Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 09:42 PM JST

PDB ID	:	5Y2Z
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:

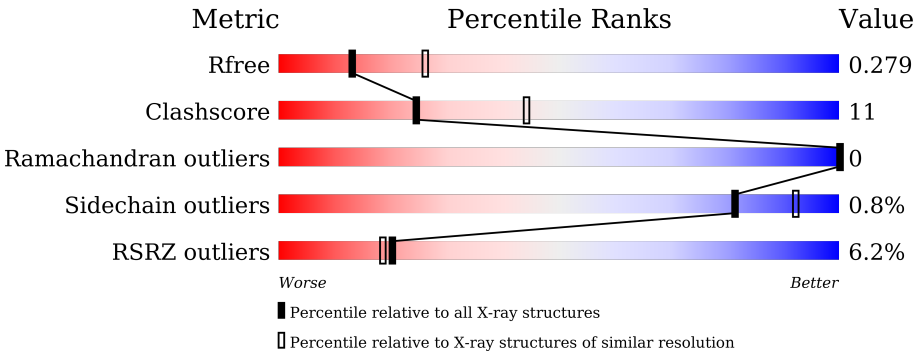
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (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 <=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	6% 75% 20% ·
1	C	504	12% 73% 21% 6%
1	E	504	8% 75% 17% · 7%
1	G	504	11% 76% 16% 8%
1	I	504	7% 79% 17% 5%
1	K	504	11% 78% 19% ·

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Mol	Chain	Length	Quality of chain
2	B	347	64% 29% 5%
2	D	347	68% 26% 5%
2	F	347	68% 27% 5%
2	H	347	65% 30% 5%
2	J	347	67% 27% 5%
2	L	347	67% 27% 5%
3	M	2	50% 50%
3	O	2	100%
3	Q	2	100%
3	T	2	100%
4	N	4	50% 50%
4	S	4	75% 25%
5	P	3	67% 33%
5	U	3	67% 33%
5	V	3	67% 33%
6	R	2	100%

2 Entry composition (i)

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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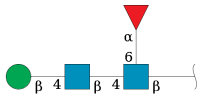
Chain	Residue	Modelled	Actual	Comment	Reference
H	221	GLN	-	expression tag	UNP O95970
H	222	PRO	-	expression tag	UNP O95970
H	223	ALA	-	expression tag	UNP O95970
H	558	LYS	-	expression tag	UNP O95970
H	559	HIS	-	expression tag	UNP O95970
H	560	HIS	-	expression tag	UNP O95970
H	561	HIS	-	expression tag	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.

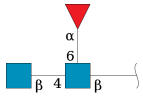
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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			

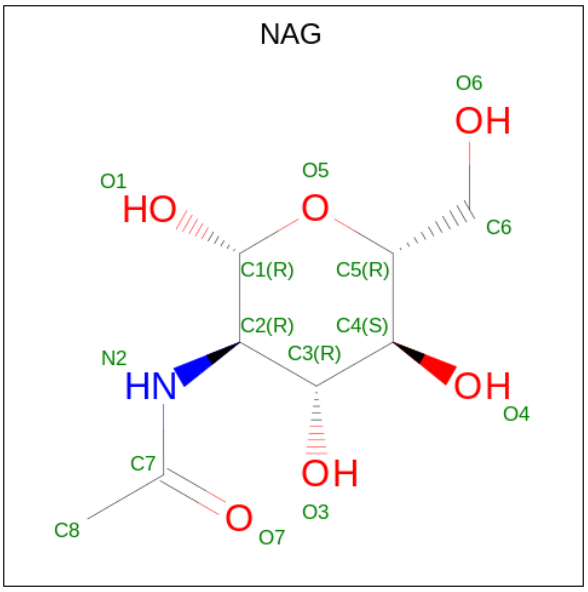
- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is water.

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

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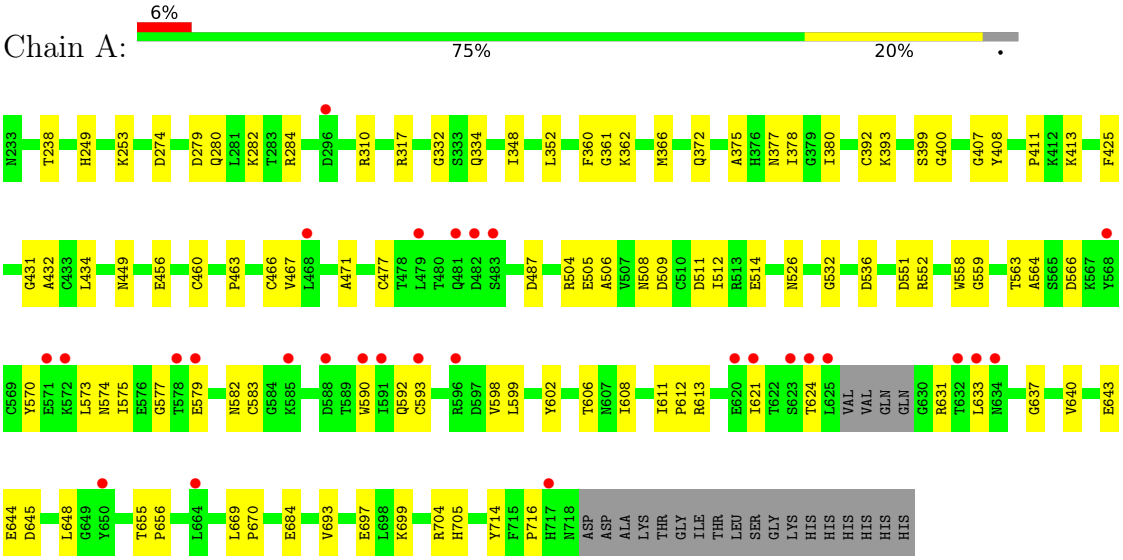
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	J	67	Total O 67 67	0	0
9	L	59	Total O 59 59	0	0

3 Residue-property plots (i)

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

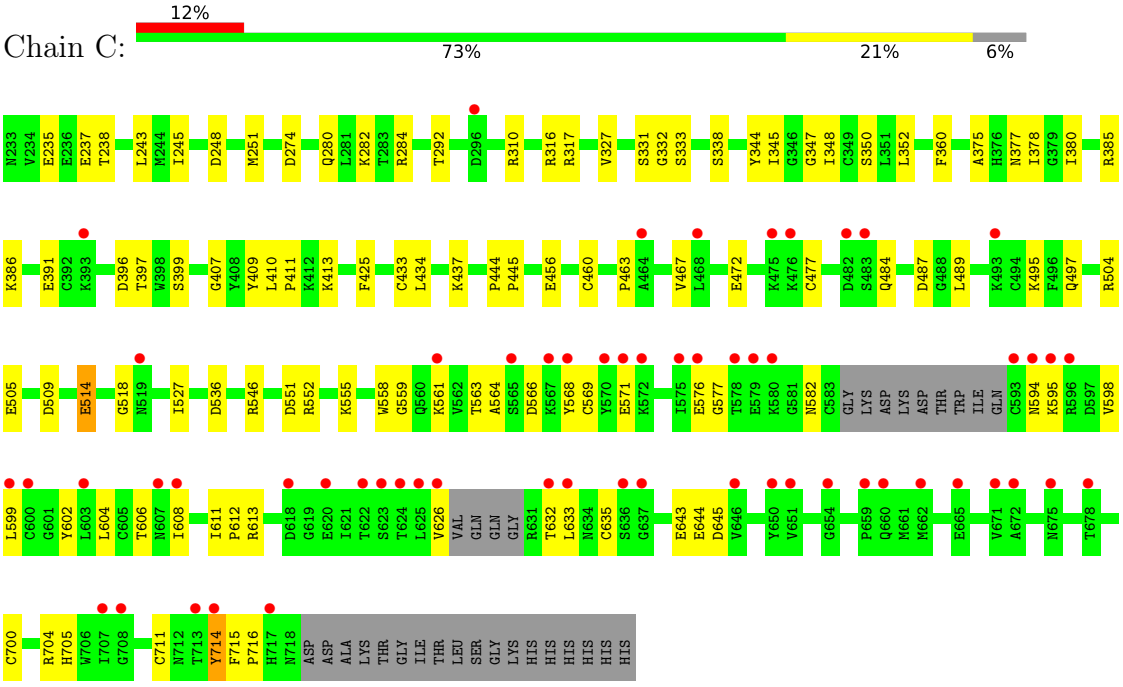
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

Chain A:



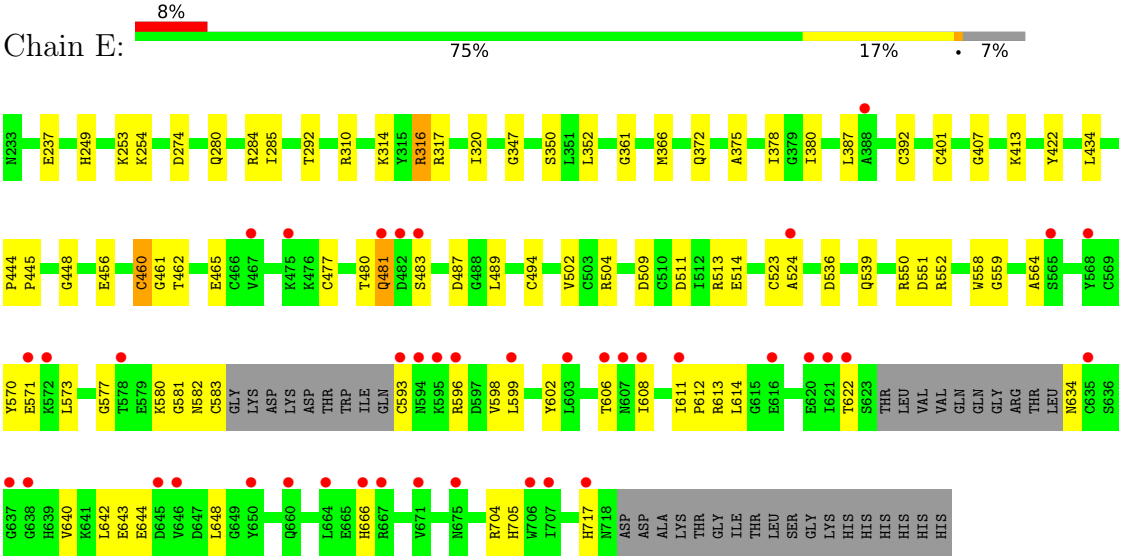
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

Chain C:



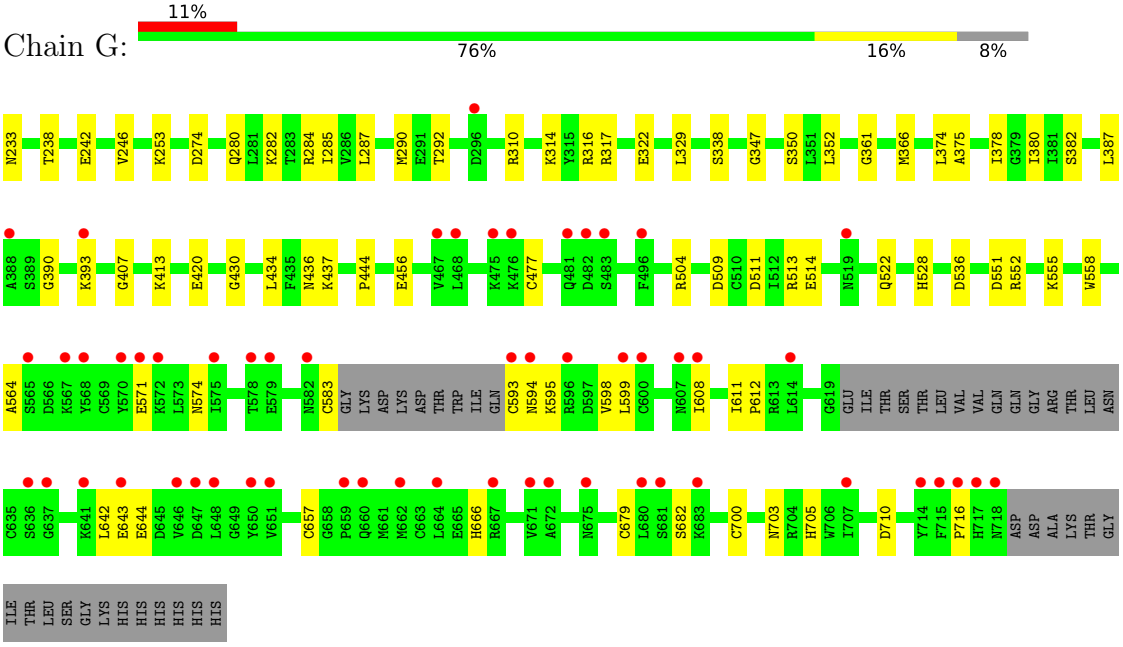
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

Chain E:



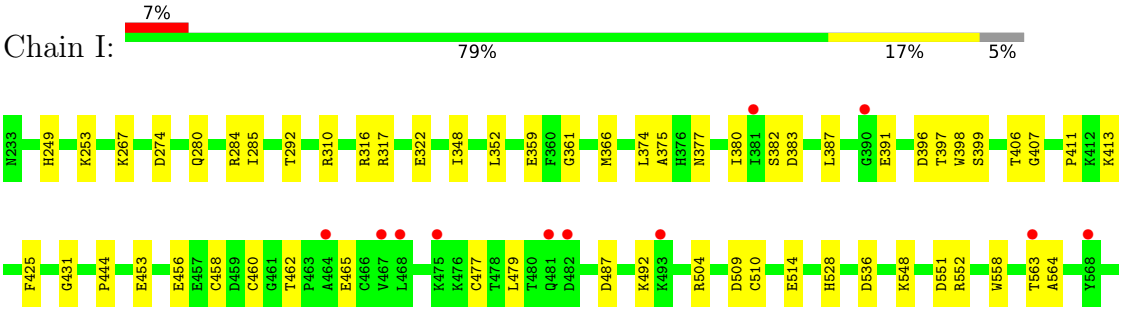
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

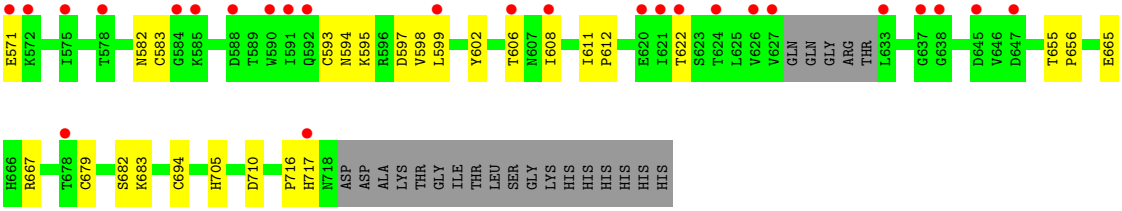
Chain G:



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

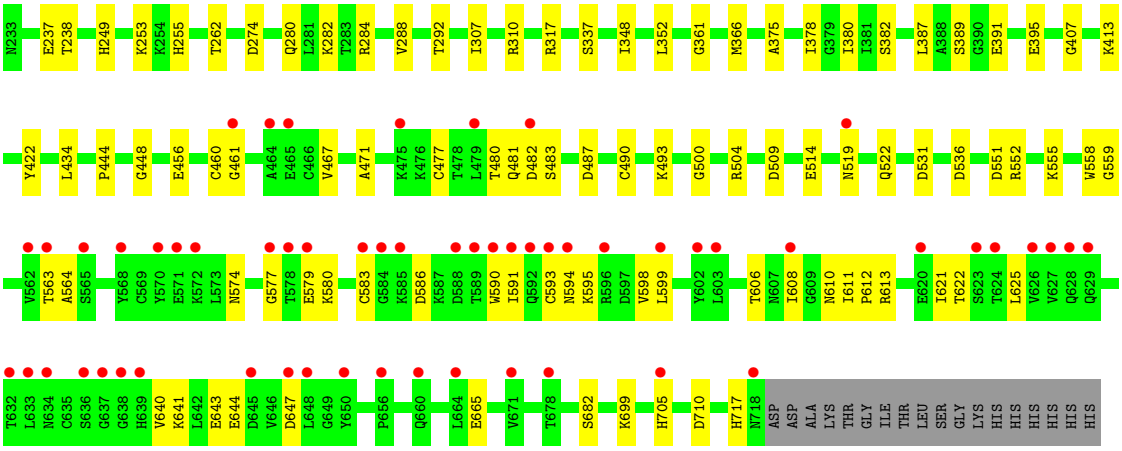
Chain I:





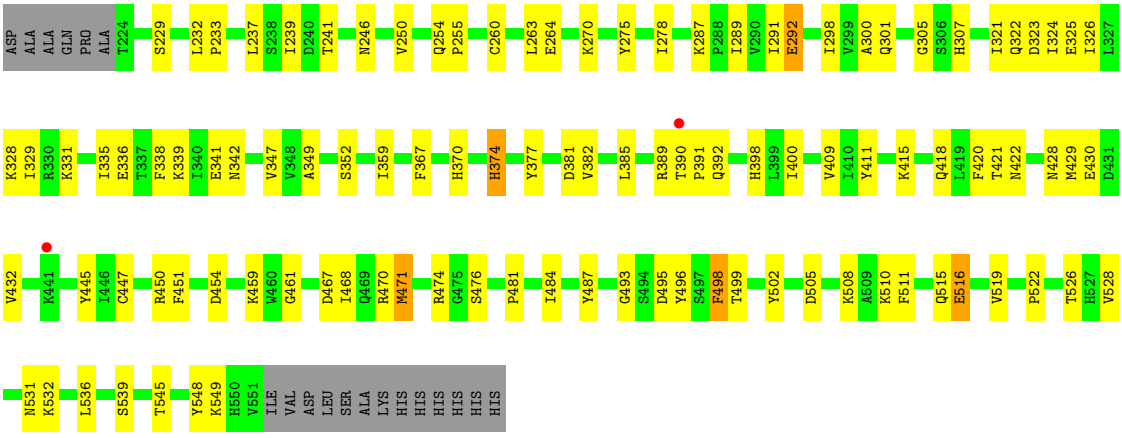
• Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

Chain K:



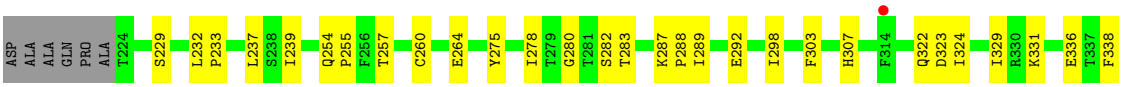
• Molecule 2: Leucine-rich glioma-inactivated protein 1

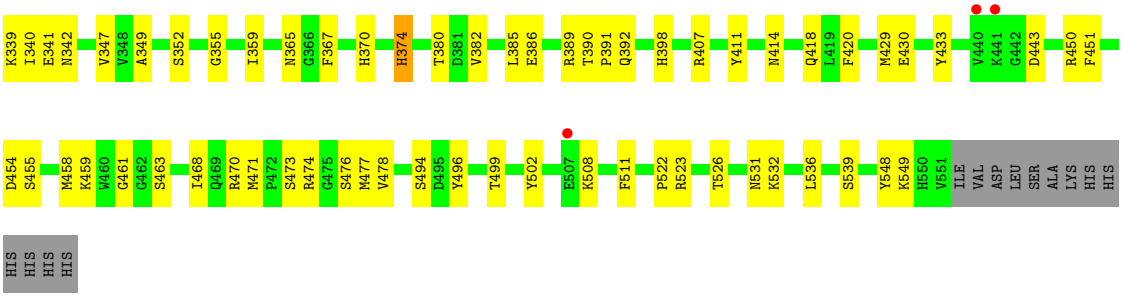
Chain B:



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

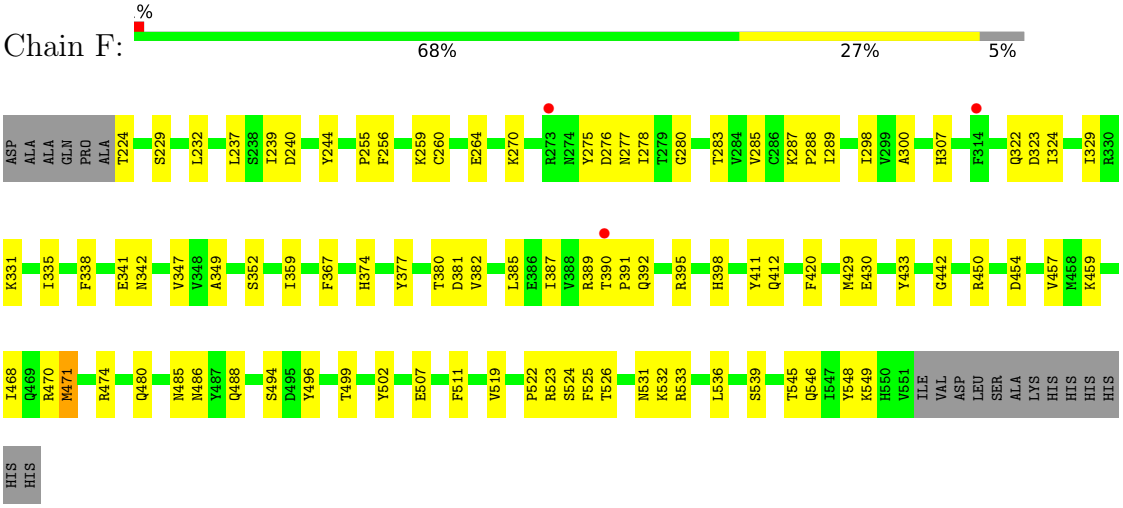
Chain D:





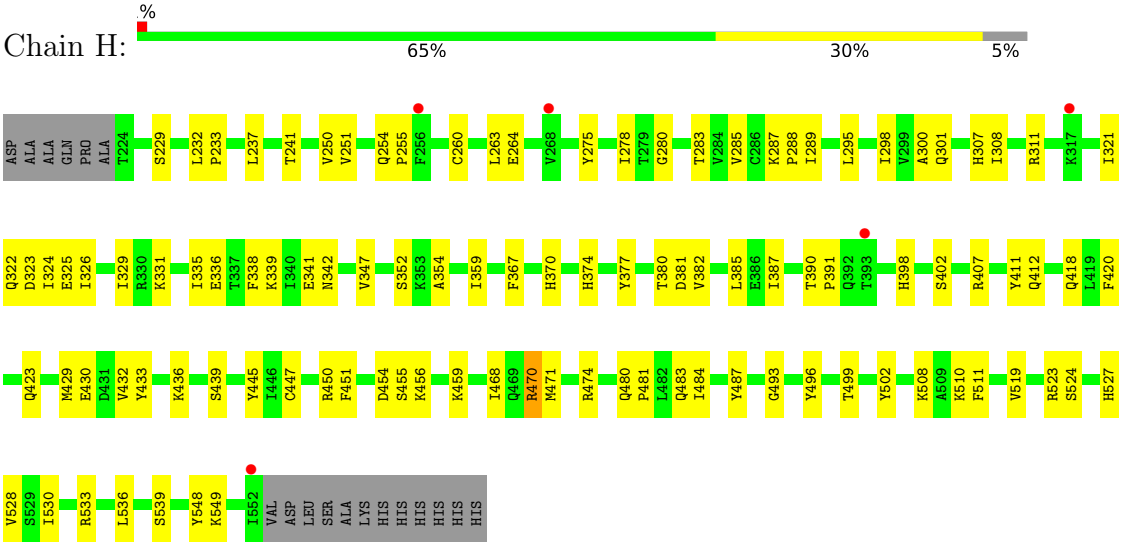
• Molecule 2: Leucine-rich glioma-inactivated protein 1

Chain F:



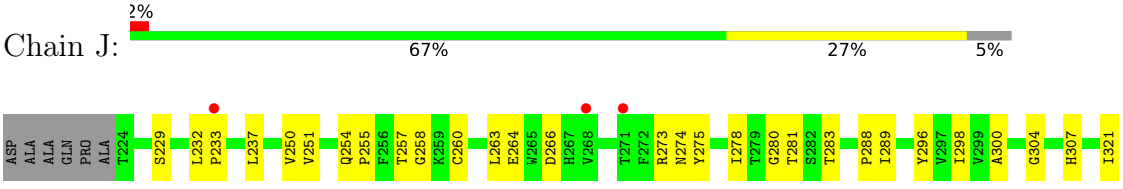
• Molecule 2: Leucine-rich glioma-inactivated protein 1

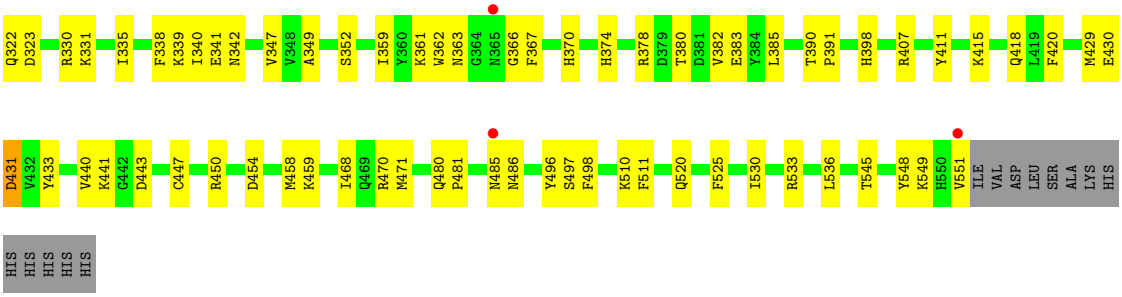
Chain H:



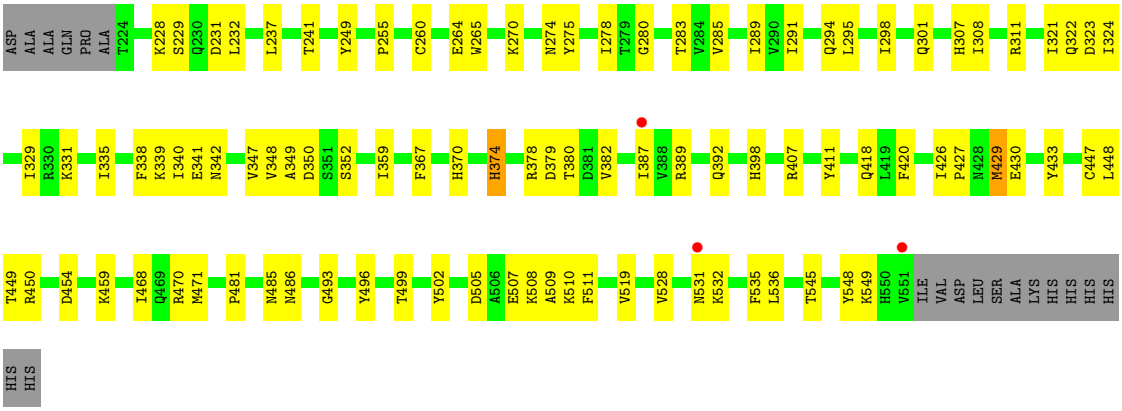
• Molecule 2: Leucine-rich glioma-inactivated protein 1

