	0.47
1:K:167:LEU:C	1:K:167:LEU:HD23	2.39	0.47
2:L:59:MET:HE1	2:L:92:TRP:CZ3	2.50	0.47
2:H:94:TYR:CE1	2:J:59:MET:HB2	2.50	0.47
1:A:106:GLU:O	1:A:110:GLN:HG3	2.15	0.47
1:A:125:LYS:HD3	1:A:258:ARG:NH1	2.29	0.47
1:E:125:LYS:HB2	1:E:258:ARG:NH1	2.30	0.47
1:G:206:PHE:CZ	1:K:223:ARG:HG3	2.47	0.47
1:G:224:PRO:HG2	1:I:209:SER:CA	2.44	0.47
1:G:327:ILE:CG2	1:G:328:PRO:CD	2.91	0.47
1:K:9:LEU:HD12	2:L:152:VAL:HG11	1.97	0.47
1:C:72:GLU:CG	5:C:602:NAG:H82	2.45	0.47
1:A:155:ILE:HG22	1:A:157:LEU:HD13	1.97	0.46
2:D:158:ASP:OD2	2:D:160:PRO:HD2	2.14	0.46
1:E:101:PHE:HB3	1:E:104:TYR:HB2	1.97	0.46
1:E:312:TYR:HD2	2:F:89:LEU:HD13	1.80	0.46
1:G:197:LEU:HD11	3:Q:4:SIA:H92	1.97	0.46
1:I:101:PHE:HB3	1:I:104:TYR:HB2	1.98	0.46
2:J:162:TYR:CE1	7:J:212:HOH:O	2.48	0.46
1:K:258:ARG:HE	1:K:259:TYR:HE1	1.62	0.46
1:A:13:TYR:O	2:B:14:TRP:N	2.37	0.46
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.50	0.46
2:F:4:GLY:O	2:F:8:GLY:HA3	2.15	0.46
2:H:79:ASN:HB2	2:J:68:LYS:HE3	1.97	0.46
2:J:5:ALA:HB3	2:J:112:ASP:OD2	2.15	0.46
1:G:145:ALA:C	1:G:147:ALA:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:HIS:CE1	3:Q:4:SIA:H91	2.49	0.46
1:I:11:ILE:CG1	2:J:24:TYR:HD2	2.27	0.46
2:J:28:ASN:HD22	2:J:28:ASN:N	2.08	0.46
1:K:159:LYS:HD2	1:K:199:GLN:HG2	1.96	0.46
1:C:324:LEU:HB3	2:D:111:HIS:CG	2.50	0.46
1:E:258:ARG:HE	1:E:259:TYR:HE1	1.63	0.46
3:P:4:SIA:O7	3:P:4:SIA:H113	2.16	0.46
1:A:145:ALA:C	1:A:147:ALA:H	2.24	0.46
1:C:198:TYR:O	1:C:199:GLN:CB	2.61	0.46
1:I:125:LYS:HB2	1:I:258:ARG:NH1	2.31	0.46
1:K:145:ALA:C	1:K:147:ALA:H	2.24	0.46
1:A:183:TRP:HZ3	1:A:238:THR:HG22	1.81	0.46
1:G:161:GLY:O	1:G:162:ASN:HB2	2.15	0.46
1:C:8:THR:CB	7:D:204:HOH:O	2.06	0.46
1:E:34:HIS:CE1	2:F:21:TRP:HE1	2.34	0.46
1:I:11:ILE:HG12	2:J:24:TYR:CE2	2.47	0.46
1:I:14:HIS:CD2	1:I:15:ALA:N	2.83	0.46
2:J:9:PHE:CE1	2:J:10:ILE:HG13	2.51	0.46
2:B:59:MET:O	2:B:59:MET:HG3	2.16	0.46
1:A:164:TYR:HE2	7:A:919:HOH:O	1.78	0.46
1:C:183:TRP:HZ3	1:C:238:THR:HG22	1.81	0.46
1:E:183:TRP:HZ3	1:E:238:THR:HG22	1.81	0.46
1:I:9:LEU:HA	2:J:26:HIS:HA	1.98	0.46
1:I:324:LEU:CD2	2:J:21:TRP:CG	2.99	0.46
2:J:129:ASN:CB	7:J:219:HOH:O	2.59	0.46
1:K:101:PHE:HB3	1:K:104:TYR:HB2	1.98	0.46
1:A:224:PRO:HG2	1:C:209:SER:CA	2.45	0.46
1:C:13:TYR:HA	2:D:21:TRP:O	2.15	0.46
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.51	0.46
1:I:162:ASN:HA	1:I:199:GLN:HG3	1.98	0.46
1:K:183:TRP:HZ3	1:K:238:THR:HG22	1.81	0.46
1:K:324:LEU:HB3	2:L:111:HIS:CG	2.51	0.46
2:L:4:GLY:O	2:L:8:GLY:HA3	2.16	0.46
1:E:11:ILE:N	2:F:136:GLY:O	2.47	0.45
1:G:159:LYS:NZ	1:G:199:GLN:HG2	2.30	0.45
1:K:44:ASN:C	1:K:44:ASN:HD22	2.24	0.45
2:B:4:GLY:O	2:B:8:GLY:HA3	2.15	0.45
2:D:59:MET:O	2:D:59:MET:HG3	2.16	0.45
2:F:28:ASN:HD22	2:F:28:ASN:N	2.09	0.45
2:J:142:HIS:CE1	7:J:205:HOH:O	2.69	0.45
2:L:89:LEU:HB2	7:L:201:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:GLY:O	2:H:8:GLY:HA3	2.16	0.45
1:I:307:GLY:HA2	2:J:63:PHE:CE1	2.51	0.45
1:A:113:SER:C	7:A:913:HOH:O	2.08	0.45
1:E:42:LYS:HE3	1:E:42:LYS:HB2	1.81	0.45
2:F:5:ALA:HB3	2:F:112:ASP:OD2	2.16	0.45
1:G:101:PHE:HB3	1:G:104:TYR:HB2	1.98	0.45
1:K:125:LYS:HB2	1:K:258:ARG:NH1	2.32	0.45
1:C:145:ALA:C	1:C:147:ALA:H	2.25	0.45
1:C:155:ILE:HG22	1:C:157:LEU:HD13	1.98	0.45
1:E:44:ASN:C	1:E:44:ASN:HD22	2.24	0.45
2:F:19:ASP:HB2	2:F:36:ALA:CB	2.47	0.45
1:G:162:ASN:HD22	1:G:162:ASN:HA	1.56	0.45
2:H:79:ASN:HB3	2:J:68:LYS:HE3	1.98	0.45
1:I:44:ASN:HD22	1:I:44:ASN:C	2.24	0.45
2:H:9:PHE:CE1	2:H:10:ILE:HG13	2.52	0.45
1:I:145:ALA:C	1:I:147:ALA:H	2.25	0.45
1:E:14:HIS:CD2	1:E:15:ALA:N	2.85	0.45
1:E:145:ALA:C	1:E:147:ALA:H	2.24	0.45
1:E:308:LYS:HE2	2:F:61:THR:O	2.17	0.45
2:F:59:MET:O	2:F:59:MET:HG3	2.17	0.45
2:H:151:SER:HB2	2:H:157:TYR:HA	1.98	0.45
2:J:143:LYS:HE2	2:J:143:LYS:HA	1.98	0.45
1:A:101:PHE:HB3	1:A:104:TYR:HB2	1.99	0.45
1:A:125:LYS:HB2	1:A:258:ARG:NH1	2.32	0.45
1:G:125:LYS:HB2	1:G:258:ARG:NH1	2.31	0.45
1:I:49:LYS:C	7:I:714:HOH:O	2.58	0.45
1:K:197:LEU:HD21	6:K:603:SIA:H111	1.99	0.45
1:A:225:LYS:HD2	1:G:80:SER:HB3	1.99	0.45
1:A:312:TYR:HD2	2:B:89:LEU:HD13	1.80	0.45
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.52	0.45
1:C:125:LYS:HB2	1:C:258:ARG:NH1	2.31	0.45
1:E:9:LEU:CD1	2:F:152:VAL:HG11	2.47	0.45
1:E:167:LEU:C	1:E:167:LEU:HD23	2.42	0.45
1:G:14:HIS:CD2	1:G:15:ALA:N	2.84	0.45
1:G:42:LYS:HE3	1:G:42:LYS:HB2	1.81	0.45
2:H:28:ASN:HD22	2:H:28:ASN:N	2.08	0.45
2:J:59:MET:O	2:J:59:MET:HG3	2.17	0.45
2:B:151:SER:HB2	2:B:157:TYR:HA	1.99	0.45
1:I:155:ILE:HG22	1:I:157:LEU:HD13	1.98	0.45
2:D:151:SER:HB2	2:D:157:TYR:HA	2.00	0.44
2:D:160:PRO:O	2:D:161:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:CYS:HB3	1:E:281:CYS:O	2.17	0.44
1:E:106:GLU:O	1:E:110:GLN:HG3	2.17	0.44
1:I:292:ILE:HG22	1:I:294:THR:HG22	2.00	0.44
1:K:308:LYS:HE2	2:L:61:THR:O	2.17	0.44
2:L:9:PHE:CE1	2:L:10:ILE:HG13	2.52	0.44
1:E:51:ARG:HB2	1:E:52:GLY:H	1.61	0.44
1:G:307:GLY:HA2	2:H:63:PHE:CD1	2.52	0.44
2:D:5:ALA:HB3	2:D:112:ASP:OD2	2.17	0.44
1:E:8:THR:C	7:E:709:HOH:O	2.54	0.44
1:E:13:TYR:CE1	2:F:6:ILE:HG23	2.51	0.44
2:J:151:SER:HB2	2:J:157:TYR:HA	1.99	0.44
1:K:14:HIS:CD2	1:K:15:ALA:N	2.86	0.44
1:G:297:PRO:HG3	2:H:56:ILE:HA	1.99	0.44
2:H:151:SER:HB2	2:H:156:THR:O	2.18	0.44
1:A:8:THR:O	2:B:27:GLN:N	2.49	0.44
1:C:159:LYS:NZ	1:C:199:GLN:CG	2.63	0.44
1:G:10:CYS:N	2:H:137:CYS:SG	2.85	0.44
1:I:11:ILE:CD1	2:J:24:TYR:CE2	3.01	0.44
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.17	0.44
1:E:25:VAL:CG2	2:F:102:LEU:HD12	2.46	0.44
1:K:42:LYS:HE3	1:K:42:LYS:HB2	1.80	0.44
1:A:11:ILE:HA	2:B:14:TRP:HH2	1.83	0.44
1:C:118:GLU:O	1:C:118:GLU:HG3	2.18	0.44
2:D:123:ARG:HH12	2:F:123:ARG:HH22	1.66	0.44
2:D:132:GLU:HG2	2:D:138:PHE:HE2	1.83	0.44
2:H:40:SER:CA	7:H:205:HOH:O	2.63	0.44
1:A:25:VAL:HG22	2:B:101:LEU:HB3	2.00	0.44
1:A:228:GLU:OE1	1:G:80:SER:OG	2.28	0.44
1:C:9:LEU:N	7:D:204:HOH:O	2.50	0.44
1:C:44:ASN:HD22	1:C:45:GLY:N	2.16	0.44
1:I:14:HIS:HB2	2:J:21:TRP:HA	2.00	0.44
1:I:106:GLU:O	1:I:110:GLN:HG3	2.18	0.44
1:I:118:GLU:O	1:I:118:GLU:HG3	2.17	0.44
2:J:132:GLU:HG2	2:J:138:PHE:HE2	1.82	0.44
1:K:269:SER:N	7:K:703:HOH:O	2.50	0.44
2:L:5:ALA:HB3	2:L:112:ASP:OD2	2.18	0.44
2:L:30:GLN:HE22	2:L:145:ASP:CB	2.28	0.44
1:C:273:ILE:N	1:C:273:ILE:HD12	2.33	0.43
1:I:25:VAL:CG2	2:J:102:LEU:HA	2.48	0.43
1:I:49:LYS:O	1:I:283:THR:HG22	2.17	0.43
1:A:223:ARG:HG3	1:C:206:PHE:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:GLN:HE22	2:B:145:ASP:CB	2.28	0.43
1:C:14:HIS:CD2	1:C:15:ALA:N	2.86	0.43
1:G:51:ARG:HB3	1:G:51:ARG:HH11	1.83	0.43
1:G:66:TRP:NE1	1:G:77:SER:CB	2.76	0.43
2:L:19:ASP:HB2	2:L:36:ALA:CB	2.48	0.43
2:L:59:MET:HG3	2:L:59:MET:O	2.18	0.43
1:A:276:THR:HA	1:A:277:PRO:HD3	1.89	0.43
1:C:55:PRO:HB3	1:C:84:TYR:CZ	2.53	0.43
1:C:161:GLY:O	1:C:162:ASN:HB2	2.18	0.43
1:C:312:TYR:HD2	2:D:89:LEU:HD13	1.80	0.43
1:E:33:THR:HG23	1:E:324:LEU:O	2.18	0.43
1:E:113:SER:CA	7:E:717:HOH:O	2.66	0.43
2:H:30:GLN:HE22	2:H:145:ASP:CB	2.29	0.43
1:A:305:THR:HG22	2:B:66:VAL:HG23	1.99	0.43
1:E:162:ASN:HD22	1:E:162:ASN:HA	1.55	0.43
1:G:63:ILE:HD11	1:G:85:ILE:HG21	2.01	0.43
1:I:8:THR:O	2:J:27:GLN:N	2.45	0.43
2:B:145:ASP:O	2:B:148:CYS:HB3	2.19	0.43
1:E:118:GLU:O	1:E:118:GLU:HG3	2.19	0.43
1:G:183:TRP:HZ3	1:G:238:THR:HG22	1.83	0.43
2:H:59:MET:O	2:H:59:MET:HG3	2.17	0.43
1:A:55:PRO:HB3	1:A:84:TYR:CZ	2.54	0.43
2:B:132:GLU:HG2	2:B:138:PHE:HE2	1.83	0.43
1:E:198:TYR:O	1:E:199:GLN:CB	2.67	0.43
1:E:204:TYR:CD1	1:E:215:LYS:HE3	2.53	0.43
1:E:292:ILE:HG22	1:E:294:THR:HG22	2.01	0.43
1:E:307:GLY:HA2	2:F:63:PHE:CE1	2.54	0.43
1:K:8:THR:HB	2:L:138:PHE:O	2.19	0.43
1:A:11:ILE:CA	2:B:14:TRP:CH2	3.01	0.43
2:D:19:ASP:HB2	2:D:36:ALA:CB	2.47	0.43
2:D:158:ASP:CG	2:D:160:PRO:HD2	2.44	0.43
1:E:114:VAL:CG2	1:E:117:PHE:HB2	2.43	0.43
2:F:132:GLU:HG2	2:F:138:PHE:HE2	1.83	0.43
1:G:49:LYS:O	1:G:283:THR:HG22	2.19	0.43
2:H:19:ASP:HB2	2:H:36:ALA:CB	2.48	0.43
1:I:42:LYS:HB2	1:I:42:LYS:HE3	1.81	0.43
1:I:48:CYS:HB3	1:I:281:CYS:O	2.19	0.43
1:K:204:TYR:CD1	1:K:215:LYS:HE3	2.53	0.43
1:A:14:HIS:CD2	1:A:15:ALA:N	2.86	0.43
1:A:44:ASN:C	1:A:44:ASN:HD22	2.26	0.43
1:E:323:GLY:O	2:F:111:HIS:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:ILE:HD11	2:J:24:TYR:CE2	2.52	0.43
1:K:33:THR:HG23	1:K:324:LEU:O	2.19	0.43
1:E:50:LEU:HB3	1:E:83:SER:HB2	2.01	0.43
1:G:48:CYS:HB3	1:G:281:CYS:O	2.19	0.43
1:G:198:TYR:O	1:G:199:GLN:CB	2.66	0.43
1:E:159:LYS:CD	1:E:199:GLN:HG2	2.49	0.43
1:K:167:LEU:C	1:K:167:LEU:CD2	2.92	0.43
2:L:151:SER:HB2	2:L:156:THR:O	2.19	0.43
1:C:48:CYS:HB3	1:C:281:CYS:O	2.18	0.42
2:D:145:ASP:O	2:D:148:CYS:HB3	2.19	0.42
1:E:22:VAL:HG21	1:E:321:ALA:HB2	2.01	0.42
1:E:49:LYS:O	1:E:283:THR:HG22	2.19	0.42
1:E:51:ARG:HB3	1:E:51:ARG:HH11	1.84	0.42
1:E:63:ILE:HD11	1:E:85:ILE:HG21	2.01	0.42
2:H:145:ASP:O	2:H:148:CYS:HB3	2.19	0.42
