



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:21 PM UTC

PDB ID : 5Y2Z / pdb_00005y2z
Title : Crystal structure of human LGI1 EPTP-ADAM22 complex
Authors : Yamagata, A.; Fukai, S.
Deposited on : 2017-07-27
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

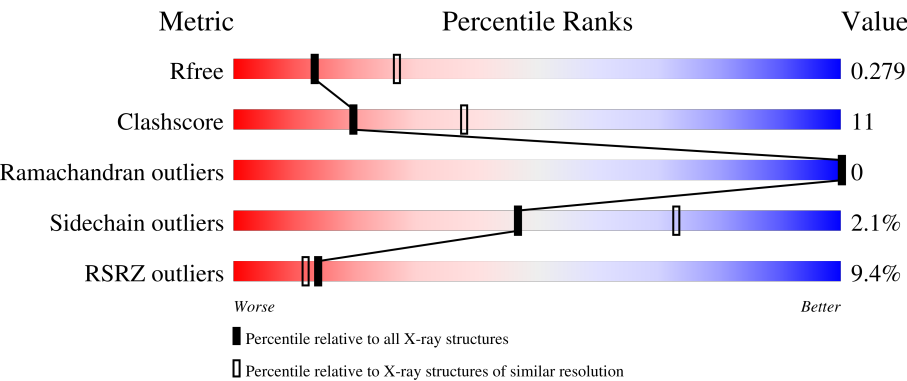
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.67 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	504	8% 72% 23% • •
1	C	504	17% 71% 22% • 6%
1	E	504	16% 72% 20% • 7%
1	G	504	15% 74% 16% • 8%
1	I	504	9% 77% 18% • 5%

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Mol	Chain	Length	Quality of chain
1	K	504	
2	B	347	
2	D	347	
2	F	347	
2	H	347	
2	J	347	
2	L	347	
3	M	2	
3	O	2	
3	Q	2	
3	T	2	
4	N	4	
4	S	4	
5	P	3	
5	U	3	
5	V	3	
6	R	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 39417 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3696	2283	637	725	51			
1	C	473	Total	C	N	O	S	0	0	0
			3623	2238	624	710	51			
1	E	467	Total	C	N	O	S	0	0	0
			3575	2207	615	702	51			
1	G	462	Total	C	N	O	S	0	0	0
			3537	2185	609	692	51			
1	I	481	Total	C	N	O	S	0	0	0
			3688	2281	633	723	51			
1	K	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	LYS	-	expression tag	UNP Q9P0K1
A	731	HIS	-	expression tag	UNP Q9P0K1
A	732	HIS	-	expression tag	UNP Q9P0K1
A	733	HIS	-	expression tag	UNP Q9P0K1
A	734	HIS	-	expression tag	UNP Q9P0K1
A	735	HIS	-	expression tag	UNP Q9P0K1
A	736	HIS	-	expression tag	UNP Q9P0K1
C	730	LYS	-	expression tag	UNP Q9P0K1
C	731	HIS	-	expression tag	UNP Q9P0K1
C	732	HIS	-	expression tag	UNP Q9P0K1
C	733	HIS	-	expression tag	UNP Q9P0K1
C	734	HIS	-	expression tag	UNP Q9P0K1
C	735	HIS	-	expression tag	UNP Q9P0K1
C	736	HIS	-	expression tag	UNP Q9P0K1
E	730	LYS	-	expression tag	UNP Q9P0K1
E	731	HIS	-	expression tag	UNP Q9P0K1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	732	HIS	-	expression tag	UNP Q9P0K1
E	733	HIS	-	expression tag	UNP Q9P0K1
E	734	HIS	-	expression tag	UNP Q9P0K1
E	735	HIS	-	expression tag	UNP Q9P0K1
E	736	HIS	-	expression tag	UNP Q9P0K1
G	730	LYS	-	expression tag	UNP Q9P0K1
G	731	HIS	-	expression tag	UNP Q9P0K1
G	732	HIS	-	expression tag	UNP Q9P0K1
G	733	HIS	-	expression tag	UNP Q9P0K1
G	734	HIS	-	expression tag	UNP Q9P0K1
G	735	HIS	-	expression tag	UNP Q9P0K1
G	736	HIS	-	expression tag	UNP Q9P0K1
I	730	LYS	-	expression tag	UNP Q9P0K1
I	731	HIS	-	expression tag	UNP Q9P0K1
I	732	HIS	-	expression tag	UNP Q9P0K1
I	733	HIS	-	expression tag	UNP Q9P0K1
I	734	HIS	-	expression tag	UNP Q9P0K1
I	735	HIS	-	expression tag	UNP Q9P0K1
I	736	HIS	-	expression tag	UNP Q9P0K1
K	730	LYS	-	expression tag	UNP Q9P0K1
K	731	HIS	-	expression tag	UNP Q9P0K1
K	732	HIS	-	expression tag	UNP Q9P0K1
K	733	HIS	-	expression tag	UNP Q9P0K1
K	734	HIS	-	expression tag	UNP Q9P0K1
K	735	HIS	-	expression tag	UNP Q9P0K1
K	736	HIS	-	expression tag	UNP Q9P0K1

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	328	Total	C	N	O	S	0	0	0
			2708	1753	450	498	7			
2	D	328	Total	C	N	O	S	0	0	0
			2708	1753	450	498	7			
2	F	328	Total	C	N	O	S	0	0	0
			2708	1753	450	498	7			
2	H	329	Total	C	N	O	S	0	0	0
			2716	1759	451	499	7			
2	J	328	Total	C	N	O	S	0	0	0
			2708	1753	450	498	7			
2	L	328	Total	C	N	O	S	0	0	0
			2708	1753	450	498	7			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	218	ASP	-	expression tag	UNP O95970
B	219	ALA	-	expression tag	UNP O95970
B	220	ALA	-	expression tag	UNP O95970
B	221	GLN	-	expression tag	UNP O95970
B	222	PRO	-	expression tag	UNP O95970
B	223	ALA	-	expression tag	UNP O95970
B	558	LYS	-	expression tag	UNP O95970
B	559	HIS	-	expression tag	UNP O95970
B	560	HIS	-	expression tag	UNP O95970
B	561	HIS	-	expression tag	UNP O95970
B	562	HIS	-	expression tag	UNP O95970
B	563	HIS	-	expression tag	UNP O95970
B	564	HIS	-	expression tag	UNP O95970
D	218	ASP	-	expression tag	UNP O95970
D	219	ALA	-	expression tag	UNP O95970
D	220	ALA	-	expression tag	UNP O95970
D	221	GLN	-	expression tag	UNP O95970
D	222	PRO	-	expression tag	UNP O95970
D	223	ALA	-	expression tag	UNP O95970
D	558	LYS	-	expression tag	UNP O95970
D	559	HIS	-	expression tag	UNP O95970
D	560	HIS	-	expression tag	UNP O95970
D	561	HIS	-	expression tag	UNP O95970
D	562	HIS	-	expression tag	UNP O95970
D	563	HIS	-	expression tag	UNP O95970
D	564	HIS	-	expression tag	UNP O95970
F	218	ASP	-	expression tag	UNP O95970
F	219	ALA	-	expression tag	UNP O95970
F	220	ALA	-	expression tag	UNP O95970
F	221	GLN	-	expression tag	UNP O95970
F	222	PRO	-	expression tag	UNP O95970
F	223	ALA	-	expression tag	UNP O95970
F	558	LYS	-	expression tag	UNP O95970
F	559	HIS	-	expression tag	UNP O95970
F	560	HIS	-	expression tag	UNP O95970
F	561	HIS	-	expression tag	UNP O95970
F	562	HIS	-	expression tag	UNP O95970
F	563	HIS	-	expression tag	UNP O95970
F	564	HIS	-	expression tag	UNP O95970
H	218	ASP	-	expression tag	UNP O95970
H	219	ALA	-	expression tag	UNP O95970
H	220	ALA	-	expression tag	UNP O95970

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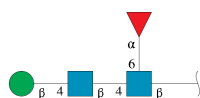
Chain	Residue	Modelled	Actual	Comment	Reference
H	221	GLN	-	expression tag	UNP O95970
H	222	PRO	-	expression tag	UNP O95970
H	223	ALA	-	expression tag	UNP O95970
H	558	LYS	-	expression tag	UNP O95970
H	559	HIS	-	expression tag	UNP O95970
H	560	HIS	-	expression tag	UNP O95970
H	561	HIS	-	expression tag	UNP O95970
H	562	HIS	-	expression tag	UNP O95970
H	563	HIS	-	expression tag	UNP O95970
H	564	HIS	-	expression tag	UNP O95970
J	218	ASP	-	expression tag	UNP O95970
J	219	ALA	-	expression tag	UNP O95970
J	220	ALA	-	expression tag	UNP O95970
J	221	GLN	-	expression tag	UNP O95970
J	222	PRO	-	expression tag	UNP O95970
J	223	ALA	-	expression tag	UNP O95970
J	558	LYS	-	expression tag	UNP O95970
J	559	HIS	-	expression tag	UNP O95970
J	560	HIS	-	expression tag	UNP O95970
J	561	HIS	-	expression tag	UNP O95970
J	562	HIS	-	expression tag	UNP O95970
J	563	HIS	-	expression tag	UNP O95970
J	564	HIS	-	expression tag	UNP O95970
L	218	ASP	-	expression tag	UNP O95970
L	219	ALA	-	expression tag	UNP O95970
L	220	ALA	-	expression tag	UNP O95970
L	221	GLN	-	expression tag	UNP O95970
L	222	PRO	-	expression tag	UNP O95970
L	223	ALA	-	expression tag	UNP O95970
L	558	LYS	-	expression tag	UNP O95970
L	559	HIS	-	expression tag	UNP O95970
L	560	HIS	-	expression tag	UNP O95970
L	561	HIS	-	expression tag	UNP O95970
L	562	HIS	-	expression tag	UNP O95970
L	563	HIS	-	expression tag	UNP O95970
L	564	HIS	-	expression tag	UNP O95970

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



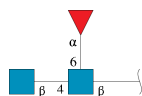
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	S	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	U	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	V	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	R	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Ca	0	0
			3	3		
7	C	3	Total	Ca	0	0
			3	3		
7	E	3	Total	Ca	0	0
			3	3		
7	G	3	Total	Ca	0	0
			3	3		
7	I	3	Total	Ca	0	0
			3	3		
7	K	3	Total	Ca	0	0
			3	3		
7	B	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		
7	F	1	Total	Ca	0	0
			1	1		
7	H	1	Total	Ca	0	0
			1	1		
7	J	1	Total	Ca	0	0
			1	1		
7	L	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			14	8	1	5		
8	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	91	Total	O	0	0
			91	91		
9	C	73	Total	O	0	0
			73	73		
9	E	78	Total	O	0	0
			78	78		
9	G	72	Total	O	0	0
			72	72		
9	I	91	Total	O	0	0
			91	91		
9	K	83	Total	O	0	0
			83	83		
9	B	94	Total	O	0	0
			94	94		
9	D	78	Total	O	0	0
			78	78		
9	F	62	Total	O	0	0
			62	62		
9	H	66	Total	O	0	0
			66	66		

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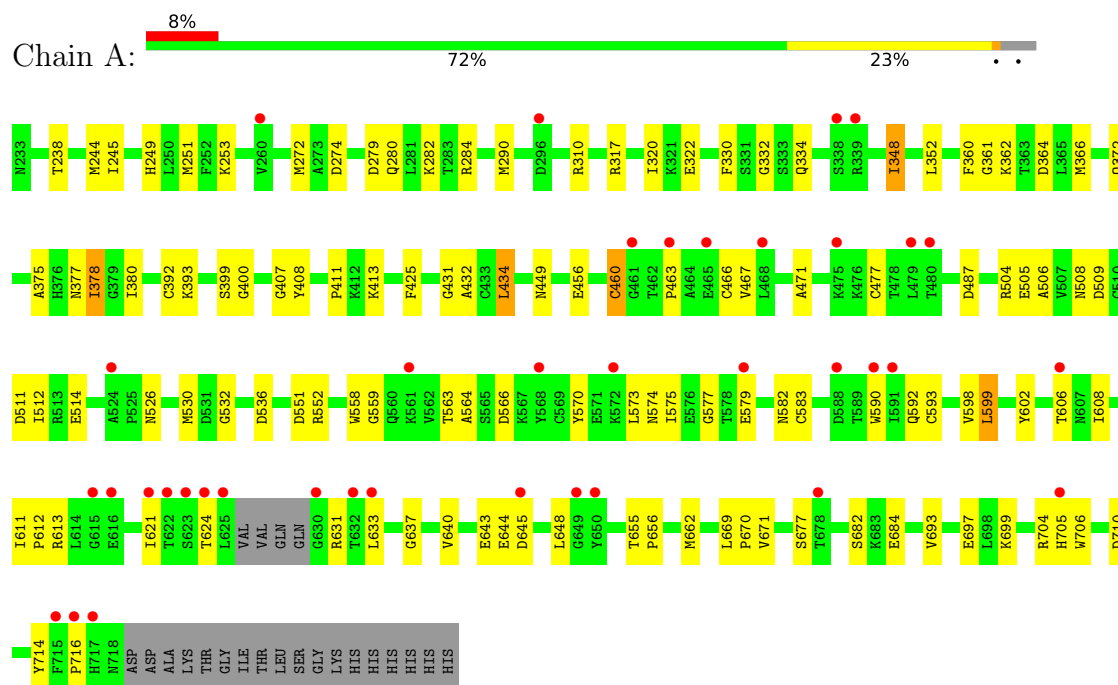
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	67	Total	O	0	0
			67	67		
9	L	59	Total	O	0	0
			59	59		

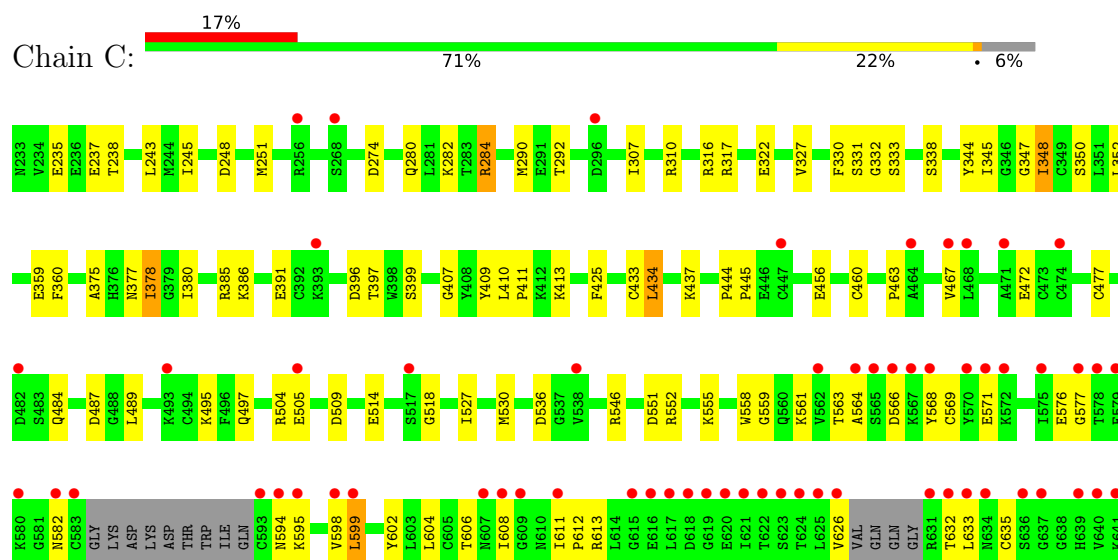
3 Residue-property plots [i](#)

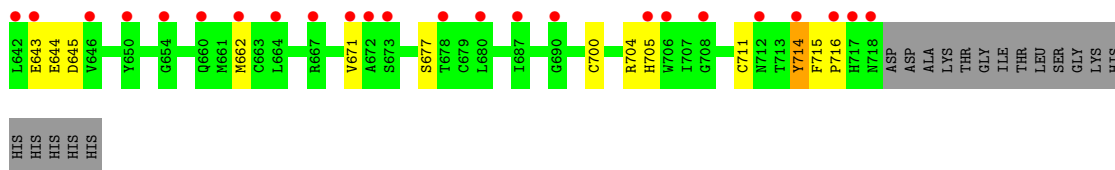
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Disintegrin and metalloproteinase domain-containing protein 22

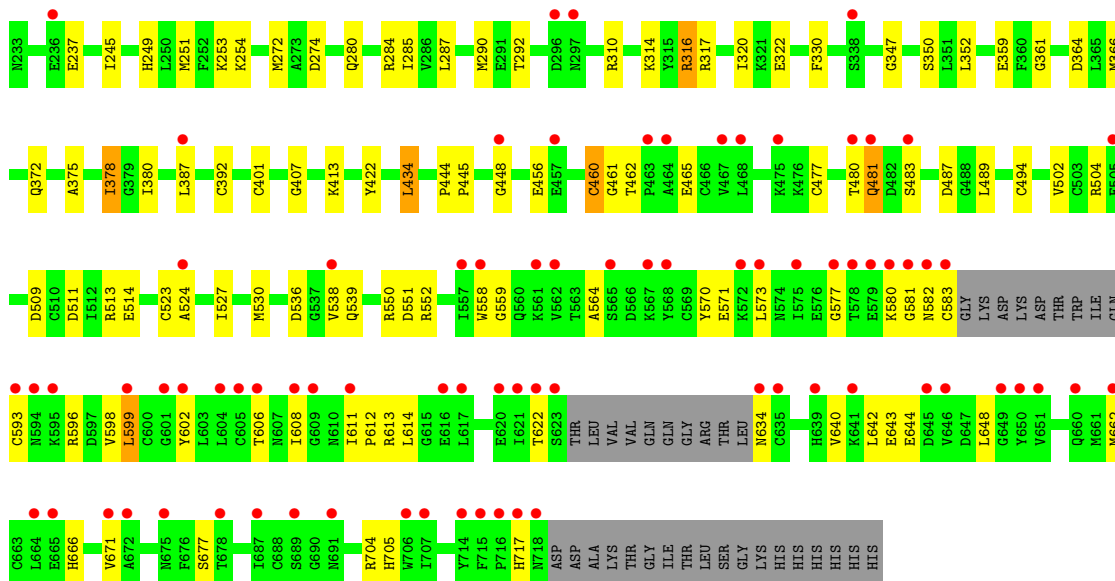


- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

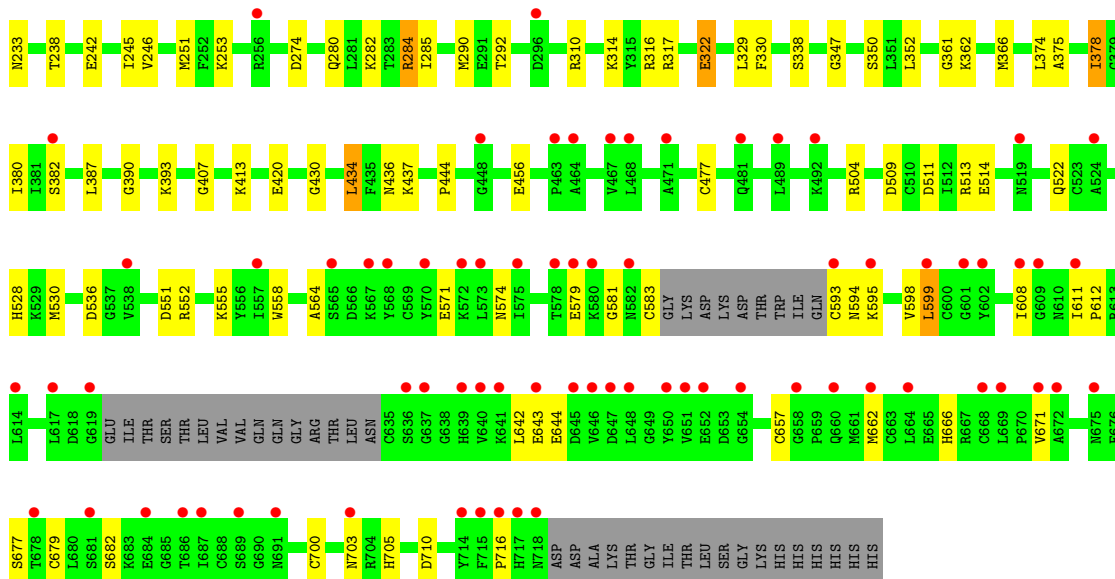
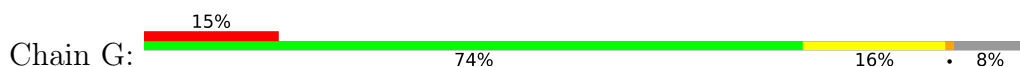




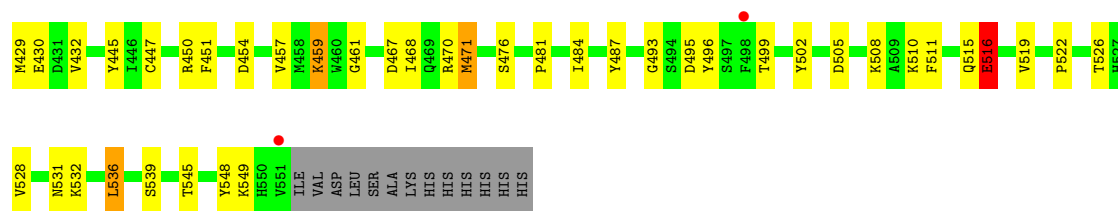
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22



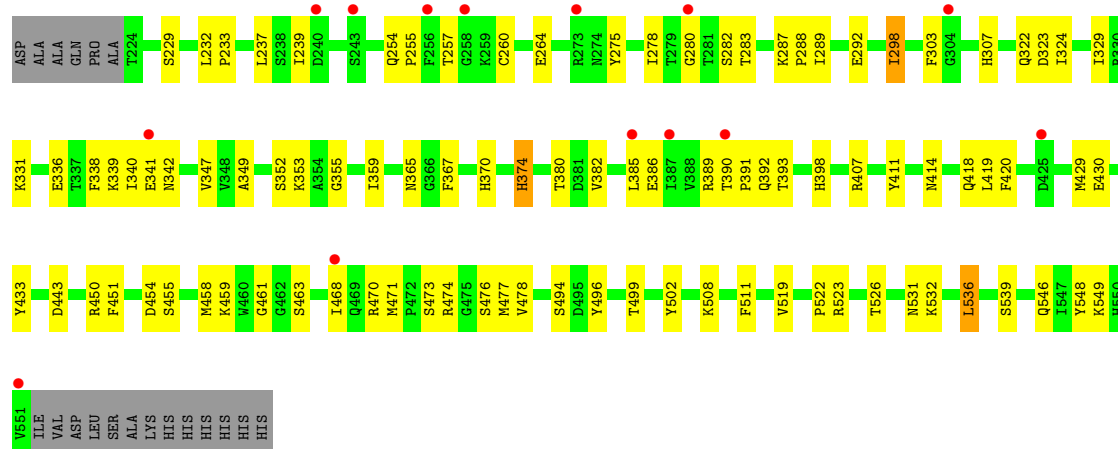
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22