Chain J:





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



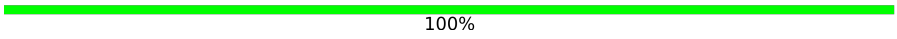
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

• 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 T:

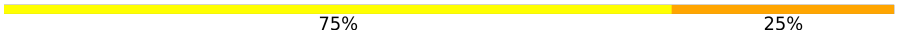


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• 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:

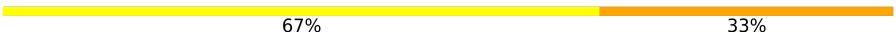


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

• 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:

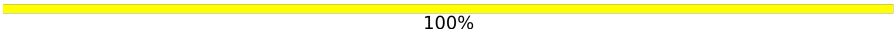


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

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

Chain R:



NAG1
FUC2

4 Data and refinement statistics (i)

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) 90.5 (48.83-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [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 (5.10%)	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 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/3759	0.43	0/5058
1	C	0.30	1/3683 (0.0%)	0.45	0/4955
1	E	0.29	0/3635	0.46	0/4889
1	G	0.27	0/3597	0.43	0/4837
1	I	0.28	0/3751	0.44	0/5049
1	K	0.27	0/3792	0.43	0/5105
2	B	0.44	3/2783 (0.1%)	0.57	5/3775 (0.1%)
2	D	0.29	0/2783	0.45	0/3775
2	F	0.29	0/2783	0.47	0/3775
2	H	0.29	0/2791	0.45	0/3786
2	J	0.29	0/2783	0.47	0/3775
2	L	0.29	0/2783	0.46	0/3775
All	All	0.30	4/38923 (0.0%)	0.46	5/52554 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	516	GLU	CD-OE1	-10.55	1.14	1.25
2	B	498	PHE	CD1-CE1	-7.18	1.24	1.39
2	B	516	GLU	CG-CD	-6.86	1.41	1.51
1	C	514	GLU	CB-CG	6.45	1.64	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	474	ARG	NE-CZ-NH2	-8.95	115.82	120.30
2	B	516	GLU	CG-CD-OE2	8.25	134.80	118.30
2	B	516	GLU	CG-CD-OE1	-7.31	103.69	118.30
2	B	498	PHE	CD1-CE1-CZ	6.08	127.40	120.10
2	B	474	ARG	NE-CZ-NH1	5.29	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3696	0	3548	82	0
1	C	3623	0	3480	79	0
1	E	3575	0	3422	72	0
1	G	3537	0	3387	50	0
1	I	3688	0	3543	67	0
1	K	3728	0	3583	77	0
2	B	2708	0	2635	77	0
2	D	2708	0	2635	68	0
2	F	2708	0	2635	65	0
2	H	2716	0	2646	70	0
2	J	2708	0	2635	66	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	28	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	15	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	822	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 (822) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:253:LYS:NZ	9:G:904:HOH:O	2.01	0.83
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
2:F:457:VAL:HG23	2:F:471:MET:HE1	1.64	0.79
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:253:LYS:NZ	9:K:902:HOH:O	1.92	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
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:A:714:TYR:OH	9:A:908:HOH:O	2.08	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
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:A:704:ARG:NH2	9:A:916:HOH:O	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:532:LYS:NZ	9:D:711:HOH:O	2.22	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: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
2:J:340:ILE:HG22	2:J:341:GLU:HG2	1.75	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:597:ASP:OD2	9:I:907:HOH:O	2.14	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
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
1:G:361:GLY:H	1:G:366:MET:HE2	1.62	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
2:H:445:TYR:HE2	2:H:459:LYS:HZ1	1.44	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
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
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
2:J:266:ASP:CG	2:J:273:ARG:HH12	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
1:K:361:GLY:H	1:K:366:MET:HE2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:361:GLY:H	1:A:366:MET:HE2	1.66	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: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:K:456:GLU:HB2	1:K:477:CYS:HB3	1.85	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:J:254:GLN:OE1	2:J:257:THR:OG1	2.20	0.59
1:A:362:LYS:NZ	9:A:919:HOH:O	2.26	0.59
1:I:361:GLY:H	1:I:366:MET:HE2	1.68	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:D:508:LYS:NZ	9:D:718:HOH:O	2.33	0.58
2:B:510:LYS:NZ	2:B:511:PHE:O	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:429:MET:HE2	2:L:448:LEU:HG	1.87	0.56
2:B:445:TYR:HE2	2:B:459:LYS:HZ1	1.52	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
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: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
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:705:HIS:HD2	1:A:716:PRO:HA	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:454:ASP:N	2:H:454:ASP:OD1	2.38	0.55
1:C:437:LYS:NZ	9:C:919:HOH:O	2.35	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
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: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:361:GLY:H	1:E:366:MET:HE2	1.72	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
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:I:453:GLU:HB3	9:I:917:HOH:O	2.07	0.54
2:D:474:ARG:O	2:D:494:SER:OG	2.25	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:287:LYS:HZ1	2:D:336:GLU:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:K:699:LYS:NZ	9:K:928:HOH:O	2.43	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:A:699:LYS:NZ	9:A:928:HOH:O	2.41	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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:287:LYS:NZ	9:B:713:HOH:O	2.14	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
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
1:K:480:THR:C	9:K:918:HOH:O	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:310:ARG:HB2	1:A:310:ARG:CZ	2.41	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: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
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:643:GLU:HG2	1:C:644:GLU:N	2.28	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:K:558:TRP:CE2	1:K:608:ILE:HD11	2.48	0.48
2:B:447:CYS:SG	2:B:481:PRO:HG3	2.53	0.48
1:I:267:LYS:NZ	9:I:926:HOH:O	2.47	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:429:MET:HE1	2:L:448:LEU:HG	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:I:583:CYS:N	1:I:593:CYS:SG	2.87	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: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:D:429:MET:HE1	2:D:458:MET:SD	2.55	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:333:SER:OG	9:C:912:HOH:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:235:GLU:HG2	9:C:943:HOH:O	2.16	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
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
1:G:242:GLU:OE1	1:G:436:ASN:ND2	2.49	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:337:SER:HB2	9:K:978:HOH:O	2.17	0.45
2:F:519:VAL:HG12	2:F:546:GLN:CD	2.36	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:C:444:PRO:HG3	2:F:496:TYR:CZ	2.52	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
1:C:509:ASP:N	1:C:509:ASP:OD1	2.42	0.45
1:I:310:ARG:CZ	1:I:310:ARG:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:GLY:N	1:G:366:MET:HE2	2.29	0.44
1:G:551:ASP:OD2	1:G:555:LYS:HE2	2.18	0.44
2:B:287:LYS:HZ1	2:B:336:GLU:HA	1.83	0.44
2:F:390:THR:HA	2:F:391:PRO:HA	1.78	0.44
2:J:429:MET:HE1	2:J:458:MET:SD	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:280:GLY:O	2:D:283:THR:HG23	2.17	0.44
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:A:361:GLY:N	1:A:366:MET:HE2	2.32	0.44
1:E:705:HIS:HD2	1:E:717:HIS:H	1.65	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: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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:524:SER:N	2:F:539:SER:HG	2.17	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
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
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: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: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:H:451:PHE:HE2	2:H:496:TYR:HH	1.65	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: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
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:G:287:LEU:HD11	1:G:290:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:285:VAL:HG11	2:H:335:ILE:HB	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
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
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
2:F:531:ASN:O	2:F:532:LYS:HB2	2.20	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
2:F:533:ARG:NH2	2:F:549:LYS:HZ1	2.19	0.41
4:S:1:NAG:H5	4:S:4:FUC:O2	2.20	0.41
1:E:310:ARG:HG2	1:E:314:LYS:HE3	2.03	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:J:258:GLY:HA2	2:J:280:GLY:O	2.20	0.41
2:J:296:TYR:HH	2:J:362:TRP:HH2	1.69	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:K:310:ARG:HH11	1:K:643:GLU:CD	2.24	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:470:ARG:HA	2:B:471:MET:HE2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:495:ASP:C	9:B:722:HOH:O	2.59	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:B:381:ASP:OD1	9:B:716:HOH:O	2.21	0.40
2:D:478:VAL:HG21	2:D:523:ARG:C	2.42	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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/435 (96%)	415 (100%)	1 (0%)	93	98
1	C	409/435 (94%)	406 (99%)	3 (1%)	84	93
1	E	403/435 (93%)	399 (99%)	4 (1%)	76	90
1	G	398/435 (92%)	397 (100%)	1 (0%)	92	97
1	I	416/435 (96%)	414 (100%)	2 (0%)	88	95
1	K	420/435 (97%)	420 (100%)	0	100	100
2	B	300/315 (95%)	296 (99%)	4 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	300/315 (95%)	298 (99%)	2 (1%)	84 93
2	F	300/315 (95%)	296 (99%)	4 (1%)	69 86
2	H	301/315 (96%)	299 (99%)	2 (1%)	84 93
2	J	300/315 (95%)	297 (99%)	3 (1%)	76 90
2	L	300/315 (95%)	294 (98%)	6 (2%)	55 79
All	All	4263/4500 (95%)	4231 (99%)	32 (1%)	81 92

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	LYS
1	C	576	GLU
1	C	714	TYR
1	C	715	PHE
1	E	316	ARG
1	E	460	CYS
1	E	480	THR
1	E	481	GLN
1	G	316	ARG
1	I	316	ARG
1	I	683	LYS
2	B	292	GLU
2	B	374	HIS
2	B	471	MET
2	B	498	PHE
2	D	374	HIS
2	D	471	MET
2	F	374	HIS
2	F	429	MET
2	F	430	GLU
2	F	471	MET
2	H	374	HIS
2	H	470	ARG
2	J	374	HIS
2	J	431	ASP
2	J	471	MET
2	L	374	HIS
2	L	429	MET
2	L	449	THR
2	L	471	MET

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Mol	Chain	Res	Type
2	L	507	GLU
2	L	510	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	334	GLN
1	A	705	HIS
1	C	705	HIS
1	E	247	ASN
1	E	481	GLN
1	E	539	GLN
1	E	705	HIS
1	G	247	ASN
1	G	334	GLN
1	I	247	ASN
1	I	705	HIS
1	K	249	HIS
1	K	574	ASN
1	K	705	HIS
2	B	342	ASN
2	B	406	GLN
2	B	412	GLN
2	B	418	GLN
2	D	406	GLN
2	D	412	GLN
2	D	437	HIS
2	F	342	ASN
2	F	412	GLN
2	F	485	ASN
2	H	301	GLN
2	H	342	ASN
2	H	412	GLN
2	H	418	GLN
2	J	274	ASN
2	J	342	ASN
2	J	406	GLN
2	J	412	GLN
2	J	418	GLN
2	J	437	HIS
2	J	485	ASN

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Mol	Chain	Res	Type
2	L	342	ASN
2	L	406	GLN
2	L	412	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	3,2	14,14,15	0.33	0	17,19,21	0.62	0
3	NAG	M	2	3	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	N	1	4,2	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	0.51	0
4	BMA	N	3	4	11,11,12	1.10	2 (18%)	15,15,17	1.69	4 (26%)
4	FUC	N	4	4	10,10,11	1.20	1 (10%)	14,14,16	1.51	3 (21%)
3	NAG	O	1	3,2	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	O	2	3	14,14,15	0.33	0	17,19,21	0.36	0
5	NAG	P	1	5,2	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	P	2	5	14,14,15	0.57	0	17,19,21	1.40	2 (11%)
5	FUC	P	3	5	10,10,11	1.34	2 (20%)	14,14,16	1.65	1 (7%)
3	NAG	Q	1	3,2	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	Q	2	3	14,14,15	0.31	0	17,19,21	0.41	0
6	NAG	R	1	6,2	14,14,15	0.38	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	FUC	R	2	6	10,10,11	1.54	2 (20%)	14,14,16	2.02	3 (21%)
4	NAG	S	1	4,2	14,14,15	0.63	0	17,19,21	0.81	0
4	NAG	S	2	4	14,14,15	0.88	1 (7%)	17,19,21	0.94	1 (5%)
4	BMA	S	3	4	11,11,12	2.12	4 (36%)	15,15,17	1.62	4 (26%)
4	FUC	S	4	4	10,10,11	1.61	3 (30%)	14,14,16	2.01	4 (28%)
3	NAG	T	1	3,2	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	T	2	3	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	U	1	5,2	14,14,15	0.68	1 (7%)	17,19,21	0.85	1 (5%)
5	NAG	U	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	FUC	U	3	5	10,10,11	2.06	2 (20%)	14,14,16	2.09	4 (28%)
5	NAG	V	1	5,2	14,14,15	0.26	0	17,19,21	0.49	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.54	0
5	FUC	V	3	5	10,10,11	1.38	1 (10%)	14,14,16	2.49	4 (28%)

