



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 07:25 PM EDT

PDB ID : 4JU0
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

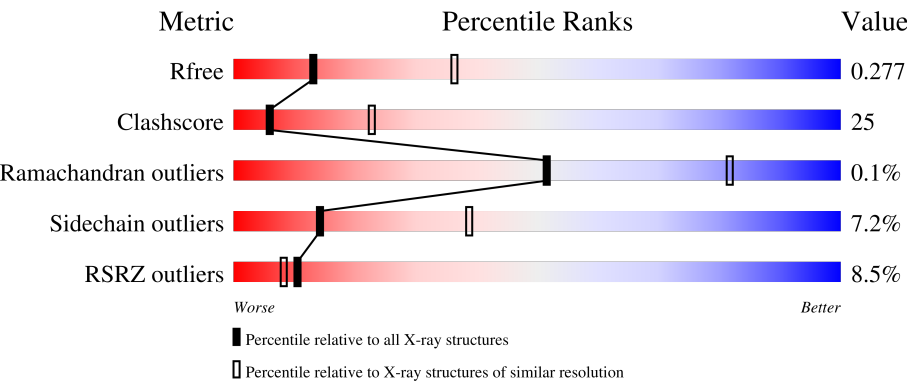
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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	
1	C	322	
1	E	322	
1	G	322	
1	I	322	

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAL	P	1	-	-	-	X

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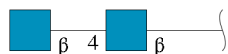
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	J	164	Total	C	N	O	S	0	0	0
			1315	826	221	262	6			
2	L	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			

- 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.



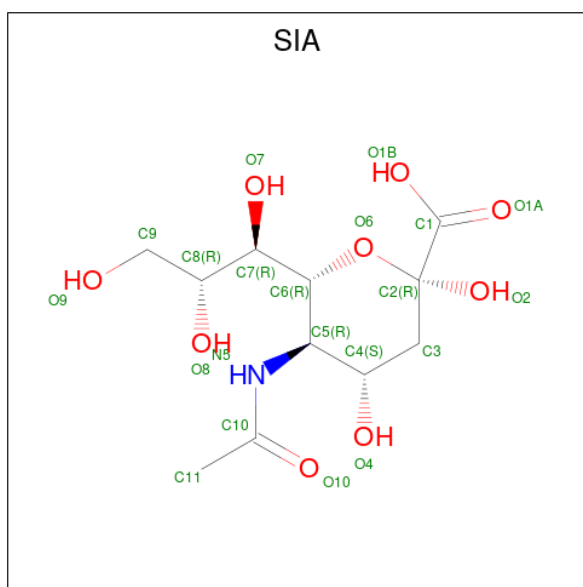
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: 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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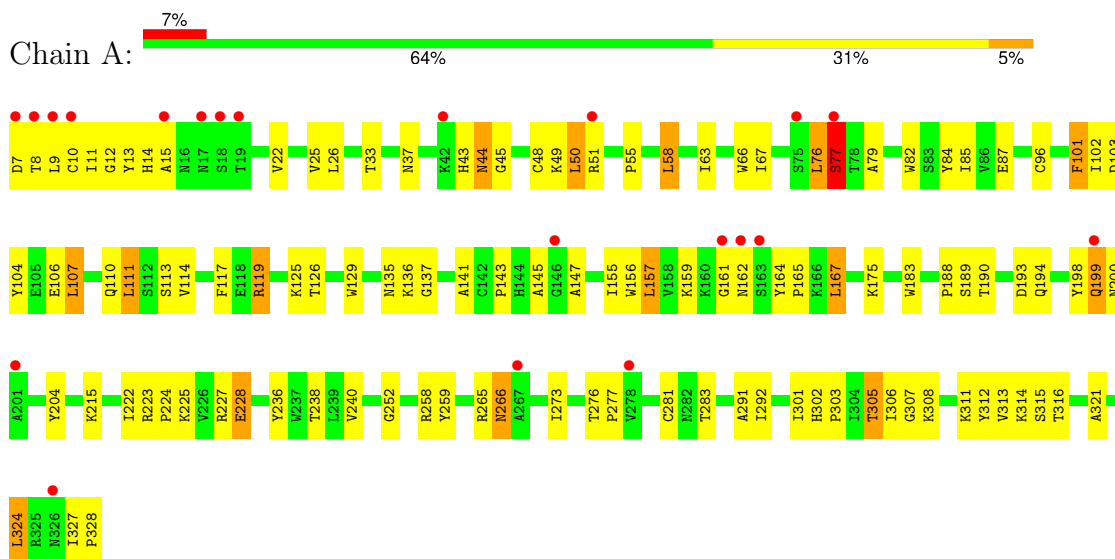
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	8	Total	O	0	0
			8	8		

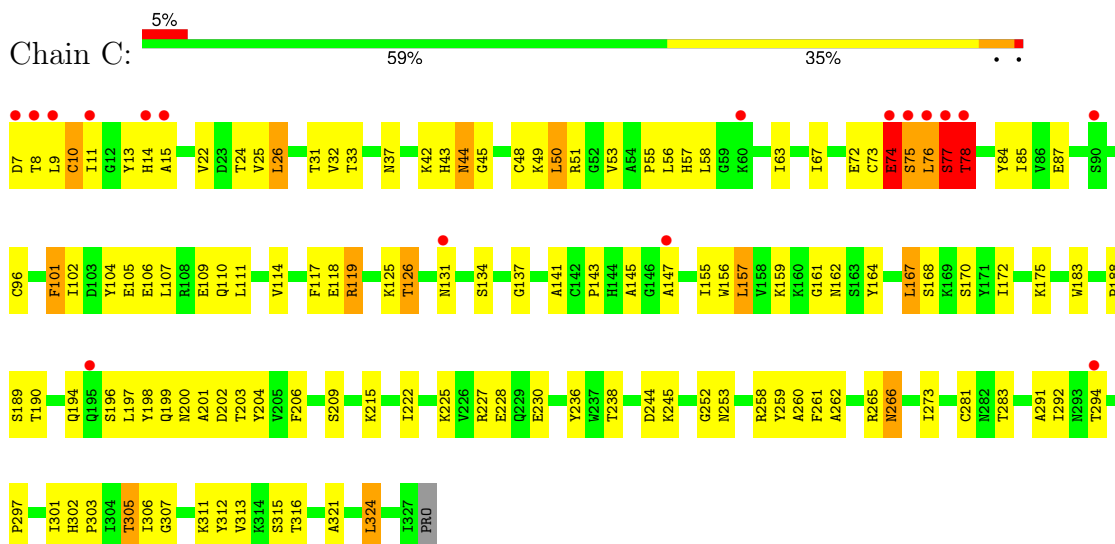
3 Residue-property plots [i](#)