1:A:204:TYR:CD1	1:A:215:LYS:HE3	2.54	0.42
2:B:151:SER:HB2	2:B:156:THR:O	2.19	0.42
1:C:14:HIS:CE1	2:D:18:VAL:HA	2.53	0.42
1:C:33:THR:HG23	1:C:324:LEU:O	2.19	0.42
1:C:292:ILE:HG22	1:C:294:THR:HG22	2.01	0.42
1:I:51:ARG:HB2	1:I:52:GLY:H	1.59	0.42
1:I:63:ILE:HD11	1:I:85:ILE:HG21	2.01	0.42
1:K:50:LEU:CD2	1:K:306:ILE:HG22	2.49	0.42
1:A:273:ILE:HD12	1:A:273:ILE:N	2.34	0.42
1:G:204:TYR:CD1	1:G:215:LYS:HE3	2.54	0.42
1:K:273:ILE:HD12	1:K:273:ILE:N	2.35	0.42
1:A:48:CYS:HB3	1:A:281:CYS:O	2.19	0.42
1:C:63:ILE:HD11	1:C:85:ILE:HG21	2.02	0.42
2:D:159:TYR:N	2:D:160:PRO:HD2	2.34	0.42
1:G:118:GLU:O	1:G:118:GLU:HG3	2.18	0.42
2:H:88:PHE:CZ	2:L:87:GLY:HA3	2.55	0.42
1:I:33:THR:HG23	1:I:324:LEU:O	2.20	0.42
1:I:257:PRO:C	7:I:709:HOH:O	2.57	0.42
1:K:266:ASN:ND2	1:K:266:ASN:N	2.67	0.42
1:A:302:HIS:HA	1:A:303:PRO:HD3	1.86	0.42
2:B:19:ASP:HB2	2:B:36:ALA:CB	2.47	0.42
1:C:44:ASN:ND2	1:C:44:ASN:C	2.78	0.42
1:C:204:TYR:CD1	1:C:215:LYS:HE3	2.54	0.42
2:H:132:GLU:HG2	2:H:138:PHE:HE2	1.83	0.42
1:I:55:PRO:HB3	1:I:84:TYR:CZ	2.54	0.42
1:I:183:TRP:HZ3	1:I:238:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:204:TYR:CD1	1:I:215:LYS:HE3	2.54	0.42
1:K:13:TYR:C	7:K:723:HOH:O	2.55	0.42
7:K:723:HOH:O	2:L:13:GLY:HA3	2.06	0.42
1:E:13:TYR:HB3	2:F:115:VAL:HG21	2.01	0.42
1:E:50:LEU:CD2	1:E:306:ILE:HG22	2.48	0.42
1:G:66:TRP:HE1	1:G:77:SER:HB3	1.81	0.42
2:J:87:GLY:HA3	2:L:88:PHE:CZ	2.55	0.42
2:J:145:ASP:O	2:J:148:CYS:HB3	2.19	0.42
1:K:44:ASN:HD22	1:K:45:GLY:N	2.17	0.42
1:K:49:LYS:O	1:K:283:THR:HG22	2.19	0.42
1:K:67:ILE:CA	7:K:725:HOH:O	2.60	0.42
1:A:162:ASN:HD22	1:A:162:ASN:HA	1.56	0.42
2:B:143:LYS:HE2	2:B:143:LYS:HA	2.02	0.42
1:E:28:LYS:HD3	7:E:707:HOH:O	2.19	0.42
1:E:162:ASN:HA	1:E:199:GLN:HG3	2.02	0.42
1:G:118:GLU:HG2	1:G:262:ALA:HB3	2.02	0.42
1:I:44:ASN:HD22	1:I:45:GLY:N	2.18	0.42
1:K:63:ILE:HD11	1:K:85:ILE:HG21	2.01	0.42
1:K:302:HIS:HA	1:K:303:PRO:HD3	1.88	0.42
1:A:63:ILE:HD11	1:A:85:ILE:HG21	2.01	0.42
1:G:70:ASN:HA	1:G:71:PRO:HD3	1.96	0.42
2:J:38:LEU:C	7:J:202:HOH:O	2.62	0.42
2:J:144:CYS:HB2	7:J:205:HOH:O	2.19	0.42
1:K:161:GLY:O	1:K:162:ASN:HB2	2.20	0.42
2:L:143:LYS:HE2	2:L:143:LYS:HA	2.02	0.42
1:A:49:LYS:O	1:A:283:THR:HG22	2.20	0.42
2:D:143:LYS:HE2	2:D:143:LYS:HA	2.02	0.42
2:F:123:ARG:HG3	2:F:138:PHE:CE2	2.55	0.42
1:G:55:PRO:HB3	1:G:84:TYR:CZ	2.55	0.42
1:K:50:LEU:HB3	1:K:83:SER:HB2	2.01	0.42
1:K:55:PRO:HB3	1:K:84:TYR:CZ	2.54	0.42
1:C:42:LYS:HE3	1:C:42:LYS:HB2	1.80	0.42
1:E:8:THR:CA	7:E:709:HOH:O	2.67	0.42
1:E:266:ASN:H	1:E:266:ASN:HD22	1.67	0.42
1:E:273:ILE:N	1:E:273:ILE:HD12	2.34	0.42
1:G:273:ILE:HD12	1:G:273:ILE:N	2.35	0.42
1:G:292:ILE:CD1	1:G:301:ILE:HD12	2.50	0.42
2:H:87:GLY:HA3	2:J:88:PHE:CZ	2.55	0.42
1:I:51:ARG:HB3	1:I:51:ARG:HH11	1.84	0.42
2:B:88:PHE:CZ	2:F:87:GLY:HA3	2.55	0.41
1:C:128:SER:C	1:C:130:PRO:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:OD2	1:C:245:LYS:N	2.53	0.41
2:D:151:SER:HB2	2:D:156:THR:O	2.19	0.41
2:F:145:ASP:O	2:F:148:CYS:HB3	2.19	0.41
1:G:25:VAL:O	2:J:51:LYS:HA	2.20	0.41
1:K:118:GLU:O	1:K:118:GLU:HG3	2.19	0.41
2:L:123:ARG:HG3	2:L:138:PHE:CE2	2.55	0.41
1:C:297:PRO:HG3	2:D:56:ILE:HA	2.01	0.41
2:F:143:LYS:HA	2:F:143:LYS:HE2	2.02	0.41
2:F:151:SER:HB2	2:F:156:THR:O	2.20	0.41
1:G:33:THR:HG23	1:G:324:LEU:O	2.20	0.41
1:G:44:ASN:C	1:G:44:ASN:HD22	2.27	0.41
2:J:123:ARG:C	2:J:125:GLN:H	2.28	0.41
1:K:119:ARG:HB2	1:K:261:PHE:CE2	2.56	0.41
1:A:22:VAL:HG21	1:A:321:ALA:HB2	2.01	0.41
1:C:50:LEU:HD23	1:C:50:LEU:HA	1.84	0.41
1:E:47:LEU:HD12	1:E:286:GLN:NE2	2.35	0.41
1:G:22:VAL:HG21	1:G:321:ALA:HB2	2.02	0.41
1:I:119:ARG:HB2	1:I:261:PHE:CE2	2.55	0.41
1:I:244:ASP:OD2	1:I:245:LYS:N	2.53	0.41
1:K:51:ARG:HB3	1:K:51:ARG:HH11	1.85	0.41
2:L:122:VAL:HG22	2:L:138:PHE:CE1	2.55	0.41
1:A:33:THR:HG23	1:A:324:LEU:O	2.20	0.41
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.84	0.41
1:C:49:LYS:O	1:C:283:THR:HG22	2.20	0.41
1:C:105:GLU:OE2	2:D:71:ASN:HB3	2.19	0.41
1:I:22:VAL:HG21	1:I:321:ALA:HB2	2.01	0.41
1:K:48:CYS:HB3	1:K:281:CYS:O	2.20	0.41
1:K:118:GLU:HG2	1:K:262:ALA:HB3	2.03	0.41
1:A:292:ILE:CD1	1:A:301:ILE:HD12	2.51	0.41
1:C:302:HIS:HA	1:C:303:PRO:HD3	1.87	0.41
2:D:123:ARG:C	2:D:125:GLN:H	2.28	0.41
2:D:159:TYR:H	2:D:160:PRO:HD2	1.86	0.41
1:E:128:SER:C	1:E:130:PRO:HD3	2.46	0.41
1:G:266:ASN:ND2	1:G:266:ASN:N	2.66	0.41
2:J:151:SER:HB2	2:J:156:THR:O	2.20	0.41
2:L:145:ASP:O	2:L:148:CYS:HB3	2.20	0.41
1:E:55:PRO:HB3	1:E:84:TYR:CZ	2.55	0.41
1:G:50:LEU:CD1	1:G:306:ILE:HG22	2.51	0.41
2:H:110:TYR:CE1	1:K:26:LEU:HD13	2.55	0.41
2:H:143:LYS:HA	2:H:143:LYS:HE2	2.03	0.41
2:J:19:ASP:HB2	2:J:36:ALA:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:GLN:HE22	2:J:145:ASP:CB	2.29	0.41
1:K:47:LEU:HD13	1:K:276:THR:CG2	2.50	0.41
2:L:132:GLU:HG2	2:L:138:PHE:HE2	1.85	0.41
1:E:244:ASP:OD2	1:E:245:LYS:N	2.53	0.41
1:E:302:HIS:HA	1:E:303:PRO:HD3	1.86	0.41
2:H:5:ALA:HB3	2:H:112:ASP:OD2	2.21	0.41
1:A:308:LYS:HE2	2:B:61:THR:O	2.21	0.41
1:C:225:LYS:HG2	1:C:230:GLU:HG2	2.03	0.41
1:G:327:ILE:HG22	1:G:328:PRO:HD2	2.01	0.41
1:I:271:ILE:HD12	2:J:69:GLU:OE1	2.20	0.41
1:I:296:LEU:HA	1:I:297:PRO:HD3	1.86	0.41
1:K:13:TYR:CZ	2:L:6:ILE:HG23	2.56	0.41
1:A:327:ILE:CG2	1:A:328:PRO:CD	2.98	0.41
1:C:22:VAL:HG21	1:C:321:ALA:HB2	2.02	0.41
1:C:118:GLU:HG2	1:C:262:ALA:HB3	2.03	0.41
1:C:159:LYS:HZ2	1:C:199:GLN:HE21	1.69	0.41
2:D:123:ARG:HG3	2:D:138:PHE:CE2	2.55	0.41
1:E:44:ASN:HD22	1:E:45:GLY:N	2.17	0.41
1:E:118:GLU:HG2	1:E:262:ALA:HB3	2.03	0.41
1:E:324:LEU:HB3	2:F:111:HIS:CB	2.50	0.41
2:F:122:VAL:HG22	2:F:138:PHE:CE1	2.56	0.41
1:G:128:SER:C	1:G:130:PRO:HD3	2.46	0.41
1:G:266:ASN:H	1:G:266:ASN:HD22	1.69	0.41
1:I:118:GLU:HG2	1:I:262:ALA:HB3	2.03	0.41
1:I:292:ILE:CD1	1:I:301:ILE:HD12	2.50	0.41
2:J:123:ARG:HG3	2:J:138:PHE:CE2	2.56	0.41
2:J:159:TYR:H	2:J:160:PRO:CD	2.34	0.41
1:K:292:ILE:CD1	1:K:301:ILE:HD12	2.50	0.41
1:A:314:LYS:HB2	1:A:314:LYS:HE3	1.78	0.41
1:A:327:ILE:CG2	1:A:328:PRO:N	2.84	0.41
1:E:319:ARG:CZ	7:E:711:HOH:O	2.29	0.41
1:G:302:HIS:HA	1:G:303:PRO:HD3	1.88	0.41
1:I:305:THR:O	2:J:66:VAL:HG13	2.21	0.41
2:J:11:GLU:HB3	7:J:217:HOH:O	2.19	0.41
1:C:245:LYS:HZ2	1:G:264:GLU:CD	2.23	0.40
2:D:128:ASN:HB3	2:D:162:TYR:CE1	2.56	0.40
2:F:133:ILE:CG2	7:F:205:HOH:O	2.69	0.40
1:G:12:GLY:N	2:H:14:TRP:CH2	2.88	0.40
1:I:107:LEU:HB2	1:I:237:TRP:CE2	2.56	0.40
1:I:128:SER:C	1:I:130:PRO:HD3	2.46	0.40
1:K:22:VAL:HG21	1:K:321:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LYS:HA	1:E:25:VAL:O	2.21	0.40
2:B:123:ARG:C	2:B:125:GLN:H	2.29	0.40
1:C:119:ARG:HB2	1:C:261:PHE:CE2	2.57	0.40
1:E:66:TRP:NE1	1:E:77:SER:HB3	2.32	0.40
1:K:44:ASN:ND2	1:K:44:ASN:C	2.79	0.40
1:K:128:SER:C	1:K:130:PRO:HD3	2.46	0.40
1:A:44:ASN:HD22	1:A:45:GLY:N	2.18	0.40
1:C:292:ILE:CD1	1:C:301:ILE:HD12	2.52	0.40
2:D:30:GLN:HE22	2:D:145:ASP:CB	2.29	0.40
1:I:11:ILE:HA	2:J:24:TYR:HA	2.02	0.40
1:C:126:THR:CB	1:K:92:ASP:CG	2.94	0.40
2:D:94:TYR:CE1	2:F:59:MET:HB2	2.57	0.40
1:I:302:HIS:HA	1:I:303:PRO:HD3	1.87	0.40
1:K:131:ASN:CA	7:K:719:HOH:O	2.57	0.40
2:L:123:ARG:C	2:L:125:GLN:H	2.29	0.40
1:A:26:LEU:HB3	2:D:47:GLU:HB3	2.02	0.40
1:C:326:ASN:C	1:C:327:ILE:HG13	2.46	0.40
1:E:324:LEU:HD13	2:F:6:ILE:HD13	2.02	0.40
1:G:314:LYS:HB2	1:G:314:LYS:HE3	1.78	0.40
2:H:123:ARG:HG3	2:H:138:PHE:CE2	2.56	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	320/322 (99%)	296 (92%)	24 (8%)	0	100	100
1	C	319/322 (99%)	297 (93%)	22 (7%)	0	100	100
1	E	319/322 (99%)	297 (93%)	22 (7%)	0	100	100
1	G	320/322 (99%)	298 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	319/322 (99%)	298 (93%)	21 (7%)	0	100	100
1	K	319/322 (99%)	297 (93%)	22 (7%)	0	100	100
2	B	160/164 (98%)	149 (93%)	10 (6%)	1 (1%)	21	51
2	D	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	21	51
2	F	159/164 (97%)	148 (93%)	11 (7%)	0	100	100
2	H	160/164 (98%)	149 (93%)	10 (6%)	1 (1%)	21	51
2	J	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	21	51
2	L	159/164 (97%)	147 (92%)	12 (8%)	0	100	100
All	All	2878/2916 (99%)	2675 (93%)	199 (7%)	4 (0%)	48	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	160	PRO
2	H	160	PRO
2	J	160	PRO
2	D	159	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/283 (100%)	260 (92%)	22 (8%)	11	35
1	C	282/283 (100%)	259 (92%)	23 (8%)	10	32
1	E	282/283 (100%)	263 (93%)	19 (7%)	15	43
1	G	282/283 (100%)	263 (93%)	19 (7%)	15	43
1	I	282/283 (100%)	261 (93%)	21 (7%)	13	38
1	K	282/283 (100%)	263 (93%)	19 (7%)	15	43
2	B	139/141 (99%)	133 (96%)	6 (4%)	26	60
2	D	140/141 (99%)	131 (94%)	9 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	139/141 (99%)	126 (91%)	13 (9%)	8	26
2	H	139/141 (99%)	133 (96%)	6 (4%)	26	60
2	J	140/141 (99%)	131 (94%)	9 (6%)	16	44
2	L	139/141 (99%)	126 (91%)	13 (9%)	8	26
All	All	2528/2544 (99%)	2349 (93%)	179 (7%)	13	40