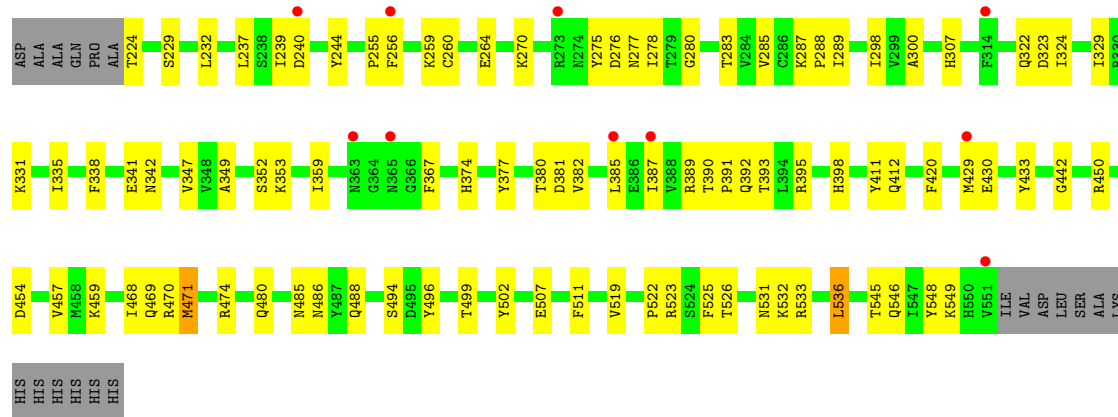
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22



• Molecule 2: Leucine-rich glioma-inactivated protein 1

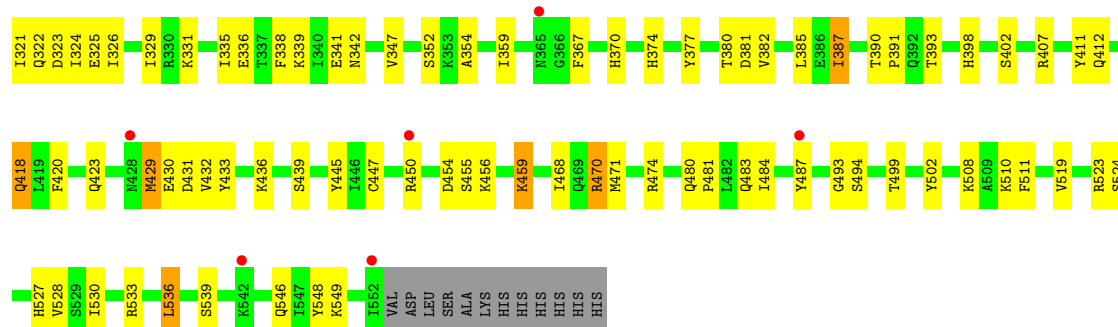


• Molecule 2: Leucine-rich glioma-inactivated protein 1



• Molecule 2: Leucine-rich glioma-inactivated protein 1

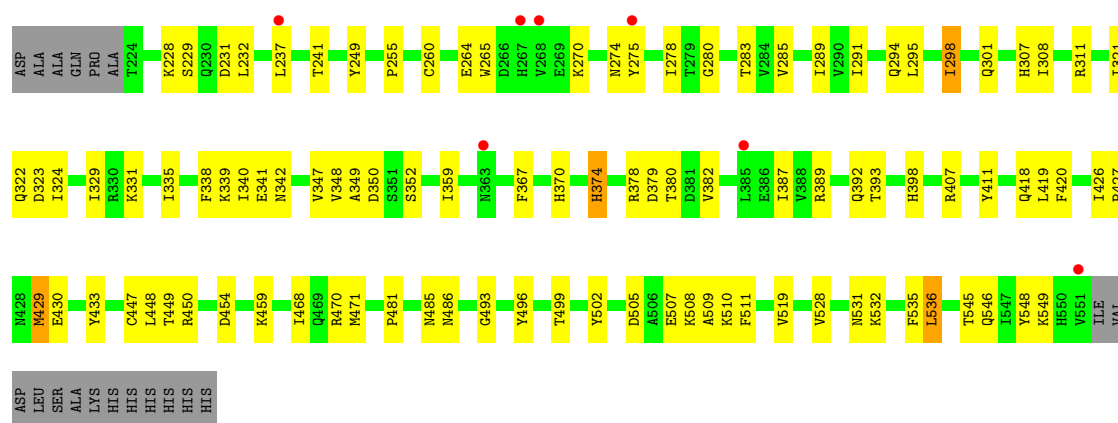




• Molecule 2: Leucine-rich glioma-inactivated protein 1



• Molecule 2: Leucine-rich glioma-inactivated protein 1



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 100%



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

Chain N: 50% 50%



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

Chain S: 75% 25%

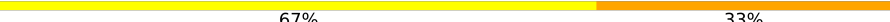


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  67% 33%

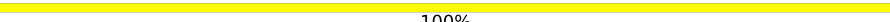
MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  67% 33%