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

• Molecule 1: Hemagglutinin

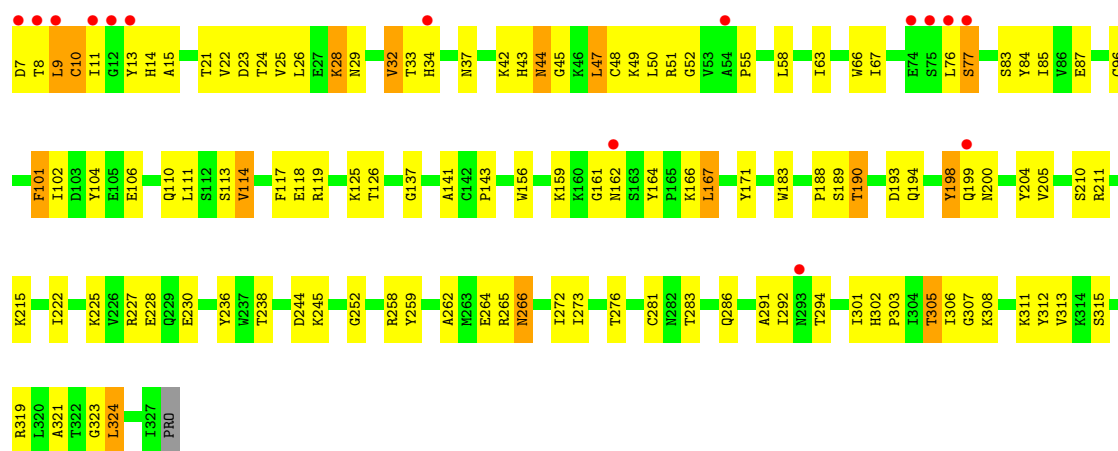


• Molecule 1: Hemagglutinin

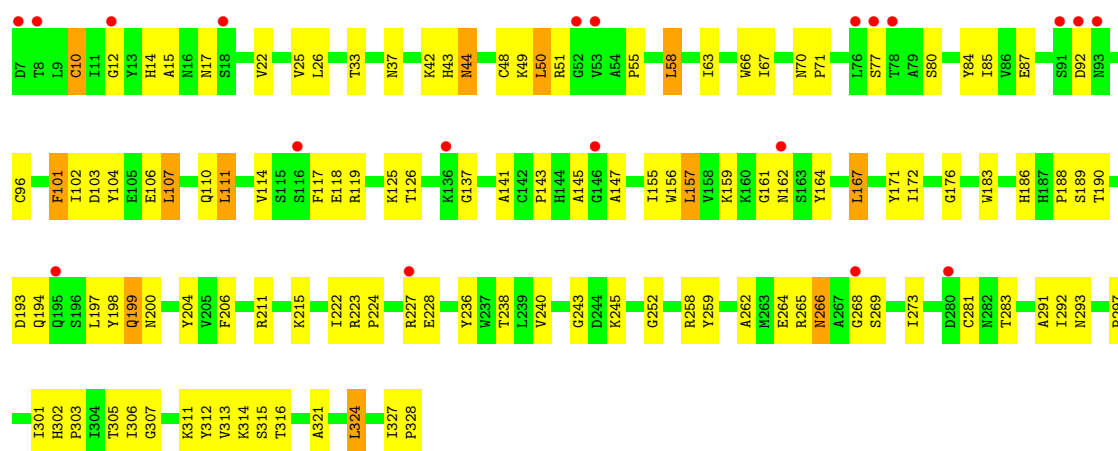


• Molecule 1: Hemagglutinin

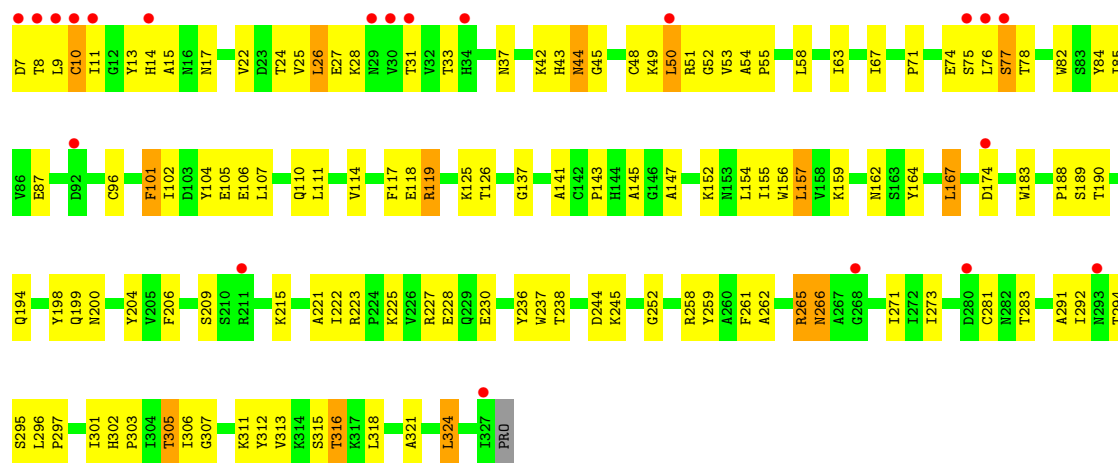




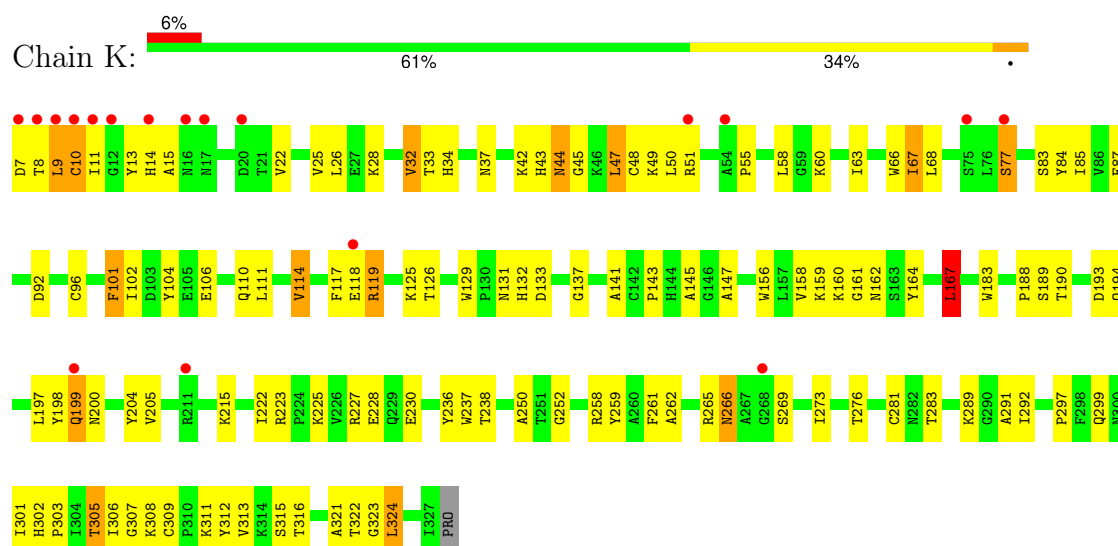
• Molecule 1: Hemagglutinin



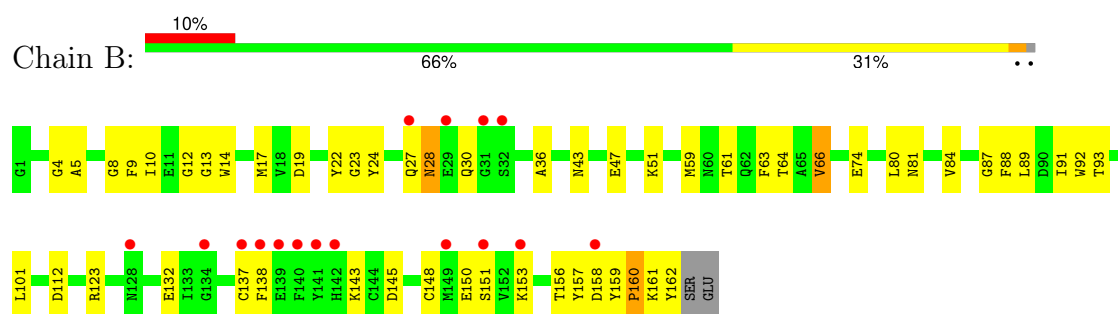
• Molecule 1: Hemagglutinin



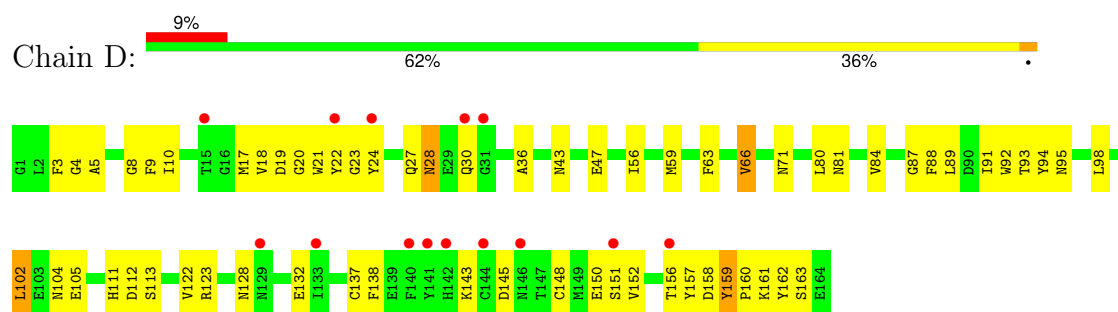
• Molecule 1: Hemagglutinin



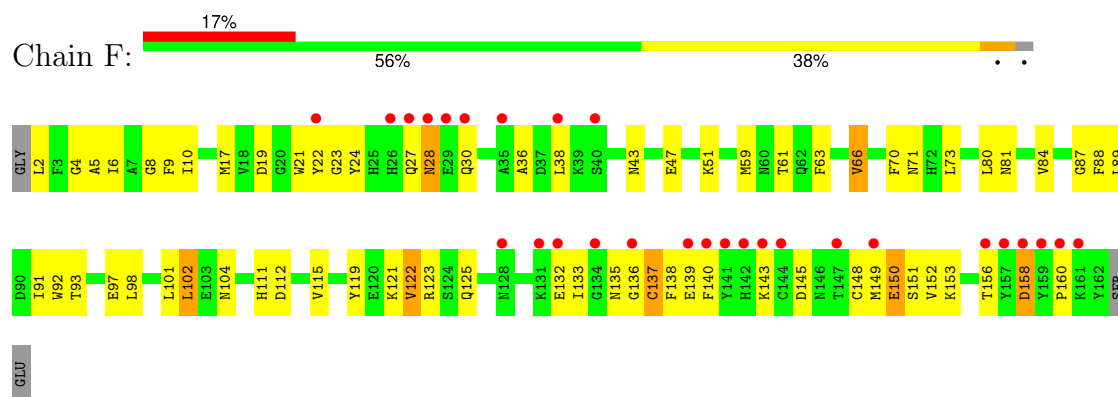
• Molecule 2: Hemagglutinin



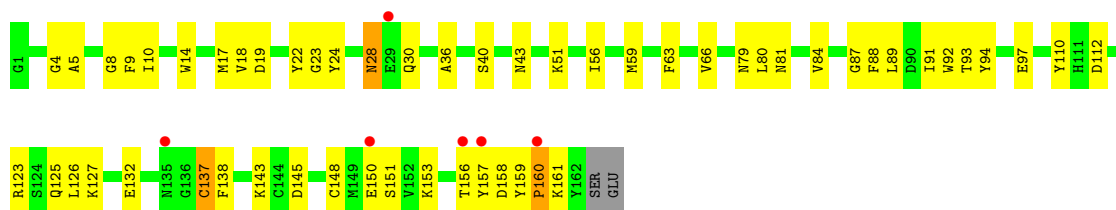
• Molecule 2: Hemagglutinin



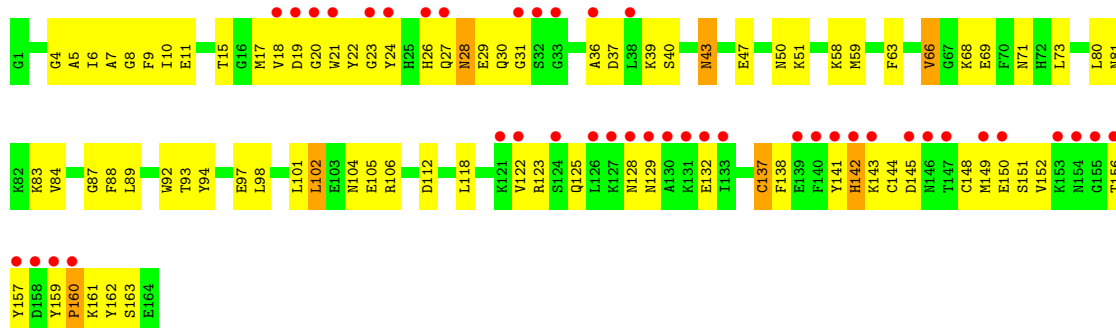
• Molecule 2: Hemagglutinin



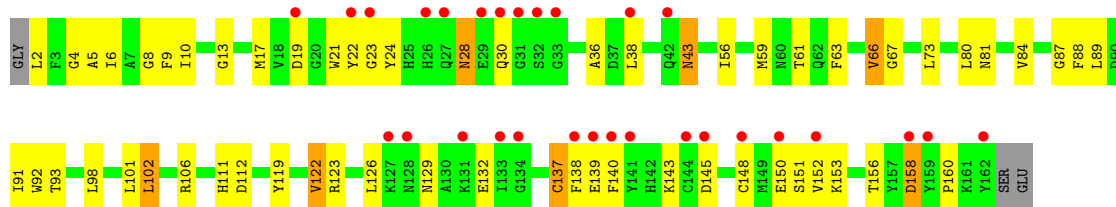
- Molecule 2: Hemagglutinin



- 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

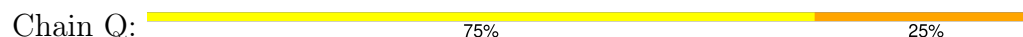




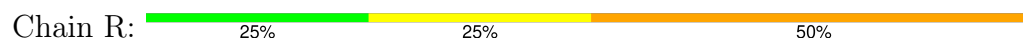
- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- 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



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



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 40.23 – 2.91	Depositor EDS
% Data completeness (in resolution range)	88.2 (40.22-2.91) 94.3 (40.23-2.91)	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 (5.04%)	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)	0.30 , 54.0	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	0.25	0/2577	0.71	8/3501 (0.2%)
1	C	0.29	1/2573 (0.0%)	0.68	9/3494 (0.3%)
1	E	0.24	0/2573	0.60	8/3494 (0.2%)
1	G	0.26	0/2577	0.70	6/3501 (0.2%)
1	I	0.25	0/2573	0.60	6/3494 (0.2%)
1	K	0.24	0/2573	0.65	8/3494 (0.2%)
2	B	0.24	0/1333	0.54	1/1797 (0.1%)
2	D	0.26	0/1343	0.48	1/1811 (0.1%)
2	F	0.24	0/1330	0.49	0/1794
2	H	0.24	0/1333	0.50	1/1797 (0.1%)
2	J	0.24	0/1343	0.47	1/1811 (0.1%)
2	L	0.24	0/1330	0.49	0/1794
All	All	0.25	1/23458 (0.0%)	0.61	49/31782 (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	CB-SG	-5.76	1.72	1.81