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	3,2	-	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	3,2	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
5	NAG	P	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	P	2	5	-	3/6/23/26	0/1/1/1
5	FUC	P	3	5	-	-	0/1/1/1
3	NAG	Q	1	3,2	-	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	6,2	-	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
4	BMA	S	3	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	S	4	4	-	-	0/1/1/1
3	NAG	T	1	3,2	-	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	5,2	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	FUC	U	3	5	-	-	0/1/1/1
5	NAG	V	1	5,2	-	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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	3	FUC	O2-C2	5.08	1.54	1.43
4	S	3	BMA	C2-C3	4.75	1.59	1.52
4	S	3	BMA	C1-C2	3.85	1.61	1.52
5	V	3	FUC	C1-C2	3.72	1.60	1.52
4	S	4	FUC	C2-C3	-3.53	1.47	1.52
6	R	2	FUC	C1-C2	3.51	1.60	1.52
6	R	2	FUC	C2-C3	3.14	1.57	1.52
4	N	4	FUC	C1-C2	3.13	1.59	1.52
5	P	3	FUC	C1-C2	3.11	1.59	1.52
4	S	2	NAG	O5-C1	-2.99	1.38	1.43
4	N	3	BMA	C2-C3	2.51	1.56	1.52
5	U	1	NAG	O5-C1	-2.46	1.39	1.43
4	S	3	BMA	O5-C5	-2.44	1.38	1.43
5	P	3	FUC	C2-C3	2.43	1.56	1.52
5	U	3	FUC	C1-C2	2.39	1.57	1.52
4	S	4	FUC	O5-C1	2.34	1.47	1.43
4	N	3	BMA	C1-C2	2.31	1.57	1.52
4	S	3	BMA	C4-C3	2.30	1.58	1.52
4	S	4	FUC	C1-C2	2.07	1.56	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	V	3	FUC	C1-C2-C3	6.79	118.01	109.67
6	R	2	FUC	C1-C2-C3	5.56	116.50	109.67
5	P	3	FUC	C1-C2-C3	4.95	115.75	109.67
5	P	2	NAG	C2-N2-C7	4.49	129.29	122.90
5	U	3	FUC	O2-C2-C1	4.39	118.14	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	2	NAG	C2-N2-C7	4.38	129.14	122.90
4	S	4	FUC	C1-O5-C5	4.04	121.93	112.78
4	S	4	FUC	C1-C2-C3	3.72	114.24	109.67
6	R	2	FUC	O5-C1-C2	3.70	116.48	110.77
5	U	3	FUC	O2-C2-C3	3.65	117.45	110.14
4	S	4	FUC	O5-C1-C2	3.65	116.41	110.77
4	S	3	BMA	C2-C3-C4	3.63	117.17	110.89
4	N	3	BMA	C1-O5-C5	3.53	116.97	112.19
5	V	3	FUC	C1-O5-C5	3.38	120.44	112.78
4	N	4	FUC	C1-O5-C5	3.36	120.40	112.78
4	N	3	BMA	C1-C2-C3	3.29	113.71	109.67
5	V	3	FUC	C2-C3-C4	3.26	116.54	110.89
4	S	3	BMA	O5-C5-C4	-2.81	103.99	110.83
4	S	3	BMA	C1-C2-C3	2.78	113.08	109.67
4	N	3	BMA	O5-C1-C2	2.73	114.98	110.77
6	R	2	FUC	C1-O5-C5	2.68	118.85	112.78
5	U	3	FUC	O5-C5-C4	2.63	114.24	109.52
4	N	4	FUC	O5-C1-C2	2.49	114.62	110.77
4	S	3	BMA	C1-O5-C5	-2.46	108.86	112.19
5	U	1	NAG	C1-O5-C5	-2.40	108.94	112.19
4	S	4	FUC	O5-C5-C4	2.38	113.78	109.52
4	S	2	NAG	O3-C3-C2	-2.37	104.56	109.47
5	U	3	FUC	C1-C2-C3	-2.37	106.76	109.67
5	U	2	NAG	C1-C2-N2	2.30	114.42	110.49
5	V	3	FUC	O5-C1-C2	2.27	114.27	110.77
4	N	3	BMA	O5-C5-C4	-2.15	105.60	110.83
5	U	2	NAG	C1-O5-C5	2.12	115.06	112.19
4	N	4	FUC	C1-C2-C3	2.03	112.16	109.67
5	P	2	NAG	C1-C2-N2	2.03	113.96	110.49

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
4	N	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	R	1	NAG	C4-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
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	P	1	NAG	C4-C5-C6-O6
5	V	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	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C1-C2-N2-C7
3	O	2	NAG	C1-C2-N2-C7
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
4	N	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
5	P	2	NAG	C3-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
5	P	2	NAG	2	0
5	U	2	NAG	1	0
6	R	1	NAG	1	0
4	S	4	FUC	1	0

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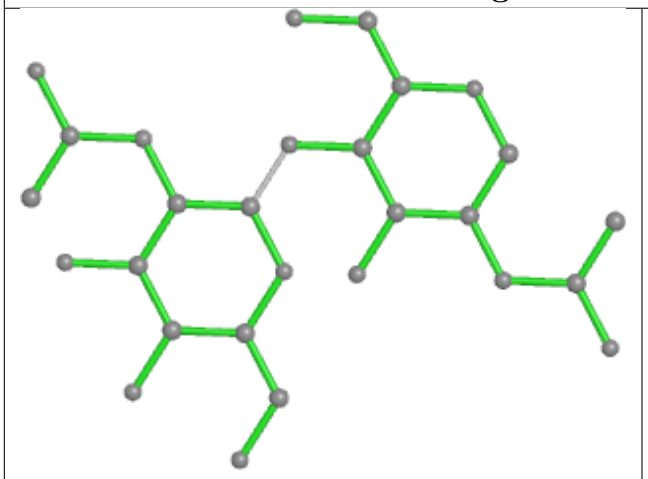
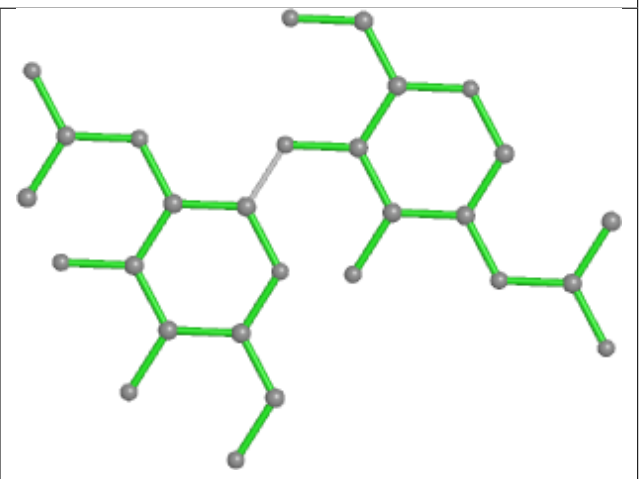
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0
5	P	1	NAG	2	0
3	M	2	NAG	1	0