MAG1
MAG2
FUC3

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.58Å 83.61Å 293.54Å 86.40° 88.17° 59.95°	Depositor
Resolution (Å)	48.83 – 2.67 48.83 – 2.67	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.83-2.67) 90.7 (48.83-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.279 0.245 , 0.279	Depositor DCC
R_{free} test set	9035 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.049 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	39417	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/3759	0.73	1/5058 (0.0%)
1	C	0.35	0/3683	0.74	1/4955 (0.0%)
1	E	0.35	0/3635	0.74	1/4889 (0.0%)
1	G	0.33	0/3597	0.71	0/4837
1	I	0.34	0/3751	0.73	1/5049 (0.0%)
1	K	0.33	0/3792	0.72	1/5105 (0.0%)
2	B	0.43	1/2783 (0.0%)	0.79	4/3775 (0.1%)
2	D	0.32	0/2783	0.70	0/3775
2	F	0.32	0/2783	0.72	0/3775
2	H	0.32	0/2791	0.72	1/3786 (0.0%)
2	J	0.33	0/2783	0.73	1/3775 (0.0%)
2	L	0.33	0/2783	0.72	0/3775
All	All	0.34	1/38923 (0.0%)	0.73	11/52554 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	516	GLU	CD-OE1	-5.95	1.14	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	516	GLU	CG-CD-OE2	7.13	134.80	118.40
1	K	460	CYS	N-CA-C	6.95	118.85	111.28
1	I	460	CYS	N-CA-C	6.69	118.58	111.28
2	B	516	GLU	N-CA-C	6.66	119.37	108.52
1	A	460	CYS	N-CA-C	6.51	119.19	111.71
2	B	516	GLU	CG-CD-OE1	-6.40	103.69	118.40
2	H	429	MET	N-CA-C	5.54	117.88	108.02
2	J	281	THR	N-CA-C	5.54	116.99	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	538	VAL	N-CA-C	-5.43	107.69	112.90
2	B	281	THR	N-CA-C	5.18	117.60	111.33
1	C	307	ILE	CB-CA-C	-5.04	105.51	111.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3696	0	3548	91	0
1	C	3623	0	3480	84	0
1	E	3575	0	3422	81	0
1	G	3537	0	3387	55	0
1	I	3688	0	3543	73	0
1	K	3728	0	3583	83	0
2	B	2708	0	2635	79	0
2	D	2708	0	2635	70	0
2	F	2708	0	2635	67	0
2	H	2716	0	2646	73	0
2	J	2708	0	2635	67	0
2	L	2708	0	2635	63	0
3	M	28	0	25	1	0
3	O	28	0	25	0	0
3	Q	28	0	25	0	0
3	T	28	0	25	0	0
4	N	49	0	43	0	0
4	S	49	0	43	1	0
5	P	38	0	34	3	0
5	U	38	0	33	1	0
5	V	38	0	34	0	0
6	R	24	0	22	1	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	3	0	0	0	0
7	F	1	0	0	0	0
7	G	3	0	0	0	0
7	H	1	0	0	0	0
7	I	3	0	0	0	0
7	J	1	0	0	0	0
7	K	3	0	0	0	0
7	L	1	0	0	0	0
8	H	14	0	13	0	0
8	L	14	0	13	1	0
9	A	91	0	0	30	0
9	B	94	0	0	21	1
9	C	73	0	0	18	0
9	D	78	0	0	18	0
9	E	78	0	0	23	0
9	F	62	0	0	17	0
9	G	72	0	0	10	0
9	H	66	0	0	16	0
9	I	91	0	0	27	0
9	J	67	0	0	14	0
9	K	83	0	0	32	1
9	L	59	0	0	12	0
All	All	39417	0	37119	868	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (868) 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:E:513:ARG:NH1	9:E:901:HOH:O	1.85	1.07
2:L:307:HIS:NE2	9:L:701:HOH:O	1.91	1.01
1:I:458:CYS:SG	9:I:949:HOH:O	2.20	0.99
2:B:377:TYR:O	9:B:701:HOH:O	1.81	0.97
2:H:377:TYR:O	9:H:701:HOH:O	1.81	0.96
1:K:665:GLU:OE1	9:K:901:HOH:O	1.84	0.95
1:C:409:TYR:O	9:C:901:HOH:O	1.85	0.95
1:E:580:LYS:HD2	1:E:622:THR:HG23	1.49	0.94
1:G:253:LYS:NZ	9:G:904:HOH:O	2.01	0.94
2:B:307:HIS:NE2	9:B:707:HOH:O	2.00	0.94
2:H:381:ASP:OD1	9:H:702:HOH:O	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:322:GLU:OE1	9:I:901:HOH:O	1.85	0.93
2:B:325:GLU:O	9:B:702:HOH:O	1.85	0.93
2:B:519:VAL:O	9:B:703:HOH:O	1.87	0.92
1:E:598:VAL:O	9:E:902:HOH:O	1.88	0.91
1:E:401:CYS:O	9:E:903:HOH:O	1.90	0.89
2:J:366:GLY:O	9:J:701:HOH:O	1.91	0.89
1:K:490:CYS:SG	9:K:943:HOH:O	2.28	0.89
2:H:474:ARG:NH2	9:H:706:HOH:O	2.07	0.85
1:G:430:GLY:O	9:G:901:HOH:O	1.95	0.85
1:A:310:ARG:NH2	9:A:909:HOH:O	2.09	0.84
2:H:429:MET:SD	2:H:450:ARG:NH2	2.50	0.84
1:A:624:THR:OG1	9:A:902:HOH:O	1.95	0.84
2:L:289:ILE:HD11	2:L:298:ILE:HD11	1.61	0.83
2:B:289:ILE:HD11	2:B:298:ILE:HD11	1.61	0.83
2:B:301:GLN:O	9:B:704:HOH:O	1.96	0.83
1:E:581:GLY:HA3	9:E:905:HOH:O	1.78	0.83
2:L:429:MET:HE2	2:L:448:LEU:HG	1.60	0.82
1:K:551:ASP:OD2	9:K:904:HOH:O	1.97	0.82
2:F:289:ILE:HD11	2:F:298:ILE:HD11	1.61	0.82
1:A:334:GLN:NE2	9:A:910:HOH:O	2.12	0.82
1:G:420:GLU:OE2	9:G:902:HOH:O	1.98	0.81
1:K:622:THR:HB	9:K:906:HOH:O	1.80	0.81
1:C:566:ASP:HB3	1:C:633:LEU:HD13	1.62	0.81
2:H:289:ILE:HD11	2:H:298:ILE:HD11	1.62	0.81
1:A:463:PRO:O	9:A:903:HOH:O	1.99	0.80
1:K:389:SER:OG	9:K:903:HOH:O	1.97	0.80
2:B:461:GLY:O	9:B:706:HOH:O	1.99	0.80
1:K:237:GLU:OE2	9:K:905:HOH:O	1.99	0.80
2:D:289:ILE:HD11	2:D:298:ILE:HD11	1.60	0.80
2:F:474:ARG:NH2	9:F:707:HOH:O	2.13	0.80
1:K:519:ASN:ND2	9:K:911:HOH:O	2.14	0.80
1:A:407:GLY:HA3	2:B:331:LYS:HG2	1.64	0.80
1:I:456:GLU:O	9:I:902:HOH:O	2.00	0.80
2:J:289:ILE:HD11	2:J:298:ILE:HD11	1.64	0.80
1:I:694:CYS:SG	9:I:922:HOH:O	2.40	0.79
1:G:703:ASN:OD1	9:G:903:HOH:O	2.01	0.79
1:E:539:GLN:NE2	9:E:909:HOH:O	2.15	0.79
2:L:519:VAL:O	9:L:702:HOH:O	1.99	0.78
1:K:444:PRO:O	9:K:907:HOH:O	2.01	0.78
1:A:631:ARG:NH2	9:A:912:HOH:O	2.17	0.78
1:C:345:ILE:O	9:C:903:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:602:TYR:OH	9:K:906:HOH:O	1.99	0.77
1:A:399:SER:O	9:A:904:HOH:O	2.01	0.77
9:I:906:HOH:O	2:J:378:ARG:NH1	2.18	0.76
2:J:361:LYS:O	9:J:701:HOH:O	2.04	0.76
2:B:429:MET:SD	9:B:788:HOH:O	2.42	0.76
2:B:291:ILE:HG22	2:B:292:GLU:HG2	1.68	0.75
1:A:449:ASN:O	9:A:905:HOH:O	2.04	0.75
2:F:377:TYR:O	9:F:703:HOH:O	2.04	0.74
1:A:372:GLN:NE2	9:A:915:HOH:O	2.20	0.74
2:H:301:GLN:NE2	9:H:712:HOH:O	2.19	0.74
2:D:455:SER:HG	2:D:473:SER:HG	1.34	0.74
2:F:232:LEU:HB2	2:F:545:THR:HG23	1.70	0.74
1:C:385:ARG:NE	9:C:911:HOH:O	2.20	0.74
1:E:407:GLY:HA3	2:F:331:LYS:HG2	1.69	0.74
2:H:321:ILE:HD12	2:H:322:GLN:HB2	1.69	0.74
1:K:531:ASP:OD1	9:K:908:HOH:O	2.05	0.74
2:J:441:LYS:O	9:J:703:HOH:O	2.05	0.73
1:C:407:GLY:HA3	2:D:331:LYS:HG2	1.69	0.73
1:K:407:GLY:HA3	2:L:331:LYS:HG2	1.69	0.73
1:E:573:LEU:HB3	9:E:905:HOH:O	1.88	0.73
2:B:430:GLU:H	2:B:450:ARG:HH21	1.37	0.73
2:F:229:SER:HB2	2:F:549:LYS:HG3	1.70	0.73
2:B:237:LEU:O	9:B:709:HOH:O	2.07	0.72
2:H:519:VAL:O	9:H:705:HOH:O	2.06	0.72
1:I:514:GLU:OE1	9:I:905:HOH:O	2.06	0.72
2:D:414:ASN:OD1	9:D:702:HOH:O	2.06	0.72
2:H:339:LYS:HE2	2:H:342:ASN:HA	1.72	0.72
2:B:229:SER:HB2	2:B:549:LYS:HG3	1.71	0.72
1:A:505:GLU:OE1	9:A:907:HOH:O	2.07	0.72
1:G:407:GLY:HA3	2:H:331:LYS:HG2	1.70	0.72
2:D:463:SER:OG	9:D:701:HOH:O	2.06	0.72
1:C:505:GLU:OE2	9:C:906:HOH:O	2.08	0.72
2:F:412:GLN:OE1	9:F:705:HOH:O	2.08	0.72
2:F:450:ARG:NH1	2:F:454:ASP:O	2.23	0.71
1:A:361:GLY:H	1:A:366:MET:HE2	1.54	0.71
2:B:260:CYS:HB2	2:B:278:ILE:HB	1.73	0.71
2:F:412:GLN:NE2	6:R:1:NAG:O7	2.23	0.71
1:G:322:GLU:OE1	9:G:905:HOH:O	2.07	0.71
1:G:583:CYS:N	1:G:593:CYS:SG	2.63	0.71
1:C:563:THR:OG1	1:C:606:THR:OG1	2.09	0.71
1:E:580:LYS:O	9:E:905:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396:ASP:OD1	9:I:903:HOH:O	2.09	0.71
2:D:461:GLY:O	9:D:703:HOH:O	2.08	0.70
2:J:304:GLY:O	9:J:704:HOH:O	2.10	0.70
2:L:407:ARG:HG3	2:L:430:GLU:HG3	1.73	0.70
2:L:274:ASN:OD1	9:L:703:HOH:O	2.07	0.70
2:D:477:MET:SD	9:D:774:HOH:O	2.49	0.70
1:K:361:GLY:H	1:K:366:MET:HE2	1.57	0.70
2:J:266:ASP:CG	2:J:273:ARG:HH12	2.00	0.70
1:A:704:ARG:NH2	9:A:916:HOH:O	2.20	0.70
2:J:407:ARG:HG3	2:J:430:GLU:HG3	1.73	0.69
1:E:280:GLN:HE22	1:E:413:LYS:HA	1.57	0.69
2:H:260:CYS:HB2	2:H:278:ILE:HB	1.74	0.69
1:C:251:MET:N	9:C:905:HOH:O	2.24	0.69
1:C:472:GLU:HB2	9:C:915:HOH:O	1.92	0.69
2:B:229:SER:OG	9:B:711:HOH:O	2.10	0.69
1:I:359:GLU:OE2	9:I:906:HOH:O	2.09	0.69
2:J:260:CYS:HB2	2:J:278:ILE:HB	1.74	0.69
2:B:232:LEU:HB2	2:B:545:THR:HG23	1.73	0.69
2:B:467:ASP:OD2	9:B:710:HOH:O	2.10	0.69
1:E:361:GLY:H	1:E:366:MET:HE2	1.58	0.69
1:K:395:GLU:OE1	9:K:909:HOH:O	2.10	0.69
2:F:224:THR:N	9:F:713:HOH:O	2.26	0.69
2:F:381:ASP:OD1	9:F:706:HOH:O	2.11	0.69
2:L:379:ASP:OD2	9:L:705:HOH:O	2.11	0.69
1:E:511:ASP:OD2	9:E:906:HOH:O	2.10	0.69
1:I:407:GLY:HA3	2:J:331:LYS:HG2	1.75	0.68
1:I:622:THR:HB	9:I:923:HOH:O	1.93	0.68
1:E:292:THR:O	2:D:470:ARG:NH1	2.26	0.68
1:K:641:LYS:HA	9:K:916:HOH:O	1.92	0.68
2:J:450:ARG:NH1	2:J:454:ASP:O	2.26	0.68
2:H:229:SER:HB2	2:H:549:LYS:HG3	1.76	0.68
1:A:251:MET:HE3	1:A:330:PHE:HB3	1.76	0.68
2:J:340:ILE:HG22	2:J:341:GLU:HG2	1.75	0.68
1:G:361:GLY:H	1:G:366:MET:HE2	1.59	0.68
2:D:454:ASP:OD2	9:D:704:HOH:O	2.10	0.68
1:I:383:ASP:HB2	9:I:919:HOH:O	1.94	0.67
2:L:241:THR:HG21	2:L:528:VAL:HG22	1.77	0.67
2:L:339:LYS:HE2	2:L:342:ASN:HA	1.77	0.67
1:K:288:VAL:O	9:K:910:HOH:O	2.12	0.67
1:E:666:HIS:NE2	9:E:913:HOH:O	2.24	0.67
1:I:536:ASP:OD2	1:I:552:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ARG:HD3	1:C:352:LEU:HD21	1.77	0.67
1:E:704:ARG:NH1	9:E:918:HOH:O	2.27	0.66
1:A:511:ASP:OD2	9:A:911:HOH:O	2.14	0.66
1:C:348:ILE:HG12	1:C:378:ILE:HD12	1.78	0.66
1:G:292:THR:O	2:B:470:ARG:NH1	2.29	0.66
2:D:355:GLY:O	9:D:705:HOH:O	2.12	0.66
2:F:507:GLU:N	9:F:704:HOH:O	2.28	0.66
2:H:439:SER:O	9:H:707:HOH:O	2.11	0.66
1:K:574:ASN:HD22	1:K:598:VAL:HA	1.60	0.66
1:G:251:MET:HE3	1:G:330:PHE:HB3	1.77	0.66
2:B:246:ASN:OD1	9:B:712:HOH:O	2.14	0.66
2:H:474:ARG:NH1	9:H:704:HOH:O	2.06	0.66
1:I:597:ASP:OD2	9:I:907:HOH:O	2.14	0.66
2:D:532:LYS:NZ	9:D:711:HOH:O	2.22	0.66
2:L:260:CYS:HB2	2:L:278:ILE:HB	1.78	0.66
2:L:374:HIS:O	9:L:705:HOH:O	2.14	0.66
2:H:445:TYR:HE2	2:H:459:LYS:HZ1	1.43	0.66
1:K:647:ASP:HA	9:K:916:HOH:O	1.96	0.65
1:E:523:CYS:O	9:E:908:HOH:O	2.14	0.65
2:D:407:ARG:HG3	2:D:430:GLU:HG3	1.77	0.65
1:C:292:THR:O	2:F:470:ARG:NH1	2.30	0.65
2:B:445:TYR:HE2	2:B:459:LYS:HZ1	1.42	0.65
2:F:469:GLN:HG3	2:F:471:MET:HE1	1.78	0.65
1:C:338:SER:N	9:C:909:HOH:O	2.16	0.65
1:K:483:SER:N	9:K:918:HOH:O	2.29	0.65
2:J:229:SER:HB2	2:J:549:LYS:HG3	1.79	0.65
1:I:667:ARG:HG2	9:I:907:HOH:O	1.95	0.65
2:B:237:LEU:HB2	2:B:255:PRO:HG3	1.78	0.65
2:D:229:SER:HB2	2:D:549:LYS:HG3	1.79	0.65
1:C:251:MET:HE3	1:C:330:PHE:HB3	1.76	0.65
2:J:363:ASN:N	9:J:701:HOH:O	2.30	0.64
2:D:347:VAL:HG22	2:D:359:ILE:HG12	1.80	0.64
2:B:510:LYS:NZ	2:B:511:PHE:O	2.29	0.64
1:C:248:ASP:OD1	9:C:905:HOH:O	2.15	0.64
1:C:577:GLY:O	9:C:908:HOH:O	2.15	0.64
2:L:378:ARG:NH1	9:L:714:HOH:O	2.30	0.64
1:K:598:VAL:HG13	1:K:599:LEU:HD22	1.80	0.64
2:B:459:LYS:HB2	2:B:468:ILE:HD11	1.79	0.64
2:D:459:LYS:HB2	2:D:468:ILE:HD11	1.80	0.64
2:F:459:LYS:HB2	2:F:468:ILE:HD11	1.79	0.64
2:H:536:LEU:HB3	2:H:548:TYR:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:459:LYS:HB2	2:J:468:ILE:HD11	1.79	0.64
1:A:378:ILE:HD11	1:A:434:LEU:HD21	1.79	0.64
1:A:392:CYS:SG	9:A:983:HOH:O	2.55	0.64
2:F:341:GLU:O	2:F:342:ASN:ND2	2.31	0.64
2:D:237:LEU:HB2	2:D:255:PRO:HG3	1.81	0.63
2:H:508:LYS:HB3	2:H:510:LYS:HG2	1.81	0.63
2:B:536:LEU:HB3	2:B:548:TYR:HB2	1.79	0.63
1:K:280:GLN:HE22	1:K:413:LYS:HA	1.62	0.63
8:L:602:NAG:H5	9:L:703:HOH:O	1.97	0.63
1:G:310:ARG:NH2	1:G:643:GLU:OE1	2.31	0.63
1:I:280:GLN:HE22	1:I:413:LYS:HA	1.61	0.63
1:C:378:ILE:HD11	1:C:434:LEU:HD21	1.80	0.63
1:K:391:GLU:N	9:K:919:HOH:O	2.23	0.63
2:F:237:LEU:HB2	2:F:255:PRO:HG3	1.81	0.63
1:G:598:VAL:HG13	1:G:599:LEU:HD22	1.81	0.63
2:B:287:LYS:NZ	9:B:713:HOH:O	2.14	0.63
2:F:536:LEU:HB3	2:F:548:TYR:HB2	1.81	0.63
1:E:705:HIS:HE1	9:E:907:HOH:O	1.81	0.62
1:I:598:VAL:HG13	1:I:599:LEU:HD22	1.80	0.62
1:A:280:GLN:HE22	1:A:413:LYS:HA	1.64	0.62
1:C:514:GLU:OE2	1:C:527:ILE:N	2.31	0.62
1:C:598:VAL:HG13	1:C:599:LEU:HD22	1.81	0.62
1:G:594:ASN:OD1	1:G:595:LYS:N	2.32	0.62
1:A:536:ASP:OD2	1:A:552:ARG:NH1	2.32	0.62
2:D:536:LEU:HB3	2:D:548:TYR:HB2	1.80	0.62
2:L:429:MET:CE	2:L:448:LEU:HG	2.30	0.62
2:H:423:GLN:NE2	9:H:708:HOH:O	2.14	0.62
1:A:598:VAL:HG13	1:A:599:LEU:HD22	1.80	0.62
2:F:322:GLN:NE2	2:F:367:PHE:O	2.32	0.62
1:E:274:ASP:OD2	1:E:284:ARG:NH1	2.32	0.62
1:K:245:ILE:HB	1:K:290:MET:HE2	1.80	0.62
2:H:241:THR:HG21	2:H:528:VAL:HG22	1.82	0.62
2:L:340:ILE:HG22	2:L:341:GLU:HG2	1.81	0.62
1:K:251:MET:HE3	1:K:330:PHE:HB3	1.80	0.62
2:L:347:VAL:HG22	2:L:359:ILE:HG12	1.81	0.62
1:K:504:ARG:HH11	1:K:514:GLU:HG3	1.65	0.61
2:J:347:VAL:HG22	2:J:359:ILE:HG12	1.81	0.61
1:A:245:ILE:HB	1:A:290:MET:HE2	1.83	0.61
1:A:530:MET:HE1	1:A:677:SER:O	2.00	0.61
5:P:1:NAG:O3	5:P:2:NAG:O5	2.18	0.61
2:H:456:LYS:HD2	2:H:470:ARG:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:237:LEU:HB2	2:J:255:PRO:HG3	1.81	0.61
1:A:704:ARG:HG2	1:A:705:HIS:ND1	2.15	0.61
2:D:322:GLN:NE2	2:D:367:PHE:O	2.33	0.61
1:C:280:GLN:HE22	1:C:413:LYS:HA	1.65	0.61
2:J:232:LEU:HB2	2:J:545:THR:HG23	1.81	0.61
2:D:443:ASP:OD2	9:D:706:HOH:O	2.16	0.61
1:C:568:TYR:HB3	1:C:633:LEU:HD11	1.83	0.61
2:B:430:GLU:H	2:B:450:ARG:NH2	1.97	0.61
2:F:395:ARG:NH1	9:F:716:HOH:O	2.32	0.61
2:H:459:LYS:HB2	2:H:468:ILE:HD11	1.82	0.61
1:C:561:LYS:NZ	9:C:902:HOH:O	2.02	0.61
1:K:583:CYS:N	1:K:593:CYS:SG	2.74	0.61
1:E:598:VAL:HG13	1:E:599:LEU:HD22	1.83	0.60
1:K:348:ILE:O	9:K:912:HOH:O	2.16	0.60
2:B:430:GLU:N	2:B:450:ARG:HH21	1.98	0.60
2:D:407:ARG:NH2	9:D:719:HOH:O	2.34	0.60
2:F:347:VAL:HG22	2:F:359:ILE:HG12	1.82	0.60
2:H:347:VAL:HG22	2:H:359:ILE:HG12	1.82	0.60
1:E:577:GLY:O	9:E:912:HOH:O	2.17	0.60
2:L:349:ALA:HB2	2:L:382:VAL:HG23	1.84	0.60
1:E:285:ILE:O	9:E:911:HOH:O	2.16	0.60
1:I:361:GLY:H	1:I:366:MET:HE2	1.65	0.60
2:D:508:LYS:NZ	9:D:718:HOH:O	2.33	0.60
1:A:714:TYR:OH	9:A:908:HOH:O	2.08	0.60
1:C:437:LYS:NZ	9:C:919:HOH:O	2.35	0.60
1:I:399:SER:N	9:I:903:HOH:O	2.34	0.60
2:H:483:GLN:OE1	9:H:707:HOH:O	2.17	0.60
2:J:551:VAL:HG12	9:J:763:HOH:O	2.00	0.60
2:L:232:LEU:HB2	2:L:545:THR:HG23	1.84	0.60
1:E:251:MET:HE3	1:E:330:PHE:HB3	1.84	0.60
1:I:665:GLU:OE1	9:I:908:HOH:O	2.17	0.59
2:D:307:HIS:ND1	2:D:323:ASP:OD1	2.29	0.59
1:C:463:PRO:O	1:C:467:VAL:HG23	2.02	0.59
1:G:245:ILE:HB	1:G:290:MET:HE2	1.84	0.59
1:K:456:GLU:HB2	1:K:477:CYS:HB3	1.85	0.59
1:I:251:MET:HE3	1:I:330:PHE:HB3	1.83	0.59
2:B:341:GLU:O	2:B:342:ASN:ND2	2.35	0.59
2:D:340:ILE:HG22	2:D:341:GLU:HG3	1.83	0.59
2:L:331:LYS:HB2	2:L:352:SER:HB3	1.83	0.59
2:F:470:ARG:HA	2:F:471:MET:HE2	1.85	0.59
2:J:254:GLN:OE1	2:J:257:THR:OG1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LYS:NZ	9:A:919:HOH:O	2.26	0.59
2:J:536:LEU:HB3	2:J:548:TYR:HB2	1.85	0.59
1:G:536:ASP:OD2	1:G:552:ARG:NH1	2.35	0.59
1:A:467:VAL:HG23	9:A:903:HOH:O	2.03	0.58
2:B:454:ASP:HB3	9:B:791:HOH:O	2.04	0.58
1:K:389:SER:HB2	9:K:919:HOH:O	2.03	0.58
2:D:341:GLU:O	2:D:342:ASN:ND2	2.37	0.58
1:G:504:ARG:HH11	1:G:514:GLU:HG3	1.68	0.58
1:K:577:GLY:O	1:K:590:TRP:HB2	2.03	0.58
2:F:280:GLY:HA3	9:F:711:HOH:O	2.01	0.58
2:J:331:LYS:HB2	2:J:352:SER:HB3	1.85	0.58
2:L:350:ASP:O	9:L:706:HOH:O	2.17	0.58
1:A:566:ASP:HB3	1:A:633:LEU:HD13	1.85	0.58
1:C:536:ASP:OD2	1:C:552:ARG:NH1	2.37	0.58
2:L:387:ILE:HG22	2:L:398:HIS:CE1	2.39	0.58
1:C:626:VAL:O	1:C:632:THR:HA	2.04	0.58
2:J:383:GLU:OE1	9:J:705:HOH:O	2.17	0.58
2:L:411:TYR:HB3	2:L:420:PHE:HB3	1.86	0.58
2:J:443:ASP:OD2	9:J:706:HOH:O	2.17	0.57
2:B:328:LYS:HB2	9:B:702:HOH:O	2.04	0.57
2:D:324:ILE:HG21	2:D:329:ILE:HD12	1.85	0.57
2:L:321:ILE:HD12	2:L:322:GLN:HB2	1.84	0.57
1:I:391:GLU:OE2	9:I:910:HOH:O	2.18	0.57
2:B:347:VAL:HG22	2:B:359:ILE:HG12	1.85	0.57
2:B:454:ASP:OD1	2:B:454:ASP:N	2.37	0.57
1:I:249:HIS:CD2	1:I:253:LYS:HE2	2.38	0.57
2:B:385:LEU:O	2:B:398:HIS:N	2.37	0.57
2:J:349:ALA:HB2	2:J:382:VAL:HG23	1.85	0.57
1:E:558:TRP:CE2	1:E:608:ILE:HD11	2.40	0.57
1:A:704:ARG:HE	1:A:705:HIS:CE1	2.23	0.57
1:G:280:GLN:HE22	1:G:413:LYS:HA	1.70	0.57
1:I:274:ASP:OD2	1:I:284:ARG:NH1	2.38	0.57
1:K:317:ARG:HD3	1:K:352:LEU:HD21	1.87	0.57
2:L:536:LEU:HB3	2:L:548:TYR:HB2	1.87	0.57
2:B:505:ASP:HB3	2:B:508:LYS:HB2	1.86	0.57
2:J:307:HIS:CE1	9:J:704:HOH:O	2.58	0.57
2:L:389:ARG:NH2	9:L:716:HOH:O	2.37	0.57
2:J:250:VAL:HB	2:J:263:LEU:HB2	1.86	0.56
1:E:502:VAL:HG22	9:E:901:HOH:O	2.06	0.56
9:B:714:HOH:O	3:M:2:NAG:O4	2.18	0.56
2:D:239:ILE:O	2:D:526:THR:HG21	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:321:ILE:HD12	2:J:322:GLN:HB2	1.86	0.56
2:L:454:ASP:OD2	2:L:454:ASP:N	2.38	0.56
1:G:317:ARG:HD3	1:G:352:LEU:HD21	1.88	0.56
1:K:579:GLU:OE2	9:K:913:HOH:O	2.18	0.56
2:H:480:GLN:OE1	9:H:711:HOH:O	2.18	0.56
2:D:349:ALA:HB2	2:D:382:VAL:HG23	1.87	0.56
2:H:331:LYS:HB2	2:H:352:SER:HB3	1.86	0.56
1:K:253:LYS:NZ	9:K:902:HOH:O	1.92	0.56
1:K:610:ASN:HA	1:K:621:ILE:HD11	1.88	0.56
2:L:450:ARG:NH1	2:L:454:ASP:O	2.39	0.56
1:I:317:ARG:HD3	1:I:352:LEU:HD21	1.88	0.56
1:I:551:ASP:OD2	9:I:909:HOH:O	2.17	0.56
2:D:454:ASP:OD1	2:D:454:ASP:N	2.37	0.56
1:A:577:GLY:HA3	1:A:592:GLN:HA	1.87	0.56
1:E:504:ARG:HH11	1:E:514:GLU:HG3	1.71	0.56
1:I:245:ILE:HB	1:I:290:MET:HE2	1.87	0.56
2:F:244:TYR:O	9:F:708:HOH:O	2.17	0.56
2:F:385:LEU:HD23	2:F:387:ILE:HD11	1.88	0.56
2:J:264:GLU:HB2	2:J:275:TYR:HB2	1.88	0.56
1:A:508:ASN:HB2	9:A:922:HOH:O	2.06	0.55
1:A:662:MET:HE2	1:A:671:VAL:HG12	1.88	0.55
1:A:705:HIS:HD2	1:A:716:PRO:HA	1.70	0.55
2:H:244:TYR:OH	9:H:710:HOH:O	2.17	0.55
1:C:633:LEU:O	1:C:635:CYS:N	2.38	0.55
2:J:454:ASP:OD1	2:J:454:ASP:N	2.35	0.55
2:L:270:LYS:NZ	9:L:717:HOH:O	2.40	0.55
2:L:322:GLN:NE2	2:L:367:PHE:O	2.39	0.55
1:I:662:MET:HE2	1:I:671:VAL:HG12	1.87	0.55
2:H:454:ASP:N	2:H:454:ASP:OD1	2.38	0.55
1:G:378:ILE:HD11	1:G:434:LEU:HD21	1.88	0.55
1:K:249:HIS:CD2	1:K:253:LYS:HE2	2.41	0.55
1:I:406:THR:O	9:I:911:HOH:O	2.18	0.55
1:K:378:ILE:HD11	1:K:434:LEU:HD21	1.88	0.55
1:K:391:GLU:HB2	9:K:919:HOH:O	2.06	0.55
1:A:460:CYS:HA	1:A:487:ASP:OD2	2.07	0.55
2:D:260:CYS:HB2	2:D:278:ILE:HB	1.89	0.55
2:H:264:GLU:HB2	2:H:275:TYR:HB2	1.88	0.55
1:K:310:ARG:NH1	1:K:643:GLU:OE2	2.39	0.55
2:F:352:SER:O	9:F:703:HOH:O	2.18	0.55
2:J:510:LYS:NZ	2:J:511:PHE:O	2.28	0.55
2:L:307:HIS:ND1	2:L:323:ASP:OD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:611:ILE:HD12	1:E:612:PRO:HD2	1.89	0.54
1:A:699:LYS:HB2	9:A:901:HOH:O	2.06	0.54
1:K:705:HIS:CE1	1:K:717:HIS:H	2.25	0.54
1:C:245:ILE:HB	1:C:290:MET:HE2	1.88	0.54
1:C:594:ASN:OD1	1:C:595:LYS:N	2.40	0.54
2:D:264:GLU:HB2	2:D:275:TYR:HB2	1.89	0.54
2:B:321:ILE:HD12	2:B:322:GLN:HB2	1.87	0.54
2:F:349:ALA:HB2	2:F:382:VAL:HG23	1.89	0.54
1:K:580:LYS:HA	1:K:622:THR:HG21	1.88	0.54
1:C:274:ASP:OD2	1:C:284:ARG:NH1	2.41	0.54
1:E:583:CYS:N	1:E:593:CYS:SG	2.81	0.54
1:K:522:GLN:NE2	9:K:927:HOH:O	2.41	0.54
2:B:307:HIS:ND1	2:B:323:ASP:OD1	2.35	0.54
1:I:504:ARG:HH11	1:I:514:GLU:HG3	1.72	0.54
1:K:292:THR:O	2:J:470:ARG:NH1	2.41	0.54
1:K:480:THR:C	9:K:918:HOH:O	2.51	0.54
2:F:260:CYS:HB2	2:F:278:ILE:HB	1.90	0.54
2:L:229:SER:HB2	2:L:549:LYS:HG3	1.89	0.54
5:U:2:NAG:H3	5:U:2:NAG:H83	1.90	0.54
1:A:361:GLY:N	1:A:366:MET:HE2	2.23	0.54
1:I:453:GLU:HB3	9:I:917:HOH:O	2.07	0.54
2:F:395:ARG:NH2	2:F:442:GLY:O	2.41	0.53
2:J:274:ASN:ND2	9:J:702:HOH:O	2.02	0.53
2:L:237:LEU:HB2	2:L:255:PRO:HG3	1.90	0.53
1:K:536:ASP:OD2	1:K:552:ARG:NH1	2.41	0.53
2:B:241:THR:HG21	2:B:528:VAL:HG22	1.90	0.53
2:H:530:ILE:O	2:H:533:ARG:HB2	2.08	0.53
1:A:579:GLU:HG2	1:A:590:TRP:NE1	2.22	0.53
1:I:551:ASP:HA	1:I:564:ALA:HB2	1.91	0.53
1:K:307:ILE:HD13	1:K:310:ARG:HH22	1.74	0.53
1:K:530:MET:HE1	1:K:677:SER:O	2.08	0.53
1:A:279:ASP:OD2	9:A:913:HOH:O	2.19	0.53
1:A:621:ILE:HG23	1:A:637:GLY:O	2.09	0.53
1:A:697:GLU:HB2	9:A:901:HOH:O	2.07	0.53
1:I:348:ILE:HG23	1:I:377:ASN:HB3	1.90	0.53
1:A:249:HIS:CD2	1:A:253:LYS:HE2	2.44	0.53
1:K:551:ASP:HA	1:K:564:ALA:HB2	1.91	0.53
1:I:594:ASN:OD1	1:I:595:LYS:N	2.42	0.53
2:B:339:LYS:HE2	2:B:342:ASN:HA	1.91	0.53
1:A:611:ILE:HD12	1:A:612:PRO:HD2	1.90	0.53
2:D:430:GLU:OE1	9:D:708:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:474:ARG:O	2:D:494:SER:OG	2.25	0.53
2:F:240:ASP:OD2	9:F:709:HOH:O	2.19	0.53
2:H:447:CYS:SG	2:H:481:PRO:HG3	2.49	0.53
1:A:348:ILE:HG12	1:A:378:ILE:HD12	1.90	0.53
1:E:571:GLU:HA	1:E:598:VAL:HG21	1.90	0.53
1:A:274:ASP:OD2	1:A:284:ARG:NH1	2.42	0.52
1:G:310:ARG:HG2	1:G:314:LYS:HE3	1.91	0.52
1:G:509:ASP:OD1	1:G:509:ASP:N	2.40	0.52
2:L:249:TYR:HE1	2:L:264:GLU:HG3	1.73	0.52
1:E:372:GLN:NE2	9:E:915:HOH:O	2.26	0.52
1:E:310:ARG:NH2	1:E:643:GLU:OE1	2.42	0.52
2:F:307:HIS:ND1	2:F:323:ASP:OD1	2.33	0.52
2:L:459:LYS:HB2	2:L:468:ILE:HD11	1.92	0.52
2:B:428:ASN:ND2	9:B:710:HOH:O	2.43	0.52
2:D:429:MET:HG2	2:D:450:ARG:HH22	1.75	0.52
2:H:387:ILE:HG22	2:H:398:HIS:CE1	2.45	0.52
2:J:307:HIS:ND1	2:J:323:ASP:OD1	2.43	0.52
2:H:341:GLU:O	2:H:342:ASN:ND2	2.42	0.52
1:E:483:SER:HB2	1:E:494:CYS:HB3	1.91	0.52
1:K:611:ILE:HD12	1:K:612:PRO:HD2	1.92	0.52
2:F:488:GLN:OE1	9:F:710:HOH:O	2.19	0.52
1:E:536:ASP:OD2	1:E:552:ARG:NH1	2.43	0.52
2:B:264:GLU:HB2	2:B:275:TYR:HB2	1.92	0.52
1:A:551:ASP:HA	1:A:564:ALA:HB2	1.92	0.52
2:F:411:TYR:HB3	2:F:420:PHE:HB3	1.91	0.52
1:A:348:ILE:HD11	1:A:425:PHE:CE2	2.45	0.51
1:I:679:CYS:N	9:I:922:HOH:O	2.42	0.51
2:F:338:PHE:HE1	2:F:347:VAL:HG23	1.75	0.51
2:H:322:GLN:NE2	2:H:367:PHE:O	2.43	0.51
1:E:245:ILE:HB	1:E:290:MET:HE2	1.90	0.51
2:D:336:GLU:HG2	9:D:707:HOH:O	2.10	0.51
1:C:569:CYS:SG	1:C:633:LEU:HB2	2.50	0.51
2:J:470:ARG:NH1	9:J:722:HOH:O	2.43	0.51
2:L:324:ILE:HG21	2:L:329:ILE:HD12	1.92	0.51
1:C:611:ILE:HD12	1:C:612:PRO:HD2	1.92	0.51
1:A:504:ARG:HH11	1:A:514:GLU:HG3	1.75	0.51
2:D:411:TYR:HB3	2:D:420:PHE:HB3	1.92	0.51
1:A:408:TYR:O	9:A:914:HOH:O	2.19	0.51
1:E:570:TYR:HB3	9:E:902:HOH:O	2.11	0.51
1:K:361:GLY:HA2	9:L:721:HOH:O	2.09	0.51
1:K:662:MET:HE2	1:K:671:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:411:TYR:HB3	2:H:420:PHE:HB3	1.92	0.51
1:E:254:LYS:HA	9:E:919:HOH:O	2.11	0.51
2:H:412:GLN:OE1	9:H:713:HOH:O	2.19	0.51
1:E:448:GLY:HA2	1:E:461:GLY:O	2.11	0.51
2:H:324:ILE:HG21	2:H:329:ILE:HD12	1.93	0.51
1:A:559:GLY:HA2	1:A:613:ARG:HD2	1.93	0.51
1:A:582:ASN:H	1:A:602:TYR:HB2	1.75	0.51
1:C:551:ASP:HA	1:C:564:ALA:HB2	1.93	0.51
1:G:611:ILE:HD12	1:G:612:PRO:HD2	1.93	0.51
2:D:499:THR:HG21	2:D:522:PRO:HG3	1.93	0.51
1:E:317:ARG:HD3	1:E:352:LEU:HD21	1.93	0.50
2:L:291:ILE:O	2:L:294:GLN:HB2	2.10	0.50
1:C:514:GLU:OE2	1:C:527:ILE:HG13	2.10	0.50
1:I:611:ILE:HD12	1:I:612:PRO:HD2	1.93	0.50
2:F:519:VAL:HG12	2:F:546:GLN:CD	2.36	0.50
1:C:433:CYS:HB2	9:C:914:HOH:O	2.12	0.50
1:C:484:GLN:HG3	1:C:495:LYS:HD3	1.92	0.50
1:E:530:MET:HE1	1:E:677:SER:O	2.12	0.50
1:G:530:MET:HE1	1:G:677:SER:O	2.12	0.50
1:K:482:ASP:N	9:K:918:HOH:O	2.45	0.50
2:J:266:ASP:HB2	2:J:273:ARG:NH1	2.27	0.50
2:J:411:TYR:HB3	2:J:420:PHE:HB3	1.93	0.50
1:I:717:HIS:CG	1:I:717:HIS:O	2.65	0.50
1:K:625:LEU:HB2	9:K:923:HOH:O	2.12	0.50
2:B:270:LYS:NZ	9:B:727:HOH:O	2.39	0.50
2:F:494:SER:H	2:F:499:THR:HG22	1.75	0.50
2:H:338:PHE:HE1	2:H:347:VAL:HG23	1.77	0.50
2:J:338:PHE:HE1	2:J:347:VAL:HG23	1.76	0.50
1:A:706:TRP:NE1	9:A:927:HOH:O	2.40	0.50
1:E:378:ILE:HD11	1:E:434:LEU:HD21	1.93	0.50
1:G:238:THR:OG1	1:G:282:LYS:NZ	2.45	0.50
2:L:338:PHE:HE1	2:L:347:VAL:HG23	1.76	0.50
1:A:400:GLY:HA3	9:A:904:HOH:O	2.11	0.50
2:H:336:GLU:HB2	2:H:382:VAL:HG13	1.94	0.50
1:C:546:ARG:NH2	9:C:917:HOH:O	2.33	0.50
2:B:338:PHE:HE1	2:B:347:VAL:HG23	1.76	0.50
2:B:389:ARG:NH2	9:B:731:HOH:O	2.44	0.50
2:D:282:SER:N	9:D:729:HOH:O	2.45	0.50
1:A:509:ASP:OD1	1:A:509:ASP:N	2.39	0.49
2:B:370:HIS:NE2	2:B:418:GLN:O	2.41	0.49
2:D:331:LYS:HB2	2:D:352:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:339:LYS:HE2	2:J:342:ASN:HA	1.94	0.49
2:L:341:GLU:O	2:L:342:ASN:ND2	2.45	0.49
1:G:513:ARG:NH1	9:G:923:HOH:O	2.45	0.49
1:K:509:ASP:OD1	1:K:509:ASP:N	2.43	0.49
2:D:338:PHE:HE1	2:D:347:VAL:HG23	1.77	0.49
2:H:436:LYS:HD2	9:H:757:HOH:O	2.10	0.49
2:D:386:GLU:N	9:D:724:HOH:O	2.42	0.49
2:F:324:ILE:HG21	2:F:329:ILE:HD12	1.95	0.49
1:E:551:ASP:HA	1:E:564:ALA:HB2	1.94	0.49
2:F:239:ILE:O	2:F:526:THR:HG21	2.12	0.49
1:E:504:ARG:NH1	1:E:514:GLU:HG3	2.27	0.49
1:G:375:ALA:HB1	1:G:380:ILE:HB	1.95	0.49
1:G:437:LYS:HB3	1:G:522:GLN:NE2	2.28	0.49
1:G:574:ASN:HD22	1:G:598:VAL:HA	1.77	0.49
2:B:349:ALA:HB2	2:B:382:VAL:HG23	1.95	0.49
2:B:502:TYR:HB3	2:B:511:PHE:HB3	1.95	0.49
2:J:322:GLN:NE2	2:J:367:PHE:O	2.45	0.49
1:C:456:GLU:HB2	1:C:477:CYS:HB3	1.94	0.49
1:C:504:ARG:HB3	1:C:514:GLU:HB2	1.95	0.49
1:E:456:GLU:HB2	1:E:477:CYS:HB3	1.95	0.49
1:I:456:GLU:HB2	1:I:477:CYS:HB3	1.95	0.49
1:I:479:LEU:HD12	9:I:949:HOH:O	2.12	0.49
2:B:239:ILE:O	2:B:526:THR:HG21	2.13	0.49
2:D:292:GLU:N	9:D:728:HOH:O	2.45	0.49
1:A:317:ARG:HD3	1:A:352:LEU:HD21	1.94	0.49
1:C:559:GLY:HA2	1:C:613:ARG:HD2	1.95	0.49
1:A:573:LEU:HD21	1:A:624:THR:HG21	1.95	0.49
1:E:596:ARG:HB2	9:E:934:HOH:O	2.11	0.49
1:E:606:THR:HG22	1:E:634:ASN:O	2.12	0.49
1:I:285:ILE:HD12	1:I:374:LEU:HD13	1.94	0.49
1:I:558:TRP:CE2	1:I:608:ILE:HD11	2.48	0.49
2:J:471:MET:HE1	2:J:479:PHE:HZ	1.77	0.49
1:A:310:ARG:HB2	1:A:310:ARG:CZ	2.41	0.48
1:G:361:GLY:N	1:G:366:MET:HE2	2.28	0.48
1:G:662:MET:HE2	1:G:671:VAL:HG12	1.95	0.48
2:B:331:LYS:HB2	2:B:352:SER:HB3	1.95	0.48
1:G:285:ILE:HD12	1:G:374:LEU:HD13	1.95	0.48
1:G:642:LEU:O	9:G:907:HOH:O	2.20	0.48
2:B:471:MET:HE2	2:B:471:MET:N	2.28	0.48
2:F:499:THR:HG21	2:F:522:PRO:HG3	1.94	0.48
1:A:684:GLU:OE1	2:D:532:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:456:GLU:HB2	1:G:477:CYS:HB3	1.96	0.48
2:F:380:THR:HG21	2:F:433:TYR:CD1	2.48	0.48
2:L:301:GLN:O	9:L:708:HOH:O	2.20	0.48
1:C:568:TYR:HB3	1:C:633:LEU:CD1	2.43	0.48
1:I:582:ASN:H	1:I:602:TYR:HB2	1.79	0.48
1:C:348:ILE:HG23	1:C:377:ASN:HB3	1.95	0.48
1:C:558:TRP:CE2	1:C:608:ILE:HD11	2.48	0.48
1:E:662:MET:HE2	1:E:671:VAL:HG12	1.95	0.48
1:K:558:TRP:CE2	1:K:608:ILE:HD11	2.48	0.48
2:B:429:MET:HE3	2:B:432:VAL:HG22	1.96	0.48
2:B:447:CYS:SG	2:B:481:PRO:HG3	2.53	0.48
1:C:530:MET:HE1	1:C:677:SER:O	2.14	0.48
1:I:348:ILE:HD11	1:I:425:PHE:CE2	2.49	0.48
1:I:462:THR:OG1	1:I:465:GLU:HG2	2.14	0.48
2:F:229:SER:OG	9:F:702:HOH:O	2.03	0.48
1:I:682:SER:OG	1:I:710:ASP:OD2	2.22	0.48
2:L:335:ILE:HG12	2:L:348:VAL:HG22	1.96	0.48
1:A:570:TYR:HD2	1:A:574:ASN:HD21	1.61	0.48
1:C:582:ASN:H	1:C:602:TYR:HB2	1.78	0.48
1:I:705:HIS:HD2	1:I:716:PRO:HA	1.78	0.48
1:K:274:ASP:OD2	1:K:284:ARG:NH1	2.46	0.48
2:H:370:HIS:NE2	2:H:418:GLN:O	2.37	0.48
2:L:447:CYS:SG	2:L:481:PRO:HG3	2.54	0.48
1:I:292:THR:O	2:L:470:ARG:NH1	2.47	0.48
2:F:259:LYS:HE2	9:F:723:HOH:O	2.14	0.48
2:F:502:TYR:HB3	2:F:511:PHE:HB3	1.95	0.48
1:A:643:GLU:HG2	1:A:644:GLU:N	2.29	0.47
1:G:657:CYS:O	9:G:908:HOH:O	2.20	0.47
1:A:466:CYS:N	9:A:903:HOH:O	2.46	0.47
1:I:397:THR:HG21	2:J:281:THR:CG2	2.44	0.47
1:I:460:CYS:HA	1:I:487:ASP:OD2	2.14	0.47
5:P:2:NAG:H3	5:P:2:NAG:H83	1.96	0.47
1:A:348:ILE:HD11	1:A:425:PHE:HE2	1.80	0.47
2:D:339:LYS:HE2	2:D:342:ASN:HA	1.96	0.47
2:H:385:LEU:O	2:H:398:HIS:N	2.41	0.47
1:E:361:GLY:N	1:E:366:MET:HE2	2.25	0.47
1:G:666:HIS:NE2	9:G:914:HOH:O	2.35	0.47
1:K:563:THR:OG1	1:K:606:THR:OG1	2.31	0.47
2:B:484:ILE:O	2:B:487:TYR:HB2	2.14	0.47
2:J:232:LEU:HA	2:J:233:PRO:HD3	1.75	0.47
2:L:229:SER:HA	2:L:549:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:583:CYS:N	1:I:593:CYS:SG	2.87	0.47
2:D:429:MET:HE1	2:D:458:MET:SD	2.54	0.47
1:C:643:GLU:HG2	1:C:644:GLU:N	2.28	0.47
1:K:444:PRO:HG3	2:J:496:TYR:CZ	2.50	0.47
2:B:515:GLN:HG2	2:B:516:GLU:N	2.28	0.47
2:D:429:MET:HG2	2:D:450:ARG:HH12	1.79	0.47
2:D:502:TYR:HB3	2:D:511:PHE:HB3	1.96	0.47
1:A:504:ARG:HD2	9:A:926:HOH:O	2.14	0.47
1:A:640:VAL:HB	1:A:648:LEU:HB2	1.97	0.47
1:K:467:VAL:HA	1:K:471:ALA:HB2	1.95	0.47
2:L:505:ASP:HB3	2:L:508:LYS:HB2	1.96	0.47
2:F:331:LYS:HB2	2:F:352:SER:HB3	1.96	0.47
1:E:359:GLU:OE1	2:F:353:LYS:NZ	2.41	0.47
1:E:509:ASP:OD1	1:E:509:ASP:N	2.41	0.47
2:L:493:GLY:HA2	2:L:499:THR:HG23	1.95	0.47
1:E:310:ARG:HB2	1:E:310:ARG:CZ	2.43	0.47
2:B:232:LEU:HA	2:B:233:PRO:HD3	1.75	0.47
2:J:251:VAL:HG21	2:J:288:PRO:HG3	1.96	0.47
2:L:265:TRP:CZ3	2:L:535:PHE:CZ	3.03	0.47
1:A:558:TRP:CE2	1:A:608:ILE:HD11	2.50	0.46
1:I:383:ASP:HB2	9:I:920:HOH:O	2.15	0.46
1:I:509:ASP:OD1	1:I:509:ASP:N	2.44	0.46
2:B:493:GLY:HA2	2:B:499:THR:HG23	1.96	0.46
1:C:705:HIS:ND1	1:C:716:PRO:HA	2.29	0.46
1:I:548:LYS:HG2	9:I:980:HOH:O	2.15	0.46
1:I:571:GLU:HA	1:I:598:VAL:HG21	1.97	0.46
2:F:300:ALA:HB2	2:F:335:ILE:HD11	1.97	0.46
2:L:264:GLU:HB2	2:L:275:TYR:HB2	1.97	0.46
1:C:359:GLU:OE1	2:D:353:LYS:NZ	2.43	0.46
1:C:571:GLU:HA	1:C:598:VAL:HG21	1.97	0.46
2:B:322:GLN:NE2	2:B:367:PHE:O	2.48	0.46
2:D:374:HIS:HE1	9:D:716:HOH:O	1.98	0.46
1:K:500:GLY:O	9:K:915:HOH:O	2.21	0.46
2:F:259:LYS:NZ	9:F:723:HOH:O	2.48	0.46
2:H:280:GLY:O	2:H:283:THR:HG23	2.15	0.46
2:D:329:ILE:HG22	9:D:740:HOH:O	2.14	0.46
2:H:300:ALA:HB2	2:H:335:ILE:HD11	1.97	0.46
1:C:332:GLY:HA2	1:C:360:PHE:HB2	1.96	0.46
1:K:640:VAL:O	9:K:916:HOH:O	2.21	0.46
2:J:367:PHE:HA	9:J:701:HOH:O	2.14	0.46
1:A:574:ASN:HB2	1:A:598:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:494:SER:H	2:D:499:THR:HG22	1.81	0.46
2:B:429:MET:HB3	2:B:432:VAL:CG2	2.46	0.46
2:H:307:HIS:ND1	2:H:323:ASP:OD1	2.36	0.46
1:C:375:ALA:HB1	1:C:380:ILE:HB	1.98	0.46
1:E:705:HIS:CD2	1:E:717:HIS:H	2.33	0.46
1:G:274:ASP:OD2	1:G:284:ARG:NH1	2.49	0.46
2:B:324:ILE:HG21	2:B:329:ILE:HD12	1.97	0.46
1:A:238:THR:OG1	1:A:282:LYS:NZ	2.49	0.46
1:A:348:ILE:HG13	1:A:377:ASN:O	2.16	0.46
1:A:530:MET:HE2	9:A:941:HOH:O	2.15	0.46
1:C:235:GLU:HG2	9:C:943:HOH:O	2.16	0.46
1:E:287:LEU:HD21	1:E:290:MET:HE3	1.98	0.46
1:E:634:ASN:ND2	9:E:932:HOH:O	2.48	0.46
2:D:370:HIS:NE2	2:D:418:GLN:O	2.44	0.46
2:D:429:MET:HE3	2:D:429:MET:HB2	1.60	0.46
1:C:662:MET:HE2	1:C:671:VAL:HG12	1.98	0.45
1:E:483:SER:CB	1:E:494:CYS:HB3	2.45	0.45
1:E:582:ASN:H	1:E:602:TYR:HB2	1.81	0.45
2:F:485:ASN:O	2:F:486:ASN:HB2	2.17	0.45
2:H:484:ILE:HG22	2:H:527:HIS:CG	2.51	0.45
2:L:295:LEU:HB3	2:L:311:ARG:HB3	1.98	0.45
1:A:704:ARG:HE	1:A:705:HIS:HE1	1.64	0.45
1:C:310:ARG:CZ	1:C:310:ARG:HB2	2.46	0.45
1:K:310:ARG:HH11	1:K:643:GLU:CD	2.24	0.45
1:K:337:SER:HB2	9:K:978:HOH:O	2.17	0.45
2:H:260:CYS:N	2:H:278:ILE:O	2.42	0.45
2:L:502:TYR:HB3	2:L:511:PHE:HB3	1.97	0.45
1:C:332:GLY:N	9:C:905:HOH:O	2.04	0.45
1:E:375:ALA:HB1	1:E:380:ILE:HB	1.98	0.45
2:B:415:LYS:O	2:B:418:GLN:NE2	2.50	0.45
2:F:454:ASP:OD1	2:F:454:ASP:N	2.49	0.45
1:A:682:SER:OG	1:A:710:ASP:OD2	2.30	0.45
1:C:444:PRO:HG3	2:F:496:TYR:CZ	2.52	0.45
2:B:495:ASP:C	9:B:722:HOH:O	2.59	0.45
2:J:330:ARG:O	9:J:707:HOH:O	2.21	0.45
1:C:316:ARG:HD3	1:C:327:VAL:HG21	1.99	0.45
1:C:397:THR:HG23	2:D:303:PHE:CD2	2.51	0.45
1:E:666:HIS:CD2	9:E:913:HOH:O	2.69	0.45
2:B:411:TYR:HB3	2:B:420:PHE:HB3	1.98	0.45
2:D:478:VAL:HG21	2:D:523:ARG:C	2.42	0.45
1:C:509:ASP:N	1:C:509:ASP:OD1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:ARG:CZ	1:I:310:ARG:HB2	2.46	0.45
1:A:456:GLU:HB2	1:A:477:CYS:HB3	1.99	0.45
1:C:348:ILE:HD11	1:C:425:PHE:CE2	2.52	0.45
1:K:460:CYS:SG	9:K:979:HOH:O	2.61	0.45
1:A:563:THR:OG1	1:A:606:THR:OG1	2.32	0.45
1:C:460:CYS:HA	1:C:487:ASP:OD2	2.16	0.45
1:I:602:TYR:HE2	9:I:923:HOH:O	2.00	0.45
2:B:374:HIS:NE2	2:B:409:VAL:HG21	2.32	0.45
2:F:287:LYS:HA	2:F:288:PRO:HD3	1.81	0.45
2:J:530:ILE:O	2:J:533:ARG:HB2	2.16	0.45
2:L:280:GLY:O	2:L:283:THR:HG23	2.16	0.45
1:E:378:ILE:HG13	1:E:422:TYR:CE1	2.51	0.45
1:G:444:PRO:HG3	2:B:496:TYR:CZ	2.51	0.45
1:I:492:LYS:HD3	1:I:492:LYS:HA	1.85	0.45
2:D:232:LEU:HA	2:D:233:PRO:HD3	1.78	0.45
2:F:385:LEU:O	2:F:398:HIS:N	2.45	0.45
2:J:480:GLN:HG2	2:J:525:PHE:O	2.17	0.45
1:E:705:HIS:NE2	1:E:717:HIS:O	2.51	0.44
1:K:481:GLN:N	9:K:932:HOH:O	2.49	0.44
2:L:285:VAL:HG11	2:L:335:ILE:HB	1.99	0.44
1:A:375:ALA:HB1	1:A:380:ILE:HB	1.99	0.44
1:I:382:SER:OG	1:I:387:LEU:HD11	2.18	0.44
1:K:480:THR:OG1	9:K:918:HOH:O	2.21	0.44
2:J:497:SER:OG	2:J:498:PHE:N	2.50	0.44
1:A:348:ILE:HD13	1:A:431:GLY:HA2	1.98	0.44
1:G:682:SER:OG	1:G:710:ASP:OD2	2.29	0.44
1:K:559:GLY:HA2	1:K:613:ARG:HD2	1.99	0.44
2:B:451:PHE:HA	2:B:476:SER:O	2.18	0.44
1:A:332:GLY:HA2	1:A:360:PHE:HB2	2.00	0.44
1:C:280:GLN:NE2	1:C:413:LYS:HA	2.33	0.44
1:I:397:THR:HG21	2:J:281:THR:HG22	1.99	0.44
2:H:493:GLY:HA2	2:H:499:THR:HG23	1.98	0.44
1:G:551:ASP:HA	1:G:564:ALA:HB2	2.00	0.44
1:G:643:GLU:HG2	1:G:644:GLU:N	2.31	0.44
1:I:280:GLN:NE2	1:I:413:LYS:HA	2.30	0.44
1:G:551:ASP:OD2	1:G:555:LYS:HE2	2.18	0.44
2:F:390:THR:HA	2:F:391:PRO:HA	1.78	0.44
2:H:474:ARG:O	2:H:494:SER:OG	2.33	0.44
1:C:714:TYR:CE1	1:C:716:PRO:HG3	2.53	0.44
1:E:280:GLN:NE2	1:E:413:LYS:HA	2.27	0.44
2:D:280:GLY:O	2:D:283:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:237:LEU:HB2	2:H:255:PRO:HG3	1.99	0.44
2:H:308:ILE:HB	2:H:322:GLN:HB3	1.98	0.44
1:E:705:HIS:HD2	1:E:717:HIS:H	1.65	0.44
1:G:362:LYS:NZ	2:H:431:ASP:OD1	2.36	0.44
1:K:594:ASN:OD1	1:K:595:LYS:N	2.50	0.44
2:D:287:LYS:NZ	2:D:336:GLU:HA	2.33	0.44
2:H:524:SER:N	2:H:539:SER:OG	2.51	0.44
1:I:348:ILE:HG13	1:I:377:ASN:O	2.17	0.44
1:K:378:ILE:HG13	1:K:422:TYR:CE1	2.53	0.44
1:K:460:CYS:HA	1:K:487:ASP:OD2	2.18	0.44
2:L:228:LYS:HE2	2:L:231:ASP:OD1	2.18	0.44
1:C:704:ARG:HG2	1:C:705:HIS:CD2	2.53	0.43
1:E:462:THR:H	1:E:465:GLU:HG2	1.83	0.43
1:G:571:GLU:HA	1:G:598:VAL:HG21	1.98	0.43
1:G:579:GLU:C	1:G:581:GLY:H	2.25	0.43
1:I:530:MET:HE1	1:I:677:SER:O	2.18	0.43
1:K:280:GLN:NE2	1:K:413:LYS:HA	2.31	0.43
2:B:454:ASP:OD1	9:B:715:HOH:O	2.21	0.43
2:B:300:ALA:HB2	2:B:335:ILE:HD11	1.99	0.43
2:F:480:GLN:HG2	2:F:525:PHE:O	2.18	0.43
2:J:300:ALA:HB2	2:J:335:ILE:HD11	1.99	0.43
1:A:643:GLU:HG2	1:A:645:ASP:H	1.83	0.43
2:L:531:ASN:O	2:L:532:LYS:HB2	2.18	0.43
1:C:444:PRO:HA	1:C:445:PRO:HD3	1.90	0.43
2:B:305:GLY:HA3	2:B:326:ILE:HG22	1.98	0.43
2:H:380:THR:HG21	2:H:433:TYR:CE1	2.53	0.43
2:H:407:ARG:HG3	2:H:430:GLU:HG3	2.00	0.43
2:L:370:HIS:NE2	2:L:418:GLN:O	2.38	0.43
1:I:375:ALA:HB1	1:I:380:ILE:HB	2.00	0.43
2:B:250:VAL:HB	2:B:263:LEU:HB2	2.00	0.43
2:F:470:ARG:CA	2:F:471:MET:HE2	2.47	0.43
2:H:380:THR:HG21	2:H:433:TYR:CD1	2.53	0.43
2:L:308:ILE:HB	2:L:322:GLN:HB3	2.00	0.43
1:C:248:ASP:OD1	1:C:331:SER:HA	2.19	0.43
1:I:359:GLU:OE1	2:J:353:LYS:NZ	2.44	0.43
1:K:238:THR:OG1	1:K:282:LYS:NZ	2.51	0.43
2:H:523:ARG:HD3	2:H:523:ARG:HA	1.81	0.43
1:E:316:ARG:HB2	1:E:320:ILE:HD12	2.00	0.43
1:K:251:MET:HE2	1:K:331:SER:C	2.43	0.43
2:J:280:GLY:O	2:J:283:THR:HG23	2.18	0.43
1:E:444:PRO:HA	1:E:445:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:640:VAL:HB	1:E:648:LEU:HB2	1.99	0.43
2:D:254:GLN:OE1	2:D:257:THR:OG1	2.22	0.43
2:D:390:THR:HA	2:D:391:PRO:HA	1.81	0.43
2:J:520:GLN:HB3	9:J:721:HOH:O	2.17	0.43
1:C:243:LEU:HD21	1:C:245:ILE:HD11	2.01	0.43
1:E:614:LEU:HD12	1:E:642:LEU:HD21	2.00	0.43
2:D:522:PRO:HA	2:D:539:SER:O	2.19	0.43
1:A:272:MET:HE1	1:A:364:ASP:CG	2.44	0.43
1:A:504:ARG:NH1	1:A:514:GLU:HG3	2.34	0.43
2:H:254:GLN:HA	2:H:255:PRO:HD3	1.91	0.43
2:J:370:HIS:NE2	2:J:418:GLN:O	2.41	0.43
2:J:380:THR:HG21	2:J:433:TYR:CD1	2.54	0.43
1:A:467:VAL:HA	1:A:471:ALA:HB2	2.01	0.42
1:E:237:GLU:HG2	1:E:489:LEU:HD11	2.00	0.42
1:I:348:ILE:HD13	1:I:431:GLY:HA2	2.01	0.42
1:K:287:LEU:HD21	1:K:290:MET:HE3	2.00	0.42
2:B:522:PRO:HA	2:B:539:SER:O	2.19	0.42
2:F:389:ARG:O	2:F:392:GLN:HB2	2.19	0.42
2:F:457:VAL:HG23	2:F:471:MET:CE	2.49	0.42
1:C:237:GLU:HG2	1:C:489:LEU:HD11	2.01	0.42
1:C:317:ARG:NH1	9:C:928:HOH:O	2.51	0.42
1:C:333:SER:OG	9:C:912:HOH:O	2.21	0.42
1:G:347:GLY:O	1:G:350:SER:HB3	2.19	0.42
1:I:398:TRP:N	9:I:903:HOH:O	2.52	0.42
1:I:572:LYS:NZ	9:I:927:HOH:O	2.52	0.42
1:K:551:ASP:OD2	1:K:555:LYS:HE2	2.19	0.42
2:F:256:PHE:HB2	9:F:738:HOH:O	2.19	0.42
2:H:250:VAL:HB	2:H:263:LEU:HB2	2.01	0.42
2:H:251:VAL:HG21	2:H:288:PRO:HG3	2.00	0.42
2:J:431:ASP:OD1	2:J:431:ASP:N	2.53	0.42
1:A:512:ILE:HD11	1:A:693:VAL:HG11	2.01	0.42
1:E:387:LEU:HD23	1:E:392:CYS:O	2.20	0.42
1:G:705:HIS:HD2	1:G:716:PRO:HA	1.84	0.42
1:A:411:PRO:HD3	9:A:925:HOH:O	2.19	0.42
1:C:344:TYR:HA	9:C:948:HOH:O	2.19	0.42
1:C:348:ILE:H	1:C:348:ILE:HG13	1.66	0.42
1:K:375:ALA:HB1	1:K:380:ILE:HB	2.02	0.42
2:D:519:VAL:HG12	2:D:546:GLN:CD	2.45	0.42
2:J:415:LYS:O	2:J:418:GLN:NE2	2.53	0.42
1:C:348:ILE:HG13	1:C:377:ASN:O	2.18	0.42
1:K:493:LYS:HB3	1:K:493:LYS:HE3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:338:SER:HB3	2:H:354:ALA:HB2	2.01	0.42
1:I:444:PRO:HG3	2:L:496:TYR:CZ	2.54	0.42
2:H:232:LEU:HA	2:H:233:PRO:HD3	1.75	0.42
2:L:528:VAL:HB	2:L:535:PHE:HB2	2.02	0.42
1:I:348:ILE:HD11	1:I:425:PHE:HE2	1.84	0.42
1:I:563:THR:OG1	1:I:606:THR:OG1	2.36	0.42
2:B:400:ILE:HA	2:B:409:VAL:O	2.19	0.42
2:H:285:VAL:HG11	2:H:335:ILE:HB	2.01	0.42
1:A:244:MET:HE1	1:A:320:ILE:HD12	2.01	0.42
1:A:432:ALA:O	1:A:526:ASN:HB3	2.19	0.42
1:E:347:GLY:O	1:E:350:SER:HB3	2.20	0.42
2:B:450:ARG:O	2:B:476:SER:HB3	2.20	0.42
2:F:280:GLY:O	2:F:283:THR:HG23	2.19	0.42
2:J:385:LEU:O	2:J:398:HIS:N	2.51	0.42
5:P:1:NAG:HO3	5:P:1:NAG:C7	2.28	0.42
1:A:579:GLU:HG2	1:A:590:TRP:CE2	2.55	0.42
1:C:386:LYS:HB3	1:C:391:GLU:HB3	2.01	0.42
1:C:700:CYS:HB3	1:C:711:CYS:SG	2.60	0.42
1:E:444:PRO:HG3	2:D:496:TYR:CZ	2.54	0.42
1:K:643:GLU:HG2	1:K:644:GLU:N	2.35	0.42
2:L:519:VAL:HG12	2:L:546:GLN:CD	2.45	0.42
1:C:569:CYS:HB3	1:C:604:LEU:HD13	2.02	0.42
1:E:559:GLY:HA2	1:E:613:ARG:HD2	2.01	0.42
1:E:644:GLU:H	1:E:644:GLU:CD	2.28	0.42
2:H:483:GLN:HA	2:H:487:TYR:O	2.20	0.42
2:J:440:VAL:HG22	2:J:441:LYS:HG3	2.01	0.42
1:C:396:ASP:OD1	1:C:399:SER:N	2.50	0.41
1:E:460:CYS:HA	1:E:487:ASP:OD2	2.20	0.41
1:E:643:GLU:HG2	1:E:644:GLU:N	2.34	0.41
2:B:531:ASN:O	2:B:532:LYS:HB2	2.20	0.41
2:F:523:ARG:HA	2:F:523:ARG:HD3	1.77	0.41
1:A:575:ILE:HG23	9:A:938:HOH:O	2.20	0.41
1:G:390:GLY:CA	1:G:393:LYS:HE3	2.50	0.41
2:B:389:ARG:O	2:B:392:GLN:HB2	2.21	0.41
2:B:390:THR:HA	2:B:391:PRO:HA	1.80	0.41
4:S:1:NAG:H5	4:S:4:FUC:O2	2.20	0.41
1:A:279:ASP:CG	9:A:913:HOH:O	2.63	0.41
1:E:310:ARG:HG2	1:E:314:LYS:HE3	2.03	0.41
1:G:242:GLU:OE1	1:G:436:ASN:ND2	2.49	0.41
2:F:380:THR:HG21	2:F:433:TYR:CE1	2.55	0.41
1:A:378:ILE:HD12	1:A:378:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:THR:HA	1:A:656:PRO:HD3	1.95	0.41
1:E:249:HIS:CD2	1:E:253:LYS:HE2	2.55	0.41
1:E:514:GLU:HB3	1:E:524:ALA:HB3	2.02	0.41
1:I:411:PRO:HD3	9:I:952:HOH:O	2.20	0.41
1:I:594:ASN:ND2	9:I:912:HOH:O	2.20	0.41
2:B:457:VAL:HG23	2:B:471:MET:HE1	2.01	0.41
2:D:287:LYS:HA	2:D:288:PRO:HD3	1.84	0.41
2:F:264:GLU:HB2	2:F:275:TYR:HB2	2.02	0.41
2:H:325:GLU:HG3	9:H:727:HOH:O	2.20	0.41
2:H:429:MET:HB3	2:H:432:VAL:CG2	2.51	0.41
1:C:497:GLN:O	1:C:518:GLY:HA2	2.21	0.41
1:G:679:CYS:HB3	1:G:700:CYS:SG	2.61	0.41
1:K:255:HIS:ND1	1:K:262:THR:HG22	2.35	0.41
1:K:586:ASP:HB2	1:K:591:ILE:HD11	2.02	0.41
2:D:389:ARG:O	2:D:392:GLN:HB2	2.20	0.41
2:D:451:PHE:HA	2:D:476:SER:O	2.19	0.41
2:F:531:ASN:O	2:F:532:LYS:HB2	2.20	0.41
2:L:485:ASN:O	2:L:486:ASN:HB2	2.19	0.41
1:E:666:HIS:N	9:E:931:HOH:O	2.47	0.41
1:K:504:ARG:NH1	1:K:514:GLU:HG3	2.33	0.41
2:F:285:VAL:HG11	2:F:335:ILE:HB	2.03	0.41
2:J:390:THR:HA	2:J:391:PRO:HA	1.85	0.41
1:A:532:GLY:HA3	9:A:941:HOH:O	2.21	0.41
1:A:669:LEU:HA	1:A:670:PRO:HD3	1.95	0.41
1:C:238:THR:OG1	1:C:282:LYS:NZ	2.53	0.41
1:C:410:LEU:HA	1:C:411:PRO:HD3	1.89	0.41
1:K:382:SER:OG	1:K:387:LEU:HD11	2.21	0.41
2:D:380:THR:HG21	2:D:433:TYR:CD1	2.55	0.41
2:D:531:ASN:O	2:D:532:LYS:HB2	2.21	0.41
2:H:326:ILE:N	9:H:727:HOH:O	2.54	0.41
1:E:704:ARG:HG2	1:E:705:HIS:ND1	2.36	0.41
1:G:246:VAL:O	1:G:329:LEU:HD12	2.21	0.41
2:D:385:LEU:O	2:D:398:HIS:N	2.48	0.41
1:A:280:GLN:NE2	1:A:413:LYS:HA	2.32	0.41
1:E:272:MET:HE1	1:E:364:ASP:CG	2.46	0.41
1:G:233:ASN:O	9:G:909:HOH:O	2.22	0.41
1:G:382:SER:OG	1:G:387:LEU:HD11	2.21	0.41
1:G:558:TRP:CE2	1:G:608:ILE:HD11	2.56	0.41
1:K:682:SER:OG	1:K:710:ASP:OD2	2.27	0.41
2:H:390:THR:HA	2:H:391:PRO:HA	1.83	0.41
2:H:502:TYR:HB3	2:H:511:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:258:GLY:HA2	2:J:280:GLY:O	2.20	0.41
2:L:380:THR:HG21	2:L:433:TYR:CD1	2.56	0.41
1:C:551:ASP:OD2	1:C:555:LYS:HE2	2.21	0.41
1:C:644:GLU:HG2	1:C:645:ASP:N	2.36	0.41
1:E:481:GLN:HE21	1:E:481:GLN:HB2	1.66	0.41
1:I:287:LEU:HD21	1:I:290:MET:HE3	2.02	0.41
1:A:583:CYS:N	1:A:593:CYS:SG	2.93	0.40
1:C:348:ILE:HD11	1:C:425:PHE:HE2	1.86	0.40
2:B:291:ILE:C	2:B:292:GLU:HG2	2.46	0.40
2:H:402:SER:HA	9:H:736:HOH:O	2.20	0.40
1:A:506:ALA:HB3	9:A:907:HOH:O	2.21	0.40
1:G:511:ASP:OD1	1:G:528:HIS:HB3	2.21	0.40
1:I:510:CYS:O	1:I:528:HIS:HB2	2.21	0.40
1:I:655:THR:HA	1:I:656:PRO:HD3	1.96	0.40
2:B:421:THR:HB	2:B:422:ASN:H	1.77	0.40
2:D:380:THR:HG21	2:D:433:TYR:CE1	2.56	0.40
2:F:276:ASP:OD1	2:F:277:ASN:N	2.53	0.40
2:J:478:VAL:HG21	2:J:523:ARG:C	2.46	0.40
2:B:381:ASP:OD1	9:B:716:HOH:O	2.21	0.40
2:F:270:LYS:HE3	9:F:726:HOH:O	2.22	0.40
2:F:533:ARG:HH21	2:F:549:LYS:NZ	2.19	0.40
2:H:295:LEU:HB3	2:H:311:ARG:HB3	2.04	0.40
2:J:447:CYS:SG	2:J:481:PRO:HG3	2.62	0.40
2:J:485:ASN:O	2:J:486:ASN:HB2	2.21	0.40
2:L:426:ILE:HA	2:L:427:PRO:HD3	1.91	0.40
1:C:347:GLY:O	1:C:350:SER:HB3	2.21	0.40
1:K:448:GLY:HA2	1:K:461:GLY:O	2.21	0.40
2:B:254:GLN:HA	2:B:255:PRO:HD3	1.85	0.40
2:H:455:SER:N	2:H:471:MET:O	2.54	0.40
2:H:519:VAL:HG12	2:H:546:GLN:CD	2.47	0.40
2:J:341:GLU:O	2:J:342:ASN:ND2	2.54	0.40
2:L:389:ARG:O	2:L:392:GLN:HB2	2.22	0.40
1:E:550:ARG:NH2	9:E:909:HOH:O	2.54	0.40
1:K:481:GLN:HG2	9:K:981:HOH:O	2.22	0.40
2:D:365:ASN:ND2	9:D:712:HOH:O	2.27	0.40
2:H:287:LYS:NZ	2:H:336:GLU:HA	2.37	0.40
2:L:505:ASP:O	2:L:509:ALA:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:959:HOH:O	9:B:783:HOH:O[1_554]	1.93	0.27