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	119	ARG	NE-CZ-NH1	-16.32	112.14	120.30
1	A	119	ARG	NE-CZ-NH1	-16.20	112.20	120.30
1	A	119	ARG	NE-CZ-NH2	16.09	128.34	120.30
1	G	119	ARG	NE-CZ-NH2	15.81	128.21	120.30
1	K	199	GLN	CB-CA-C	-14.58	81.24	110.40
1	C	78	THR	N-CA-C	12.11	143.70	111.00
1	C	76	LEU	CB-CA-C	-11.03	89.24	110.20
1	C	77	SER	N-CA-CB	-10.25	95.13	110.50
1	I	77	SER	CB-CA-C	-9.63	91.80	110.10
1	C	119	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	K	119	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	G	200	ASN	N-CA-C	-8.09	89.15	111.00
1	I	119	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	119	ARG	CD-NE-CZ	8.03	134.85	123.60
1	G	119	ARG	CD-NE-CZ	7.97	134.76	123.60
1	C	75	SER	CB-CA-C	-7.95	95.00	110.10
1	I	119	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	A	76	LEU	N-CA-CB	-7.59	95.22	110.40
1	C	119	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	K	119	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	E	119	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	K	200	ASN	N-CA-C	-7.46	90.86	111.00
1	A	77	SER	N-CA-C	7.04	130.02	111.00
1	I	78	THR	N-CA-CB	-6.77	97.44	110.30
1	E	119	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	G	200	ASN	N-CA-CB	6.37	122.06	110.60
1	A	76	LEU	N-CA-C	6.33	128.08	111.00
1	A	200	ASN	N-CA-C	-6.30	93.97	111.00
1	E	167	LEU	CA-CB-CG	6.06	129.25	115.30
1	C	200	ASN	N-CA-C	-5.97	94.89	111.00
1	K	167	LEU	CA-CB-CG	5.90	128.86	115.30
1	G	199	GLN	CB-CA-C	-5.77	98.86	110.40
1	I	200	ASN	N-CA-C	-5.60	95.87	111.00
1	E	167	LEU	CB-CG-CD2	5.41	120.20	111.00
2	B	66	VAL	CB-CA-C	-5.39	101.17	111.40
1	E	200	ASN	N-CA-C	-5.38	96.48	111.00
2	H	66	VAL	CB-CA-C	-5.31	101.31	111.40
1	K	167	LEU	CB-CG-CD2	5.31	120.03	111.00
1	E	198	TYR	CB-CA-C	5.22	120.85	110.40
1	I	75	SER	CB-CA-C	5.22	120.02	110.10
1	A	77	SER	CB-CA-C	-5.19	100.23	110.10
1	C	74	GLU	N-CA-C	-5.13	97.15	111.00
1	E	28	LYS	CB-CA-C	-5.12	100.16	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	32	VAL	CG1-CB-CG2	5.09	119.04	110.90
1	K	32	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	C	78	THR	CB-CA-C	-5.07	97.92	111.60
1	K	200	ASN	N-CA-CB	5.07	119.72	110.60
2	J	142	HIS	N-CA-C	5.04	124.61	111.00
2	D	163	SER	N-CA-C	5.03	124.59	111.00

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	118	0
1	C	2510	0	2452	160	0
1	E	2510	0	2453	130	0
1	G	2513	0	2455	117	0
1	I	2510	0	2452	166	0
1	K	2510	0	2452	150	0
2	B	1305	0	1228	54	0
2	D	1315	0	1227	70	0
2	F	1302	0	1226	84	0
2	H	1305	0	1228	59	0
2	J	1315	0	1227	155	0
2	L	1302	0	1226	81	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	32	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	32	0
7	F	11	0	0	23	0
7	G	16	0	0	15	0
7	H	6	0	0	12	0
7	I	25	0	0	50	0
7	J	22	0	0	54	0
7	K	26	0	0	51	0
7	L	8	0	0	17	0
All	All	23507	0	22438	1137	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 25.

All (1137) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:113:SER:N	7:D:202:HOH:O	1.94	1.01
1:K:131:ASN:C	7:K:719:HOH:O	1.97	1.00
1:E:24:THR:CA	7:E:714:HOH:O	2.09	1.00
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:97:GLU:CD	7:J:221:HOH:O	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:106:GLU:CD	7:K:718:HOH:O	2.05	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
1:E:21:THR:HB	1:E:29:ASN:OD1	1.68	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
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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:101:LEU:C	7:L:208:HOH:O	2.09	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
2:J:84:VAL:C	7:J:213:HOH:O	2.09	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
2:J:97:GLU:OE2	7:J:221:HOH:O	1.90	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
1:E:10:CYS:HA	2:F:137:CYS:HA	1.56	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:E:8:THR:OG1	7:E:709:HOH:O	1.92	0.87
1:I:265:ARG:C	7:I:718:HOH:O	2.12	0.87
1:C:57:HIS:ND1	7:C:720:HOH:O	2.08	0.86
2:L:126:LEU:C	7:L:207:HOH:O	2.13	0.86
2:J:73:LEU:C	7:K:718:HOH:O	2.14	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
1:I:27:GLU:HA	7:I:719:HOH:O	1.78	0.84
1:C:106:GLU:C	7:C:711:HOH:O	2.16	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:L:101:LEU:O	7:L:208:HOH:O	1.97	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
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:A:114:VAL:C	7:A:922:HOH:O	2.18	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: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
2:F:149:MET:C	7:F:204:HOH:O	2.19	0.80
1:I:315:SER:CA	7:I:724:HOH:O	2.29	0.80
2:H:125:GLN:C	7:H:204:HOH:O	2.19	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:ILE:O	7:K:724:HOH:O	2.00	0.80
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:A:159:LYS:HZ2	1:A:199:GLN:HG3	1.46	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
1:I:159:LYS:HZ2	1:I:199:GLN:HG2	1.48	0.78
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
1:I:55:PRO:C	7:I:720:HOH:O	2.23	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
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:E:159:LYS:HZ2	1:E:199:GLN:HG2	1.50	0.76
1:G:172:ILE:HA	7:G:516:HOH:O	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:LEU:HA	7:F:206:HOH:O	1.85	0.75
1:K:322:THR:OG1	7:K:720:HOH:O	1.93	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:L:30:GLN:HE22	2:L:145:ASP:HB2	1.53	0.74
2:J:157:TYR:CE2	7:J:219:HOH:O	2.40	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
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
1:K:159:LYS:HZ2	1:K:199:GLN:HE21	1.37	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:A:159:LYS:HZ2	1:A:199:GLN:CG	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:6:ILE:C	7:J:211:HOH:O	2.23	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:J:31:GLY:C	7:J:214:HOH:O	2.30	0.69
2:D:123:ARG:HD2	2:D:132:GLU:OE1	1.91	0.69
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:I:26:LEU:HD22	2:J:105:GLU:CD	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:66:VAL:CA	7:L:206:HOH:O	2.38	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:K:67:ILE:C	7:K:725:HOH:O	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:84:VAL:O	7:J:213:HOH:O	2.13	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
1:G:269:SER:C	7:G:515:HOH:O	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:81:ASN:O	2:L:84:VAL:HG12	1.99	0.63
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
1:C:9:LEU:C	7:C:708:HOH:O	2.37	0.62
2:H:18:VAL:CA	7:H:206:HOH:O	2.48	0.62
2:J:37:ASP:C	7:J:202:HOH:O	2.37	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LYS:HE2	1:C:230:GLU:HG3	1.83	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
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
1:I:8:THR:HG1	2:J:27:GLN:HB3	1.66	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
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
2:D:95:ASN:ND2	7:D:205:HOH:O	2.28	0.59
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
1:I:159:LYS:HZ2	1:I:199:GLN:CG	2.16	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:J:11:GLU:C	7:J:217:HOH:O	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:CA	7:A:922:HOH:O	2.35	0.57
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: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
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:E:164:TYR:CZ	1:E:252:GLY:HA2	2.40	0.56
2:F:104:ASN:CG	7:F:207:HOH:O	2.23	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: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:E:161:GLY:O	1:E:162:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:105:GLU:CD	2:J:71:ASN:HB3	2.25	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
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
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
2:F:158:ASP:C	2:F:160:PRO:HD3	2.27	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
2:H:18:VAL:C	7:H:206:HOH:O	2.44	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:57:HIS:CD2	7:C:720:HOH:O	2.52	0.54
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
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: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
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
2:F:70:PHE:C	7:F:211:HOH:O	2.47	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:E:313:VAL:HG13	2:F:93:THR:HA	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:307:GLY:HA2	2:H:63:PHE:CE1	2.44	0.53
1:K:44:ASN:ND2	1:K:291:ALA:H	2.06	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: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
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: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: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:A:11:ILE:C	2:B:14:TRP:CH2	2.82	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
1:K:312:TYR:C	7:K:721:HOH:O	2.28	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
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: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
1:I:25:VAL:HG23	2:J:101:LEU:O	2.10	0.52
1:A:162:ASN:CG	1:A:199:GLN:NE2	2.63	0.51
1:C:126:THR:CB	1:K:92:ASP:OD1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:J:157:TYR:CZ	7:J:219:HOH:O	2.62	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
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:E:159:LYS:HZ2	1:E:199:GLN:CG	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:158:ASP:C	2:L:160:PRO:HD3	2.31	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
7:E:712:HOH:O	4:O:2:NAG:O4	2.15	0.49
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
1:K:67:ILE:CA	7:K:725:HOH:O	2.60	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:A:167:LEU:HD12	1:A:167:LEU:C	2.33	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
1:K:141:ALA:C	1:K:143:PRO:HD3	2.33	0.49
2:L:17:MET:SD	2:L:23:GLY:HA3	2.51	0.49
1:C:78:THR:CG2	1:C:78:THR:O	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:LEU:C	1:C:167:LEU:HD12	2.33	0.48
1:C:258:ARG:HE	1:C:259:TYR:HE1	1.61	0.48
1:G:141:ALA:C	1:G:143:PRO:HD3	2.34	0.48
1:G:167:LEU:HD12	1:G:167:LEU:C	2.33	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:G:293:ASN:OD1	1:G:293:ASN:C	2.50	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: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:A:141:ALA:C	1:A:143:PRO:HD3	2.34	0.48
1:C:26:LEU:HD22	2:D:105:GLU:CD	2.34	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
1:G:159:LYS:HZ2	1:G:199:GLN:HG2	1.79	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
1:G:26:LEU:O	2:J:50:ASN:HB3	2.14	0.48
1:I:167:LEU:HD12	1:I:167:LEU:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:GLY:CA	7:J:215:HOH:O	2.60	0.48
2:J:4:GLY:C	7:J:215:HOH:O	2.52	0.48
1:E:8:THR:CA	2:F:138:PHE:O	2.62	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
1:G:159:LYS:NZ	1:G:199:GLN:HG2	2.30	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:C:110:GLN:C	7:C:714:HOH:O	2.50	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
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
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: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:E:141:ALA:C	1:E:143:PRO:HD3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:141:ALA:C	1:I:143:PRO:HD3	2.35	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: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: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: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:C:141:ALA:C	1:C:143:PRO:HD3	2.35	0.46
1:A:113:SER:OG	7:A:913:HOH:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:155:ILE:HG22	1:C:157:LEU:HD13	1.98	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
2:H:9:PHE:CE1	2:H:10:ILE:HG13	2.52	0.45
1:E:14:HIS:CD2	1:E:15:ALA:N	2.85	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: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: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:HG3	2:J:59:MET:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:113:SER:C	7:A:913:HOH:O	2.08	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: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
2:J:157:TYR:OH	7:J:219:HOH:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:76:LEU:O	1:C:77:SER:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:GLY:O	2:F:111:HIS:CD2	2.72	0.43
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
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:167:LEU:C	1:K:167:LEU:HD23	2.39	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: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:HD22	1:C:44:ASN:C	2.22	0.42
1:C:204:TYR:CD1	1:C:215:LYS:HE3	2.54	0.42
1:E:8:THR:C	7:E:709:HOH:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:TRP:HZ3	1:I:238:THR:HG22	1.84	0.42
1:I:204:TYR:CD1	1:I:215:LYS:HE3	2.54	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:145:ALA:C	1:A:147:ALA:H	2.24	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
1:K:145:ALA:C	1:K:147:ALA:H	2.24	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:G:145:ALA:C	1:G:147:ALA:H	2.23	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:159:TYR:H	2:D:160:PRO:HD2	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:44:ASN:HD22	1:K:44:ASN:C	2.24	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: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
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:13:TYR:HA	2:J:17:MET:HE1	2.02	0.40
1:I:107:LEU:HB2	1:I:237:TRP:CE2	2.56	0.40
1:K:22:VAL:HG21	1:K:321:ALA:HB2	2.02	0.40
2:B:51:LYS:HA	1:E:25:VAL:O	2.21	0.40
1:C:119:ARG:HB2	1:C:261:PHE:CE2	2.57	0.40
1:C:145:ALA:C	1:C:147:ALA:H	2.25	0.40
1:E:66:TRP:NE1	1:E:77:SER:HB3	2.32	0.40
1:I:44:ASN:HD22	1:I:44:ASN:C	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:92:ASP:C	7:G:512:HOH:O	2.48	0.40
1:I:11:ILE:HA	2:J:24:TYR:HA	2.02	0.40
1:I:145:ALA:C	1:I:147:ALA:H	2.25	0.40
2:D:94:TYR:CE1	2:F:59:MET:HB2	2.57	0.40
1:I:49:LYS:C	7:I:714:HOH:O	2.58	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
1:A:26:LEU:HB3	2:D:47:GLU:HB3	2.02	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
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%)	25	58
2	D	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	58
2	F	159/164 (97%)	148 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	160/164 (98%)	149 (93%)	10 (6%)	1 (1%)	25	58
2	J	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	58
2	L	159/164 (97%)	147 (92%)	12 (8%)	0	100	100
All	All	2878/2916 (99%)	2675 (93%)	199 (7%)	4 (0%)	51	82