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

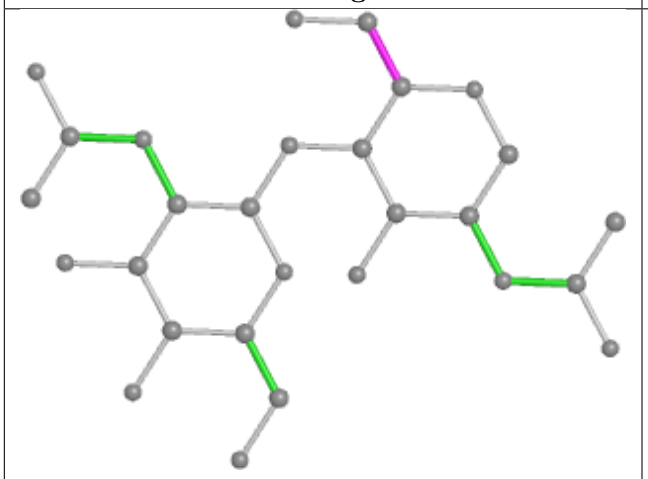
Oligosaccharide Chain M



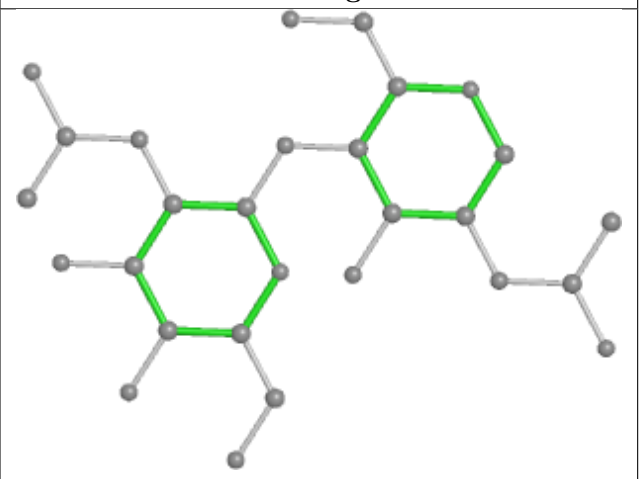
Bond lengths



Bond angles

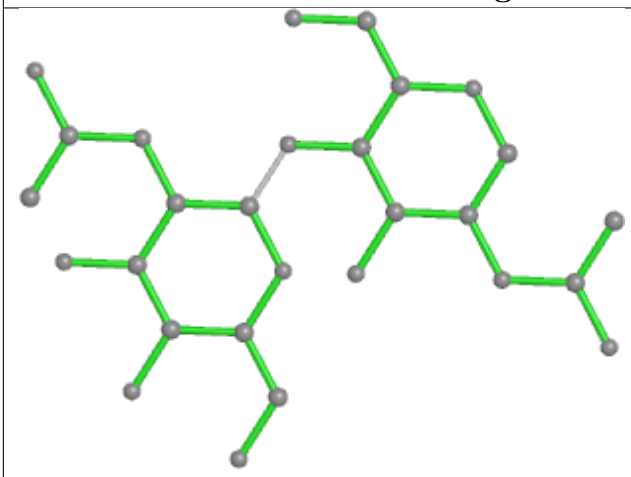


Torsions

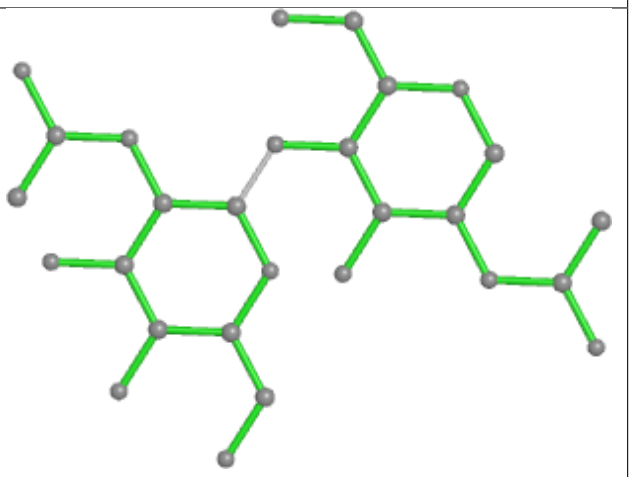


Rings

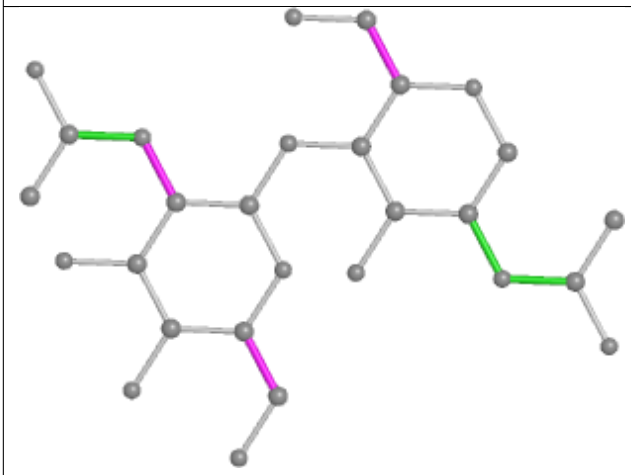
Oligosaccharide Chain O



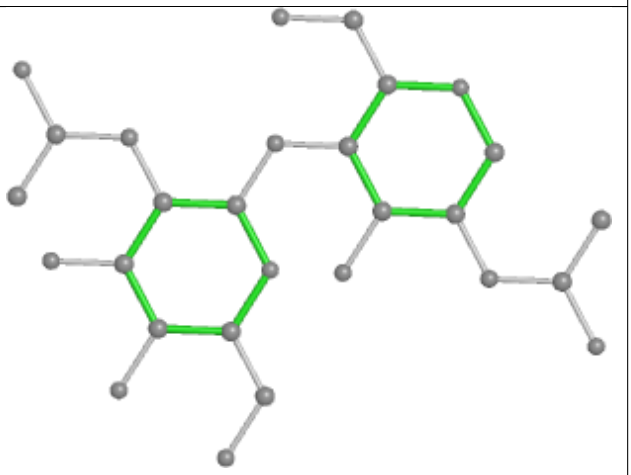
Bond lengths



Bond angles

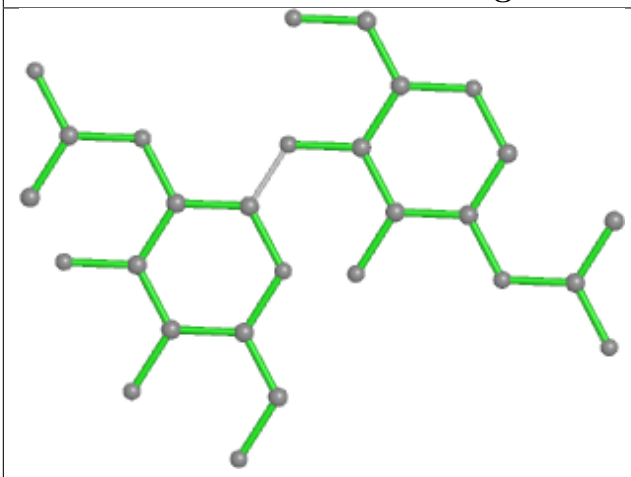


Torsions

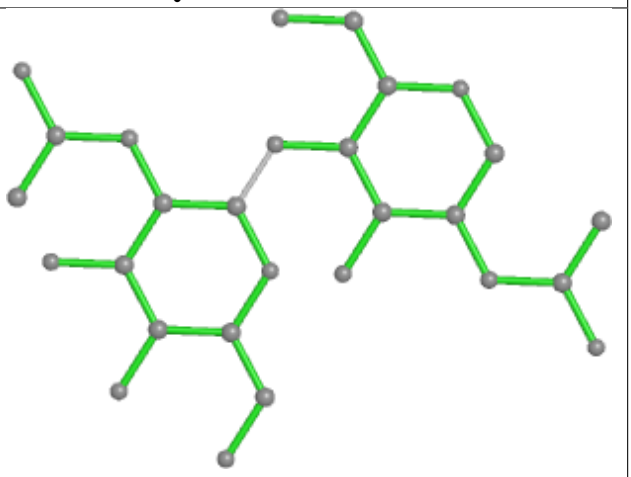


Rings

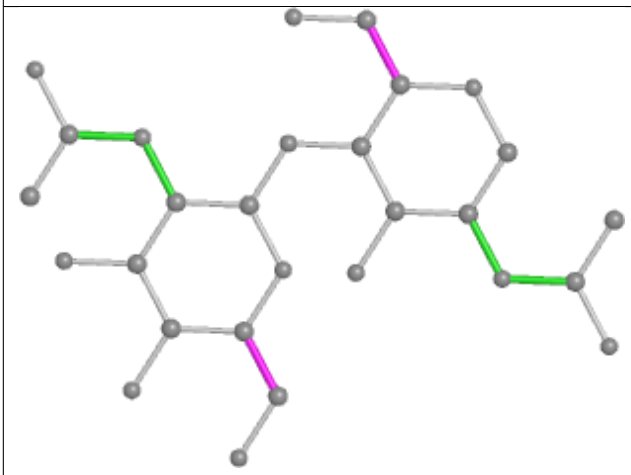
Oligosaccharide Chain Q



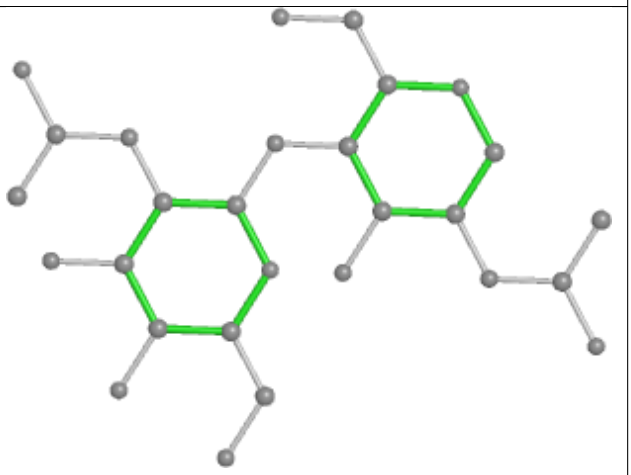
Bond lengths



Bond angles

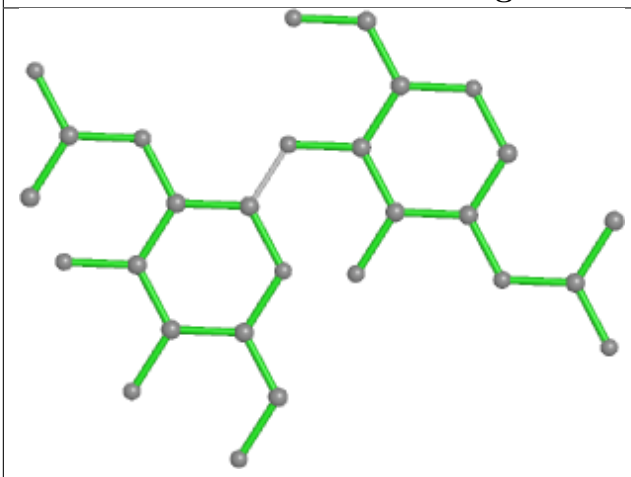


Torsions

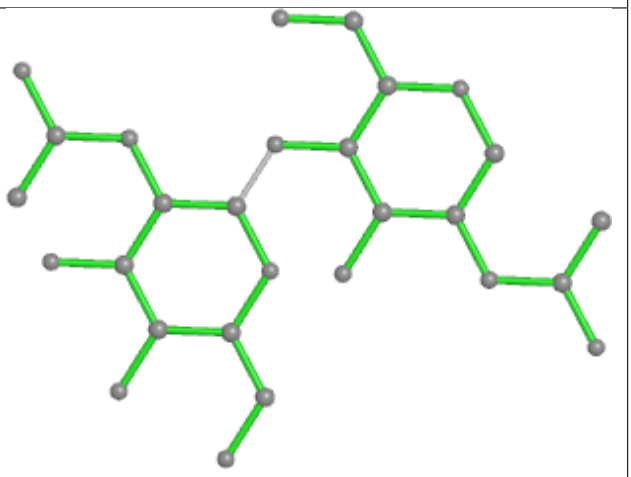


Rings

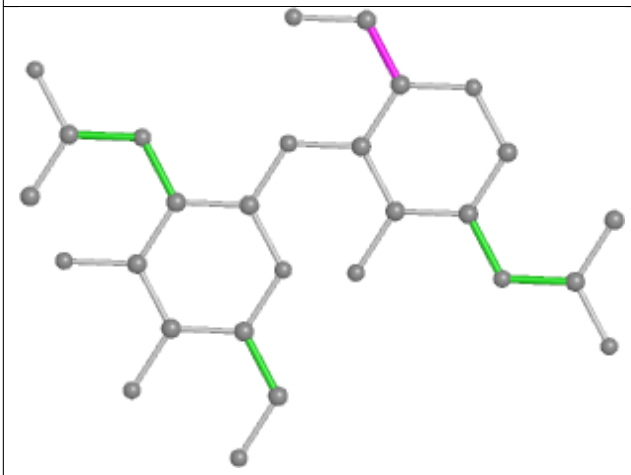
Oligosaccharide Chain T



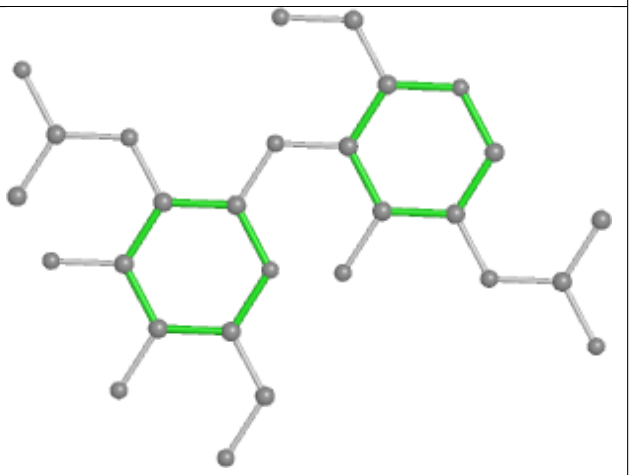
Bond lengths



Bond angles

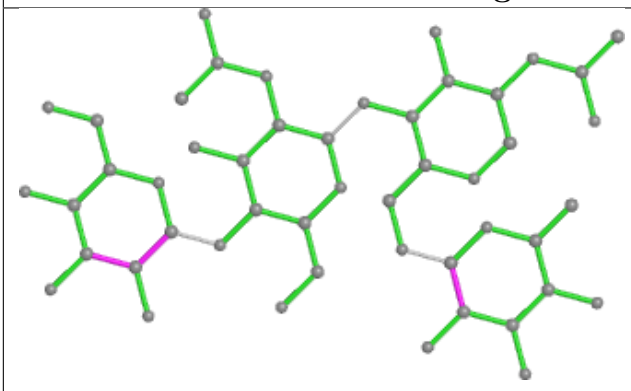


Torsions

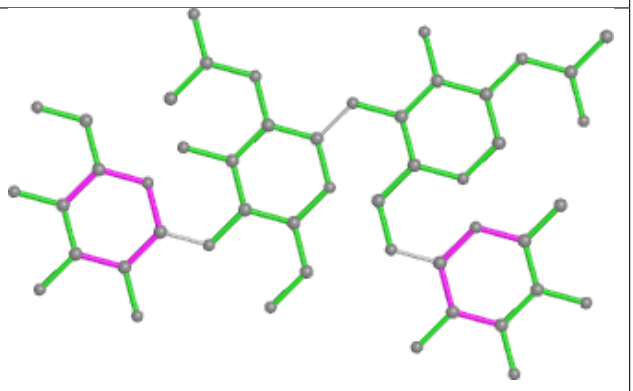


Rings

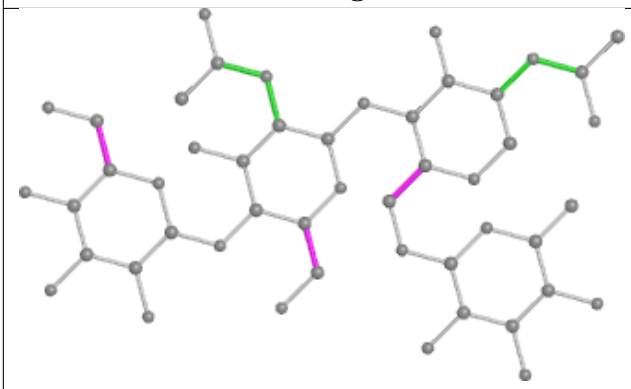
Oligosaccharide Chain N



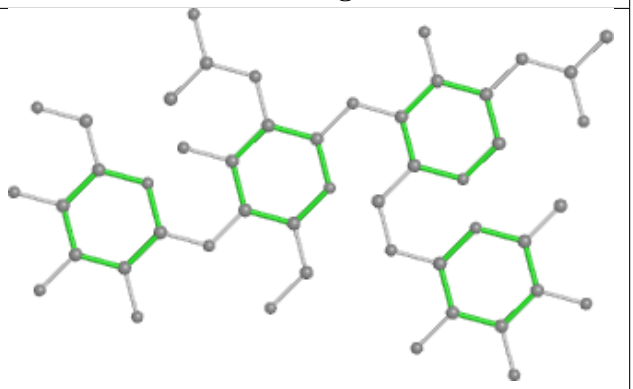
Bond lengths



Bond angles

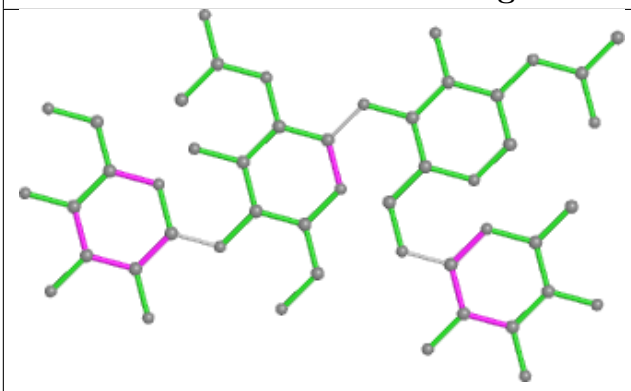


Torsions

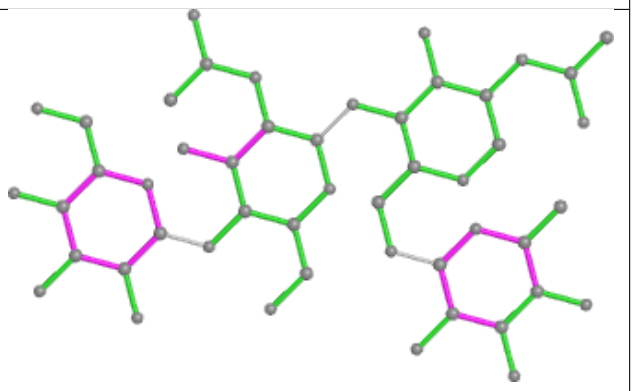


Rings

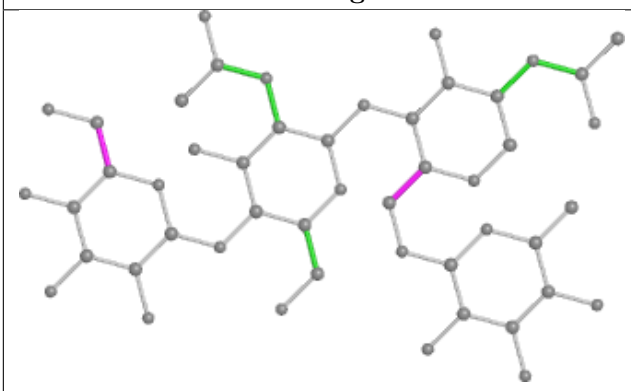
Oligosaccharide Chain S



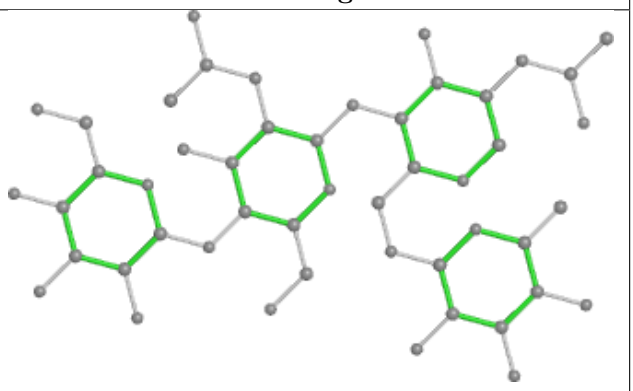
Bond lengths



Bond angles

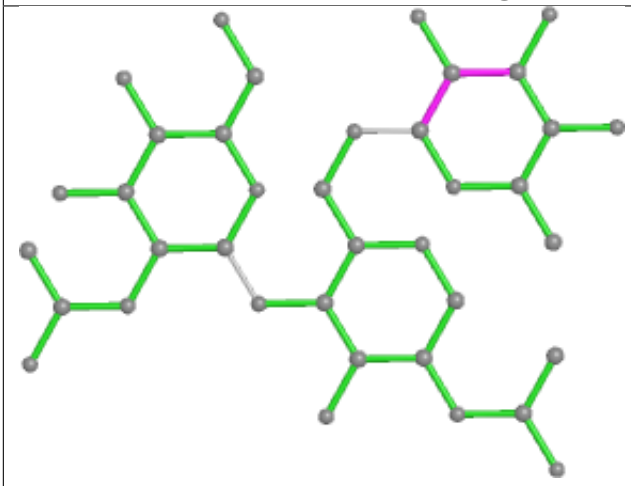


Torsions

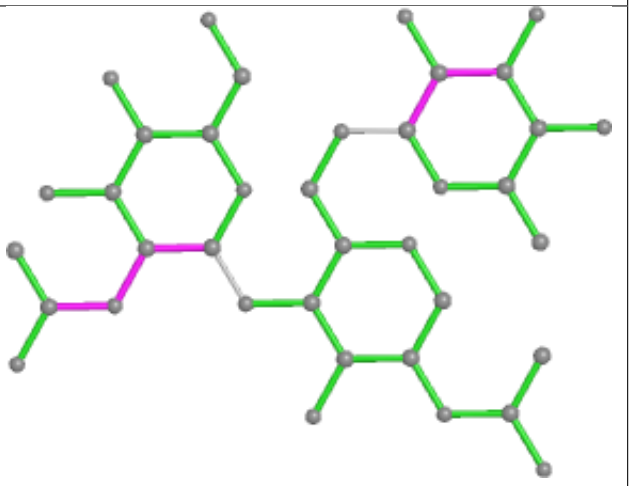


Rings

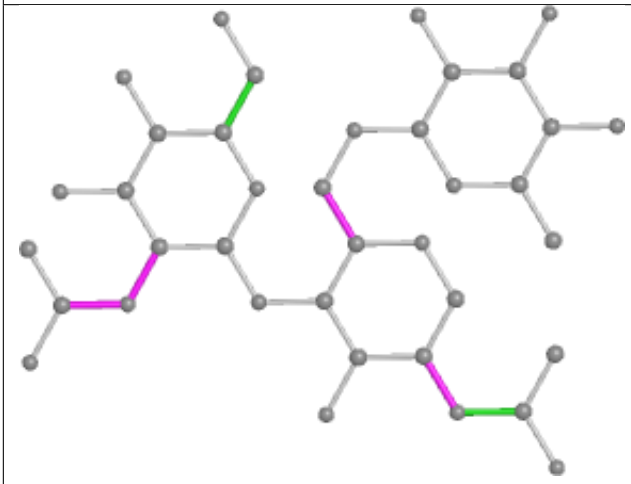
Oligosaccharide Chain P



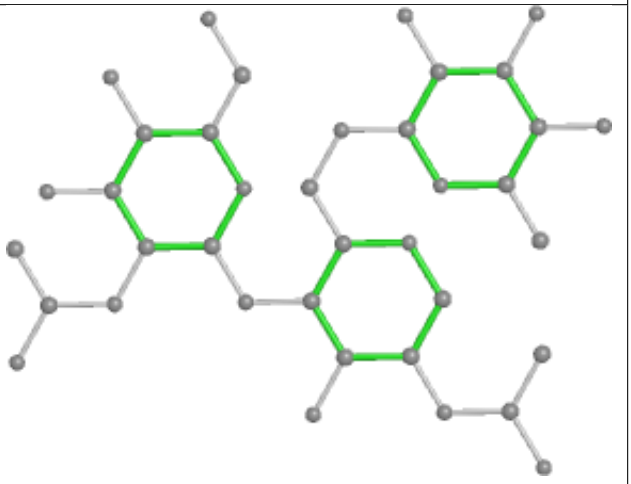
Bond lengths



Bond angles

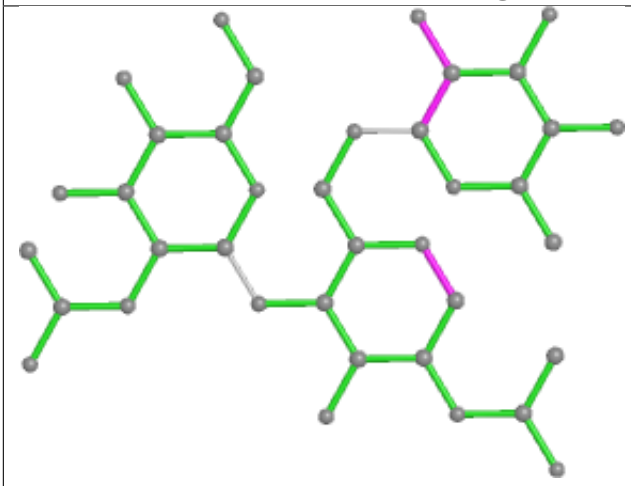


Torsions

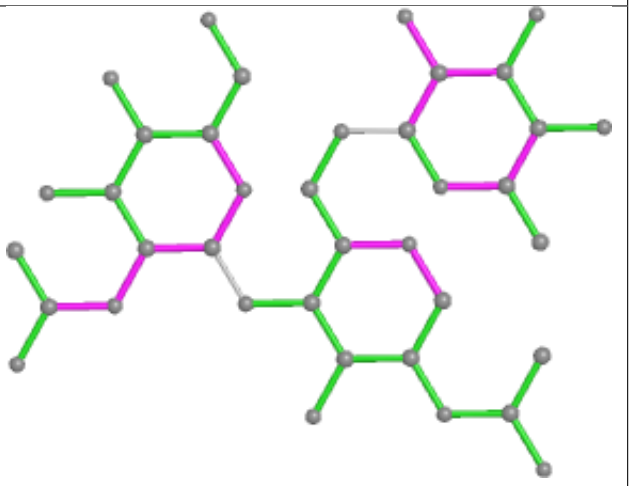


Rings

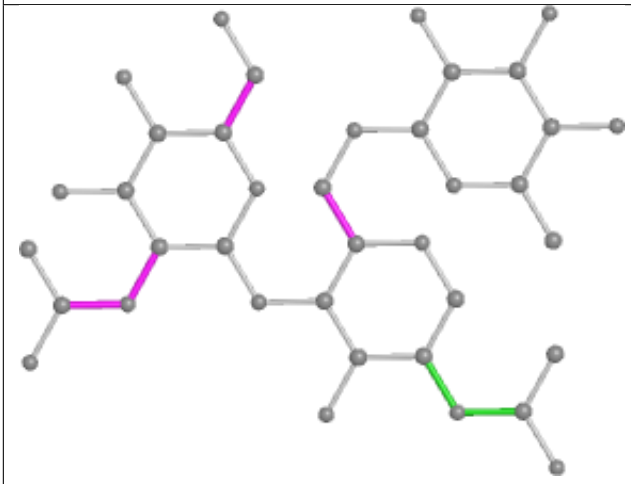
Oligosaccharide Chain U



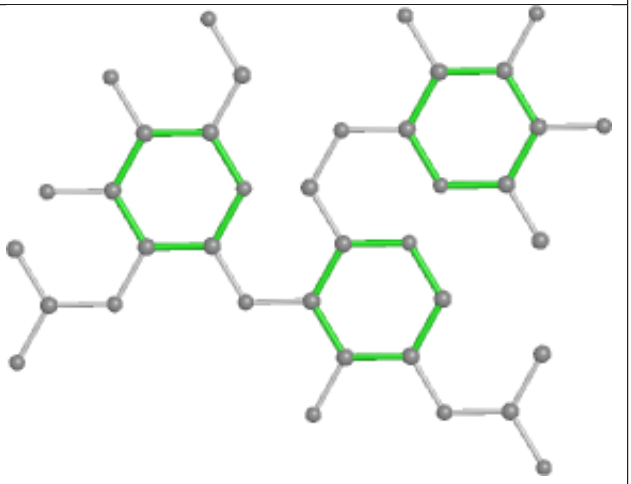
Bond lengths



Bond angles

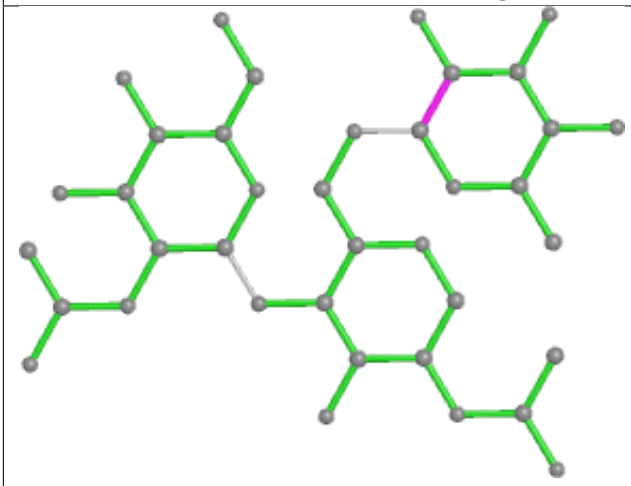


Torsions

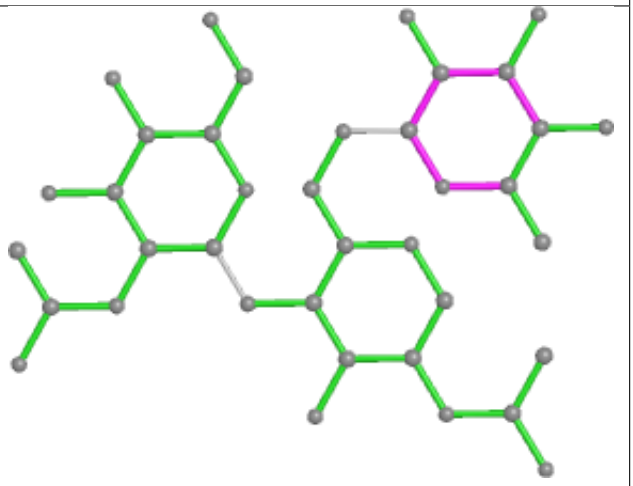


Rings

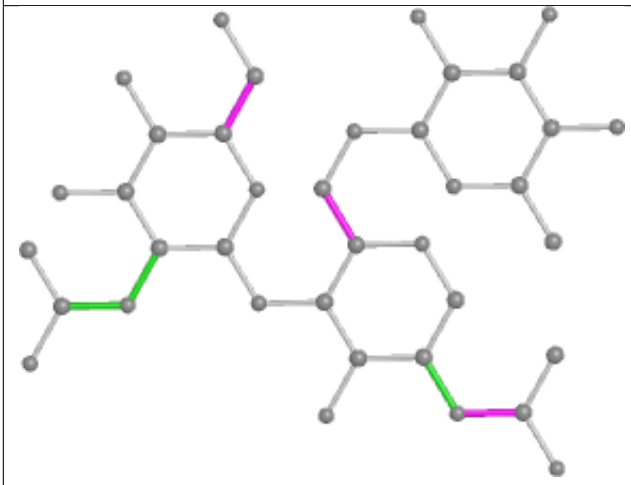
Oligosaccharide Chain V



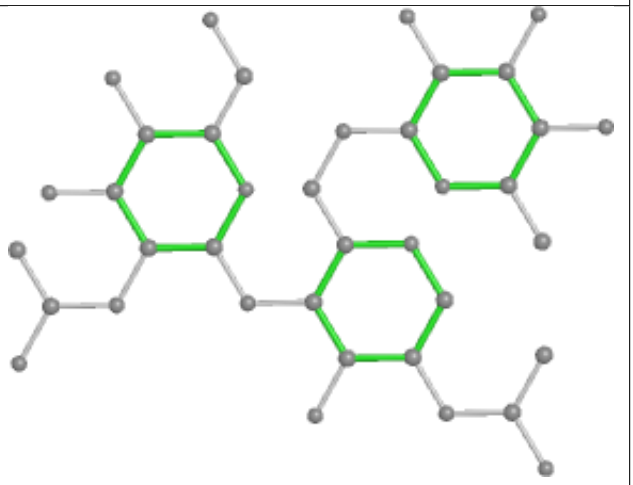
Bond lengths



Bond angles

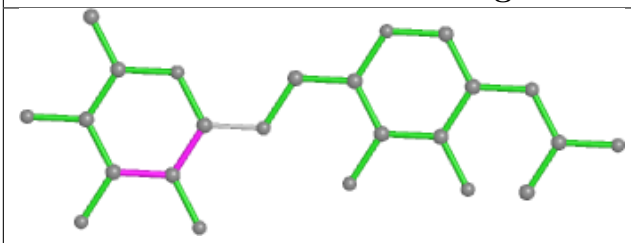


Torsions

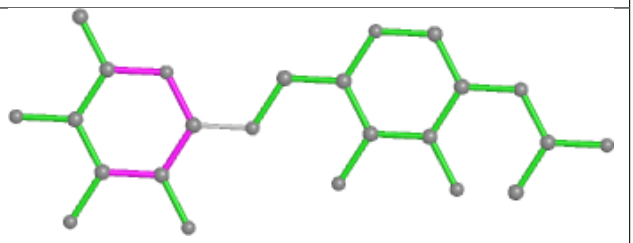


Rings

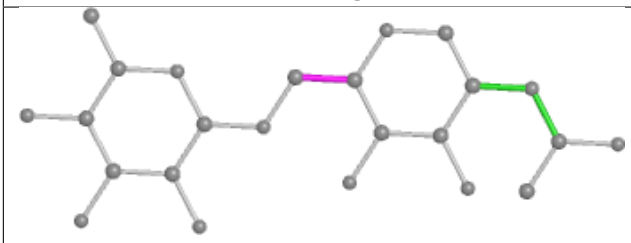
Oligosaccharide Chain R



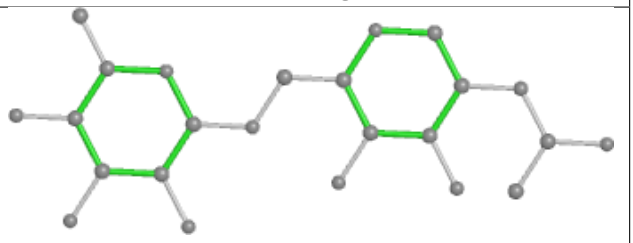
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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	0.23	0	17,19,21	0.37	0
8	NAG	H	602	2	14,14,15	0.39	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	482/504 (95%)	0.25	28 (5%) 23 21	19, 43, 89, 112	0
1	C	473/504 (93%)	0.56	59 (12%) 3 3	18, 50, 110, 133	0
1	E	467/504 (92%)	0.46	41 (8%) 10 8	18, 49, 100, 123	0
1	G	462/504 (91%)	0.56	56 (12%) 4 3	22, 51, 98, 134	0
1	I	481/504 (95%)	0.40	37 (7%) 13 11	21, 46, 92, 112	0