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/504 (95%)	461 (96%)	17 (4%)	0	100	100
1	C	467/504 (93%)	453 (97%)	14 (3%)	0	100	100
1	E	461/504 (92%)	448 (97%)	13 (3%)	0	100	100
1	G	456/504 (90%)	441 (97%)	15 (3%)	0	100	100
1	I	477/504 (95%)	462 (97%)	15 (3%)	0	100	100
1	K	484/504 (96%)	468 (97%)	16 (3%)	0	100	100
2	B	326/347 (94%)	309 (95%)	17 (5%)	0	100	100
2	D	326/347 (94%)	310 (95%)	16 (5%)	0	100	100
2	F	326/347 (94%)	312 (96%)	14 (4%)	0	100	100
2	H	327/347 (94%)	310 (95%)	17 (5%)	0	100	100
2	J	326/347 (94%)	310 (95%)	16 (5%)	0	100	100
2	L	326/347 (94%)	309 (95%)	17 (5%)	0	100	100
All	All	4780/5106 (94%)	4593 (96%)	187 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	416/435 (96%)	410 (99%)	6 (1%)	59	80
1	C	409/435 (94%)	400 (98%)	9 (2%)	45	72
1	E	403/435 (93%)	394 (98%)	9 (2%)	45	72
1	G	398/435 (92%)	392 (98%)	6 (2%)	57	79
1	I	416/435 (96%)	409 (98%)	7 (2%)	53	77
1	K	420/435 (97%)	416 (99%)	4 (1%)	68	84
2	B	300/315 (95%)	290 (97%)	10 (3%)	33	60
2	D	300/315 (95%)	294 (98%)	6 (2%)	48	74
2	F	300/315 (95%)	294 (98%)	6 (2%)	48	74
2	H	301/315 (96%)	293 (97%)	8 (3%)	39	67
2	J	300/315 (95%)	291 (97%)	9 (3%)	36	63
2	L	300/315 (95%)	290 (97%)	10 (3%)	33	60
All	All	4263/4500 (95%)	4173 (98%)	90 (2%)	47	73