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%)	259 (92%)	23 (8%)	11	32
1	C	282/283 (100%)	260 (92%)	22 (8%)	12	34
1	E	282/283 (100%)	262 (93%)	20 (7%)	14	40
1	G	282/283 (100%)	263 (93%)	19 (7%)	16	43
1	I	282/283 (100%)	261 (93%)	21 (7%)	13	38
1	K	282/283 (100%)	263 (93%)	19 (7%)	16	43
2	B	139/141 (99%)	132 (95%)	7 (5%)	24	57
2	D	140/141 (99%)	131 (94%)	9 (6%)	17	45
2	F	139/141 (99%)	126 (91%)	13 (9%)	8	26
2	H	139/141 (99%)	132 (95%)	7 (5%)	24	57
2	J	140/141 (99%)	131 (94%)	9 (6%)	17	45
2	L	139/141 (99%)	126 (91%)	13 (9%)	8	26
All	All	2528/2544 (99%)	2346 (93%)	182 (7%)	14	39

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	37	ASN
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	101	PHE
1	A	107	LEU
1	A	111	LEU
1	A	119	ARG
1	A	126	THR
1	A	157	LEU
1	A	167	LEU
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
2	B	158	ASP
1	C	10	CYS
1	C	26	LEU
1	C	37	ASN
1	C	44	ASN
1	C	50	LEU
1	C	53	VAL
1	C	67	ILE
1	C	74	GLU
1	C	77	SER
1	C	78	THR
1	C	101	PHE
1	C	111	LEU

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Mol	Chain	Res	Type
1	C	126	THR
1	C	157	LEU
1	C	167	LEU
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	37	ASN
1	E	44	ASN
1	E	47	LEU
1	E	67	ILE
1	E	76	LEU
1	E	101	PHE
1	E	111	LEU
1	E	114	VAL
1	E	126	THR
1	E	167	LEU
1	E	190	THR
1	E	205	VAL
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

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Mol	Chain	Res	Type
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	37	ASN
1	G	44	ASN
1	G	50	LEU
1	G	58	LEU
1	G	67	ILE
1	G	101	PHE
1	G	107	LEU
1	G	111	LEU
1	G	126	THR
1	G	157	LEU
1	G	167	LEU
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
2	H	150	GLU
2	H	158	ASP
1	I	10	CYS
1	I	26	LEU
1	I	37	ASN
1	I	44	ASN
1	I	50	LEU
1	I	53	VAL

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Mol	Chain	Res	Type
1	I	67	ILE
1	I	76	LEU
1	I	77	SER
1	I	101	PHE
1	I	111	LEU
1	I	126	THR
1	I	157	LEU
1	I	167	LEU
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	37	ASN
1	K	44	ASN
1	K	47	LEU
1	K	67	ILE
1	K	101	PHE
1	K	111	LEU
1	K	114	VAL
1	K	126	THR
1	K	167	LEU
1	K	205	VAL
1	K	228	GLU
1	K	265	ARG
1	K	266	ASN
1	K	305	THR
1	K	316	THR

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Mol	Chain	Res	Type
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 (96) 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	125	GLN
2	B	129	ASN
2	B	146	ASN
1	C	14	HIS
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

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Mol	Chain	Res	Type
1	C	229	GLN
1	C	253	ASN
1	C	266	ASN
2	D	28	ASN
2	D	30	GLN
2	D	95	ASN
2	D	125	GLN
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	125	GLN
2	F	129	ASN
2	F	146	ASN
1	G	37	ASN
1	G	44	ASN
1	G	93	ASN
1	G	132	HIS
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
2	H	125	GLN
2	H	129	ASN
2	H	146	ASN
1	I	14	HIS
1	I	37	ASN
1	I	44	ASN

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Mol	Chain	Res	Type
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	125	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	125	GLN
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

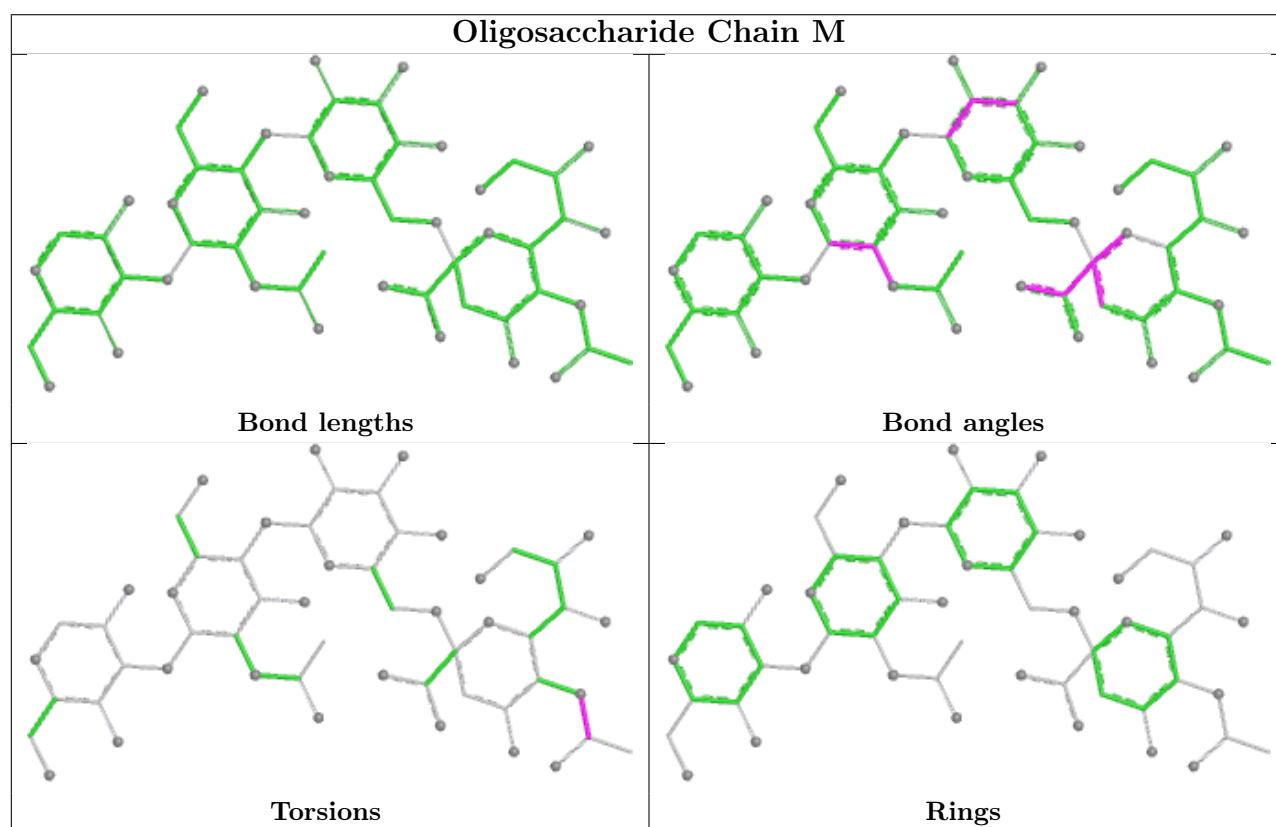
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	4	SIA	1	0