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	44	ASN
1	A	50	LEU
1	A	58	LEU
1	A	67	ILE
1	A	76	LEU
1	A	77	SER
1	A	107	LEU
1	A	111	LEU
1	A	114	VAL
1	A	126	THR
1	A	157	LEU
1	A	167	LEU
1	A	169	LYS
1	A	199	GLN
1	A	228	GLU
1	A	240	VAL
1	A	265	ARG
1	A	266	ASN
1	A	305	THR
1	A	316	THR
1	A	324	LEU
2	B	22	TYR
2	B	28	ASN
2	B	43	ASN
2	B	80	LEU
2	B	137	CYS
2	B	150	GLU
1	C	10	CYS
1	C	26	LEU
1	C	44	ASN
1	C	50	LEU

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Mol	Chain	Res	Type
1	C	53	VAL
1	C	67	ILE
1	C	74	GLU
1	C	76	LEU
1	C	77	SER
1	C	78	THR
1	C	111	LEU
1	C	114	VAL
1	C	126	THR
1	C	157	LEU
1	C	167	LEU
1	C	169	LYS
1	C	190	THR
1	C	228	GLU
1	C	265	ARG
1	C	266	ASN
1	C	305	THR
1	C	316	THR
1	C	324	LEU
2	D	22	TYR
2	D	28	ASN
2	D	43	ASN
2	D	66	VAL
2	D	80	LEU
2	D	98	LEU
2	D	102	LEU
2	D	137	CYS
2	D	150	GLU
1	E	9	LEU
1	E	10	CYS
1	E	32	VAL
1	E	44	ASN
1	E	47	LEU
1	E	67	ILE
1	E	76	LEU
1	E	111	LEU
1	E	114	VAL
1	E	126	THR
1	E	167	LEU
1	E	169	LYS
1	E	190	THR
1	E	205	VAL

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Mol	Chain	Res	Type
1	E	228	GLU
1	E	265	ARG
1	E	266	ASN
1	E	305	THR
1	E	324	LEU
2	F	2	LEU
2	F	22	TYR
2	F	28	ASN
2	F	38	LEU
2	F	43	ASN
2	F	66	VAL
2	F	80	LEU
2	F	98	LEU
2	F	102	LEU
2	F	122	VAL
2	F	137	CYS
2	F	150	GLU
2	F	158	ASP
1	G	10	CYS
1	G	44	ASN
1	G	50	LEU
1	G	58	LEU
1	G	67	ILE
1	G	107	LEU
1	G	111	LEU
1	G	114	VAL
1	G	126	THR
1	G	157	LEU
1	G	167	LEU
1	G	169	LYS
1	G	228	GLU
1	G	240	VAL
1	G	265	ARG
1	G	266	ASN
1	G	305	THR
1	G	316	THR
1	G	324	LEU
2	H	22	TYR
2	H	28	ASN
2	H	43	ASN
2	H	80	LEU
2	H	137	CYS

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Mol	Chain	Res	Type
2	H	150	GLU
1	I	10	CYS
1	I	26	LEU
1	I	44	ASN
1	I	50	LEU
1	I	53	VAL
1	I	67	ILE
1	I	76	LEU
1	I	77	SER
1	I	111	LEU
1	I	114	VAL
1	I	126	THR
1	I	157	LEU
1	I	167	LEU
1	I	169	LYS
1	I	190	THR
1	I	228	GLU
1	I	265	ARG
1	I	266	ASN
1	I	305	THR
1	I	316	THR
1	I	324	LEU
2	J	22	TYR
2	J	28	ASN
2	J	43	ASN
2	J	66	VAL
2	J	80	LEU
2	J	98	LEU
2	J	102	LEU
2	J	137	CYS
2	J	150	GLU
1	K	9	LEU
1	K	10	CYS
1	K	32	VAL
1	K	44	ASN
1	K	47	LEU
1	K	67	ILE
1	K	76	LEU
1	K	111	LEU
1	K	114	VAL
1	K	126	THR
1	K	167	LEU

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Mol	Chain	Res	Type
1	K	169	LYS
1	K	205	VAL
1	K	228	GLU
1	K	265	ARG
1	K	266	ASN
1	K	305	THR
1	K	316	THR
1	K	324	LEU
2	L	2	LEU
2	L	22	TYR
2	L	28	ASN
2	L	38	LEU
2	L	43	ASN
2	L	66	VAL
2	L	80	LEU
2	L	98	LEU
2	L	102	LEU
2	L	122	VAL
2	L	137	CYS
2	L	150	GLU
2	L	158	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	44	ASN
1	A	93	ASN
1	A	132	HIS
1	A	162	ASN
1	A	194	GLN
1	A	195	GLN
1	A	229	GLN
1	A	253	ASN
1	A	266	ASN
2	B	28	ASN
2	B	30	GLN
2	B	72	HIS
2	B	95	ASN
2	B	129	ASN
2	B	146	ASN
1	C	14	HIS

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Mol	Chain	Res	Type
1	C	37	ASN
1	C	44	ASN
1	C	131	ASN
1	C	132	HIS
1	C	162	ASN
1	C	194	GLN
1	C	195	GLN
1	C	199	GLN
1	C	229	GLN
1	C	253	ASN
1	C	266	ASN
2	D	28	ASN
2	D	30	GLN
2	D	128	ASN
2	D	129	ASN
2	D	146	ASN
1	E	37	ASN
1	E	44	ASN
1	E	132	HIS
1	E	162	ASN
1	E	194	GLN
1	E	195	GLN
1	E	229	GLN
1	E	253	ASN
1	E	266	ASN
2	F	28	ASN
2	F	30	GLN
2	F	50	ASN
2	F	129	ASN
2	F	146	ASN
1	G	37	ASN
1	G	44	ASN
1	G	93	ASN
1	G	162	ASN
1	G	194	GLN
1	G	195	GLN
1	G	199	GLN
1	G	229	GLN
1	G	253	ASN
1	G	266	ASN
2	H	28	ASN
2	H	30	GLN