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	GLU
1	A	348	ILE
1	A	378	ILE
1	A	393	LYS
1	A	434	LEU
1	A	599	LEU
1	C	284	ARG
1	C	322	GLU
1	C	348	ILE
1	C	378	ILE
1	C	434	LEU
1	C	576	GLU
1	C	599	LEU
1	C	714	TYR
1	C	715	PHE
1	E	316	ARG
1	E	322	GLU
1	E	378	ILE
1	E	434	LEU
1	E	460	CYS
1	E	480	THR
1	E	481	GLN

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Mol	Chain	Res	Type
1	E	527	ILE
1	E	599	LEU
1	G	284	ARG
1	G	316	ARG
1	G	322	GLU
1	G	378	ILE
1	G	434	LEU
1	G	599	LEU
1	I	284	ARG
1	I	316	ARG
1	I	322	GLU
1	I	348	ILE
1	I	434	LEU
1	I	599	LEU
1	I	683	LYS
1	K	322	GLU
1	K	378	ILE
1	K	434	LEU
1	K	599	LEU
2	B	292	GLU
2	B	298	ILE
2	B	374	HIS
2	B	393	THR
2	B	418	GLN
2	B	419	LEU
2	B	459	LYS
2	B	471	MET
2	B	516	GLU
2	B	536	LEU
2	D	298	ILE
2	D	374	HIS
2	D	393	THR
2	D	419	LEU
2	D	471	MET
2	D	536	LEU
2	F	374	HIS
2	F	393	THR
2	F	429	MET
2	F	430	GLU
2	F	471	MET
2	F	536	LEU
2	H	298	ILE

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Mol	Chain	Res	Type
2	H	374	HIS
2	H	387	ILE
2	H	393	THR
2	H	418	GLN
2	H	459	LYS
2	H	470	ARG
2	H	536	LEU
2	J	298	ILE
2	J	374	HIS
2	J	387	ILE
2	J	393	THR
2	J	418	GLN
2	J	419	LEU
2	J	431	ASP
2	J	471	MET
2	J	536	LEU
2	L	298	ILE
2	L	374	HIS
2	L	393	THR
2	L	419	LEU
2	L	429	MET
2	L	449	THR
2	L	471	MET
2	L	507	GLU
2	L	510	LYS
2	L	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	334	GLN
1	A	705	HIS
1	C	334	GLN
1	C	481	GLN
1	C	705	HIS
1	E	334	GLN
1	E	481	GLN
1	E	539	GLN
1	E	574	ASN
1	E	705	HIS
1	E	717	HIS

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Mol	Chain	Res	Type
1	G	261	HIS
1	G	280	GLN
1	G	334	GLN
1	G	481	GLN
1	G	705	HIS
1	I	261	HIS
1	I	271	ASN
1	I	334	GLN
1	I	574	ASN
1	I	705	HIS
1	K	247	ASN
1	K	261	HIS
1	K	334	GLN
1	K	481	GLN
1	K	574	ASN
1	K	705	HIS
2	B	274	ASN
2	B	301	GLN
2	B	342	ASN
2	B	406	GLN
2	B	412	GLN
2	B	418	GLN
2	B	423	GLN
2	D	406	GLN
2	D	412	GLN
2	D	437	HIS
2	F	342	ASN
2	F	412	GLN
2	F	423	GLN
2	F	485	ASN
2	H	301	GLN
2	H	342	ASN
2	H	406	GLN
2	H	412	GLN
2	H	418	GLN
2	J	274	ASN
2	J	301	GLN
2	J	342	ASN
2	J	406	GLN
2	J	412	GLN
2	J	418	GLN
2	J	423	GLN

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Mol	Chain	Res	Type
2	J	485	ASN
2	L	406	GLN
2	L	412	GLN
2	L	423	GLN
2	L	480	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

27 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	M	1	2,3	14,14,15	0.34	0	17,19,21	0.64	0
3	NAG	M	2	3	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	N	1	4,2	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	N	2	4	14,14,15	0.29	0	17,19,21	0.53	0
4	BMA	N	3	4	11,11,12	1.06	2 (18%)	15,15,17	1.53	3 (20%)
4	FUC	N	4	4	10,10,11	1.14	1 (10%)	14,14,16	1.36	1 (7%)
3	NAG	O	1	2,3	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	O	2	3	14,14,15	0.32	0	17,19,21	0.38	0
5	NAG	P	1	2,5	14,14,15	0.36	0	17,19,21	0.51	0
5	NAG	P	2	5	14,14,15	0.57	0	17,19,21	1.48	2 (11%)
5	FUC	P	3	5	10,10,11	1.29	2 (20%)	14,14,16	1.44	1 (7%)
3	NAG	Q	1	2,3	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.32	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	R	1	2,6	14,14,15	0.40	0	17,19,21	0.37	0
6	FUC	R	2	6	10,10,11	1.48	2 (20%)	14,14,16	1.68	3 (21%)
4	NAG	S	1	4,2	14,14,15	0.63	0	17,19,21	0.82	0
4	NAG	S	2	4	14,14,15	0.85	1 (7%)	17,19,21	0.95	1 (5%)
4	BMA	S	3	4	11,11,12	2.06	4 (36%)	15,15,17	1.55	4 (26%)
4	FUC	S	4	4	10,10,11	1.55	2 (20%)	14,14,16	1.75	4 (28%)
3	NAG	T	1	2,3	14,14,15	0.34	0	17,19,21	0.47	0
3	NAG	T	2	3	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	U	1	2,5	14,14,15	0.65	1 (7%)	17,19,21	0.85	1 (5%)
5	NAG	U	2	5	14,14,15	0.51	0	17,19,21	1.46	3 (17%)
5	FUC	U	3	5	10,10,11	2.06	2 (20%)	14,14,16	1.93	3 (21%)
5	NAG	V	1	2,5	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.56	0
5	FUC	V	3	5	10,10,11	1.33	1 (10%)	14,14,16	2.22	3 (21%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	S	3	4	-	1/2/19/22	0/1/1/1
4	FUC	S	4	4	-	-	0/1/1/1
3	NAG	T	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
5	NAG	U	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	5/6/23/26	0/1/1/1
5	FUC	U	3	5	-	-	0/1/1/1
5	NAG	V	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
5	FUC	V	3	5	-	-	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	3	FUC	O2-C2	5.14	1.54	1.43
4	S	3	BMA	C2-C3	4.58	1.59	1.52
4	S	3	BMA	C1-C2	3.68	1.61	1.52
5	V	3	FUC	C1-C2	3.55	1.60	1.52
4	S	4	FUC	C2-C3	-3.37	1.47	1.52
6	R	2	FUC	C1-C2	3.35	1.60	1.52
6	R	2	FUC	C2-C3	3.04	1.57	1.52
4	N	4	FUC	C1-C2	2.99	1.59	1.52
5	P	3	FUC	C1-C2	2.97	1.59	1.52
4	S	2	NAG	O5-C1	-2.83	1.38	1.43
4	S	3	BMA	O5-C5	-2.53	1.38	1.43
4	N	3	BMA	C2-C3	2.43	1.56	1.52
5	P	3	FUC	C2-C3	2.36	1.56	1.52
5	U	1	NAG	O5-C1	-2.32	1.39	1.43
5	U	3	FUC	C1-C2	2.28	1.57	1.52
4	S	3	BMA	C4-C3	2.25	1.58	1.52
4	S	4	FUC	O5-C1	2.24	1.47	1.43
4	N	3	BMA	C1-C2	2.20	1.57	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	3	FUC	C1-C2-C3	5.75	118.01	109.64
5	P	2	NAG	C2-N2-C7	4.77	129.29	122.90
6	R	2	FUC	C1-C2-C3	4.71	116.50	109.64
5	U	2	NAG	C2-N2-C7	4.66	129.14	122.90
5	P	3	FUC	C1-C2-C3	4.19	115.75	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	3	FUC	O2-C2-C1	3.90	118.14	109.22
4	S	4	FUC	C1-O5-C5	3.80	121.93	112.97
4	S	3	BMA	C2-C3-C4	3.59	117.17	110.86
4	N	3	BMA	C1-O5-C5	3.57	116.97	112.19
5	U	3	FUC	O2-C2-C3	3.53	117.45	110.15
5	V	3	FUC	C2-C3-C4	3.23	116.54	110.86
5	V	3	FUC	C1-O5-C5	3.17	120.44	112.97
4	S	4	FUC	C1-C2-C3	3.16	114.24	109.64
4	N	4	FUC	C1-O5-C5	3.15	120.40	112.97
4	S	3	BMA	O5-C5-C4	-2.81	103.99	110.83
4	N	3	BMA	C1-C2-C3	2.79	113.71	109.64
5	U	3	FUC	O5-C5-C4	2.60	114.24	109.55
5	U	2	NAG	C1-C2-N2	2.53	114.42	110.43
6	R	2	FUC	C1-O5-C5	2.49	118.85	112.97
4	S	3	BMA	C1-O5-C5	-2.48	108.86	112.19
5	U	1	NAG	C1-O5-C5	-2.42	108.94	112.19
6	R	2	FUC	O5-C1-C2	2.39	116.48	110.79
4	S	3	BMA	C1-C2-C3	2.36	113.08	109.64
4	S	4	FUC	O5-C1-C2	2.36	116.41	110.79
4	S	4	FUC	O5-C5-C4	2.35	113.78	109.55
4	S	2	NAG	O3-C3-C2	-2.33	104.56	109.40
5	P	2	NAG	C1-C2-N2	2.24	113.96	110.43
4	N	3	BMA	O5-C5-C4	-2.15	105.60	110.83
5	U	2	NAG	C1-O5-C5	2.15	115.06	112.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	M	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	P	1	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C1-C2-N2-C7
3	O	2	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
4	N	2	NAG	O5-C5-C6-O6
5	U	2	NAG	C1-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7

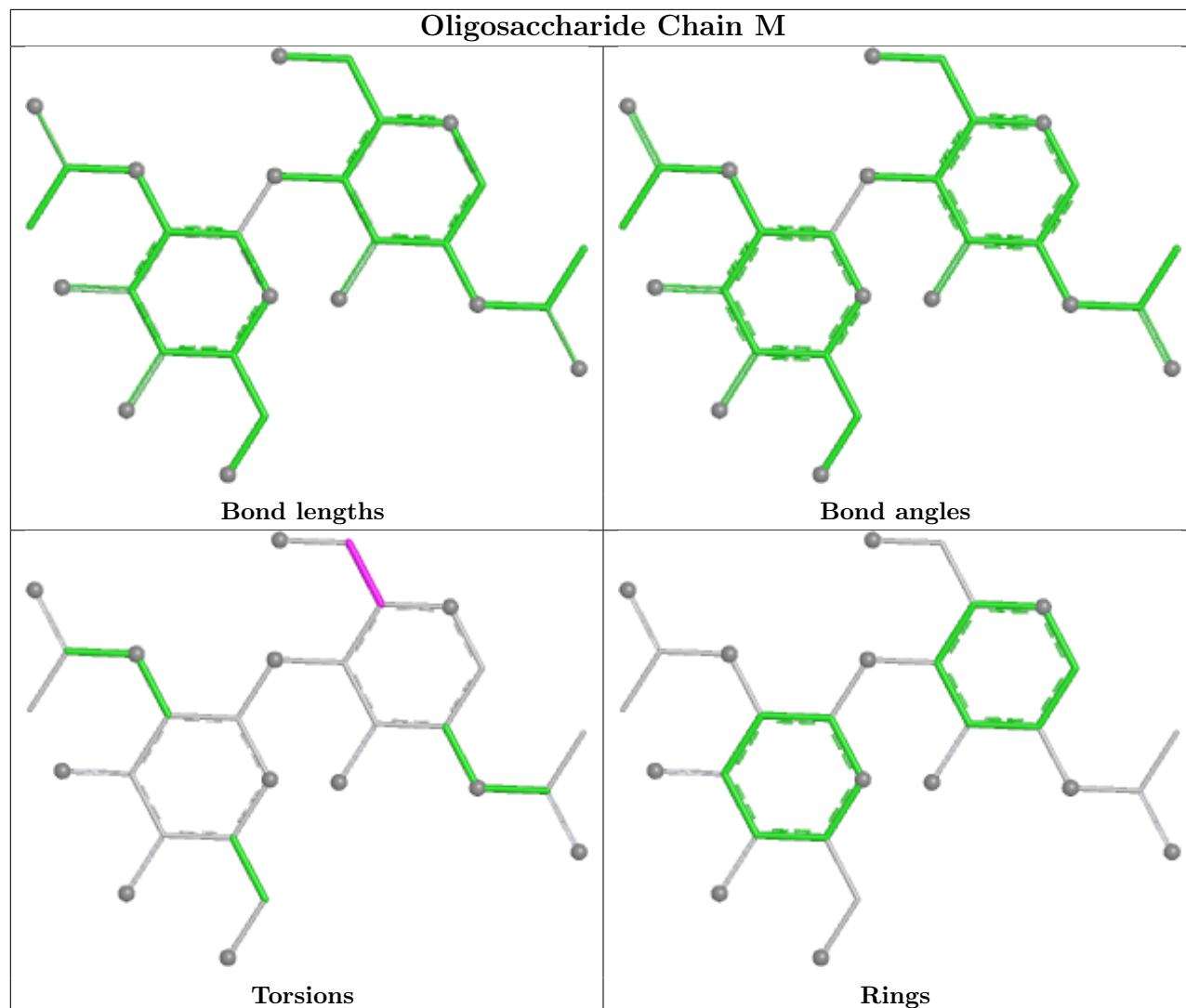
There are no ring outliers.