1	K	486/504 (96%)	0.48	57 (11%) 4 3	20, 51, 104, 137	0
2	B	328/347 (94%)	0.02	2 (0%) 89 90	21, 39, 59, 76	0
2	D	328/347 (94%)	0.08	4 (1%) 79 79	23, 38, 59, 75	0
2	F	328/347 (94%)	-0.01	3 (0%) 84 85	21, 38, 58, 87	0
2	H	329/347 (94%)	0.11	5 (1%) 73 74	22, 40, 69, 88	0
2	J	328/347 (94%)	0.15	6 (1%) 68 69	26, 42, 71, 86	0
2	L	328/347 (94%)	0.09	3 (0%) 84 85	22, 41, 68, 91	0
All	All	4820/5106 (94%)	0.30	301 (6%) 20 18	18, 43, 93, 137	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	568	TYR	8.2
1	G	637	GLY	7.9
1	E	568	TYR	7.9
1	K	626	VAL	7.5
1	I	633	LEU	7.3
1	G	578	THR	7.2
1	G	568	TYR	7.0
1	K	633	LEU	6.8
1	A	632	THR	6.7
1	C	624	THR	6.6
1	E	593	CYS	6.5

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Mol	Chain	Res	Type	RSRZ
1	C	626	VAL	6.2
1	G	593	CYS	6.2
1	C	572	LYS	5.8
1	C	636	SER	5.6
1	G	596	ARG	5.6
1	A	568	TYR	5.5
1	E	650	TYR	5.5
1	K	568	TYR	5.4
1	G	664	LEU	5.4
1	C	593	CYS	5.3
1	K	627	VAL	5.2
1	A	625	LEU	5.2
1	A	633	LEU	5.2
1	C	672	ALA	5.1
1	A	624	THR	5.1
1	I	588	ASP	4.9
1	K	571	GLU	4.9
1	E	572	LYS	4.8
1	C	625	LEU	4.7
1	G	570	TYR	4.7
1	C	637	GLY	4.7
1	C	571	GLU	4.6
1	I	482	ASP	4.6
1	G	608	ILE	4.5
1	G	636	SER	4.4
1	C	623	SER	4.4
1	K	608	ILE	4.3
1	C	475	LYS	4.3
1	G	468	LEU	4.2
1	K	628	GLN	4.2
1	G	482	ASP	4.2
1	A	572	LYS	4.2
1	E	481	GLN	4.2
1	C	595	LYS	4.1
1	E	594	ASN	4.1
1	G	572	LYS	4.1
1	I	620	GLU	4.0
1	C	671	VAL	4.0
1	G	650	TYR	4.0
1	C	596	ARG	4.0
1	C	650	TYR	4.0
1	K	638	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	621	ILE	4.0
1	E	571	GLU	4.0
1	I	585	LYS	4.0
1	E	608	ILE	3.9
1	K	637	GLY	3.9
1	I	568	TYR	3.9
1	K	590	TRP	3.9
1	A	578	THR	3.8
1	E	637	GLY	3.8
1	K	624	THR	3.8
1	G	565	SER	3.8
1	C	468	LEU	3.7
1	G	481	GLN	3.7
1	C	482	ASP	3.7
1	K	592	GLN	3.7
1	I	591	ILE	3.7
1	E	664	LEU	3.6
1	C	570	TYR	3.6
1	K	671	VAL	3.6
1	G	651	VAL	3.6
1	C	578	THR	3.6
1	I	464	ALA	3.6
1	C	620	GLU	3.6
1	E	596	ARG	3.6
1	K	632	THR	3.5
1	K	570	TYR	3.4
1	C	632	THR	3.4
1	K	664	LEU	3.4
1	K	572	LYS	3.4
1	K	678	THR	3.4
1	E	671	VAL	3.4
1	C	464	ALA	3.4
1	I	493	LYS	3.3
1	E	483	SER	3.3
1	K	596	ARG	3.3
1	K	578	THR	3.3
1	I	590	TRP	3.3
1	E	578	THR	3.3
1	C	565	SER	3.3
1	G	648	LEU	3.3
2	D	507	GLU	3.2
1	C	633	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	675	ASN	3.2
1	A	482	ASP	3.2
1	G	579	GLU	3.2
1	A	571	GLU	3.2
1	C	678	THR	3.2
1	E	707	ILE	3.2
1	I	475	LYS	3.2
1	E	646	VAL	3.1
1	I	624	THR	3.1
1	G	667	ARG	3.1
1	G	600	CYS	3.1
1	G	475	LYS	3.1
1	G	646	VAL	3.1
1	K	482	ASP	3.1
1	K	705	HIS	3.1
1	I	584	GLY	3.1
1	C	646	VAL	3.1
1	G	607	ASN	3.1
1	K	599	LEU	3.1
1	G	594	ASN	3.1
1	G	582	ASN	3.0
1	I	563	THR	3.0
1	A	296	ASP	3.0
1	C	618	ASP	3.0
1	G	681	SER	3.0
1	K	623	SER	3.0
1	C	493	LYS	3.0
1	K	588	ASP	2.9
1	G	671	VAL	2.9
1	E	475	LYS	2.9
1	K	579	GLU	2.9
1	A	591	ILE	2.9
2	H	256	PHE	2.9
1	I	606	THR	2.9
1	E	565	SER	2.9
1	C	608	ILE	2.9
1	K	636	SER	2.9
1	C	599	LEU	2.9
1	K	479	LEU	2.9
1	I	626	VAL	2.9
2	J	268	VAL	2.9