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Mol	Chain	Res	Type
2	H	50	ASN
2	H	129	ASN
2	H	146	ASN
1	I	14	HIS
1	I	37	ASN
1	I	44	ASN
1	I	93	ASN
1	I	132	HIS
1	I	162	ASN
1	I	194	GLN
1	I	195	GLN
1	I	229	GLN
1	I	253	ASN
1	I	266	ASN
2	J	28	ASN
2	J	30	GLN
2	J	129	ASN
2	J	146	ASN
1	K	37	ASN
1	K	44	ASN
1	K	132	HIS
1	K	162	ASN
1	K	194	GLN
1	K	195	GLN
1	K	199	GLN
1	K	229	GLN
1	K	253	ASN
1	K	266	ASN
2	L	28	ASN
2	L	30	GLN
2	L	43	ASN
2	L	95	ASN
2	L	117	ASN
2	L	129	ASN
2	L	146	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

22 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GAL	M	1	3	11,11,12	0.63	0	15,15,17	0.58	0
3	NAG	M	2	3	14,14,15	0.65	0	17,19,21	1.03	1 (5%)
3	GAL	M	3	3	11,11,12	0.65	0	15,15,17	0.93	1 (6%)
3	SIA	M	4	3	20,20,21	0.69	0	21,28,31	3.44	3 (14%)
3	GAL	N	1	3	11,11,12	0.64	0	15,15,17	0.49	0
3	NAG	N	2	3	14,14,15	0.58	0	17,19,21	0.81	0
3	GAL	N	3	3	11,11,12	0.62	0	15,15,17	0.78	1 (6%)
3	SIA	N	4	3	20,20,21	0.70	0	21,28,31	3.43	3 (14%)
4	NAG	O	1	1,4	14,14,15	0.57	0	17,19,21	0.67	0
4	NAG	O	2	4	14,14,15	0.47	0	17,19,21	0.71	0
3	GAL	P	1	3	11,11,12	0.61	0	15,15,17	0.55	0
3	NAG	P	2	3	14,14,15	0.62	0	17,19,21	0.73	0
3	GAL	P	3	3	11,11,12	0.71	0	15,15,17	0.83	0
3	SIA	P	4	3	20,20,21	0.59	0	21,28,31	3.65	3 (14%)
3	GAL	Q	1	3	11,11,12	0.71	0	15,15,17	1.13	1 (6%)
3	NAG	Q	2	3	14,14,15	0.59	0	17,19,21	0.96	0
3	GAL	Q	3	3	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
3	SIA	Q	4	3	20,20,21	0.67	0	21,28,31	3.37	3 (14%)
3	GAL	R	1	3	11,11,12	0.67	0	15,15,17	1.34	3 (20%)
3	NAG	R	2	3	14,14,15	0.57	0	17,19,21	0.59	0
3	GAL	R	3	3	11,11,12	0.67	0	15,15,17	1.22	2 (13%)
3	SIA	R	4	3	20,20,21	0.70	0	21,28,31	3.22	3 (14%)

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	GAL	M	1	3	-	0/2/19/22	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	GAL	M	3	3	-	0/2/19/22	0/1/1/1
3	SIA	M	4	3	-	2/18/34/38	0/1/1/1
3	GAL	N	1	3	-	0/2/19/22	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	GAL	N	3	3	-	1/2/19/22	0/1/1/1
3	SIA	N	4	3	-	3/18/34/38	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
3	GAL	P	1	3	-	0/2/19/22	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	GAL	P	3	3	-	0/2/19/22	0/1/1/1
3	SIA	P	4	3	-	3/18/34/38	0/1/1/1
3	GAL	Q	1	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	GAL	Q	3	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	4	3	-	4/18/34/38	0/1/1/1
3	GAL	R	1	3	-	0/2/19/22	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	GAL	R	3	3	-	0/2/19/22	0/1/1/1
3	SIA	R	4	3	-	4/18/34/38	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	4	SIA	O6-C2-C3	-14.49	91.08	110.56
3	N	4	SIA	O6-C2-C3	-13.24	92.76	110.56
3	M	4	SIA	O6-C2-C3	-13.21	92.80	110.56
3	Q	4	SIA	O6-C2-C3	-12.97	93.11	110.56
3	R	4	SIA	O6-C2-C3	-11.68	94.85	110.56
3	R	4	SIA	O6-C2-C1	8.29	123.36	107.72
3	M	4	SIA	O6-C2-C1	7.83	122.51	107.72
3	P	4	SIA	O6-C2-C1	7.69	122.23	107.72
3	N	4	SIA	O6-C2-C1	7.65	122.16	107.72
3	Q	4	SIA	O6-C2-C1	7.43	121.74	107.72
3	R	1	GAL	C2-C3-C4	2.85	115.88	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	3	GAL	C1-C2-C3	2.79	113.70	109.64
3	Q	1	GAL	C3-C4-C5	2.59	114.92	110.23
3	R	3	GAL	O5-C5-C6	2.43	112.40	107.66
3	Q	4	SIA	O1B-C1-C2	2.39	118.92	112.71
3	M	2	NAG	C1-C2-N2	-2.36	106.71	110.43
3	M	3	GAL	C1-C2-C3	2.31	113.00	109.64
3	R	1	GAL	C3-C4-C5	2.25	114.30	110.23
3	M	4	SIA	O1B-C1-C2	2.21	118.44	112.71
3	R	1	GAL	C1-C2-C3	2.12	112.72	109.64
3	N	4	SIA	O1B-C1-C2	2.11	118.19	112.71
3	P	4	SIA	O1B-C1-C2	2.10	118.17	112.71
3	R	3	GAL	C2-C3-C4	-2.05	107.26	110.86
3	N	3	GAL	O5-C5-C6	2.04	111.64	107.66
3	R	4	SIA	O1B-C1-C2	2.03	117.98	112.71

There are no chirality outliers.

All (19) torsion outliers are listed below:

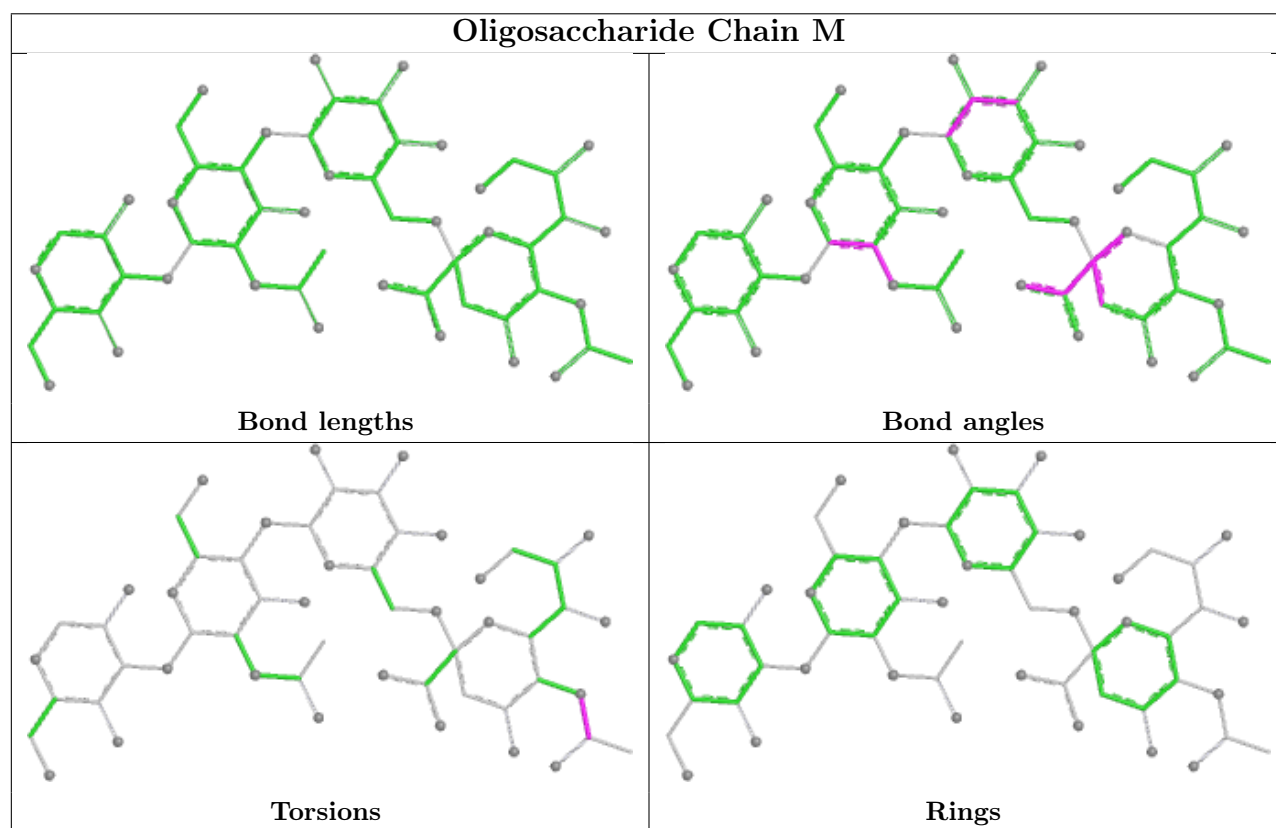
Mol	Chain	Res	Type	Atoms
3	Q	1	GAL	O5-C5-C6-O6
3	Q	1	GAL	C4-C5-C6-O6
3	Q	4	SIA	O8-C8-C9-O9
3	M	4	SIA	C11-C10-N5-C5
3	M	4	SIA	O10-C10-N5-C5
3	N	4	SIA	C11-C10-N5-C5
3	N	4	SIA	O10-C10-N5-C5
3	P	4	SIA	C11-C10-N5-C5
3	P	4	SIA	O10-C10-N5-C5
3	Q	4	SIA	C11-C10-N5-C5
3	Q	4	SIA	O10-C10-N5-C5
3	R	4	SIA	C11-C10-N5-C5
3	R	4	SIA	O10-C10-N5-C5
3	Q	4	SIA	C7-C8-C9-O9
3	N	4	SIA	O1A-C1-C2-O6
3	P	4	SIA	O1A-C1-C2-O6
3	N	3	GAL	O5-C5-C6-O6
3	R	4	SIA	O8-C8-C9-O9
3	R	4	SIA	C7-C8-C9-O9