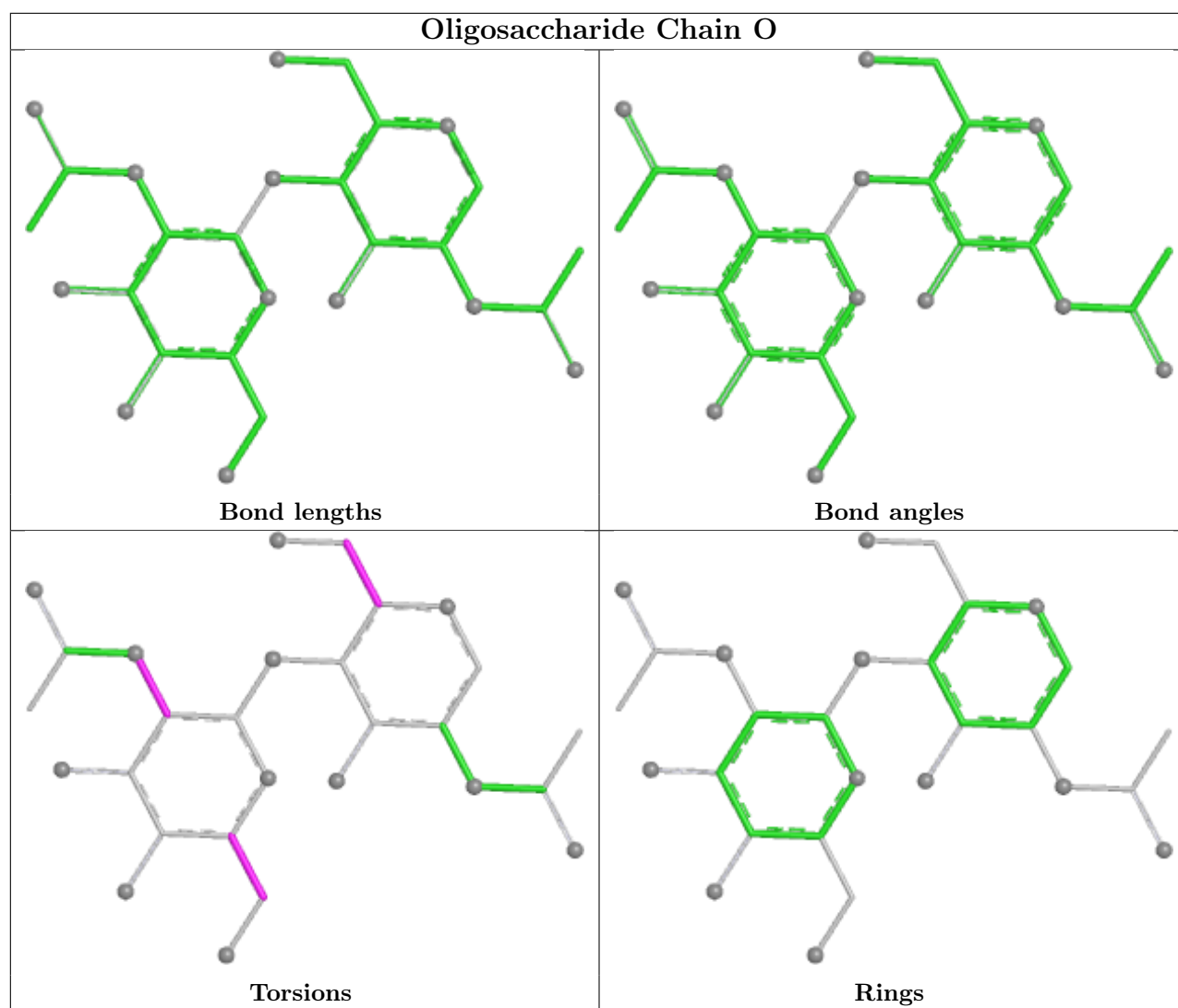
7 monomers are involved in 7 short contacts:

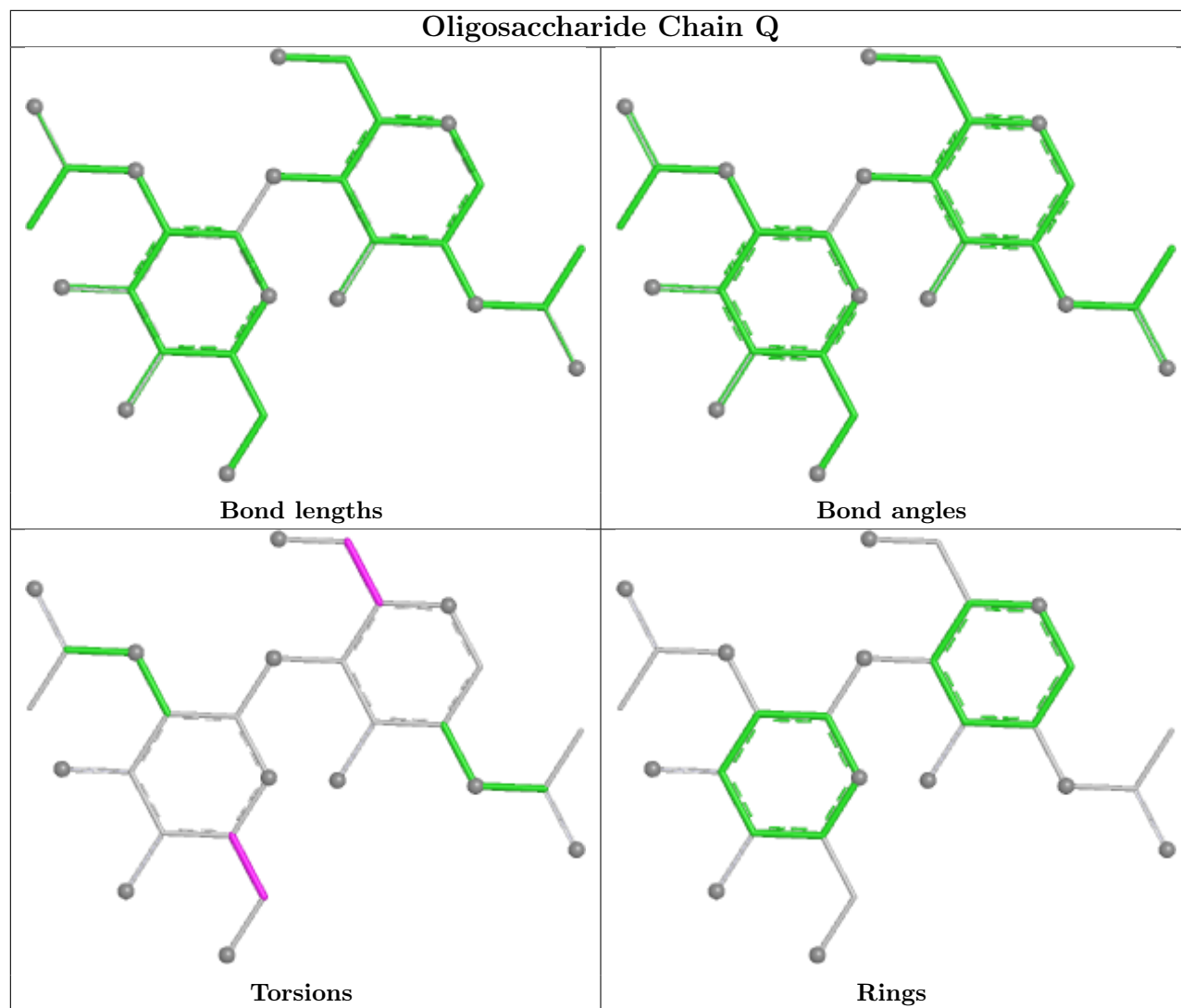
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	1	NAG	1	0
4	S	4	FUC	1	0
5	U	2	NAG	1	0
5	P	1	NAG	2	0
4	S	1	NAG	1	0
3	M	2	NAG	1	0
5	P	2	NAG	2	0

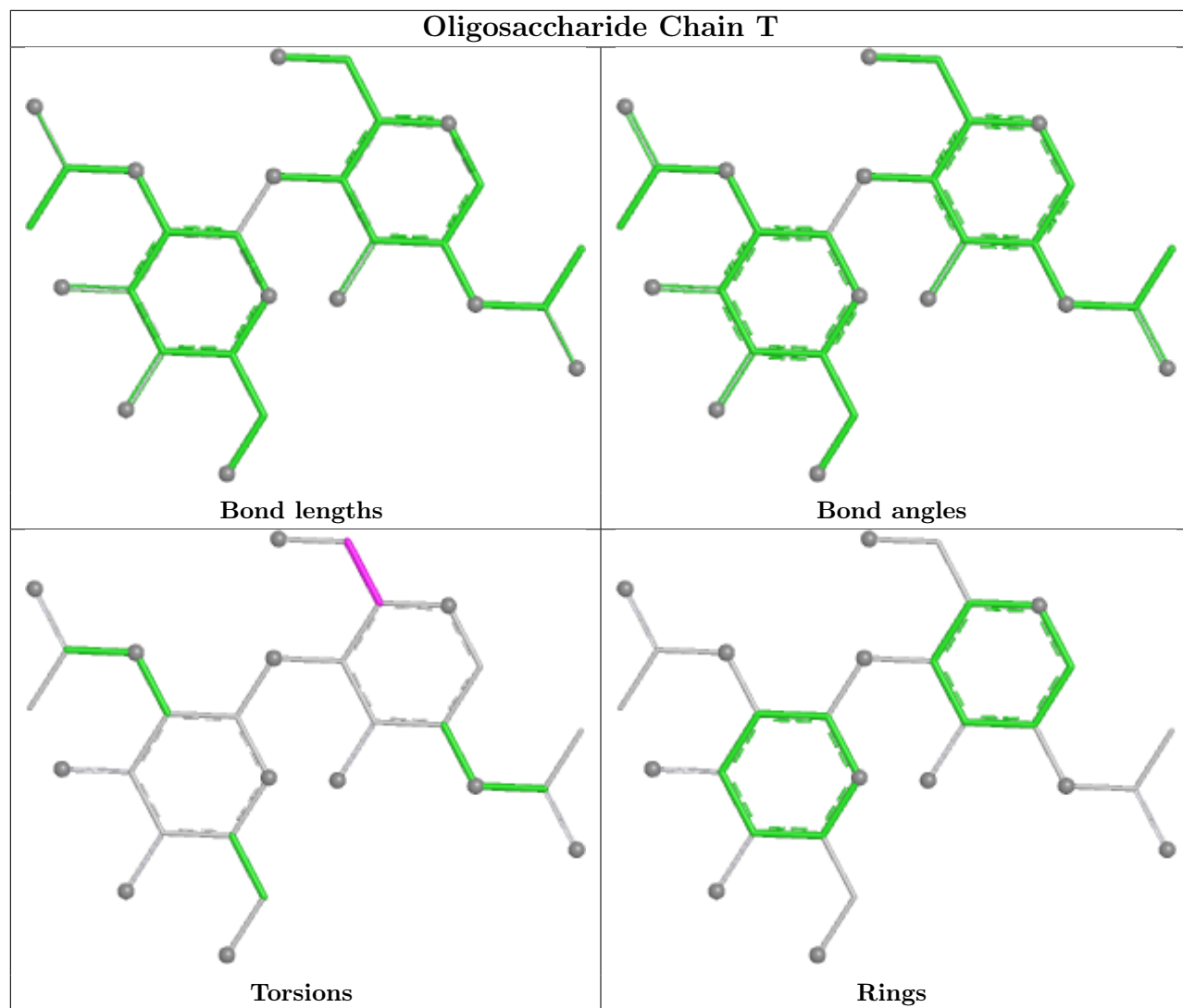
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

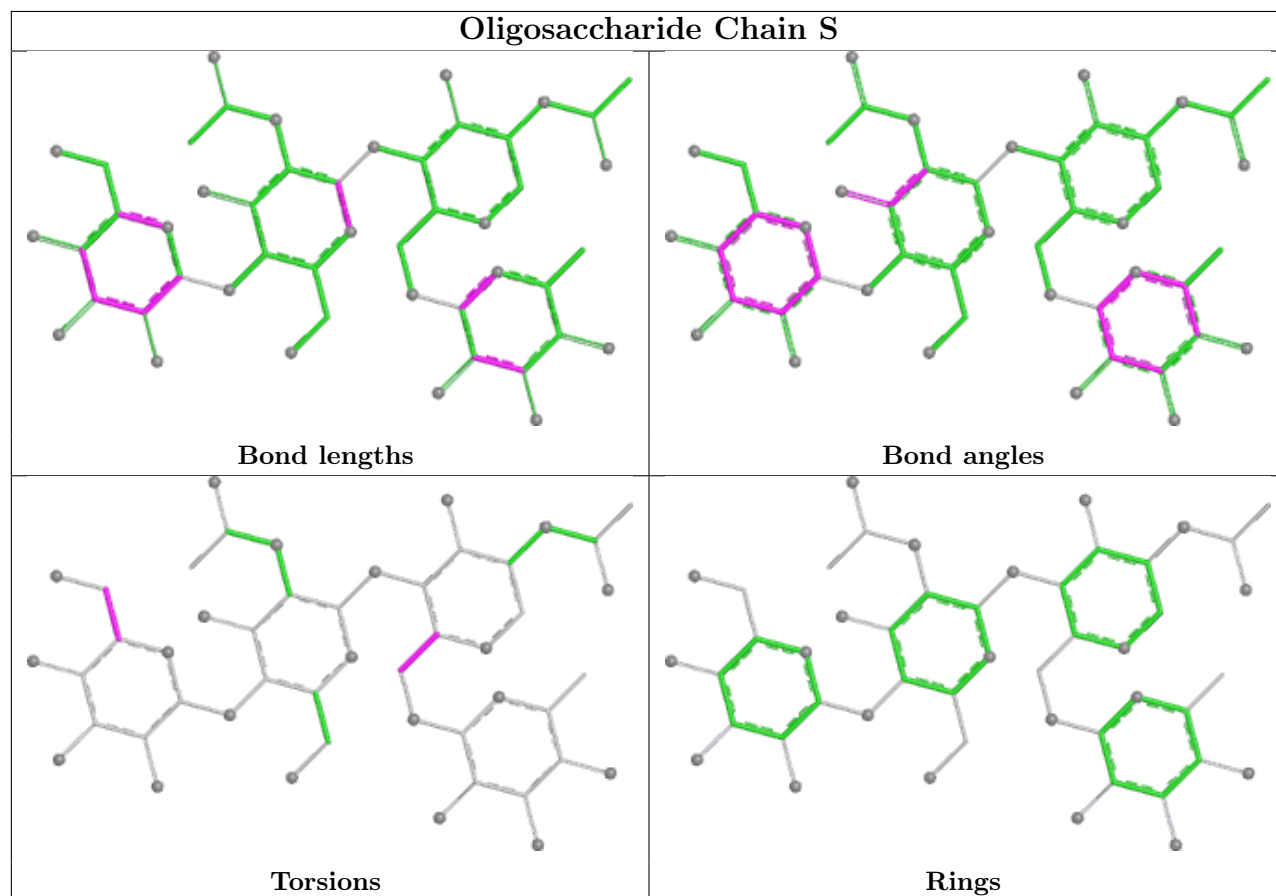
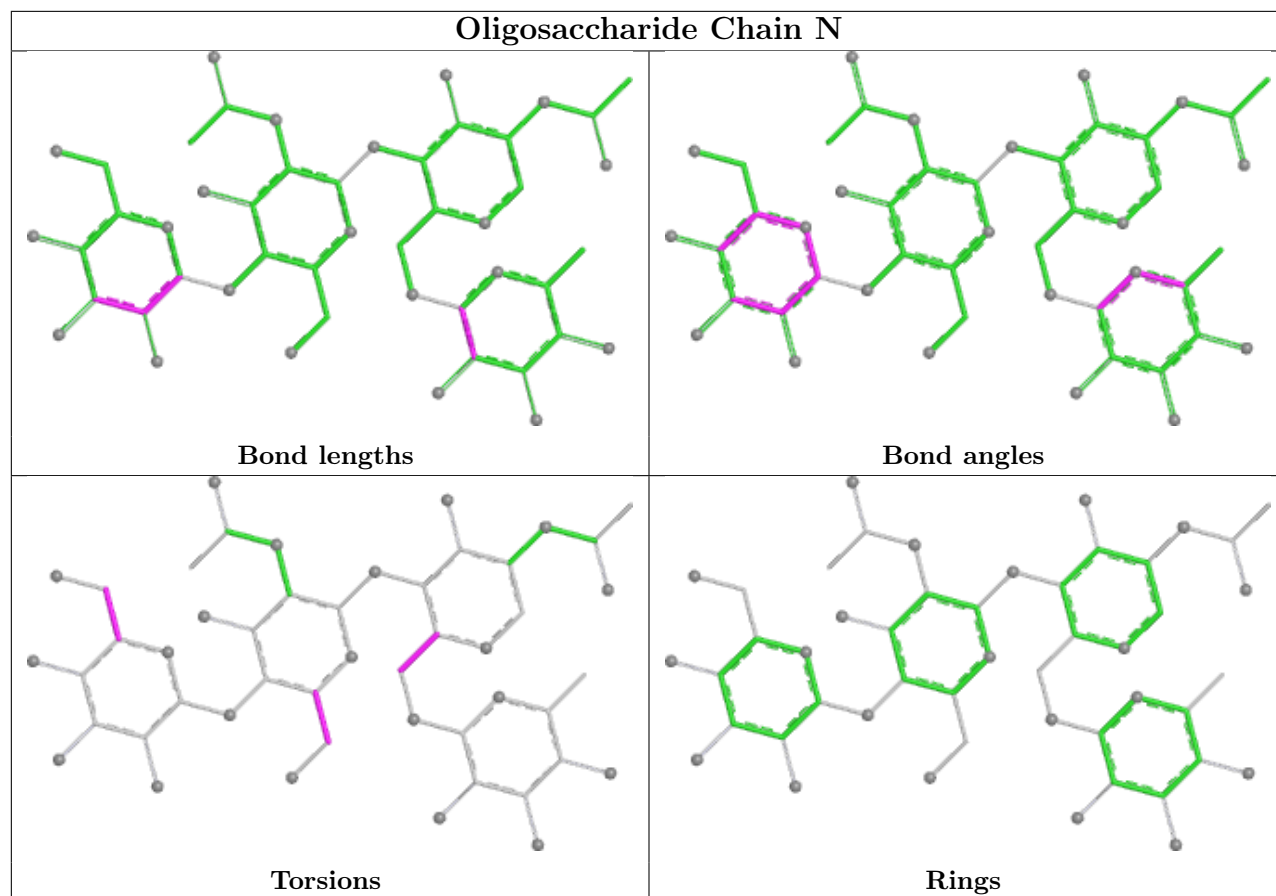
bond angles, torsion angles, and ring geometry for oligosaccharide.