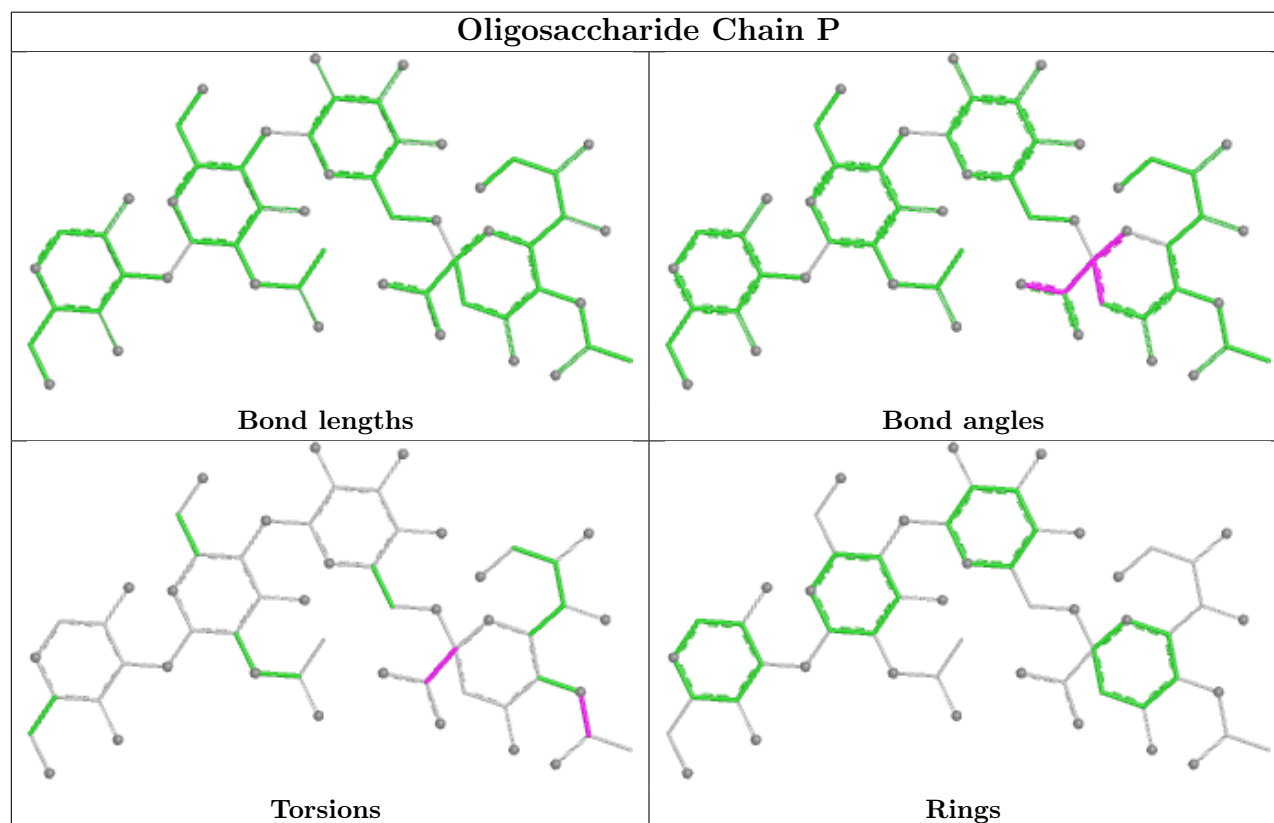
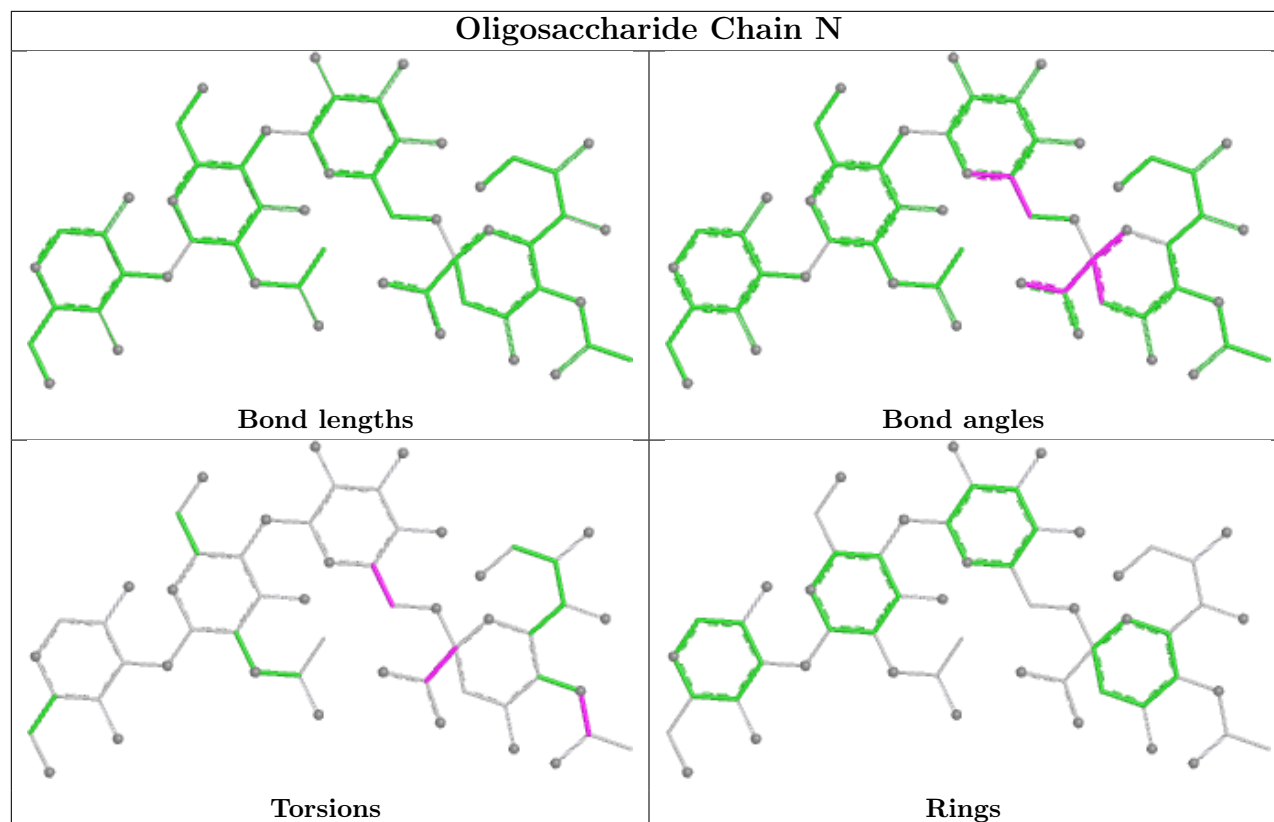
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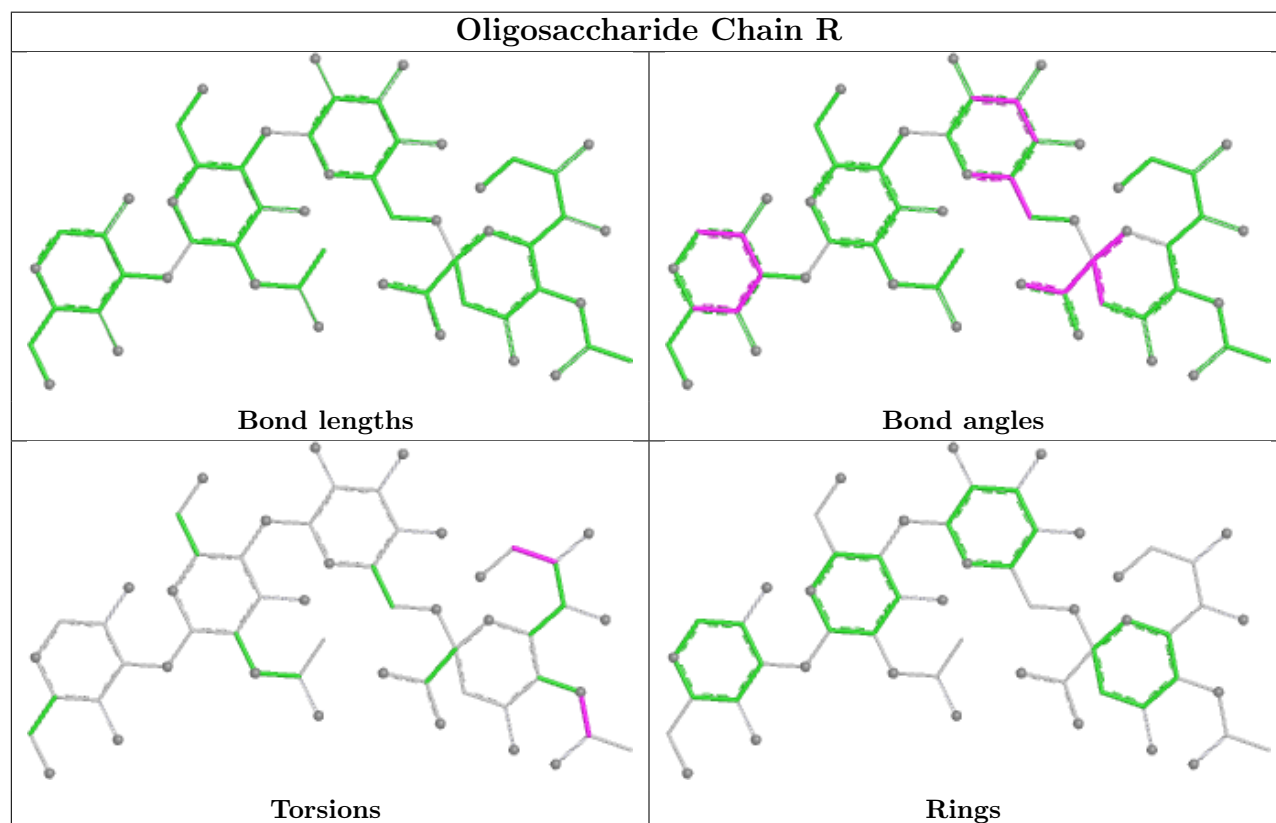
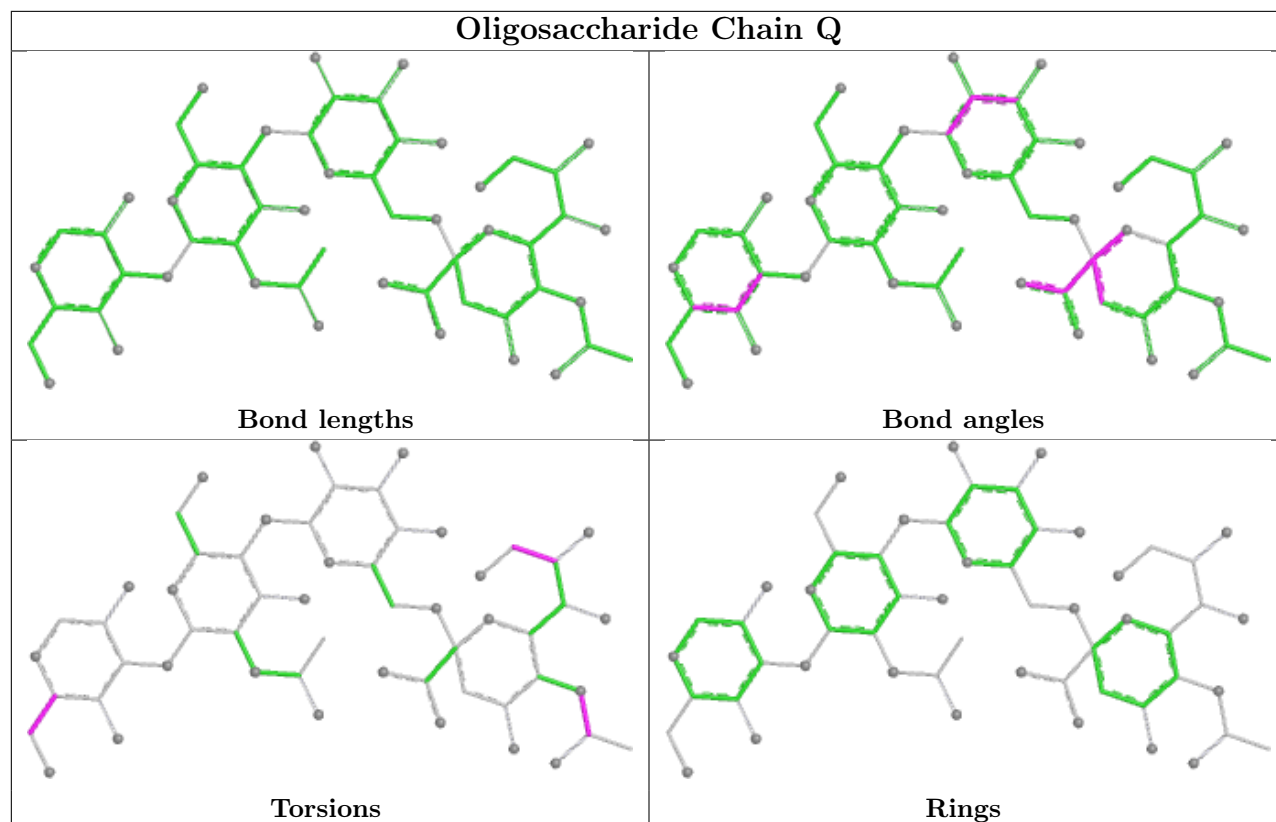
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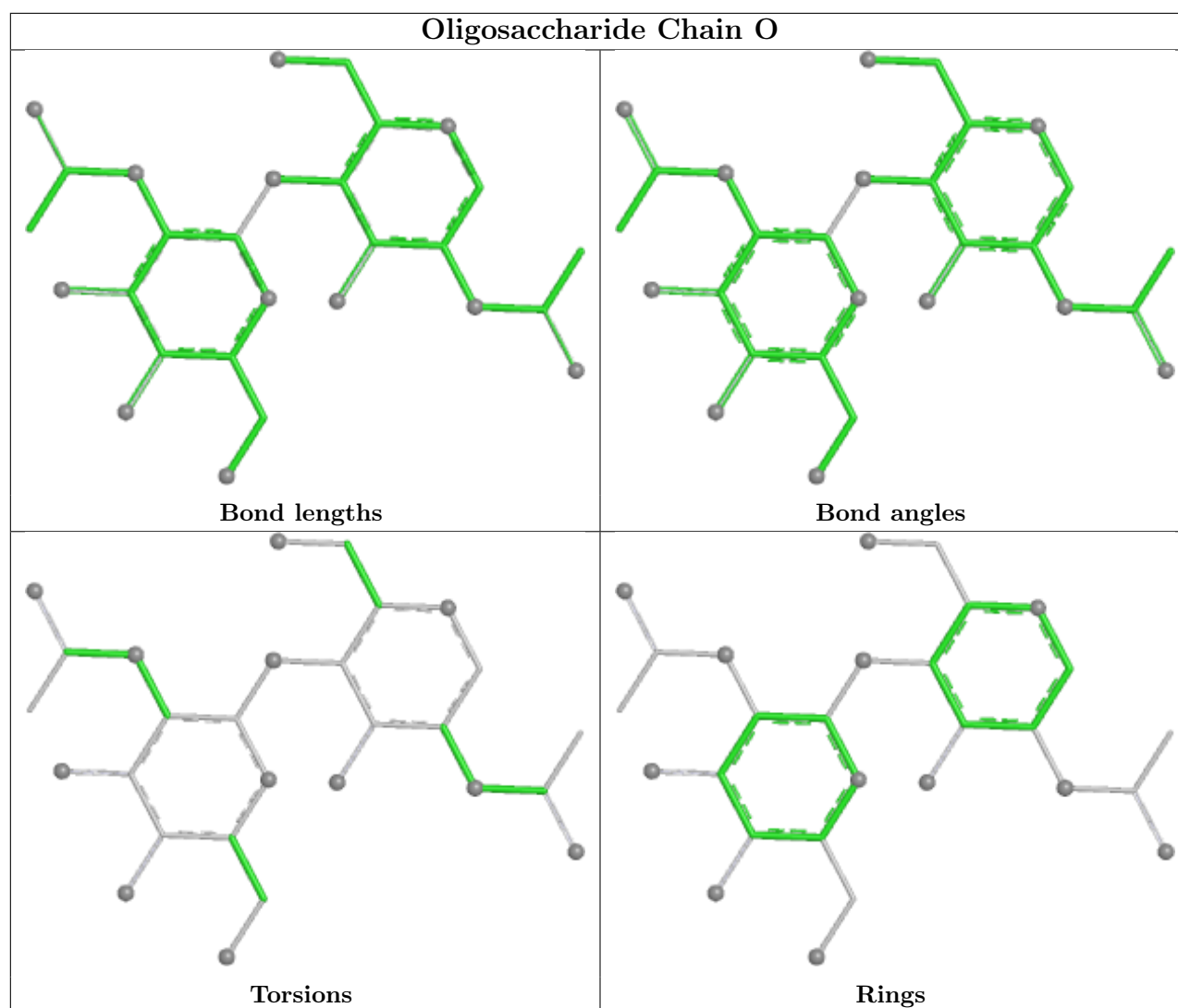
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	4	SIA	5	0
3	P	2	NAG	1	0
3	P	4	SIA	3	0
3	Q	2	NAG	2	0
4	O	2	NAG	1	0
3	N	4	SIA	2	0
3	M	2	NAG	1	0
3	M	4	SIA	2	0
3	N	2	NAG	2	0
3	R	3	GAL	1	0