1	E	717	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	660	GLN	2.8
1	C	707	ILE	2.8
1	G	599	LEU	2.8
1	G	296	ASP	2.8
1	K	585	LYS	2.8
1	A	620	GLU	2.8
1	C	579	GLU	2.8
1	A	479	LEU	2.8
1	G	715	PHE	2.8
1	E	607	ASN	2.8
1	C	576	GLU	2.8
1	I	571	GLU	2.8
1	A	588	ASP	2.7
1	I	647	ASP	2.7
1	K	565	SER	2.7
1	G	483	SER	2.7
1	G	519	ASN	2.7
1	G	716	PRO	2.7
1	E	611	ILE	2.7
1	G	714	TYR	2.7
1	K	461	GLY	2.6
1	C	607	ASN	2.6
1	I	599	LEU	2.6
1	K	475	LYS	2.6
1	C	483	SER	2.6
1	K	519	ASN	2.6
1	I	621	ILE	2.6
2	L	551	VAL	2.6
1	C	476	LYS	2.6
1	E	606	THR	2.6
1	G	393	LYS	2.6
1	K	629	GLN	2.6
1	C	580	LYS	2.6
1	I	608	ILE	2.6
1	G	660	GLN	2.6
1	I	592	GLN	2.6
1	E	645	ASP	2.6
1	E	620	GLU	2.6
1	K	562	VAL	2.6
1	G	641	LYS	2.6
1	K	639	HIS	2.6
1	K	645	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	678	THR	2.5
1	G	467	VAL	2.5
1	G	680	LEU	2.5
1	C	519	ASN	2.5
1	G	647	ASP	2.5
1	I	645	ASP	2.5
1	A	596	ARG	2.5
1	A	593	CYS	2.5
1	C	665	GLU	2.5
1	E	388	ALA	2.5
1	I	390	GLY	2.5
1	C	594	ASN	2.5
1	G	675	ASN	2.5
1	E	599	LEU	2.5
1	K	583	CYS	2.5
1	A	623	SER	2.5
1	G	388	ALA	2.5
1	C	296	ASP	2.5
1	K	620	GLU	2.4
1	C	393	LYS	2.4
1	G	707	ILE	2.4
1	I	467	VAL	2.4
1	G	571	GLU	2.4
1	E	660	GLN	2.4
1	E	706	TRP	2.4
1	G	683	LYS	2.4
1	I	481	GLN	2.4
1	I	637	GLY	2.4
1	K	650	TYR	2.4
1	K	593	CYS	2.4
1	G	614	LEU	2.4
1	K	589	THR	2.4
1	I	622	THR	2.4
1	K	591	ILE	2.4
2	J	551	VAL	2.4
1	K	465	GLU	2.4
2	H	317	LYS	2.3
1	C	651	VAL	2.3
1	K	647	ASP	2.3
1	C	622	THR	2.3
1	C	654	GLY	2.3
1	C	713	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	590	TRP	2.3
1	A	585	LYS	2.3
2	L	387	ILE	2.3
1	I	572	LYS	2.3
2	D	440	VAL	2.3
1	G	659	PRO	2.3
1	I	468	LEU	2.3
1	K	584	GLY	2.3
1	K	594	ASN	2.3
2	B	390	THR	2.3
1	G	575	ILE	2.3
1	C	561	LYS	2.3
1	C	603	LEU	2.3
1	E	524	ALA	2.3
1	G	672	ALA	2.3
2	H	393	THR	2.3
1	C	600	CYS	2.3
1	E	467	VAL	2.3
1	E	638	GLY	2.2
1	G	496	PHE	2.2
1	C	660	GLN	2.2
1	I	381	ILE	2.2
1	A	634	ASN	2.2
1	A	717	HIS	2.2
2	H	552	ILE	2.2
1	A	579	GLU	2.2
1	E	616	GLU	2.2
1	K	563	THR	2.2
1	C	714	TYR	2.2
1	G	567	LYS	2.2
2	F	314	PHE	2.2
1	G	718	ASN	2.2
1	C	717	HIS	2.2
1	E	603	LEU	2.2
2	J	271	THR	2.2
1	A	483	SER	2.1
2	D	441	LYS	2.1
2	J	365	ASN	2.1
1	E	621	ILE	2.1
1	E	666	HIS	2.1
1	K	648	LEU	2.1
2	J	233	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	464	ALA	2.1
1	C	662	MET	2.1
1	K	718	ASN	2.1
2	L	531	ASN	2.1
1	A	650	TYR	2.1
1	K	656	PRO	2.1
2	B	441	LYS	2.1
2	D	314	PHE	2.1
1	E	595	LYS	2.1
1	I	627	VAL	2.1
1	K	577	GLY	2.1
1	A	481	GLN	2.1
1	G	662	MET	2.1
1	E	667	ARG	2.1
2	F	273	ARG	2.1
1	G	717	HIS	2.1
1	I	575	ILE	2.1
1	K	634	ASN	2.1
1	E	482	ASP	2.1
1	I	638	GLY	2.1
1	G	643	GLU	2.1
1	E	622	THR	2.1
2	J	485	ASN	2.1
1	A	664	LEU	2.1
1	E	635	CYS	2.1
1	C	708	GLY	2.1
1	G	476	LYS	2.0
1	K	603	LEU	2.0
2	H	268	VAL	2.0
1	C	675	ASN	2.0
1	I	578	THR	2.0
1	A	468	LEU	2.0
1	C	575	ILE	2.0
1	K	602	TYR	2.0
2	F	390	THR	2.0
1	I	717	HIS	2.0
1	C	567	LYS	2.0
1	C	659	PRO	2.0