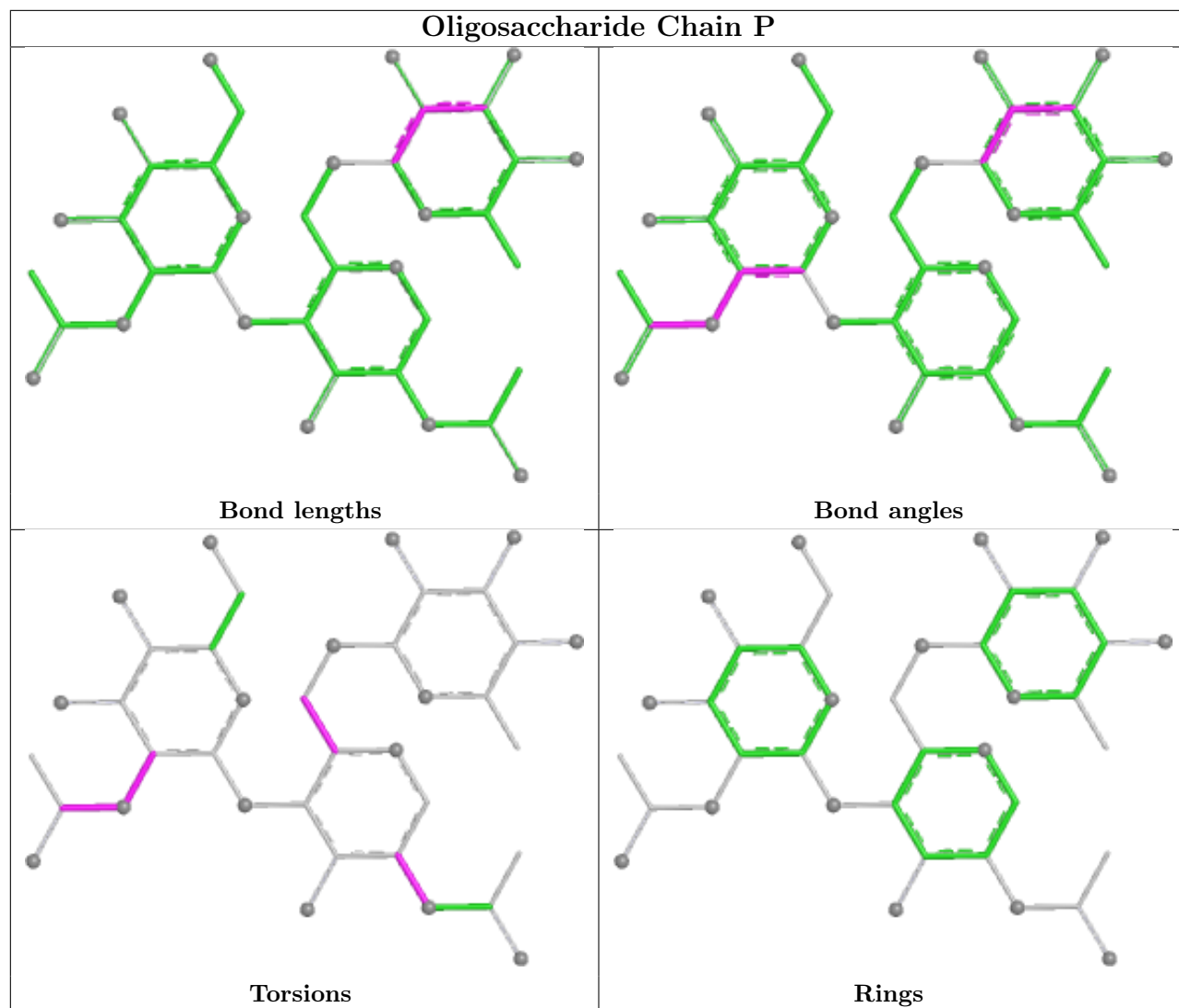


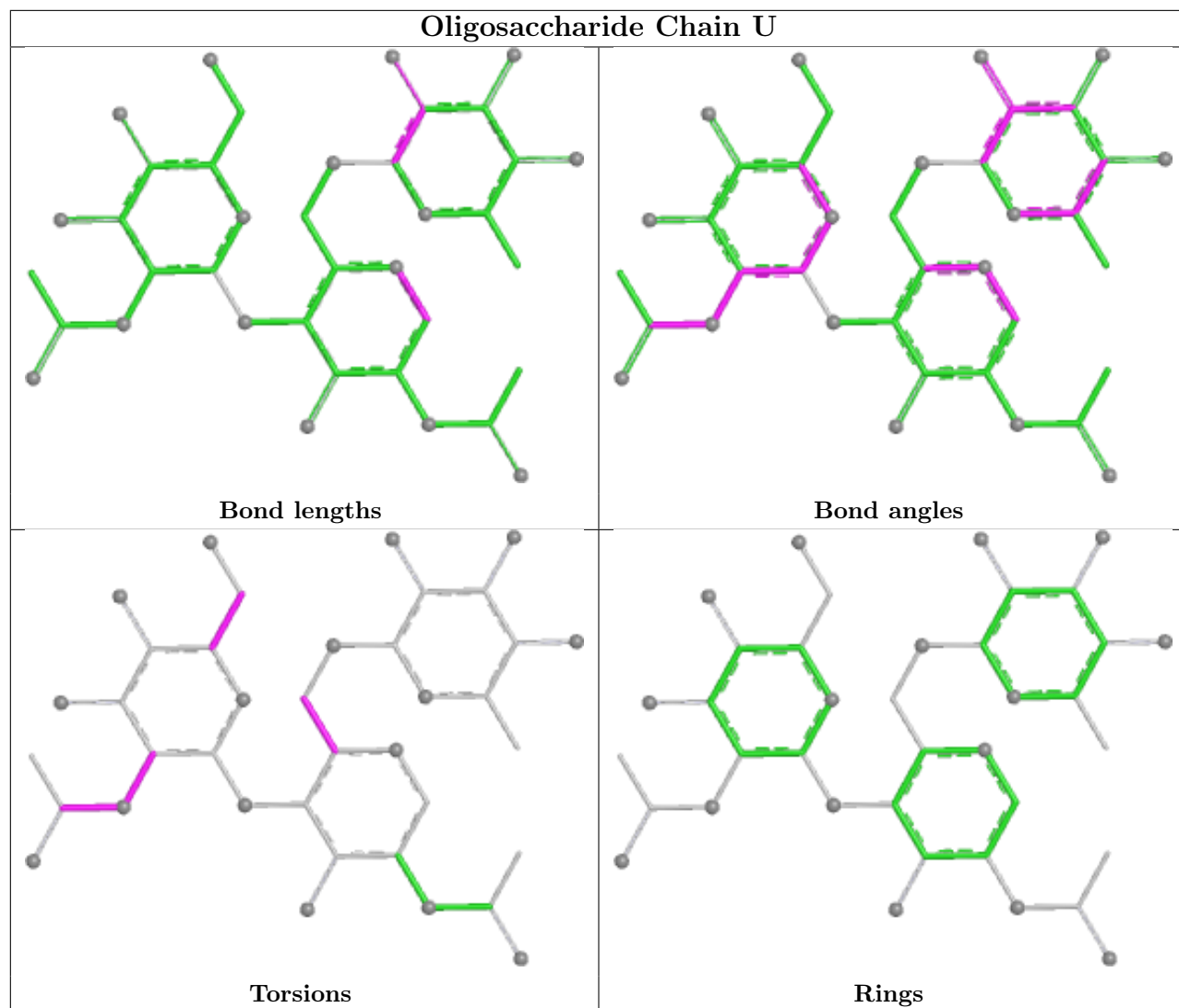


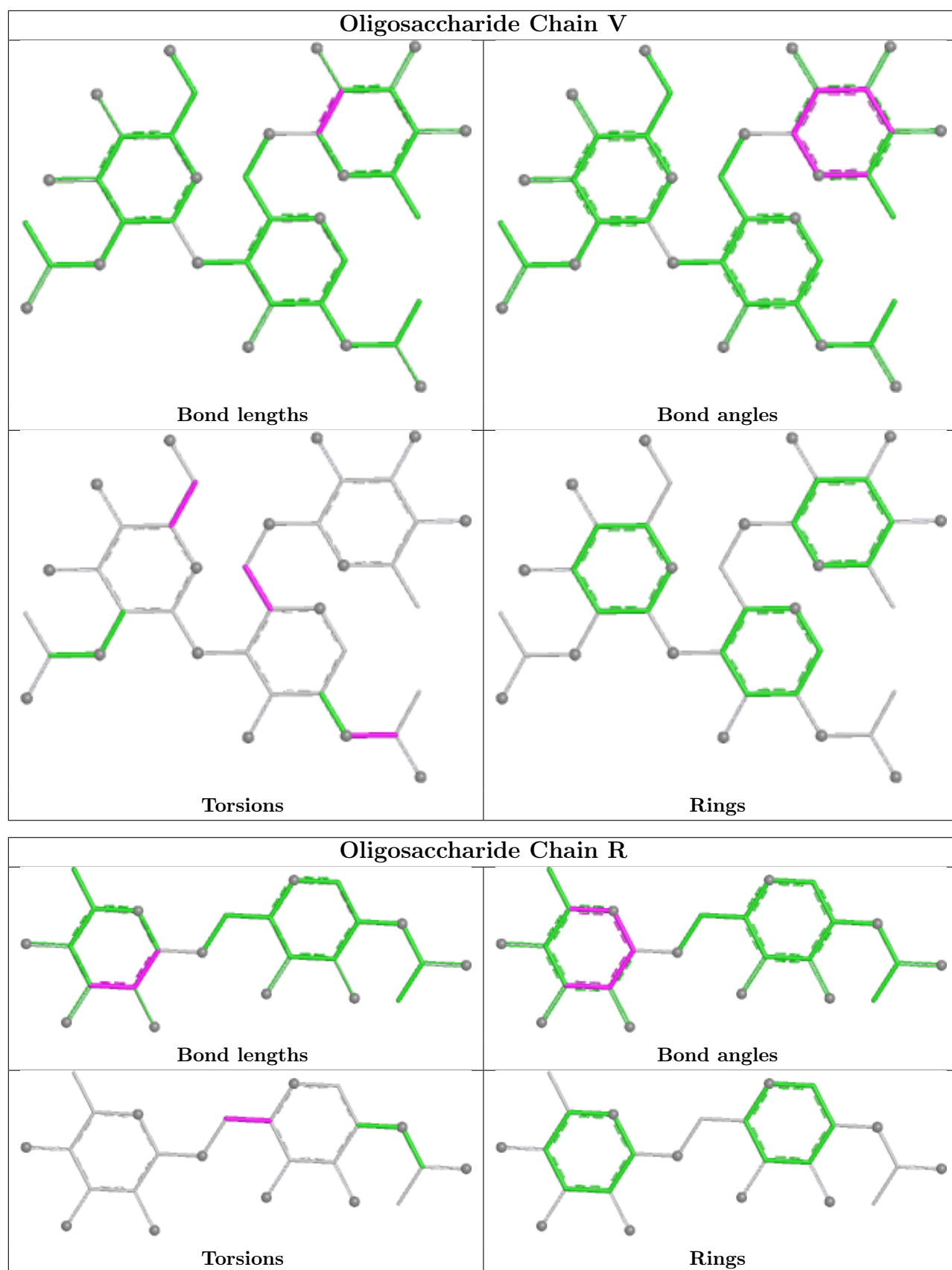












5.6 Ligand geometry

Of 26 ligands modelled in this entry, 24 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
8	NAG	L	602	2	14,14,15	0.24	0	17,19,21	0.39	0
8	NAG	H	602	2	14,14,15	0.40	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	L	602	2	-	2/6/23/26	0/1/1/1
8	NAG	H	602	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	602	NAG	O5-C5-C6-O6
8	H	602	NAG	O5-C5-C6-O6
8	L	602	NAG	C4-C5-C6-O6
8	H	602	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/504 (95%)	0.58	38 (7%) 18 15	19, 43, 89, 112	0
1	C	473/504 (93%)	0.87	85 (17%) 3 3	18, 50, 110, 133	0
1	E	467/504 (92%)	0.82	80 (17%) 4 3	18, 49, 100, 123	0
1	G	462/504 (91%)	0.92	74 (16%) 5 4	22, 51, 98, 134	0
1	I	481/504 (95%)	0.68	44 (9%) 15 12	21, 46, 92, 112	0
1	K	486/504 (96%)	0.87	74 (15%) 5 4	20, 51, 104, 137	0
2	B	328/347 (94%)	0.30	4 (1%) 76 74	21, 39, 59, 76	0
2	D	328/347 (94%)	0.38	14 (4%) 40 35	23, 38, 59, 75	0
2	F	328/347 (94%)	0.26	10 (3%) 52 48	21, 38, 58, 87	0
2	H	329/347 (94%)	0.47	12 (3%) 46 41	22, 40, 69, 88	0
2	J	328/347 (94%)	0.53	12 (3%) 45 40	26, 42, 71, 86	0
2	L	328/347 (94%)	0.45	7 (2%) 63 60	22, 41, 68, 91	0
All	All	4820/5106 (94%)	0.63	454 (9%) 14 12	18, 43, 93, 137	0

All (454) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	568	TYR	6.1
1	G	578	THR	6.0
1	G	650	TYR	5.1
1	E	593	CYS	5.0
1	K	580	LYS	4.9
1	C	672	ALA	4.9
1	K	718	ASN	4.7
1	I	638	GLY	4.6
1	K	464	ALA	4.5
1	K	577	GLY	4.4
1	C	468	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	624	THR	4.3
1	A	296	ASP	4.2
1	G	296	ASP	4.2
1	G	718	ASN	4.2
1	G	565	SER	4.2
1	C	632	THR	4.2
1	K	625	LEU	4.2
1	C	296	ASP	4.2
1	C	623	SER	4.2
1	K	590	TRP	4.1
1	G	619	GLY	4.1
1	K	638	GLY	4.1
1	G	648	LEU	4.1
1	E	650	TYR	4.0
1	A	579	GLU	4.0
1	E	568	TYR	4.0
1	E	651	VAL	4.0
1	G	637	GLY	4.0
1	E	689	SER	3.9
1	C	620	GLU	3.9
1	I	464	ALA	3.9
1	C	618	ASP	3.9
1	C	625	LEU	3.9
1	G	575	ILE	3.9
2	H	542	LYS	3.9
1	G	681	SER	3.9
1	C	619	GLY	3.9
1	A	632	THR	3.8
1	G	717	HIS	3.8
1	G	570	TYR	3.8
1	K	632	THR	3.8
2	H	552	ILE	3.8
1	C	671	VAL	3.8
1	C	580	LYS	3.8
1	G	582	ASN	3.7
1	C	650	TYR	3.7
1	E	599	LEU	3.7
1	A	461	GLY	3.7
1	K	627	VAL	3.7
1	C	568	TYR	3.7
1	I	646	VAL	3.7
1	C	579	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	647	ASP	3.7
1	K	572	LYS	3.7
1	A	716	PRO	3.7
1	C	636	SER	3.6
1	K	571	GLU	3.6
1	G	639	HIS	3.6
1	A	561	LYS	3.6
1	K	575	ILE	3.6
1	C	624	THR	3.6
1	G	593	CYS	3.6
1	E	524	ALA	3.5
1	C	660	GLN	3.5
1	K	633	LEU	3.5
1	G	716	PRO	3.5
1	E	660	GLN	3.5
1	E	565	SER	3.5
1	C	583	CYS	3.5
1	C	593	CYS	3.5
1	G	579	GLU	3.5
1	K	646	VAL	3.5
1	K	705	HIS	3.5
2	D	273	ARG	3.5
1	G	715	PHE	3.5
1	C	570	TYR	3.4
1	C	678	THR	3.4
1	K	562	VAL	3.4
1	G	599	LEU	3.4
1	I	717	HIS	3.4
1	G	572	LYS	3.4
1	K	716	PRO	3.4
1	C	599	LEU	3.4
1	C	617	LEU	3.4
1	G	651	VAL	3.4
1	E	639	HIS	3.3
1	G	524	ALA	3.3
1	G	660	GLN	3.3
1	I	627	VAL	3.3
1	I	645	ASP	3.3
1	K	570	TYR	3.3
1	E	646	VAL	3.3
1	G	641	LYS	3.2
1	G	654	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	672	ALA	3.2
1	C	634	ASN	3.2
1	K	626	VAL	3.2
2	H	256	PHE	3.2
1	C	718	ASN	3.2
1	E	671	VAL	3.2
1	I	468	LEU	3.2
1	I	563	THR	3.2
2	H	428	ASN	3.1
1	A	475	LYS	3.1
1	E	573	LEU	3.1
1	K	639	HIS	3.1
2	J	390	THR	3.1
1	C	637	GLY	3.1
1	K	642	LEU	3.1
2	F	551	VAL	3.1
1	C	567	LYS	3.1
1	E	468	LEU	3.1
1	K	579	GLU	3.1
1	A	625	LEU	3.1
1	A	465	GLU	3.1
1	I	579	GLU	3.1
1	A	649	GLY	3.1
1	K	578	THR	3.1
1	A	524	ALA	3.1
1	E	623	SER	3.1
1	E	448	GLY	3.0
1	E	578	THR	3.0
1	C	706	TRP	3.0
1	A	633	LEU	3.0
1	E	579	GLU	3.0
1	A	630	GLY	3.0
1	E	707	ILE	3.0
1	G	686	THR	3.0
1	K	461	GLY	3.0
1	A	338	SER	3.0
1	G	468	LEU	3.0
1	K	623	SER	3.0
1	A	717	HIS	3.0
1	I	647	ASP	3.0
1	A	339	ARG	3.0
1	I	648	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	665	GLU	2.9
2	D	341	GLU	2.9
1	E	475	LYS	2.9
1	A	650	TYR	2.9
1	E	714	TYR	2.9
1	G	714	TYR	2.9
2	L	551	VAL	2.9
1	G	678	THR	2.9
1	E	562	VAL	2.9
1	C	575	ILE	2.9
2	H	275	TYR	2.9
1	K	631	ARG	2.9
1	E	575	ILE	2.9
2	D	390	THR	2.9
1	C	598	VAL	2.9
1	C	633	LEU	2.9
2	D	551	VAL	2.9
2	F	314	PHE	2.9
1	A	624	THR	2.8
1	C	464	ALA	2.8
1	G	689	SER	2.8
1	C	582	ASN	2.8
1	I	294	ALA	2.8
1	G	463	PRO	2.8
1	K	382	SER	2.8
2	D	304	GLY	2.8
1	K	647	ASP	2.8
1	E	606	THR	2.8
1	E	620	GLU	2.8
2	J	275	TYR	2.8
1	C	631	ARG	2.8
1	G	675	ASN	2.8
1	G	489	LEU	2.8
1	G	640	VAL	2.8
1	K	643	GLU	2.8
1	C	393	LYS	2.7
1	K	595	LYS	2.7
1	E	621	ILE	2.7
1	G	636	SER	2.7
1	C	564	ALA	2.7
1	E	645	ASP	2.7
1	K	589	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	645	ASP	2.7
1	G	256	ARG	2.7
1	I	570	TYR	2.7
1	E	567	LYS	2.7
1	K	591	ILE	2.7
1	G	573	LEU	2.7
1	C	268	SER	2.7
1	I	461	GLY	2.7
1	C	626	VAL	2.7
1	G	580	LYS	2.7
1	E	706	TRP	2.7
2	F	273	ARG	2.7
1	K	678	THR	2.7
2	J	256	PHE	2.7
1	A	568	TYR	2.7
1	I	625	LEU	2.7
1	C	482	ASP	2.7
1	A	621	ILE	2.6
1	C	611	ILE	2.6
1	G	608	ILE	2.6
1	C	639	HIS	2.6
1	I	705	HIS	2.6
1	G	467	VAL	2.6
1	G	646	VAL	2.6
1	K	468	LEU	2.6
2	D	385	LEU	2.6
1	A	615	GLY	2.6
1	I	716	PRO	2.6
1	E	717	HIS	2.6
1	E	580	LYS	2.6
1	G	671	VAL	2.6
1	G	691	ASN	2.6
1	K	524	ALA	2.6
2	F	363	ASN	2.6
1	A	588	ASP	2.6
2	F	240	ASP	2.6
1	A	468	LEU	2.6
1	K	599	LEU	2.6
1	K	568	TYR	2.6
1	K	465	GLU	2.6
1	C	609	GLY	2.6
1	E	577	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	448	GLY	2.6
1	C	467	VAL	2.6
1	G	464	ALA	2.6
2	J	551	VAL	2.6
2	B	428	ASN	2.6
2	B	498	PHE	2.6
1	I	624	THR	2.5
2	J	281	THR	2.5
1	G	645	ASP	2.5
1	E	561	LYS	2.5
1	K	393	LYS	2.5
1	I	649	GLY	2.5
1	E	583	CYS	2.5
1	C	607	ASN	2.5
1	E	296	ASP	2.5
1	I	588	ASP	2.5
1	C	608	ILE	2.5
1	E	595	LYS	2.5
1	K	585	LYS	2.5
1	I	571	GLU	2.5
2	L	275	TYR	2.5
1	C	708	GLY	2.5
1	E	463	PRO	2.5
1	G	538	VAL	2.5
1	E	480	THR	2.5
1	I	606	THR	2.5
1	K	565	SER	2.5
1	E	641	LYS	2.5
1	I	590	TRP	2.5
2	D	240	ASP	2.5
1	K	660	GLN	2.5
1	E	572	LYS	2.5
1	K	617	LEU	2.5
1	K	636	SER	2.5
1	I	644	GLU	2.5
1	A	480	THR	2.4
1	I	634	ASN	2.4
1	K	634	ASN	2.4
1	I	642	LEU	2.4
1	K	664	LEU	2.4
1	C	517	SER	2.4
1	K	463	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	256	PHE	2.4
1	C	578	THR	2.4
1	C	642	LEU	2.4
1	C	664	LEU	2.4
1	G	687	ILE	2.4
1	I	381	ILE	2.4
1	A	623	SER	2.4
1	K	520	SER	2.4
1	I	585	LYS	2.4
1	K	475	LYS	2.4
1	E	538	VAL	2.4
2	D	387	ILE	2.4
2	L	237	LEU	2.4
1	C	717	HIS	2.4
1	G	481	GLN	2.4
1	C	640	VAL	2.4
2	D	256	PHE	2.4
1	C	565	SER	2.4
1	E	558	TRP	2.4
1	C	572	LYS	2.4
1	I	572	LYS	2.4
1	I	463	PRO	2.4
1	K	671	VAL	2.4
2	J	318	PHE	2.4
1	E	557	ILE	2.3
1	E	635	CYS	2.3
1	G	668	CYS	2.3
1	E	649	GLY	2.3
1	K	467	VAL	2.3
1	K	650	TYR	2.3
1	E	622	THR	2.3
1	C	594	ASN	2.3
1	E	634	ASN	2.3
1	A	590	TRP	2.3
1	G	658	GLY	2.3
1	K	592	GLN	2.3
1	E	687	ILE	2.3
2	J	487	TYR	2.3
1	C	643	GLU	2.3
1	E	616	GLU	2.3
1	E	718	ASN	2.3
1	G	684	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	703	ASN	2.3
1	K	582	ASN	2.3
1	G	382	SER	2.3
1	I	520	SER	2.3
2	J	243	SER	2.3
1	E	481	GLN	2.3
1	K	619	GLY	2.3
1	G	617	LEU	2.3
1	K	460	CYS	2.3
1	K	593	CYS	2.3
2	B	551	VAL	2.3
1	I	575	ILE	2.3
1	C	705	HIS	2.3
1	A	678	THR	2.3
1	C	595	LYS	2.3
1	I	462	THR	2.3
1	C	712	ASN	2.3
1	C	654	GLY	2.3
1	A	479	LEU	2.3
1	K	234	VAL	2.3
1	C	687	ILE	2.2
1	E	672	ALA	2.2
1	K	381	ILE	2.2
2	H	317	LYS	2.2
1	C	714	TYR	2.2
1	A	645	ASP	2.2
1	K	588	ASP	2.2
2	H	243	SER	2.2
1	C	577	GLY	2.2
1	E	601	GLY	2.2
1	E	609	GLY	2.2
1	G	448	GLY	2.2
1	I	633	LEU	2.2
1	C	641	LYS	2.2
1	E	611	ILE	2.2
2	B	256	PHE	2.2
2	L	267	HIS	2.2
1	C	667	ARG	2.2
2	F	365	ASN	2.2
2	H	255	PRO	2.2
1	E	338	SER	2.2
1	K	483	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	572	LYS	2.2
1	C	505	GLU	2.2
1	E	236	GLU	2.2
2	J	271	THR	2.2
1	E	675	ASN	2.2
1	E	691	ASN	2.2
1	K	519	ASN	2.2
2	H	365	ASN	2.2
1	C	615	GLY	2.2
1	E	604	LEU	2.2
1	G	492	LYS	2.2
1	I	482	ASP	2.2
2	D	280	GLY	2.2
1	A	260	VAL	2.2
1	I	620	GLU	2.2
1	C	622	THR	2.2
1	I	460	CYS	2.2
2	H	450	ARG	2.2
1	G	602	TYR	2.2
2	J	365	ASN	2.2
1	K	362	LYS	2.2
1	E	581	GLY	2.2
1	G	609	GLY	2.2
2	L	385	LEU	2.2
1	I	296	ASP	2.2
1	I	562	VAL	2.2
1	I	591	ILE	2.2
1	A	622	THR	2.1
1	C	447	CYS	2.1
1	K	466	CYS	2.1
1	C	493	LYS	2.1
1	G	567	LYS	2.1
1	C	680	LEU	2.1
1	E	662	MET	2.1
1	G	662	MET	2.1
1	E	467	VAL	2.1
2	D	425	ASP	2.1
2	J	268	VAL	2.1
2	L	268	VAL	2.1
1	C	471	ALA	2.1
1	G	471	ALA	2.1
1	C	571	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	476	LYS	2.1
1	E	617	LEU	2.1
1	G	614	LEU	2.1
2	H	237	LEU	2.1
1	I	615	GLY	2.1
2	D	258	GLY	2.1
1	A	591	ILE	2.1
1	A	705	HIS	2.1
1	C	538	VAL	2.1
1	C	562	VAL	2.1
1	G	611	ILE	2.1
1	K	608	ILE	2.1
1	A	715	PHE	2.1
1	E	483	SER	2.1
1	G	652	GLU	2.1
1	K	620	GLU	2.1
1	G	669	LEU	2.1
1	E	605	CYS	2.1
1	G	519	ASN	2.1
2	H	487	TYR	2.1
1	E	715	PHE	2.1
1	K	482	ASP	2.1
1	C	256	ARG	2.1
1	E	464	ALA	2.1
1	I	636	SER	2.1
1	E	505	GLU	2.1
1	G	643	GLU	2.1
1	G	595	LYS	2.1
2	F	429	MET	2.1
1	E	387	LEU	2.1
1	K	573	LEU	2.1
2	F	385	LEU	2.1
1	E	582	ASN	2.1
1	C	474	CYS	2.1
1	G	601	GLY	2.1
1	E	602	TYR	2.1
1	G	557	ILE	2.1
1	C	646	VAL	2.1
1	I	357	VAL	2.1
1	E	457	GLU	2.0
1	C	673	SER	2.0
2	D	243	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	606	THR	2.0
1	A	463	PRO	2.0
1	C	662	MET	2.0
1	C	716	PRO	2.0
1	E	716	PRO	2.0
1	E	297	ASN	2.0
1	E	594	ASN	2.0
1	C	690	GLY	2.0
2	D	468	ILE	2.0
1	I	568	TYR	2.0
2	J	260	CYS	2.0
1	A	616	GLU	2.0
1	C	566	ASP	2.0
1	C	616	GLU	2.0
1	E	678	THR	2.0
1	E	664	LEU	2.0
1	G	664	LEU	2.0
1	C	621	ILE	2.0
1	E	608	ILE	2.0
1	K	233	ASN	2.0
1	K	609	GLY	2.0
2	F	387	ILE	2.0
2	L	363	ASN	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($\text{\AA}^2$)	Q<0.9
4	BMA	N	3	11/12	0.32	0.20	98,102,107,110	0
5	NAG	U	2	14/15	0.50	0.21	74,90,95,96	0
4	BMA	S	3	11/12	0.63	0.16	81,105,123,131	0
3	NAG	O	2	14/15	0.63	0.17	78,85,89,90	0
4	NAG	N	2	14/15	0.67	0.16	80,90,102,103	0