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	$\# Z > 2$
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
5	NAG	C	601	1	14,14,15	0.80	0	17,19,21	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	601	1	14,14,15	0.46	0	17,19,21	1.82	4 (23%)
5	NAG	G	401	1	14,14,15	0.47	0	17,19,21	1.03	1 (5%)
5	NAG	I	601	1	14,14,15	0.59	0	17,19,21	0.90	1 (5%)
5	NAG	C	602	1	14,14,15	0.53	0	17,19,21	0.80	1 (5%)

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

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

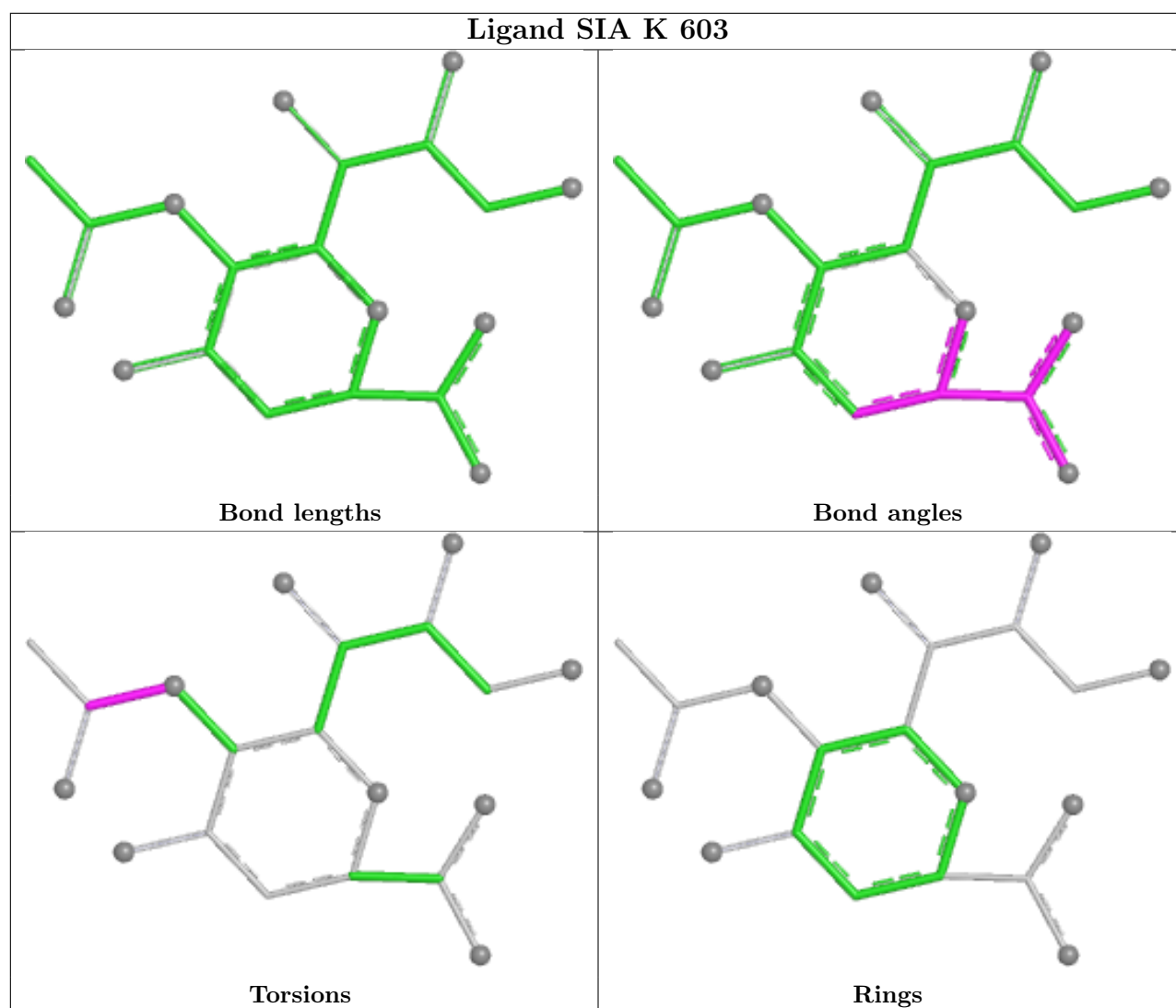
Mol	Chain	Res	Type	Atoms
5	C	601	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	K	602	NAG	O5-C5-C6-O6
5	K	602	NAG	C4-C5-C6-O6
6	K	603	SIA	C11-C10-N5-C5
6	K	603	SIA	O10-C10-N5-C5
5	G	401	NAG	C4-C5-C6-O6
5	G	401	NAG	O5-C5-C6-O6
5	C	601	NAG	C3-C2-N2-C7

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	K	601	NAG	5	0
5	C	602	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(Å²)	Q<0.9
1	A	322/322 (100%)	0.36	21 (6%)	18	14	30, 55, 103, 206	0
1	C	321/322 (99%)	0.18	17 (5%)	26	22	29, 55, 102, 249	0
1	E	321/322 (99%)	0.14	15 (4%)	31	28	24, 56, 102, 220	0
1	G	322/322 (100%)	0.22	20 (6%)	20	16	29, 58, 98, 209	0
1	I	321/322 (99%)	0.42	21 (6%)	18	14	32, 64, 124, 236	0
1	K	321/322 (99%)	0.21	18 (5%)	24	20	26, 53, 96, 165	0
2	B	162/164 (98%)	0.55	16 (9%)	7	5	32, 72, 129, 175	0
2	D	164/164 (100%)	0.51	14 (8%)	10	8	36, 74, 130, 191	0
2	F	161/164 (98%)	0.80	28 (17%)	1	1	22, 74, 155, 210	0
2	H	162/164 (98%)	0.24	6 (3%)	41	37	28, 59, 101, 138	0
2	J	164/164 (100%)	1.38	42 (25%)	0	0	29, 81, 203, 324	0
2	L	161/164 (98%)	0.74	29 (18%)	1	1	30, 63, 163, 201	0
All	All	2902/2916 (99%)	0.41	247 (8%)	10	8	22, 60, 129, 324	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	158	ASP	11.0
2	F	159	TYR	11.0
1	I	9	LEU	8.6
2	J	129	ASN	8.2
2	J	20	GLY	8.2
2	J	154	ASN	8.2
1	A	10	CYS	7.2
1	K	9	LEU	6.9
2	D	129	ASN	6.8
2	F	158	ASP	6.8
2	L	33	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
2	J	130	ALA	6.6
1	I	7	ASP	6.5
2	J	19	ASP	6.4
2	J	160	PRO	6.4
2	F	141	TYR	6.4
2	J	153	LYS	6.3
1	E	12	GLY	6.1
1	E	11	ILE	6.0
2	F	143	LYS	5.7
2	J	18	VAL	5.5
2	J	147	THR	5.5
1	K	10	CYS	5.5
2	J	156	THR	5.3
2	J	32	SER	5.3
1	A	8	THR	5.3
2	F	142	HIS	5.3
1	I	8	THR	5.2
2	H	156	THR	5.2
2	D	156	THR	5.2
2	J	149	MET	5.1
2	J	23	GLY	4.9
2	J	31	GLY	4.9
1	A	75	SER	4.8
1	A	19	THR	4.8
1	K	12	GLY	4.8
1	G	78	THR	4.7
2	J	150	GLU	4.6
2	L	32	SER	4.5
2	J	33	GLY	4.5
1	C	7	ASP	4.5
2	J	122	VAL	4.5
2	B	158	ASP	4.5
2	J	146	ASN	4.5
2	J	139	GLU	4.4
2	D	146	ASN	4.4
2	L	148	CYS	4.3
1	I	280	ASP	4.3
1	C	9	LEU	4.2
2	J	159	TYR	4.2
2	F	140	PHE	4.1
1	I	11	ILE	4.1
2	F	27	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	L	139	GLU	4.0
2	B	27	GLN	4.0
2	J	141	TYR	4.0
1	G	146	GLY	4.0
1	E	75	SER	4.0
1	C	74	GLU	4.0
1	G	162	ASN	4.0
1	K	11	ILE	4.0
2	B	140	PHE	4.0
1	I	10	CYS	3.9
2	J	27	GLN	3.9
2	L	29	GLU	3.9
1	A	161	GLY	3.9
2	D	151	SER	3.9
2	J	142	HIS	3.9
2	F	160	PRO	3.9
2	D	142	HIS	3.8
1	C	75	SER	3.8
2	L	159	TYR	3.8
1	E	9	LEU	3.8
2	D	15	THR	3.8
2	J	124	SER	3.8
2	J	140	PHE	3.8
1	C	76	LEU	3.7
1	G	52	GLY	3.7
2	L	141	TYR	3.7
1	E	7	ASP	3.7
2	L	128	ASN	3.7
1	A	163	SER	3.6
2	J	36	ALA	3.6
2	B	153	LYS	3.6
2	J	133	ILE	3.6
1	C	195	GLN	3.6
2	F	30	GLN	3.6
1	I	293	ASN	3.5
2	F	144	CYS	3.5
1	K	75	SER	3.5
2	J	132	GLU	3.5
2	J	126	LEU	3.5
2	B	134	GLY	3.5
2	J	26	HIS	3.5
2	B	32	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	211	ARG	3.4
2	J	131	LYS	3.4
1	I	50	LEU	3.4
1	A	199	GLN	3.4
2	F	147	THR	3.4
2	F	156	THR	3.4
2	L	144	CYS	3.3
2	F	132	GLU	3.3
2	L	31	GLY	3.3
1	K	8	THR	3.3
1	G	76	LEU	3.3
1	A	146	GLY	3.3
2	F	131	LYS	3.3
2	F	157	TYR	3.3
1	G	91	SER	3.2
1	E	76	LEU	3.2
1	E	77	SER	3.2
2	F	35	ALA	3.2
1	I	76	LEU	3.2
1	K	51	ARG	3.2
2	L	38	LEU	3.2
2	L	158	ASP	3.1
2	J	24	TYR	3.1
1	C	11	ILE	3.1
1	E	13	TYR	3.1
2	F	128	ASN	3.0
1	K	211	ARG	3.0
2	L	140	PHE	3.0
1	C	78	THR	3.0
2	L	152	VAL	3.0
1	C	131	ASN	3.0
1	A	201	ALA	3.0
2	L	133	ILE	3.0
1	A	77	SER	2.9
1	G	7	ASP	2.9
1	I	75	SER	2.9
1	A	326	ASN	2.9
2	B	139	GLU	2.9
1	K	268	GLY	2.9
2	F	26	HIS	2.9
2	L	19	ASP	2.9
2	J	155	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	127	LYS	2.9
1	K	17	ASN	2.8
1	E	74	GLU	2.8
1	A	267	ALA	2.8
2	J	145	ASP	2.8
1	I	30	VAL	2.8
1	E	199	GLN	2.8
2	B	128	ASN	2.8
2	F	139	GLU	2.7
2	L	27	GLN	2.7
2	J	127	LYS	2.7
1	G	12	GLY	2.7
2	J	38	LEU	2.7
2	F	29	GLU	2.7
1	G	93	ASN	2.7
2	H	160	PRO	2.7
2	L	134	GLY	2.7
1	G	8	THR	2.7
1	C	77	SER	2.6
2	L	26	HIS	2.6
1	K	7	ASP	2.6
1	I	31	THR	2.6
2	D	133	ILE	2.6
1	A	17	ASN	2.6
1	A	51	ARG	2.6
1	G	116	SER	2.6
1	E	54	ALA	2.6
1	C	60	LYS	2.6
1	G	77	SER	2.6
2	D	24	TYR	2.6
1	I	34	HIS	2.5
1	I	29	ASN	2.5
1	G	92	ASP	2.5
2	B	137	CYS	2.5
2	D	140	PHE	2.5
2	F	28	ASN	2.5
1	K	118	GLU	2.5
2	F	22	TYR	2.5
2	D	31	GLY	2.5
2	F	134	GLY	2.5
1	A	18	SER	2.4
2	B	149	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	145	ASP	2.4
1	C	8	THR	2.4
2	F	40	SER	2.4
2	B	31	GLY	2.4
1	C	294	THR	2.4
2	B	138	PHE	2.4
2	L	138	PHE	2.4
1	C	90	SER	2.4
1	C	147	ALA	2.4
1	G	53	VAL	2.4
1	A	162	ASN	2.4
1	K	77	SER	2.4
1	A	278	VAL	2.4
2	H	157	TYR	2.4
1	A	15	ALA	2.4
2	J	128	ASN	2.3
2	B	29	GLU	2.3
1	E	293	ASN	2.3
1	A	9	LEU	2.3
2	F	161	LYS	2.3
1	E	8	THR	2.3
1	G	195	GLN	2.3
2	J	21	TRP	2.3
2	J	143	LYS	2.3
2	D	141	TYR	2.3
1	I	92	ASP	2.3
2	L	30	GLN	2.3
1	I	77	SER	2.2
2	L	23	GLY	2.2
2	D	22	TYR	2.2
2	B	142	HIS	2.2
1	C	15	ALA	2.2
1	I	268	GLY	2.2
2	L	22	TYR	2.2
2	F	136	GLY	2.2
2	H	29	GLU	2.2
2	H	135	ASN	2.2
1	K	54	ALA	2.2
2	D	30	GLN	2.2
2	B	141	TYR	2.2
2	H	150	GLU	2.2
1	I	327	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	162	ASN	2.2
2	L	42	GLN	2.2
1	K	20	ASP	2.2
2	D	144	CYS	2.2
1	K	199	GLN	2.1
2	L	162	TYR	2.1
1	K	16	ASN	2.1
2	J	121	LYS	2.1
1	G	280	ASP	2.1
2	L	150	GLU	2.1
1	G	268	GLY	2.1
1	C	14	HIS	2.1
1	G	18	SER	2.1
2	J	157	TYR	2.1
1	G	227	ARG	2.1
1	K	14	HIS	2.1
2	L	131	LYS	2.1
1	I	174	ASP	2.1
1	I	14	HIS	2.0
2	F	38	LEU	2.0
2	B	151	SER	2.0
1	E	34	HIS	2.0
2	F	149	MET	2.0
1	A	42	LYS	2.0
1	A	7	ASP	2.0
1	G	136	LYS	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	0.60	0.34	99,134,164,181	0
3	GAL	P	1	11/12	0.70	0.42	122,137,149,151	0