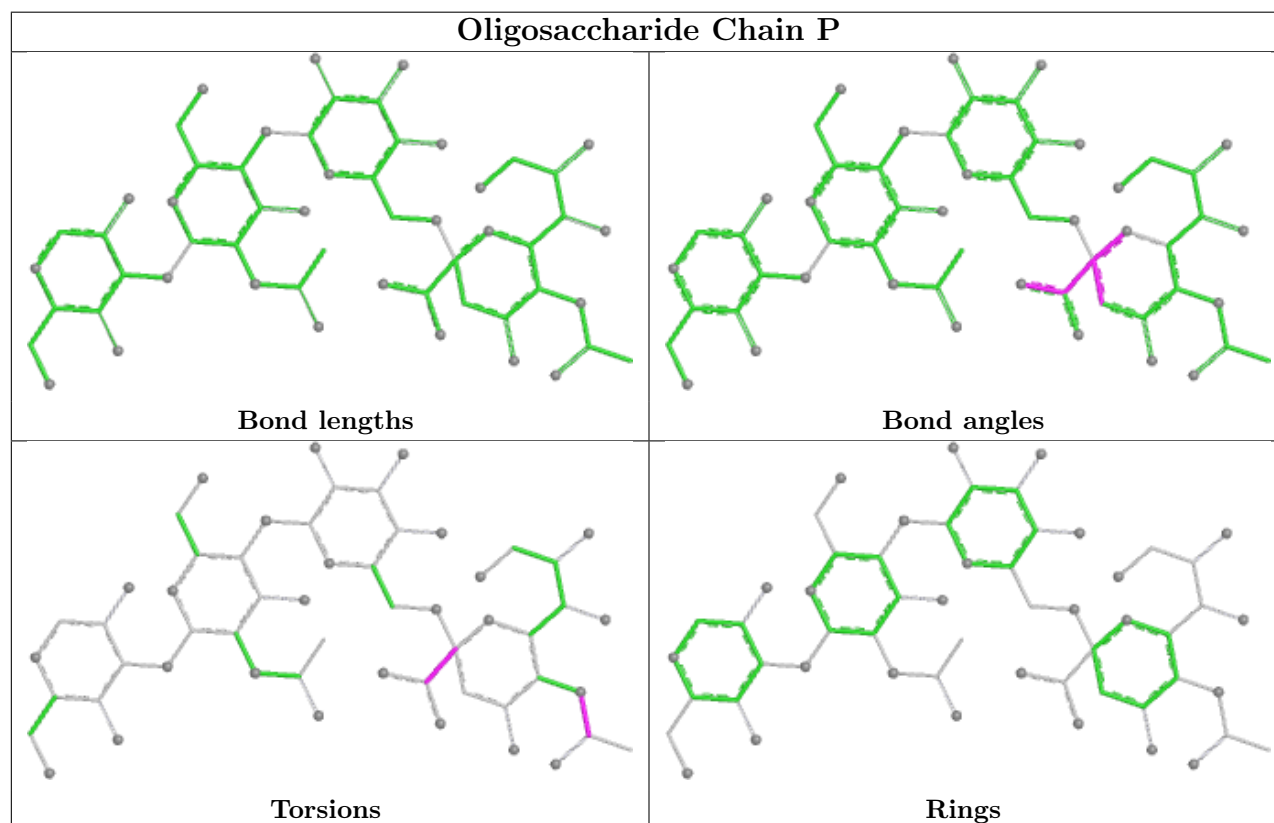
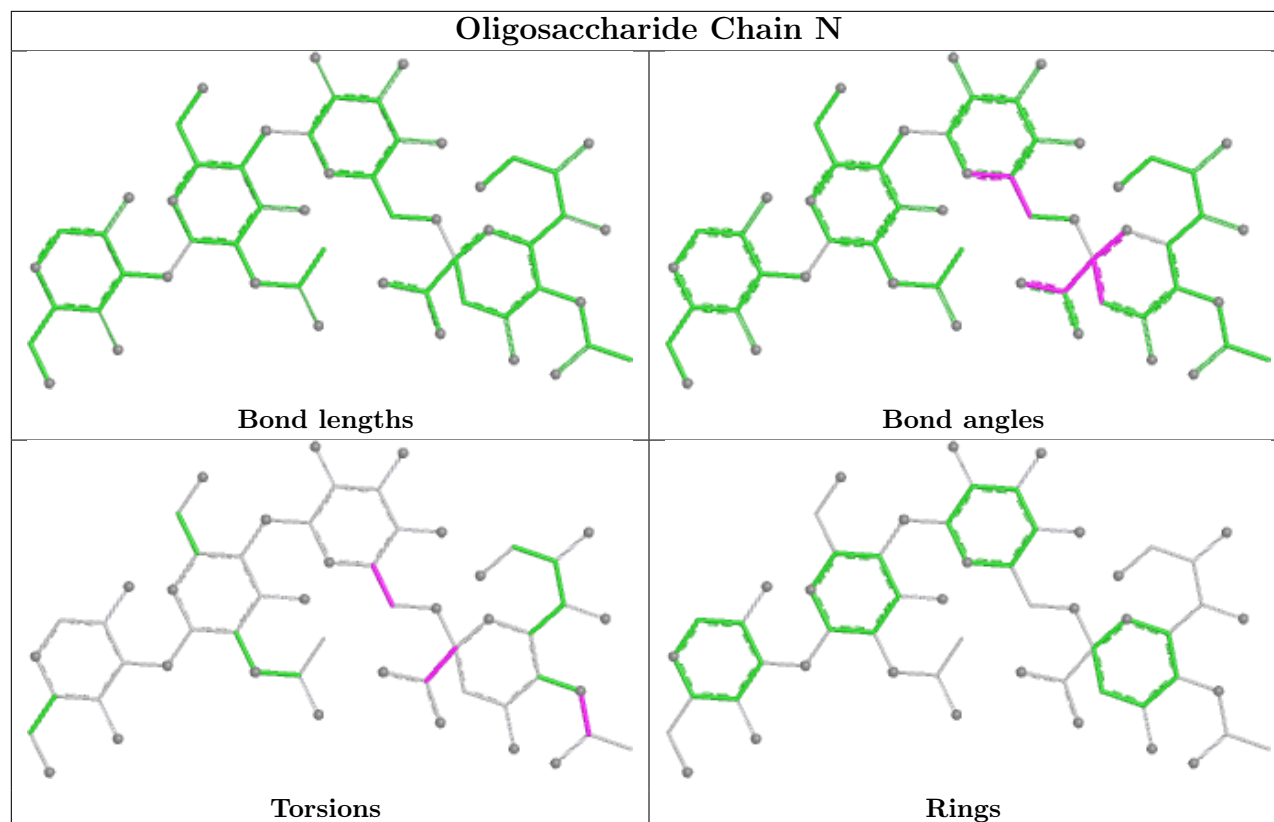
There are no ring outliers.

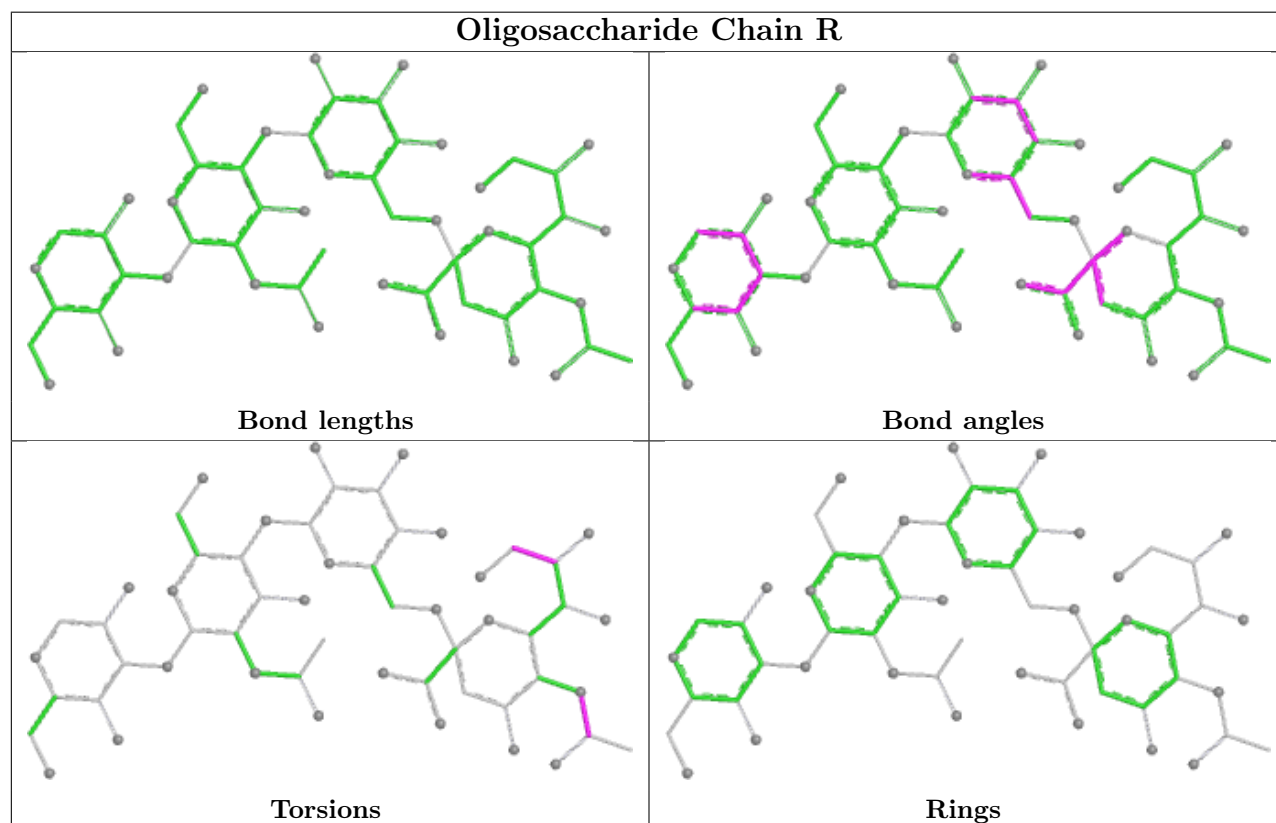
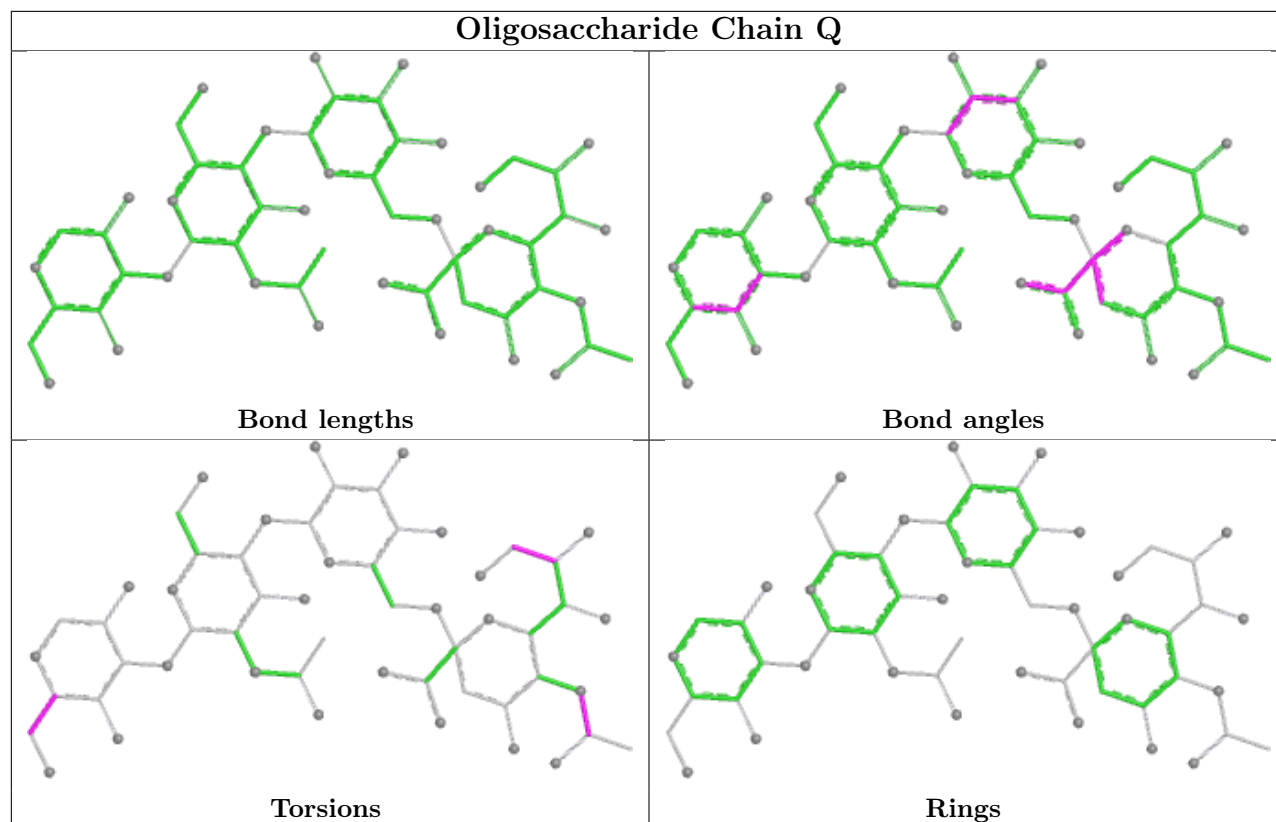
11 monomers are involved in 18 short contacts:

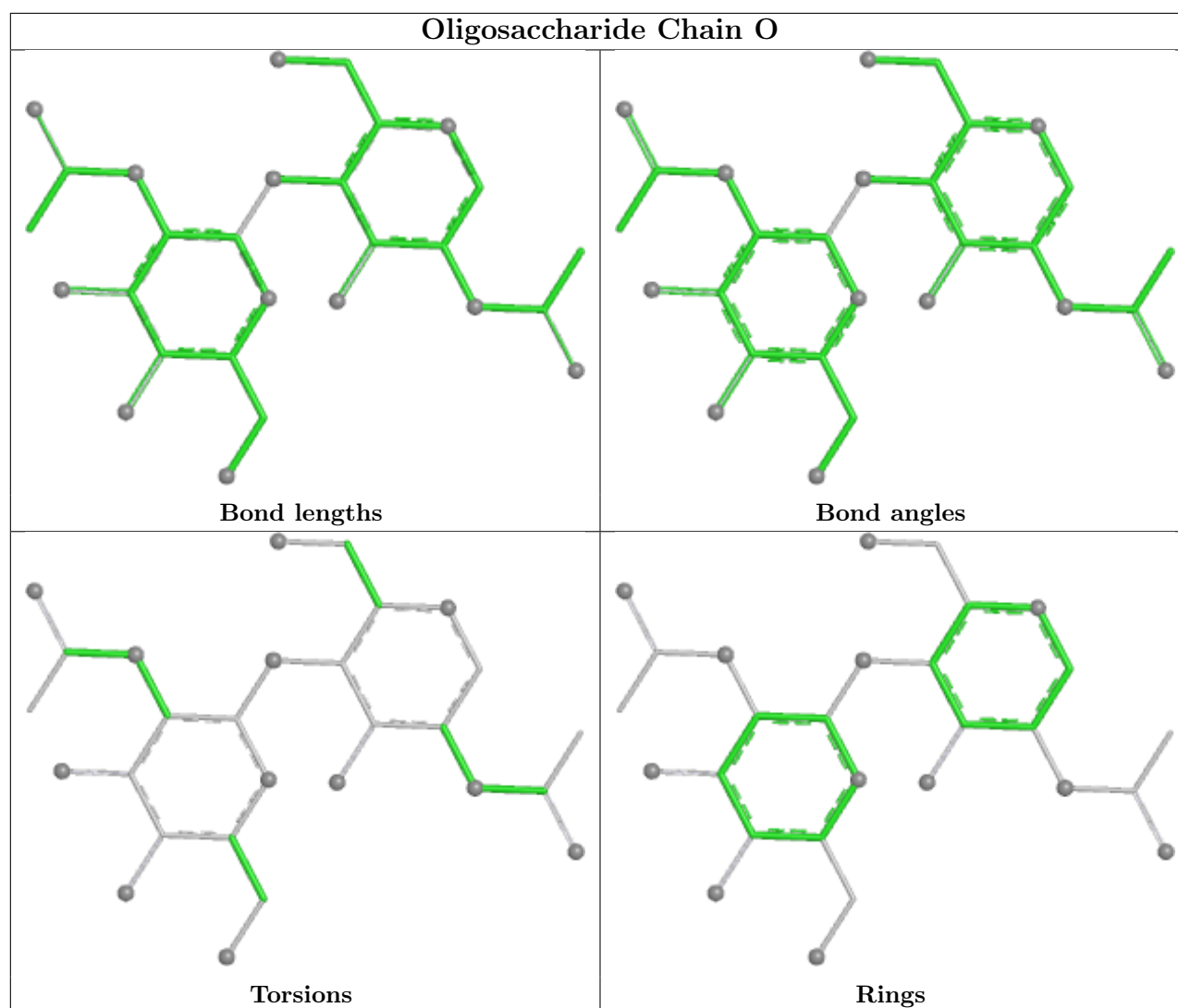
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	NAG	1	0
4	O	2	NAG	1	0
3	Q	2	NAG	2	0
3	N	2	NAG	2	0
3	P	4	SIA	3	0
3	R	4	SIA	1	0
3	Q	4	SIA	5	0
3	M	4	SIA	2	0
3	M	2	NAG	1	0
3	N	4	SIA	2	0
3	R	3	GAL	1	0