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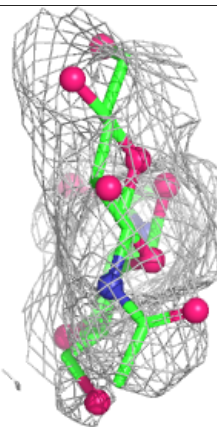
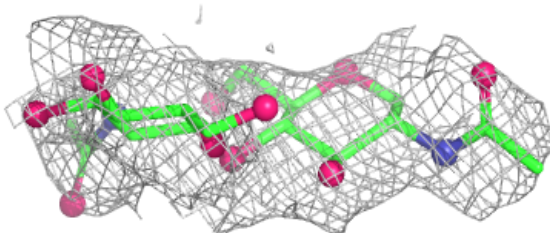
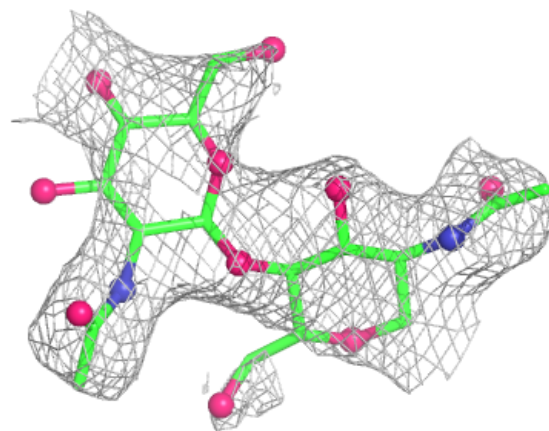
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	Q	2	14/15	0.69	0.15	71,75,80,80	0
5	NAG	P	2	14/15	0.69	0.19	79,86,90,91	0
3	NAG	T	2	14/15	0.69	0.16	73,85,91,97	0
4	FUC	N	4	10/11	0.72	0.16	72,77,81,82	0
3	NAG	T	1	14/15	0.72	0.18	60,70,77,83	0
6	FUC	R	2	10/11	0.72	0.14	58,77,80,80	0
4	NAG	S	1	14/15	0.78	0.12	49,55,67,70	0
5	FUC	U	3	10/11	0.78	0.15	58,76,79,80	0
5	FUC	P	3	10/11	0.78	0.14	70,82,89,90	0
6	NAG	R	1	14/15	0.80	0.13	51,64,71,75	0
4	NAG	S	2	14/15	0.81	0.13	62,73,87,107	0
3	NAG	M	2	14/15	0.81	0.13	73,84,85,87	0
3	NAG	M	1	14/15	0.82	0.14	56,67,72,75	0
5	NAG	U	1	14/15	0.82	0.11	54,62,72,81	0
5	NAG	P	1	14/15	0.83	0.12	60,67,72,74	0
5	NAG	V	2	14/15	0.85	0.11	55,63,67,68	0
3	NAG	Q	1	14/15	0.86	0.12	50,60,65,66	0
5	FUC	V	3	10/11	0.86	0.17	59,65,66,66	0
4	NAG	N	1	14/15	0.87	0.12	54,62,71,80	0
4	FUC	S	4	10/11	0.88	0.11	56,64,71,73	0
5	NAG	V	1	14/15	0.88	0.10	40,48,57,64	0
3	NAG	O	1	14/15	0.90	0.10	50,64,71,74	0

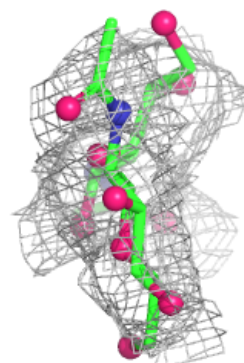
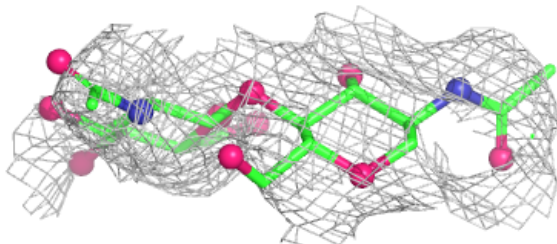
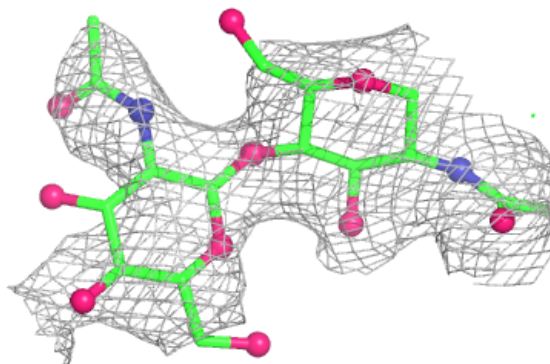
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

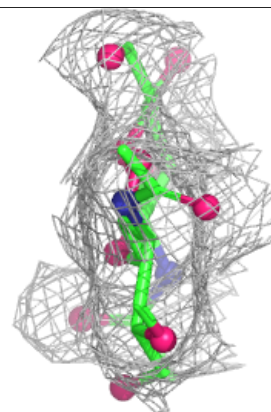
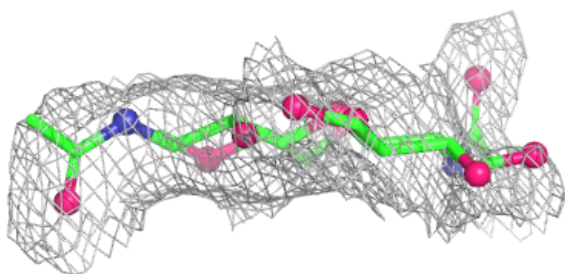
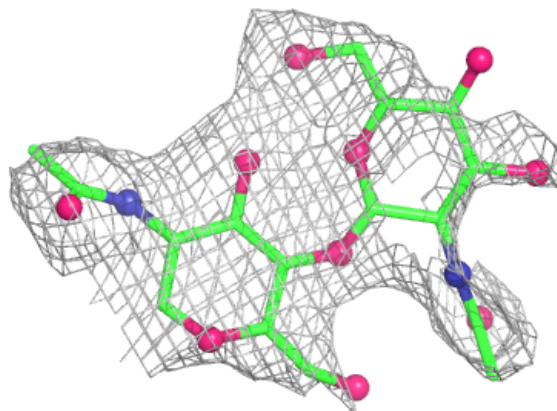
**Electron density around Chain O:**

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



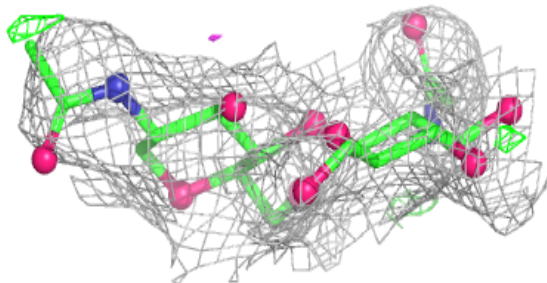
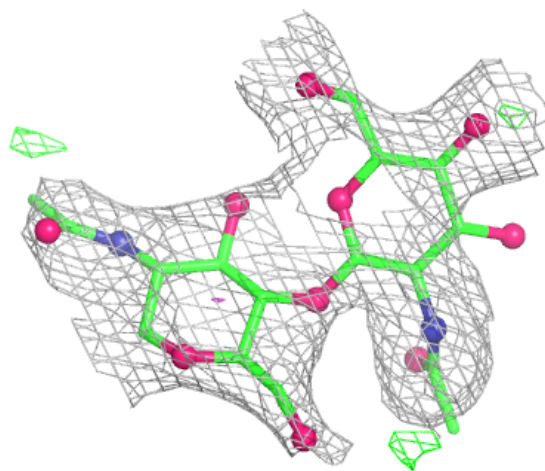
Electron density around Chain Q:

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



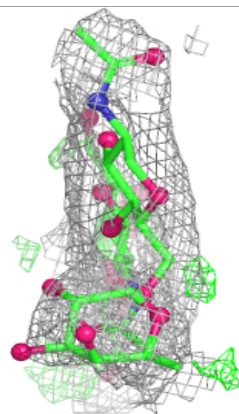
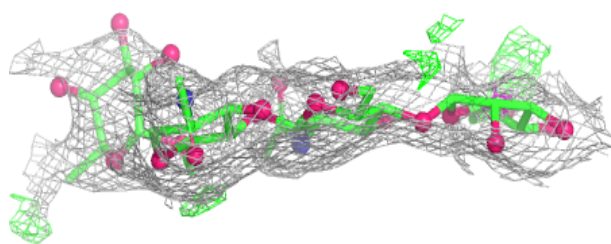
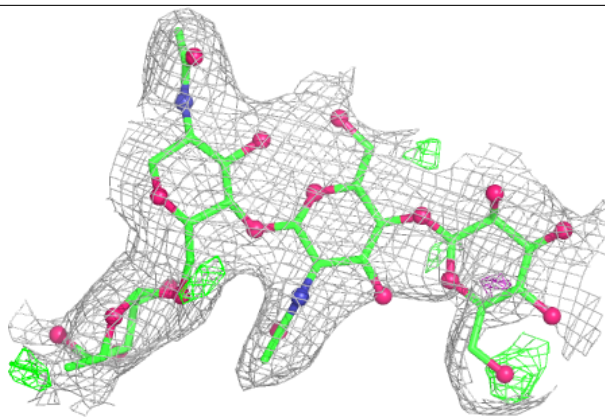
Electron density around Chain T:

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



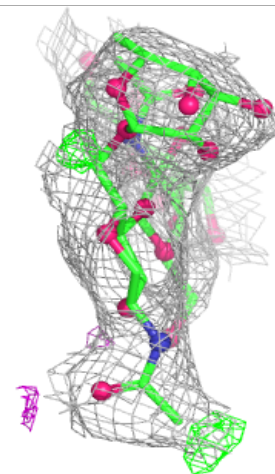
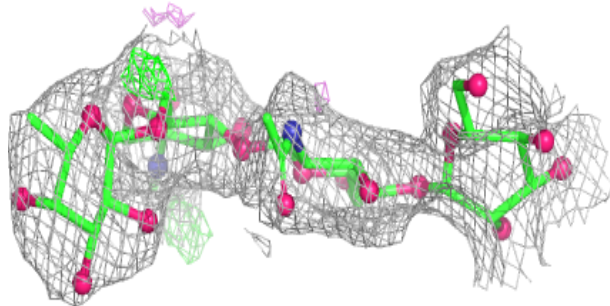
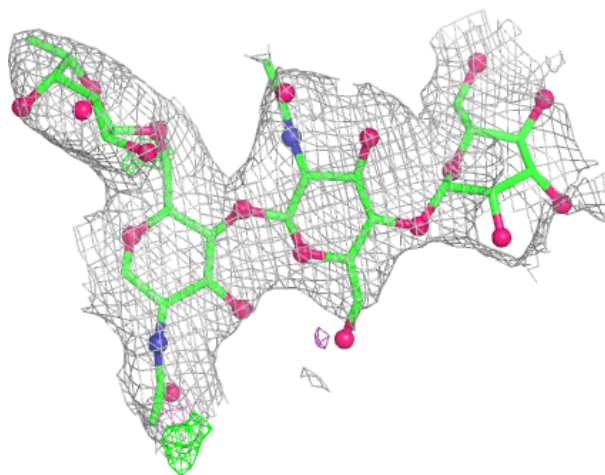
Electron density around Chain N:

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



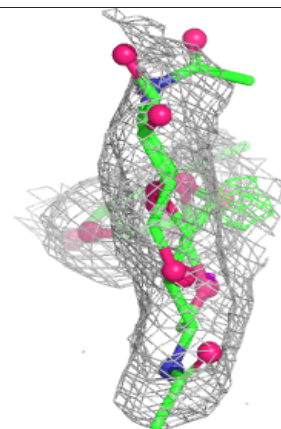
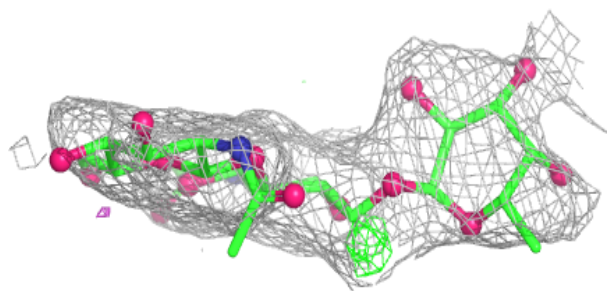
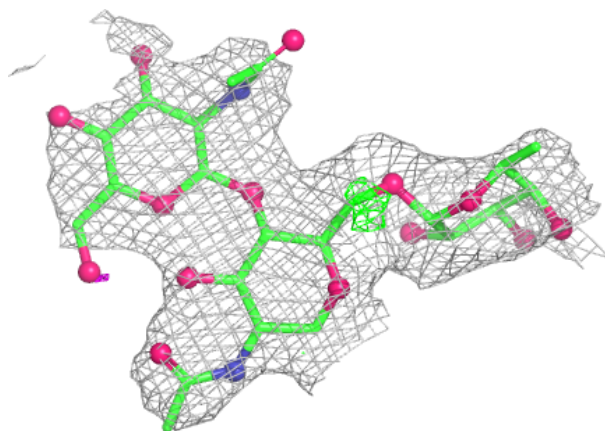
Electron density around Chain S:

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



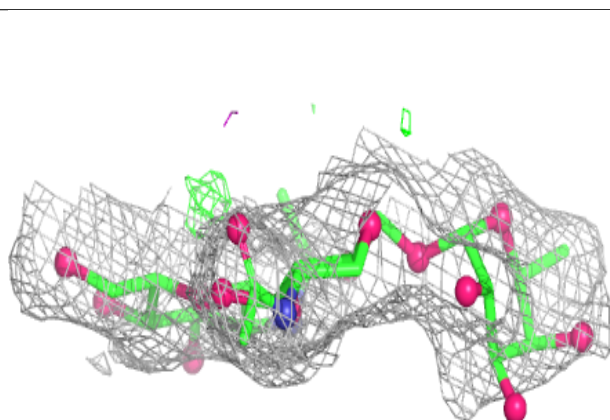
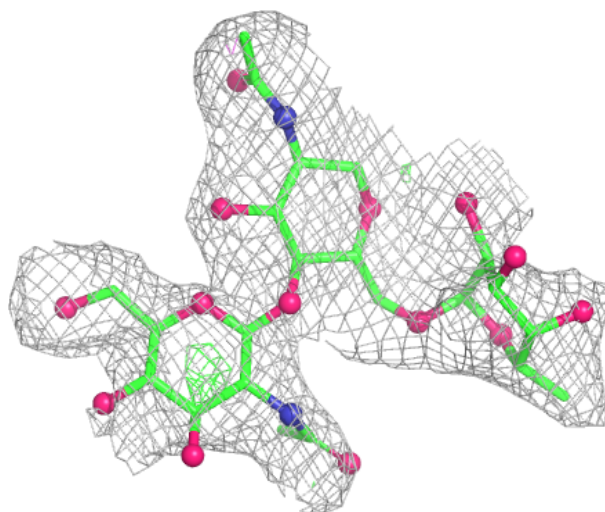
Electron density around Chain P:

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



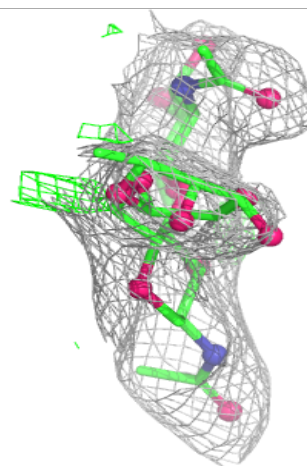
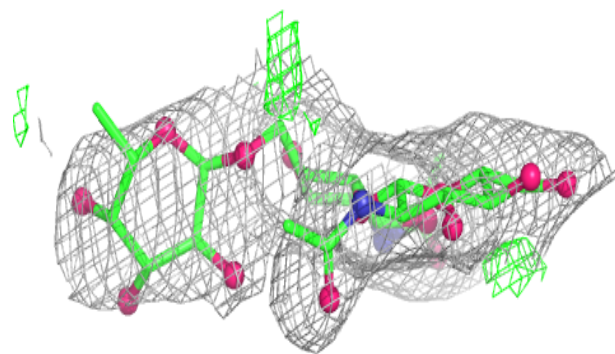
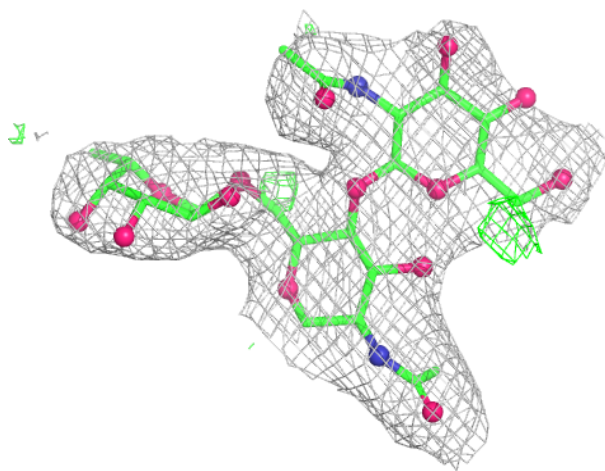
Electron density around Chain U:

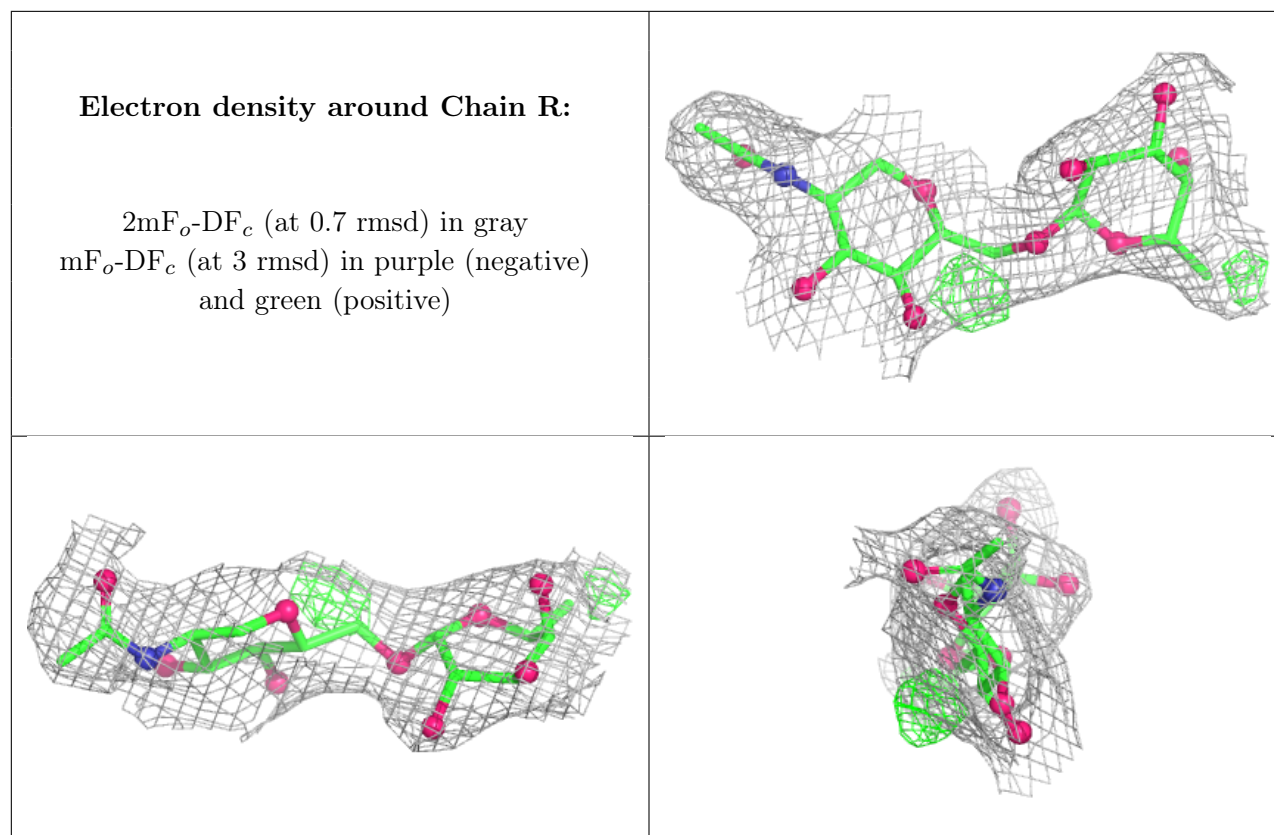
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain V:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	L	602	14/15	0.77	0.14	61,67,73,77	0
8	NAG	H	602	14/15	0.83	0.13	59,62,69,72	0
7	CA	I	801	1/1	0.87	0.09	31,31,31,31	0
7	CA	J	601	1/1	0.89	0.09	38,38,38,38	0
7	CA	E	801	1/1	0.91	0.08	28,28,28,28	0
7	CA	C	802	1/1	0.92	0.07	45,45,45,45	0
7	CA	G	803	1/1	0.92	0.07	33,33,33,33	0
7	CA	H	601	1/1	0.93	0.07	33,33,33,33	0
7	CA	B	601	1/1	0.94	0.05	37,37,37,37	0
7	CA	F	601	1/1	0.94	0.07	33,33,33,33	0
7	CA	A	801	1/1	0.94	0.06	27,27,27,27	0
7	CA	G	801	1/1	0.94	0.05	26,26,26,26	0
7	CA	I	803	1/1	0.94	0.07	37,37,37,37	0
7	CA	K	802	1/1	0.94	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	D	601	1/1	0.95	0.05	41,41,41,41	0
7	CA	E	802	1/1	0.95	0.06	41,41,41,41	0
7	CA	I	802	1/1	0.95	0.06	37,37,37,37	0
7	CA	A	802	1/1	0.95	0.06	46,46,46,46	0
7	CA	G	802	1/1	0.95	0.05	43,43,43,43	0
7	CA	A	803	1/1	0.95	0.08	29,29,29,29	0
7	CA	C	801	1/1	0.96	0.06	27,27,27,27	0
7	CA	L	601	1/1	0.96	0.05	40,40,40,40	0
7	CA	K	803	1/1	0.96	0.04	32,32,32,32	0
7	CA	K	801	1/1	0.96	0.04	27,27,27,27	0
7	CA	E	803	1/1	0.97	0.04	32,32,32,32	0
7	CA	C	803	1/1	0.98	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.