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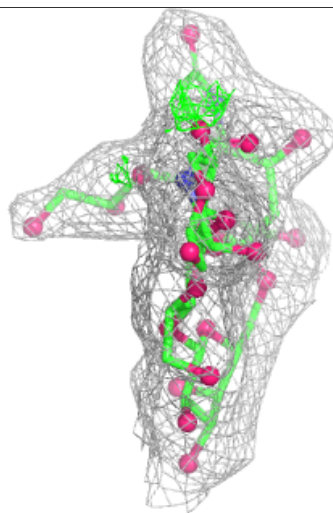
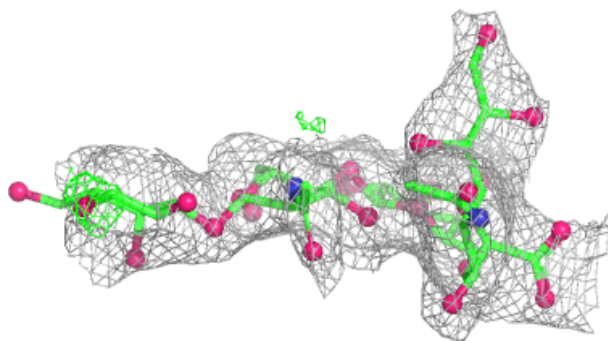
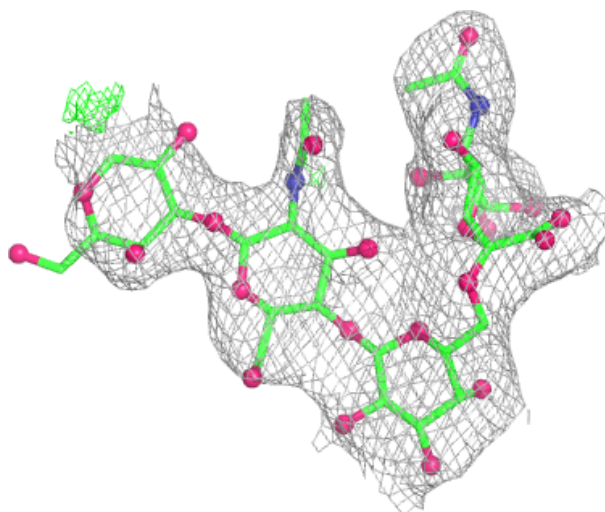
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAL	R	1	11/12	0.79	0.24	62,112,129,131	0
3	GAL	N	1	11/12	0.80	0.29	57,74,100,104	0
3	NAG	R	2	14/15	0.81	0.20	62,83,91,98	0
3	NAG	P	2	14/15	0.84	0.30	77,97,113,115	0
3	GAL	M	1	11/12	0.85	0.27	84,94,133,136	0
3	GAL	Q	3	11/12	0.86	0.19	45,65,85,103	0
3	NAG	Q	2	14/15	0.87	0.26	72,89,109,111	0
3	NAG	M	2	14/15	0.88	0.19	51,70,78,85	0
3	GAL	R	3	11/12	0.89	0.20	78,96,102,114	0
4	NAG	O	1	14/15	0.89	0.18	52,64,82,92	0
3	GAL	N	3	11/12	0.91	0.16	53,69,77,79	0
3	SIA	P	4	20/21	0.91	0.20	47,59,73,76	0
3	GAL	M	3	11/12	0.91	0.13	42,52,72,77	0
4	NAG	O	2	14/15	0.91	0.33	63,93,116,119	0
3	SIA	Q	4	20/21	0.92	0.18	44,68,95,96	0
3	SIA	N	4	20/21	0.93	0.14	41,62,76,87	0
3	GAL	P	3	11/12	0.93	0.13	53,71,89,92	0
3	NAG	N	2	14/15	0.93	0.30	60,71,84,92	0
3	SIA	R	4	20/21	0.94	0.17	38,55,67,73	0
3	SIA	M	4	20/21	0.95	0.14	34,46,60,66	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.

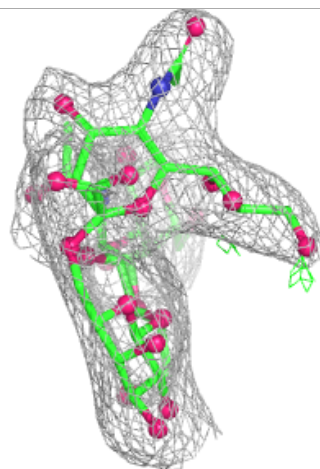
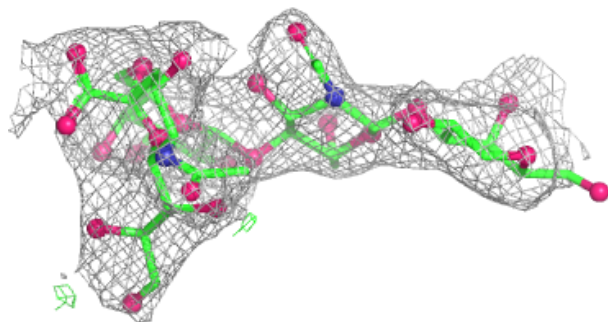
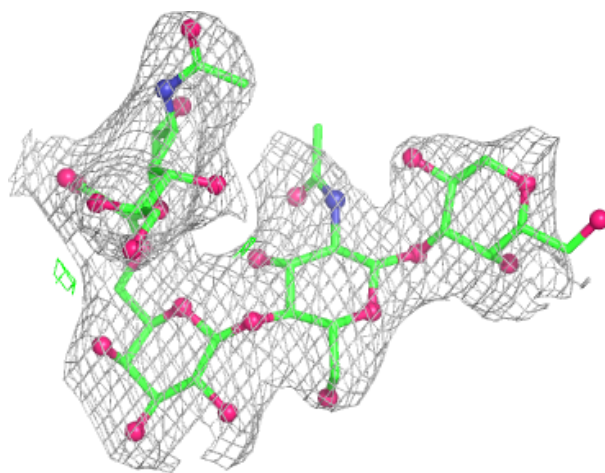
Electron density around Chain M:

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



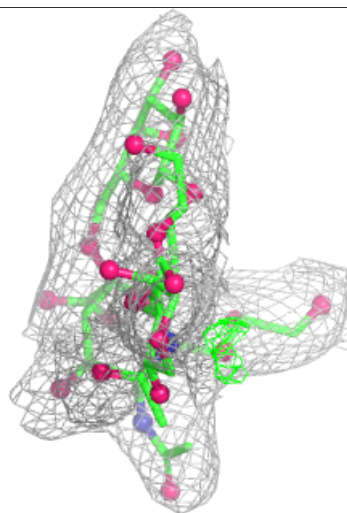
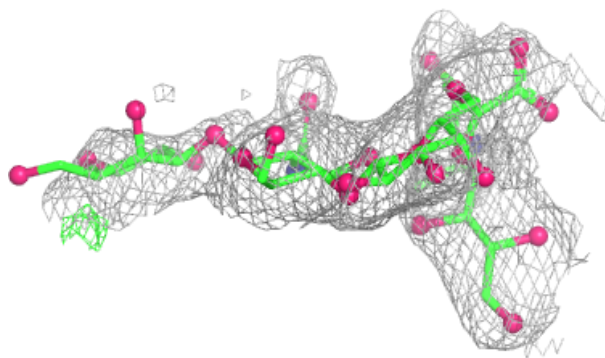
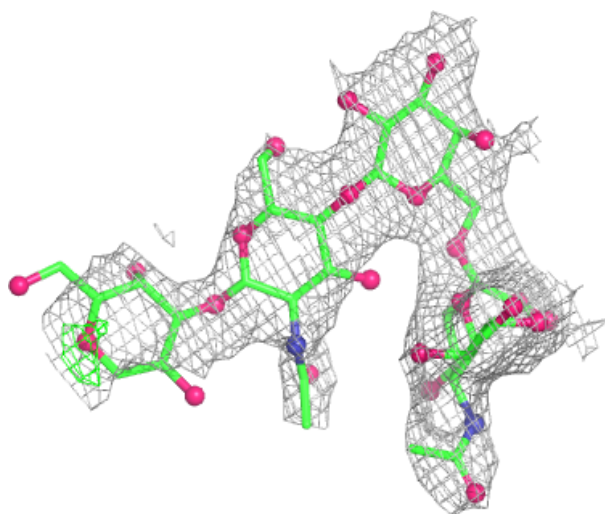
Electron density around Chain N:

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



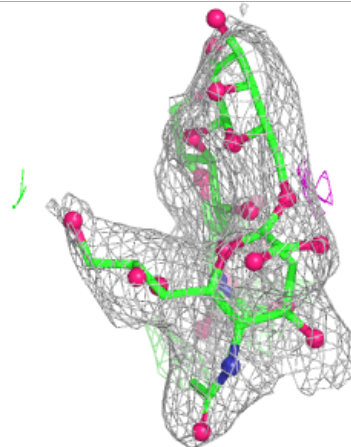
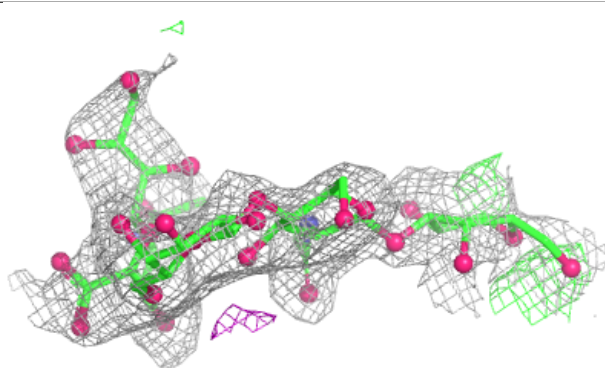
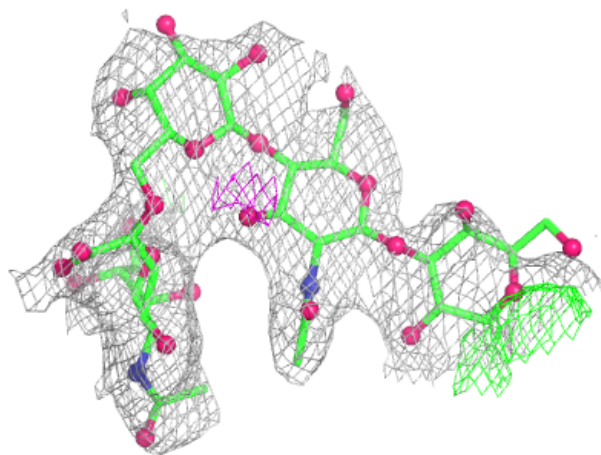
Electron density around Chain P:

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



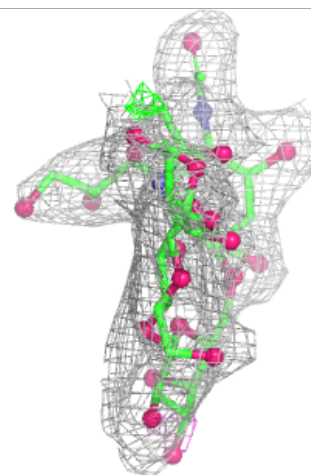
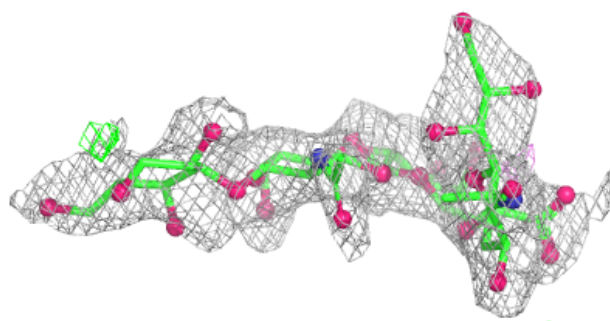
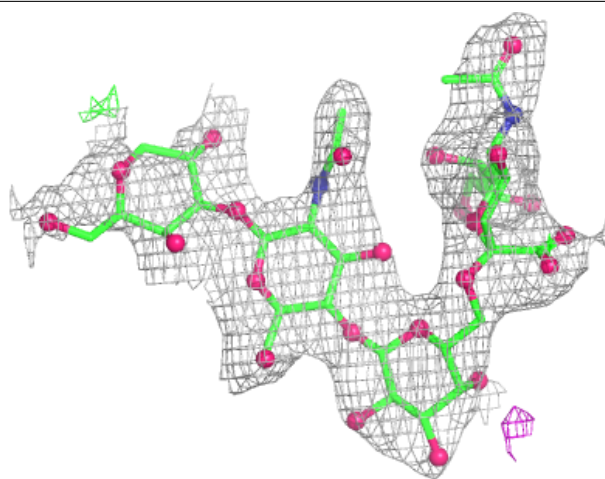
Electron density around Chain Q:

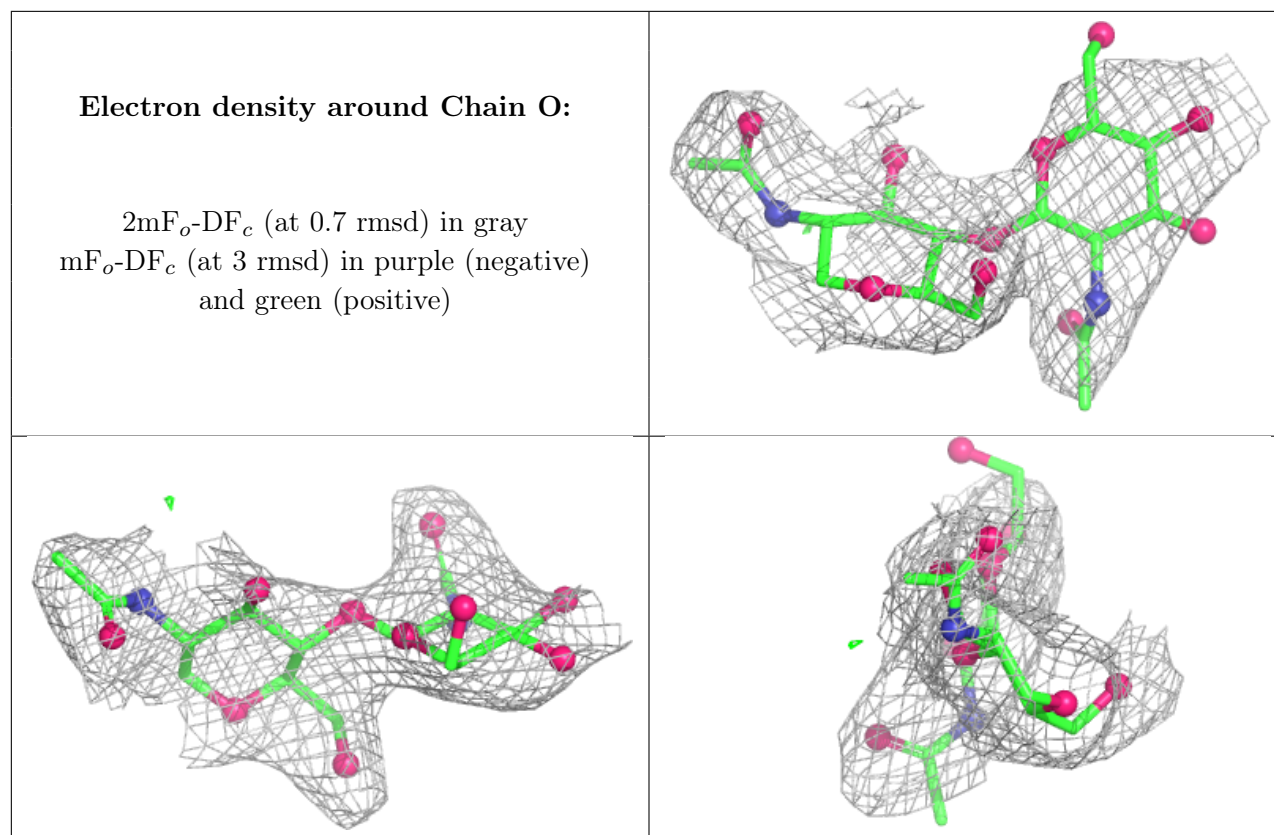
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

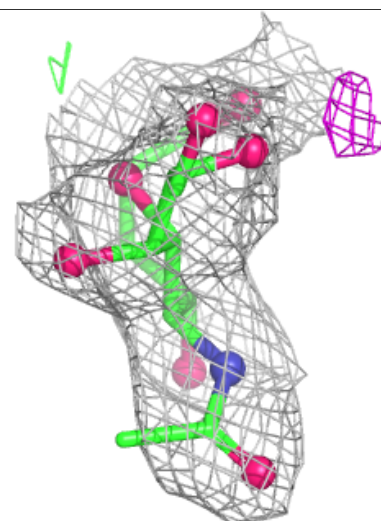
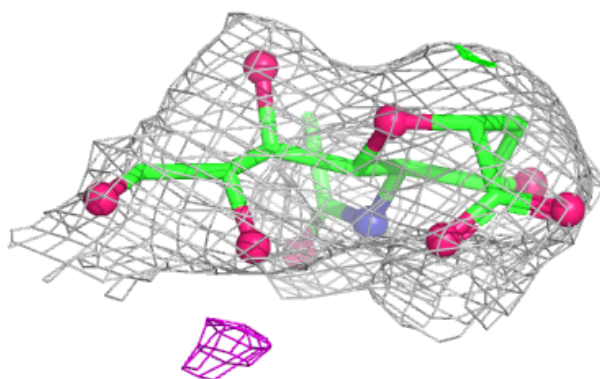
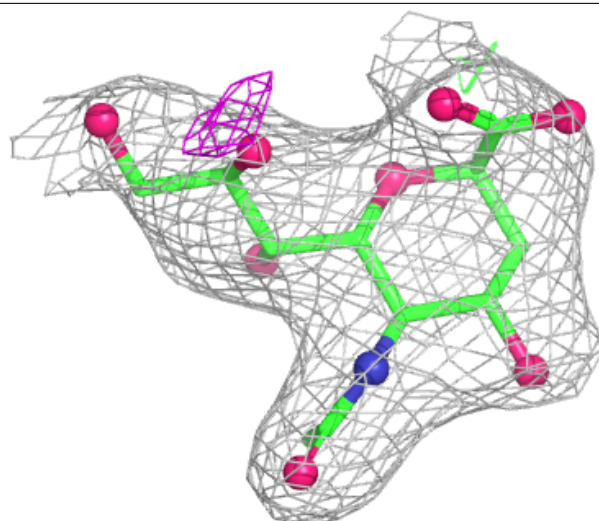
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	I	601	14/15	0.69	0.32	101,130,147,150	0
5	NAG	K	602	14/15	0.72	0.32	76,105,115,115	0
5	NAG	K	601	14/15	0.77	0.31	119,128,136,137	0
5	NAG	C	601	14/15	0.78	0.21	66,93,106,114	0
5	NAG	G	401	14/15	0.82	0.38	78,108,129,132	0
5	NAG	C	602	14/15	0.92	0.18	25,57,74,79	0
6	SIA	K	603	20/21	0.95	0.16	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.