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









5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
5	NAG	I	601	1	14,14,15	0.59	0	17,19,21	0.90	1 (5%)
6	SIA	K	603	-	20,20,21	0.63	0	21,28,31	1.08	3 (14%)
5	NAG	K	602	1	14,14,15	0.67	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	602	1	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
5	NAG	K	601	1	14,14,15	0.46	0	17,19,21	1.82	4 (23%)
5	NAG	C	601	1	14,14,15	0.80	0	17,19,21	1.25	1 (5%)
5	NAG	G	401	1	14,14,15	0.47	0	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	601	1	-	0/6/23/26	0/1/1/1
6	SIA	K	603	-	-	2/18/34/38	0/1/1/1
5	NAG	K	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	602	1	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1	-	0/6/23/26	0/1/1/1
5	NAG	C	601	1	-	3/6/23/26	0/1/1/1
5	NAG	G	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	601	NAG	C1-O5-C5	5.31	119.30	112.19
5	K	601	NAG	C6-C5-C4	-3.03	105.58	113.02
6	K	603	SIA	O6-C2-C3	2.89	114.45	110.56
5	G	401	NAG	C1-O5-C5	2.87	116.04	112.19
5	C	601	NAG	C4-C3-C2	2.61	114.84	111.02
5	I	601	NAG	C1-O5-C5	2.35	115.33	112.19
5	K	601	NAG	C4-C3-C2	-2.32	107.62	111.02
5	K	601	NAG	C2-N2-C7	-2.31	119.80	122.90
6	K	603	SIA	O1B-C1-C2	2.12	118.23	112.71
5	C	602	NAG	C1-O5-C5	2.11	115.02	112.19
6	K	603	SIA	O1A-C1-C2	-2.03	118.46	122.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

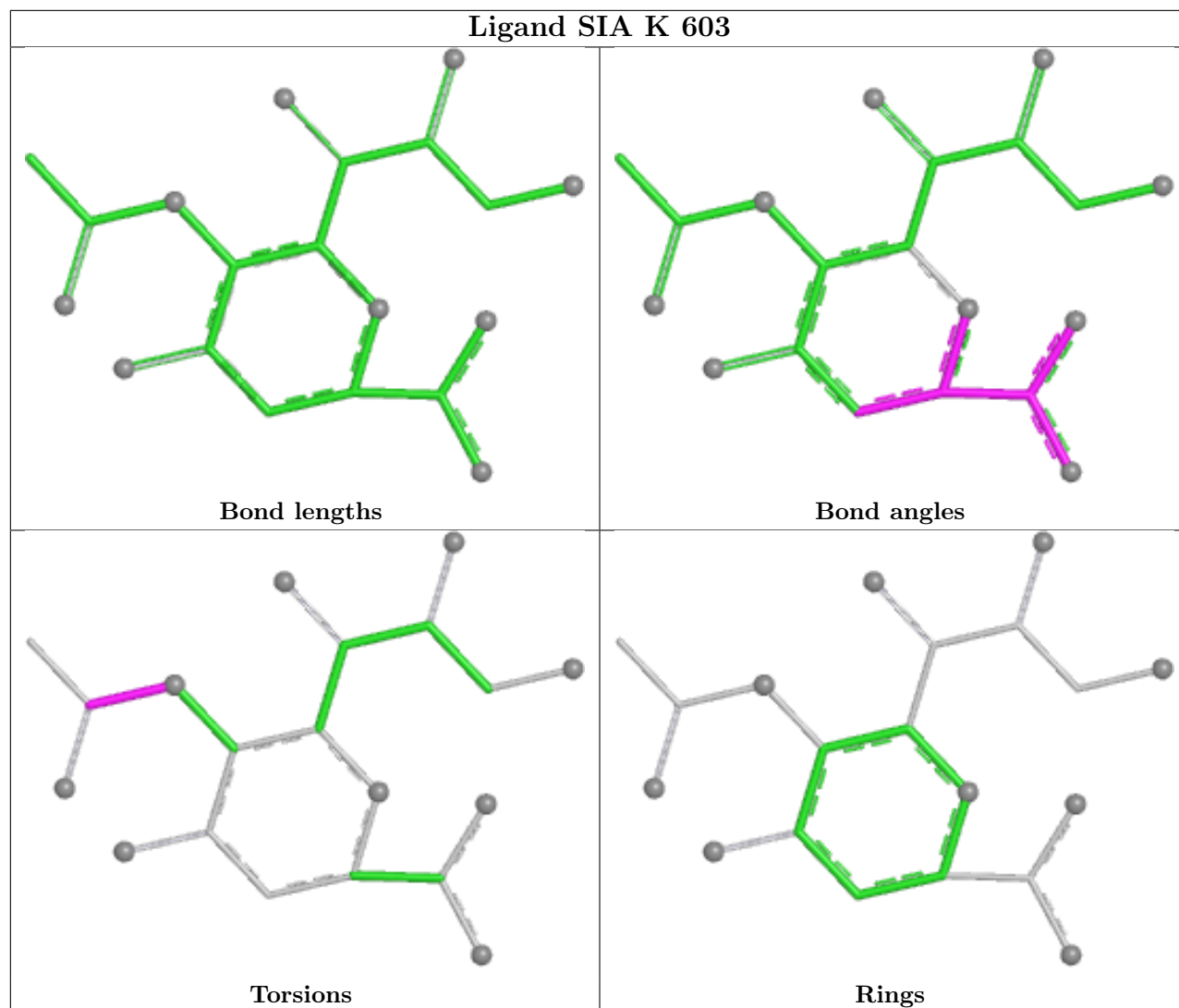
Mol	Chain	Res	Type	Atoms
5	C	601	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	K	602	NAG	O5-C5-C6-O6
5	K	602	NAG	C4-C5-C6-O6
6	K	603	SIA	C11-C10-N5-C5
6	K	603	SIA	O10-C10-N5-C5
5	G	401	NAG	C4-C5-C6-O6
5	G	401	NAG	O5-C5-C6-O6
5	C	601	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	603	SIA	1	0
5	K	602	NAG	4	0
5	C	602	NAG	5	0
5	K	601	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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	322/322 (100%)	0.79	32 (9%)	13 11	30, 55, 103, 206	0
1	C	321/322 (99%)	0.68	28 (8%)	16 13	29, 55, 102, 249	0
1	E	321/322 (99%)	0.51	20 (6%)	26 21	24, 56, 102, 220	0
1	G	322/322 (100%)	0.77	37 (11%)	9 8	29, 58, 98, 209	0
1	I	321/322 (99%)	0.80	28 (8%)	16 13	32, 64, 124, 236	0
1	K	321/322 (99%)	0.66	26 (8%)	18 15	26, 53, 96, 165	0
2	B	162/164 (98%)	0.83	22 (13%)	7 5	32, 72, 129, 175	0
2	D	164/164 (100%)	0.95	18 (10%)	10 9	36, 74, 130, 191	0
2	F	161/164 (98%)	0.77	16 (9%)	13 11	22, 74, 155, 210	0
2	H	162/164 (98%)	0.61	12 (7%)	20 17	28, 59, 101, 138	0
2	J	164/164 (100%)	1.84	67 (40%)	0 0	29, 81, 203, 324	0
2	L	161/164 (98%)	0.85	22 (13%)	6 5	30, 63, 163, 201	0
All	All	2902/2916 (99%)	0.79	328 (11%)	10 9	22, 60, 129, 324	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	9	LEU	8.0
2	J	129	ASN	7.7
2	J	130	ALA	7.6
1	K	12	GLY	7.4
2	J	122	VAL	7.0
2	J	20	GLY	6.9
1	C	9	LEU	6.6
1	E	12	GLY	6.5
1	I	327	ILE	6.4
1	I	8	THR	6.3
2	J	19	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	I	11	ILE	5.8
2	J	149	MET	5.8
1	G	7	ASP	5.5
2	D	129	ASN	5.5
1	K	9	LEU	5.4
2	J	124	SER	5.2
1	G	268	GLY	5.2
2	J	33	GLY	5.2
2	J	140	PHE	5.2
2	J	126	LEU	5.1
1	K	10	CYS	5.1
2	J	139	GLU	4.9
2	H	162	TYR	4.8
1	K	268	GLY	4.8
2	J	156	THR	4.7
1	K	11	ILE	4.7
1	G	146	GLY	4.7
1	K	75	SER	4.7
1	C	74	GLU	4.7
1	E	11	ILE	4.6
2	D	142	HIS	4.5
2	J	133	ILE	4.4
1	A	10	CYS	4.4
1	C	76	LEU	4.4
1	A	161	GLY	4.3
1	G	12	GLY	4.3
2	J	27	GLN	4.3
1	C	75	SER	4.3
1	A	8	THR	4.2
1	C	11	ILE	4.2
1	C	176	GLY	4.2
2	J	36	ALA	4.2
2	F	160	PRO	4.0
2	F	141	TYR	4.0
2	J	141	TYR	4.0
2	J	159	TYR	4.0
2	D	156	THR	3.9
1	C	327	ILE	3.9
1	G	8	THR	3.9
1	A	146	GLY	3.9
2	J	32	SER	3.9
2	L	38	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	13	TYR	3.9
1	E	75	SER	3.9
2	J	26	HIS	3.8
1	A	75	SER	3.8
2	J	160	PRO	3.8
2	J	18	VAL	3.7
2	H	29	GLU	3.7
1	A	11	ILE	3.6
2	F	40	SER	3.6
1	G	162	ASN	3.6
1	A	199	GLN	3.6
1	C	15	ALA	3.6
1	G	78	THR	3.6
2	J	142	HIS	3.5
1	G	11	ILE	3.5
2	J	38	LEU	3.5
2	J	147	THR	3.5
2	J	132	GLU	3.5
1	I	7	ASP	3.5
1	C	60	LYS	3.4
1	I	76	LEU	3.4
2	D	146	ASN	3.4
1	A	267	ALA	3.4
1	C	7	ASP	3.4
1	K	144	HIS	3.4
2	J	9	PHE	3.4
1	I	77	SER	3.3
1	E	327	ILE	3.3
2	J	158	ASP	3.3
2	J	153	LYS	3.2
1	A	326	ASN	3.2
1	I	50	LEU	3.2
2	B	134	GLY	3.2
2	J	155	GLY	3.2
1	A	7	ASP	3.2
1	I	14	HIS	3.2
2	J	131	LYS	3.2
1	G	93	ASN	3.2
2	L	33	GLY	3.2
2	D	24	TYR	3.1
1	K	17	ASN	3.1
1	E	53	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	17	MET	3.1
2	L	159	TYR	3.1
1	G	53	VAL	3.1
2	J	23	GLY	3.1
2	J	24	TYR	3.1
1	K	90	SER	3.1
2	D	134	GLY	3.1
1	A	51	ARG	3.1
1	K	152	LYS	3.1
2	L	162	TYR	3.0
2	H	160	PRO	3.0
2	J	138	PHE	3.0
1	G	99	GLY	3.0
2	J	16	GLY	3.0
1	C	78	THR	3.0
1	A	195	GLN	3.0
2	H	135	ASN	3.0
2	J	31	GLY	3.0
1	A	126	THR	3.0
1	C	131	ASN	3.0
1	I	10	CYS	3.0
2	J	121	LYS	2.9
2	J	127	LYS	2.9
2	B	16	GLY	2.9
1	A	130	PRO	2.9
2	J	146	ASN	2.9
2	H	138	PHE	2.9
2	J	25	HIS	2.9
1	G	227	ARG	2.9
1	A	266	ASN	2.9
1	G	35	SER	2.9
2	D	151	SER	2.9
1	I	78	THR	2.9
2	D	137	CYS	2.9
1	G	327	ILE	2.9
2	L	141	TYR	2.9
2	L	160	PRO	2.9
1	A	19	THR	2.8
2	J	29	GLU	2.8
1	G	145	ALA	2.8
1	I	174	ASP	2.8
1	K	200	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	2.8
2	F	38	LEU	2.8
1	K	135	ASN	2.8
2	J	15	THR	2.8
2	D	155	GLY	2.8
2	F	144	CYS	2.7
2	D	152	VAL	2.7
1	A	327	ILE	2.7
2	B	162	TYR	2.7
1	I	326	ASN	2.7
2	B	32	SER	2.7
1	A	201	ALA	2.7
2	L	154	ASN	2.7
1	G	161	GLY	2.7
1	C	10	CYS	2.7
1	G	10	CYS	2.7
2	F	162	TYR	2.7
2	J	144	CYS	2.7
1	C	195	GLN	2.7
2	B	152	VAL	2.7
2	J	164	GLU	2.7
2	L	29	GLU	2.7
1	C	147	ALA	2.6
2	J	5	ALA	2.6
1	G	279	HIS	2.6
2	B	141	TYR	2.6
1	I	267	ALA	2.6
1	G	51	ARG	2.6
1	E	10	CYS	2.6
1	A	135	ASN	2.6
2	F	19	ASP	2.6
1	C	77	SER	2.6
2	F	124	SER	2.6
1	I	34	HIS	2.6
1	A	9	LEU	2.6
1	A	282	ASN	2.6
2	B	140	PHE	2.6
2	B	19	ASP	2.6
2	J	21	TRP	2.6
1	C	163	SER	2.5
1	E	295	SER	2.5
2	L	148	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	128	ASN	2.5
2	J	135	ASN	2.5
2	J	125	GLN	2.5
2	B	135	ASN	2.5
1	G	328	PRO	2.5
1	E	78	THR	2.5
1	C	294	THR	2.5
2	D	126	LEU	2.4
1	I	137	GLY	2.4
2	J	136	GLY	2.4
2	H	124	SER	2.4
1	E	51	ARG	2.4
2	F	143	LYS	2.4
2	J	119	TYR	2.4
2	L	22	TYR	2.4
1	C	293	ASN	2.4
1	I	162	ASN	2.4
1	K	30	VAL	2.4
2	H	150	GLU	2.4
2	J	161	LYS	2.4
2	H	157	TYR	2.4
2	B	102	LEU	2.4
2	F	126	LEU	2.4
2	B	128	ASN	2.4
2	B	137	CYS	2.4
1	E	268	GLY	2.4
1	I	228	GLU	2.4
2	J	150	GLU	2.4
2	H	156	THR	2.4
1	A	50	LEU	2.4
1	I	67	ILE	2.4
1	G	131	ASN	2.4
2	J	60	ASN	2.4
2	J	154	ASN	2.4
1	A	12	GLY	2.4
1	I	32	VAL	2.4
2	B	132	GLU	2.4
2	H	139	GLU	2.4
1	C	267	ALA	2.4
2	D	141	TYR	2.4
1	K	14	HIS	2.4
1	K	324	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	67	ILE	2.4
1	I	172	ILE	2.4
2	L	134	GLY	2.3
2	J	145	ASP	2.3
1	E	118	GLU	2.3
1	K	54	ALA	2.3
1	G	90	SER	2.3
1	G	147	ALA	2.3
1	E	9	LEU	2.3
1	G	116	SER	2.3
2	D	38	LEU	2.3
2	D	133	ILE	2.3
2	F	157	TYR	2.3
2	B	138	PHE	2.3
2	F	140	PHE	2.3
2	B	38	LEU	2.3
1	C	90	SER	2.3
1	G	77	SER	2.3
1	G	91	SER	2.3
1	I	271	ILE	2.3
2	J	54	SER	2.3
2	L	15	THR	2.3
1	C	282	ASN	2.3
1	G	140	ALA	2.3
2	J	35	ALA	2.3
1	A	76	LEU	2.3
2	F	116	LYS	2.3
2	L	127	LYS	2.3
1	G	144	HIS	2.3
1	C	322	THR	2.3
1	A	328	PRO	2.3
1	C	145	ALA	2.2
1	A	149	SER	2.2
2	L	24	TYR	2.2
1	A	162	ASN	2.2
1	E	76	LEU	2.2
2	L	43	ASN	2.2
2	J	30	GLN	2.2
2	L	152	VAL	2.2
1	E	13	TYR	2.2
2	D	162	TYR	2.2
2	L	149	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	50	LEU	2.2
2	B	139	GLU	2.2
1	C	144	HIS	2.2
1	K	92	ASP	2.2
2	B	160	PRO	2.2
1	G	295	SER	2.2
2	J	157	TYR	2.2
2	J	162	TYR	2.2
1	G	228	GLU	2.2
2	D	158	ASP	2.2
1	E	294	THR	2.2
1	A	136	LYS	2.2
1	C	146	GLY	2.2
1	I	268	GLY	2.2
2	H	134	GLY	2.2
2	J	134	GLY	2.2
2	J	143	LYS	2.2
1	K	15	ALA	2.2
2	L	120	GLU	2.2
2	B	149	MET	2.1
2	F	127	LYS	2.1
1	I	12	GLY	2.1
1	I	211	ARG	2.1
1	K	211	ARG	2.1
2	D	62	GLN	2.1
2	B	49	THR	2.1
2	J	1	GLY	2.1
2	L	31	GLY	2.1
1	G	76	LEU	2.1
1	I	147	ALA	2.1
1	K	13	TYR	2.1
1	K	18	SER	2.1
2	F	132	GLU	2.1
2	L	124	SER	2.1
2	B	27	GLN	2.1
1	G	28	LYS	2.1
1	C	8	THR	2.1
1	G	79	ALA	2.1
1	K	74	GLU	2.1
2	D	124	SER	2.1
1	G	14	HIS	2.1
2	L	128	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	118	LEU	2.1
1	A	145	ALA	2.1
1	K	129	TRP	2.1
2	B	133	ILE	2.1
1	E	219	GLU	2.1
1	A	163	SER	2.0
1	G	60	LYS	2.0
1	I	149	SER	2.0
1	K	195	GLN	2.0
1	E	293	ASN	2.0
1	G	9	LEU	2.0
1	E	211	ARG	2.0
2	L	156	THR	2.0
1	A	13	TYR	2.0
2	B	153	LYS	2.0
2	J	34	TYR	2.0
1	E	162	ASN	2.0
2	F	128	ASN	2.0
1	C	12	GLY	2.0
1	E	52	GLY	2.0
1	K	327	ILE	2.0
2	H	158	ASP	2.0
2	J	22	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GAL	Q	1	11/12	0.27	0.25	99,134,164,181	0
3	GAL	P	1	11/12	0.33	0.17	122,137,149,151	0
3	GAL	N	1	11/12	0.55	0.14	57,74,100,104	0
3	GAL	R	1	11/12	0.56	0.15	62,112,129,131	0
3	GAL	M	1	11/12	0.57	0.13	84,94,133,136	0

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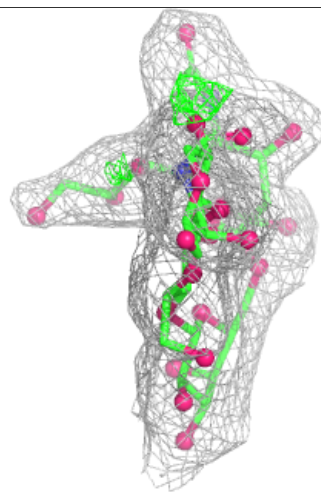
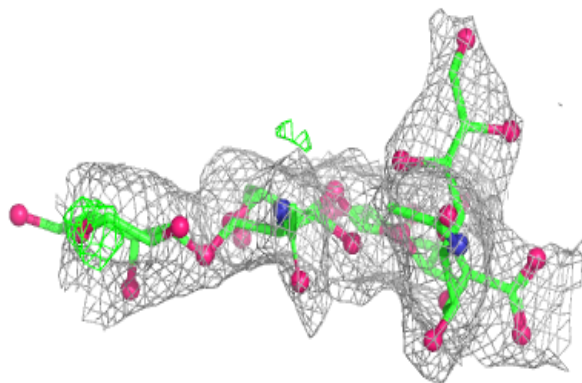
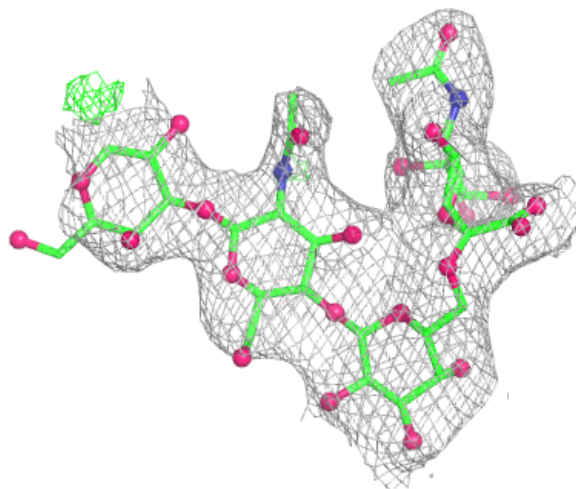
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	M	2	14/15	0.76	0.12	51,70,78,85	0
3	NAG	R	2	14/15	0.76	0.12	62,83,91,98	0
3	NAG	P	2	14/15	0.80	0.13	77,97,113,115	0
3	NAG	Q	2	14/15	0.81	0.14	72,89,109,111	0
3	GAL	R	3	11/12	0.81	0.14	78,96,102,114	0
3	GAL	M	3	11/12	0.82	0.10	42,52,72,77	0
4	NAG	O	1	14/15	0.83	0.11	52,64,82,92	0
4	NAG	O	2	14/15	0.83	0.10	63,93,116,119	0
3	SIA	P	4	20/21	0.85	0.12	47,59,73,76	0
3	GAL	Q	3	11/12	0.86	0.12	45,65,85,103	0
3	SIA	Q	4	20/21	0.87	0.12	44,68,95,96	0
3	SIA	N	4	20/21	0.87	0.11	41,62,76,87	0
3	GAL	P	3	11/12	0.87	0.09	53,71,89,92	0
3	GAL	N	3	11/12	0.89	0.09	53,69,77,79	0
3	SIA	R	4	20/21	0.90	0.10	38,55,67,73	0
3	SIA	M	4	20/21	0.92	0.09	34,46,60,66	0
3	NAG	N	2	14/15	0.92	0.09	60,71,84,92	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.

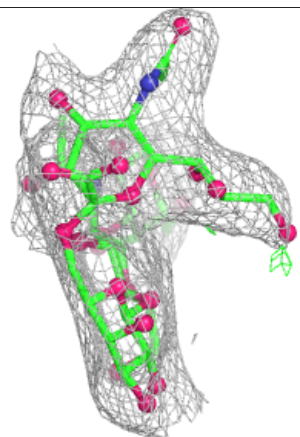
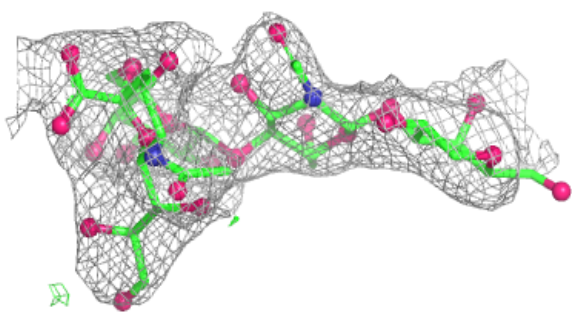
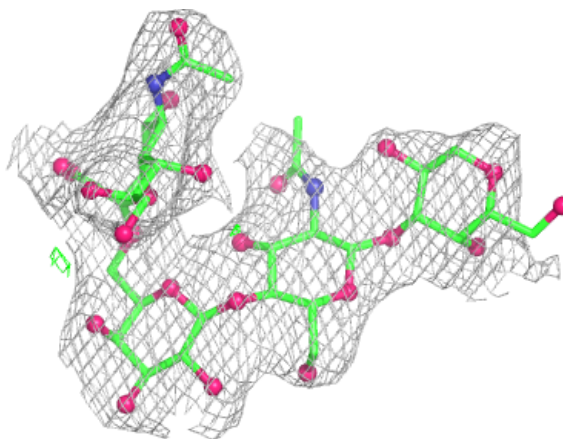
Electron density around Chain M:

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



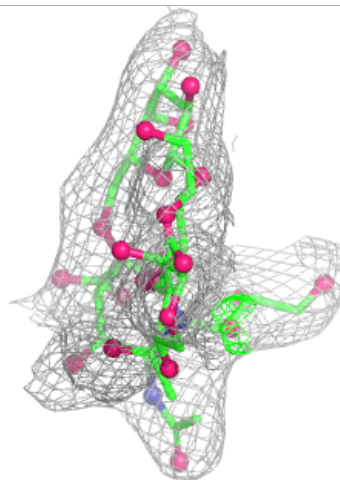
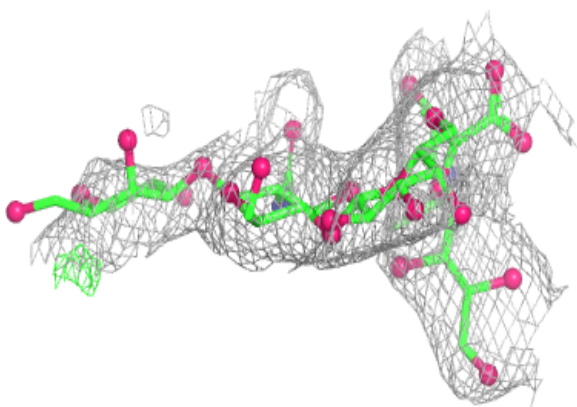
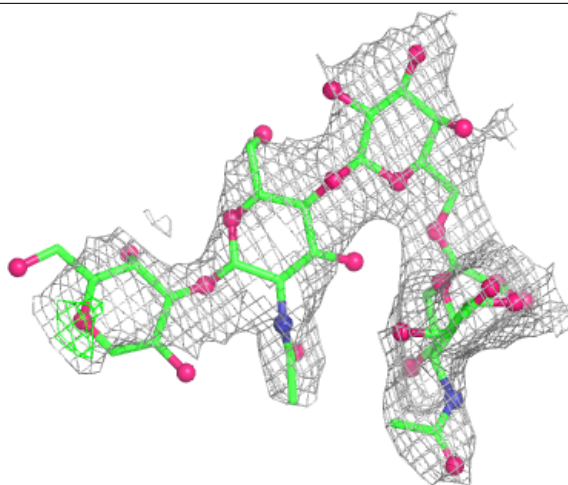
Electron density around Chain N:

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



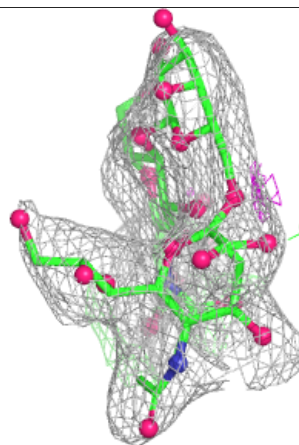
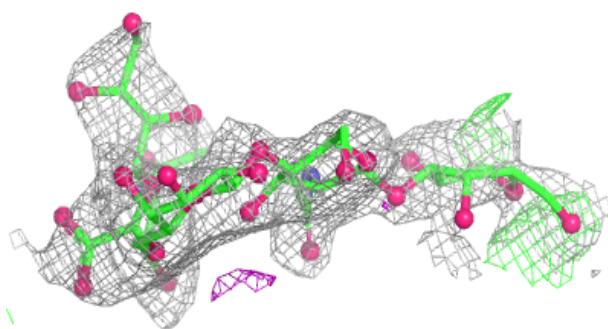
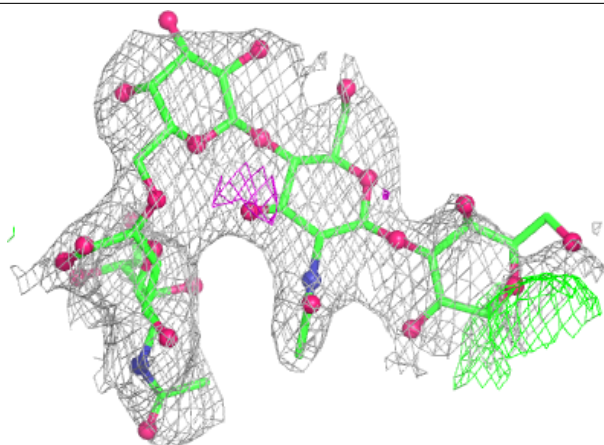
Electron density around Chain P:

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



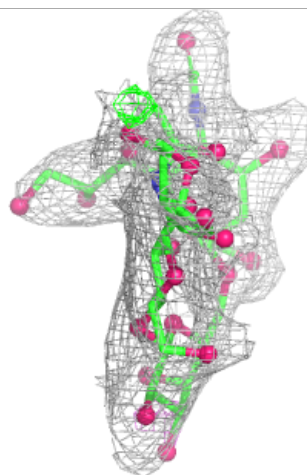
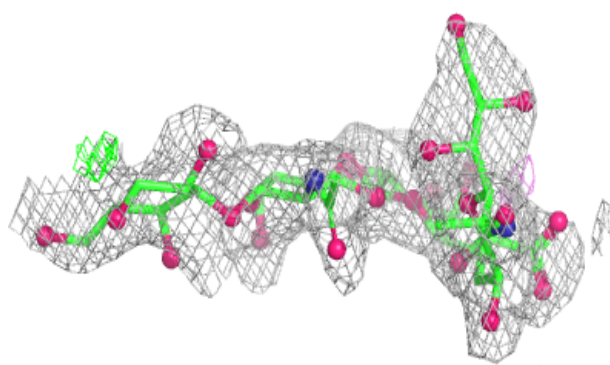
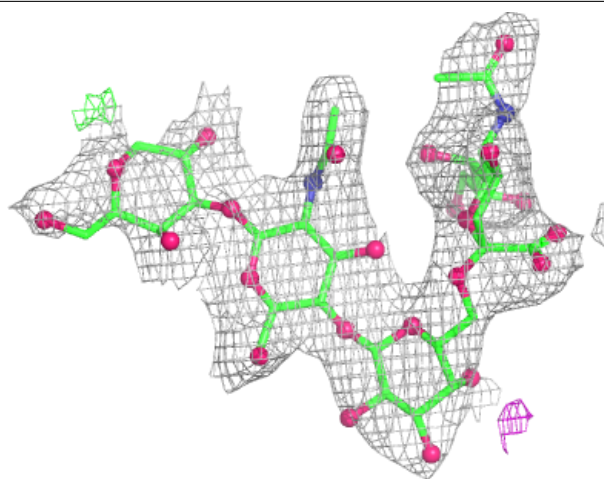
Electron density around Chain Q:

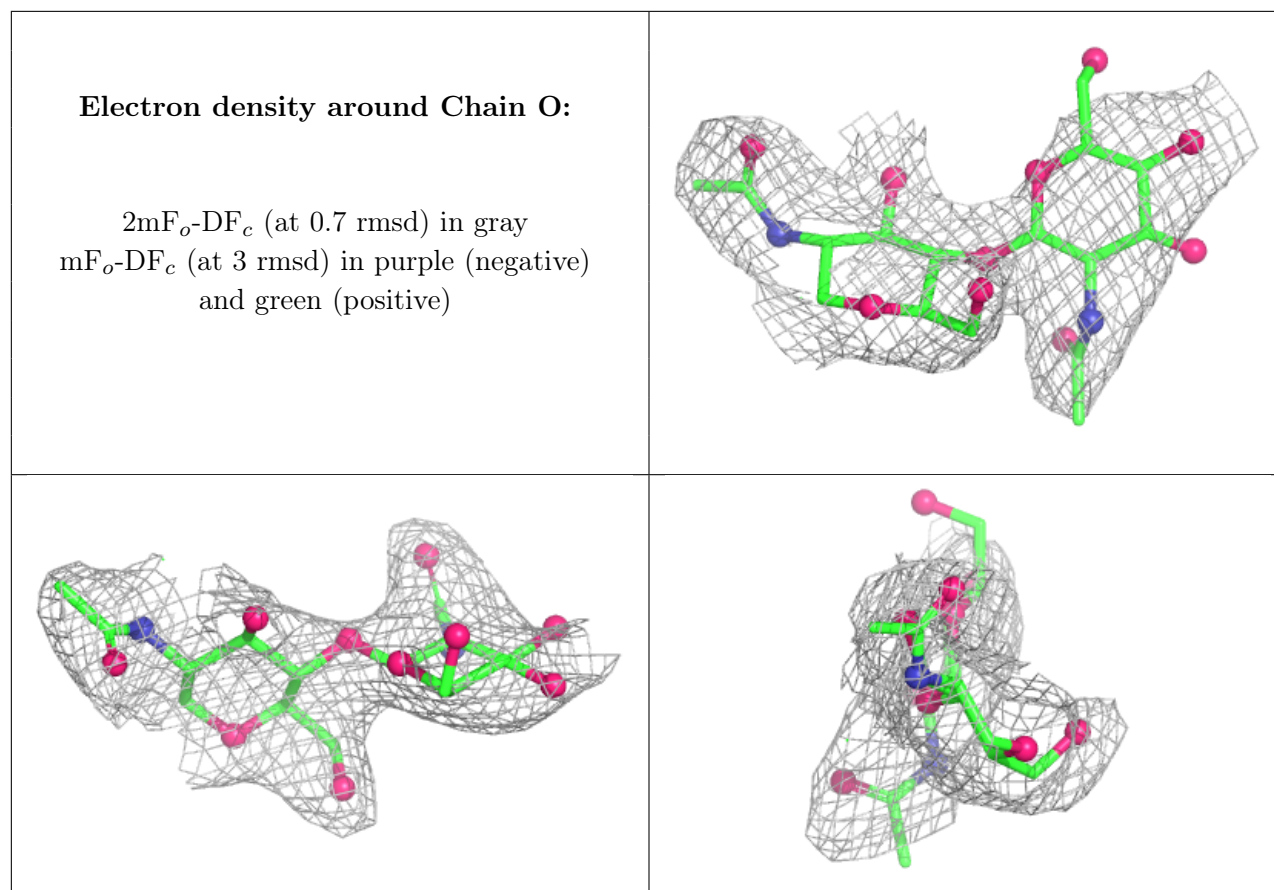
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain R:

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





6.4 Ligands ⓘ

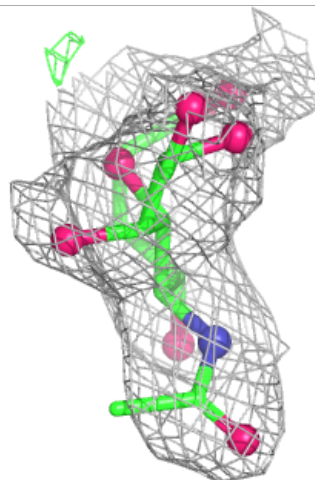
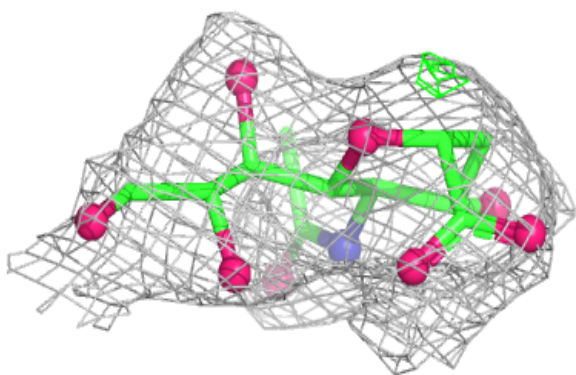
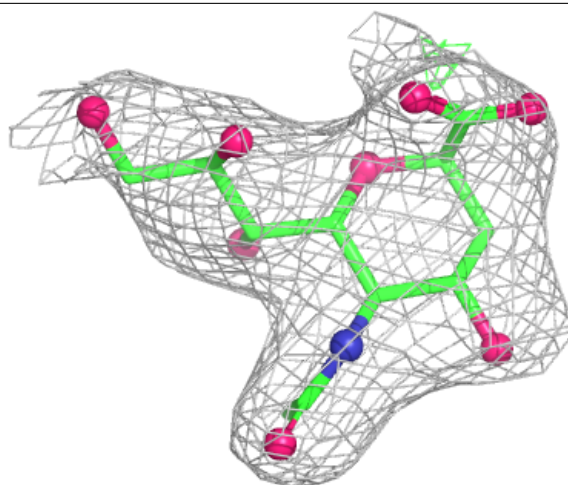
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	I	601	14/15	0.43	0.15	101,130,147,150	0
5	NAG	G	401	14/15	0.51	0.14	78,108,129,132	0
5	NAG	C	601	14/15	0.55	0.18	66,93,106,114	0
5	NAG	K	602	14/15	0.66	0.20	76,105,115,115	0
5	NAG	K	601	14/15	0.69	0.17	119,128,136,137	0
5	NAG	C	602	14/15	0.85	0.10	25,57,74,79	0
6	SIA	K	603	20/21	0.90	0.10	42,52,69,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SIA K 603:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.