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

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

6.3 Carbohydrates (i)

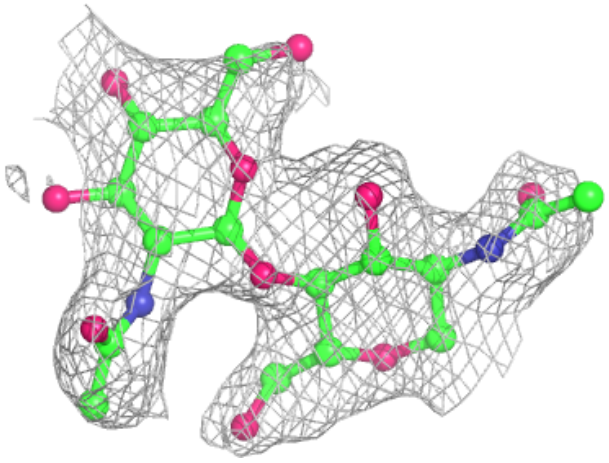
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

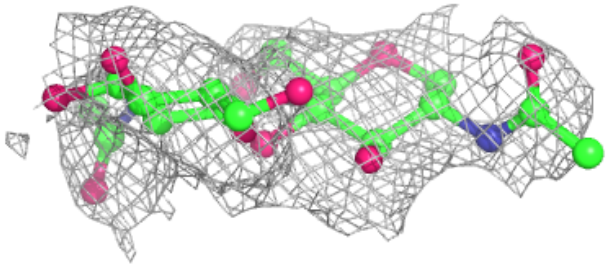
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	N	3	11/12	0.47	0.25	98,102,107,110	0
4	BMA	S	3	11/12	0.69	0.26	81,105,123,131	0
5	NAG	U	2	14/15	0.70	0.27	74,90,95,96	0
3	NAG	T	2	14/15	0.76	0.36	73,85,91,97	0
5	NAG	P	2	14/15	0.81	0.39	79,86,90,91	0
3	NAG	T	1	14/15	0.81	0.28	60,70,77,83	0
3	NAG	Q	2	14/15	0.82	0.33	71,75,80,80	0
3	NAG	M	2	14/15	0.83	0.29	73,84,85,87	0
4	NAG	N	2	14/15	0.83	0.31	80,90,102,103	0
4	NAG	S	2	14/15	0.84	0.26	62,73,87,107	0
3	NAG	O	2	14/15	0.85	0.35	78,85,89,90	0
5	FUC	U	3	10/11	0.85	0.25	58,76,79,80	0
3	NAG	M	1	14/15	0.86	0.25	56,67,72,75	0
4	NAG	S	1	14/15	0.87	0.16	49,55,67,70	0
4	FUC	N	4	10/11	0.87	0.25	72,77,81,82	0
5	FUC	P	3	10/11	0.89	0.23	70,82,89,90	0
5	FUC	V	3	10/11	0.89	0.23	59,65,66,66	0
6	NAG	R	1	14/15	0.89	0.14	51,64,71,75	0
5	NAG	U	1	14/15	0.90	0.17	54,62,72,81	0
6	FUC	R	2	10/11	0.90	0.16	58,77,80,80	0
3	NAG	O	1	14/15	0.91	0.19	50,64,71,74	0
5	NAG	P	1	14/15	0.92	0.15	60,67,72,74	0
3	NAG	Q	1	14/15	0.92	0.18	50,60,65,66	0
5	NAG	V	2	14/15	0.92	0.17	55,63,67,68	0
4	NAG	N	1	14/15	0.94	0.12	54,62,71,80	0
5	NAG	V	1	14/15	0.94	0.10	40,48,57,64	0
4	FUC	S	4	10/11	0.95	0.19	56,64,71,73	0

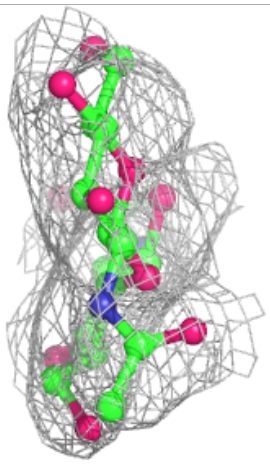
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

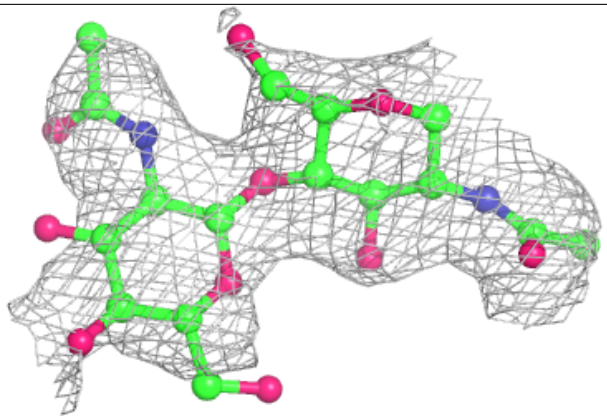


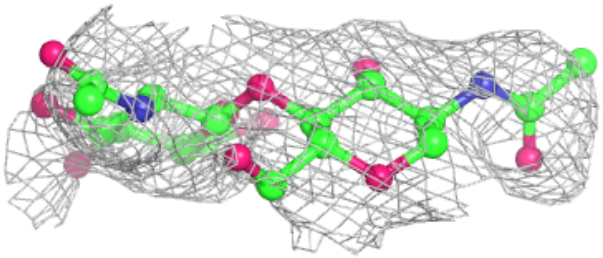


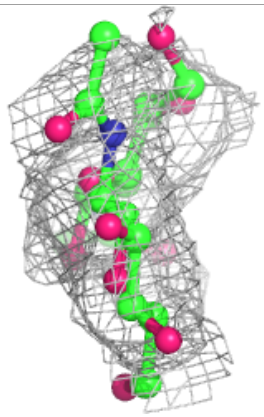


Electron density around Chain O:

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

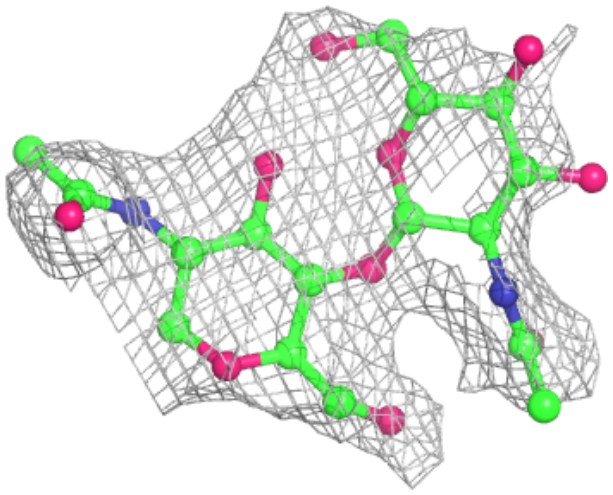


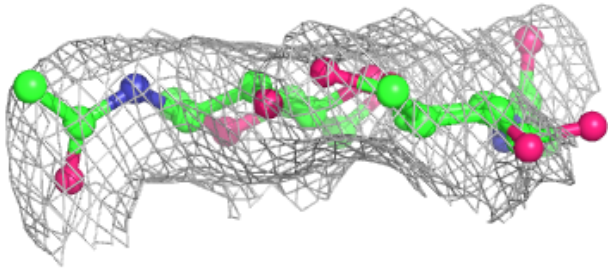


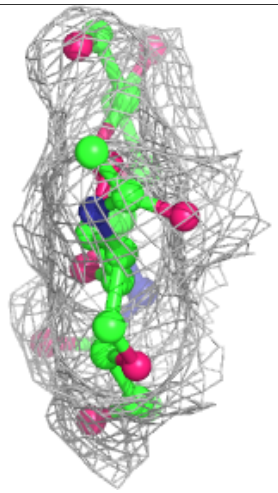


Electron density around Chain Q:

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

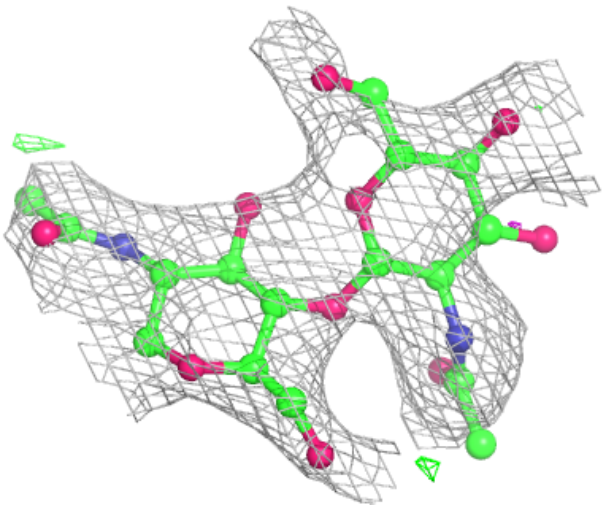


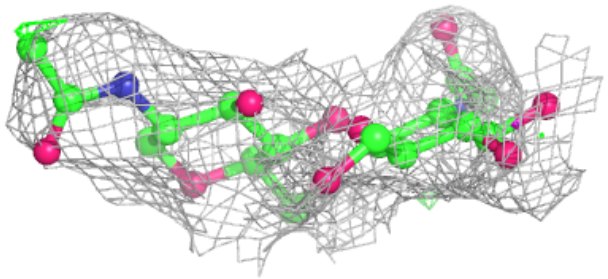


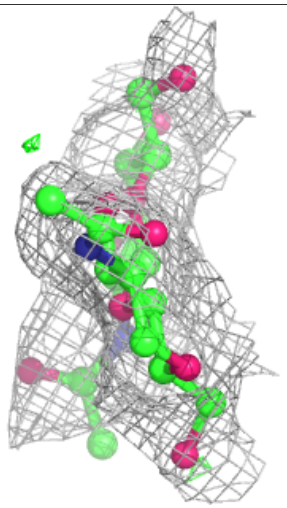


Electron density around Chain T:

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

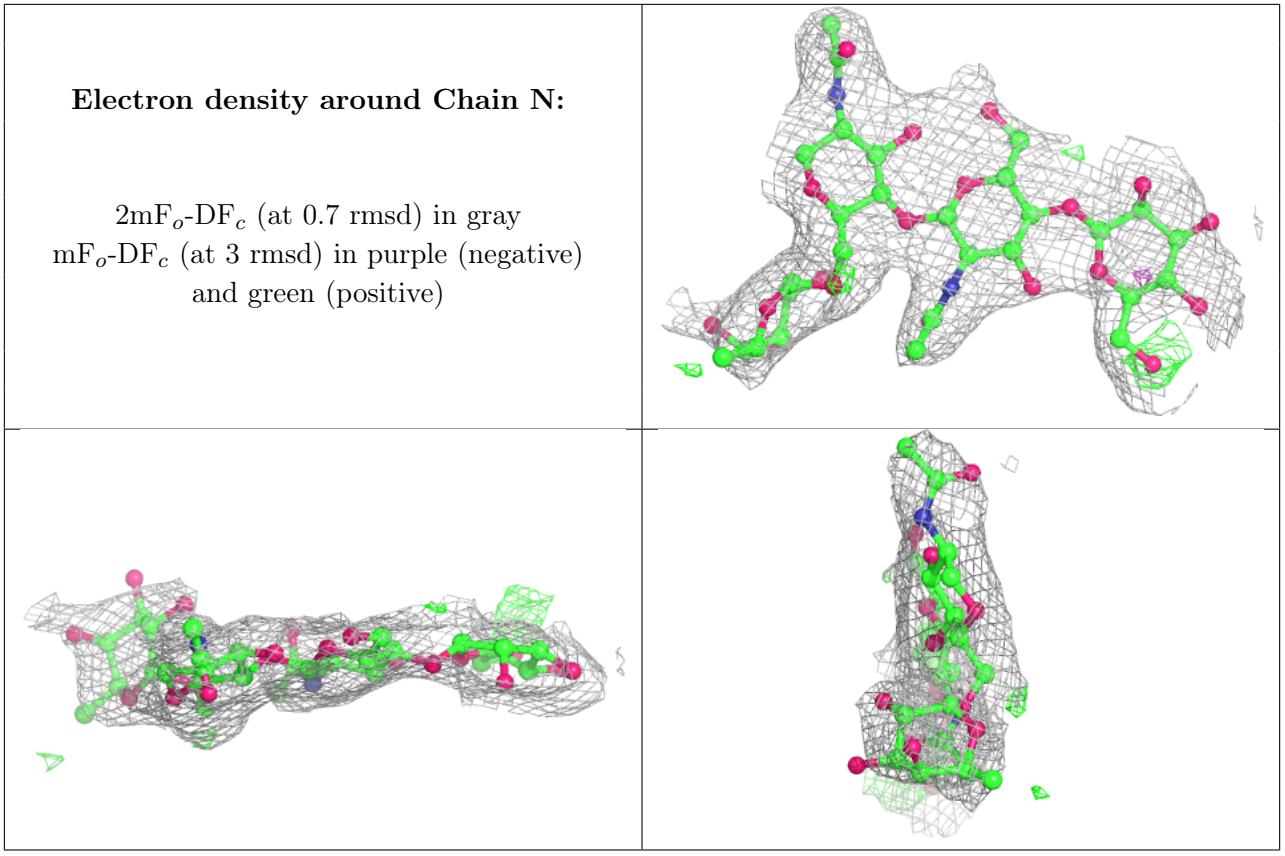






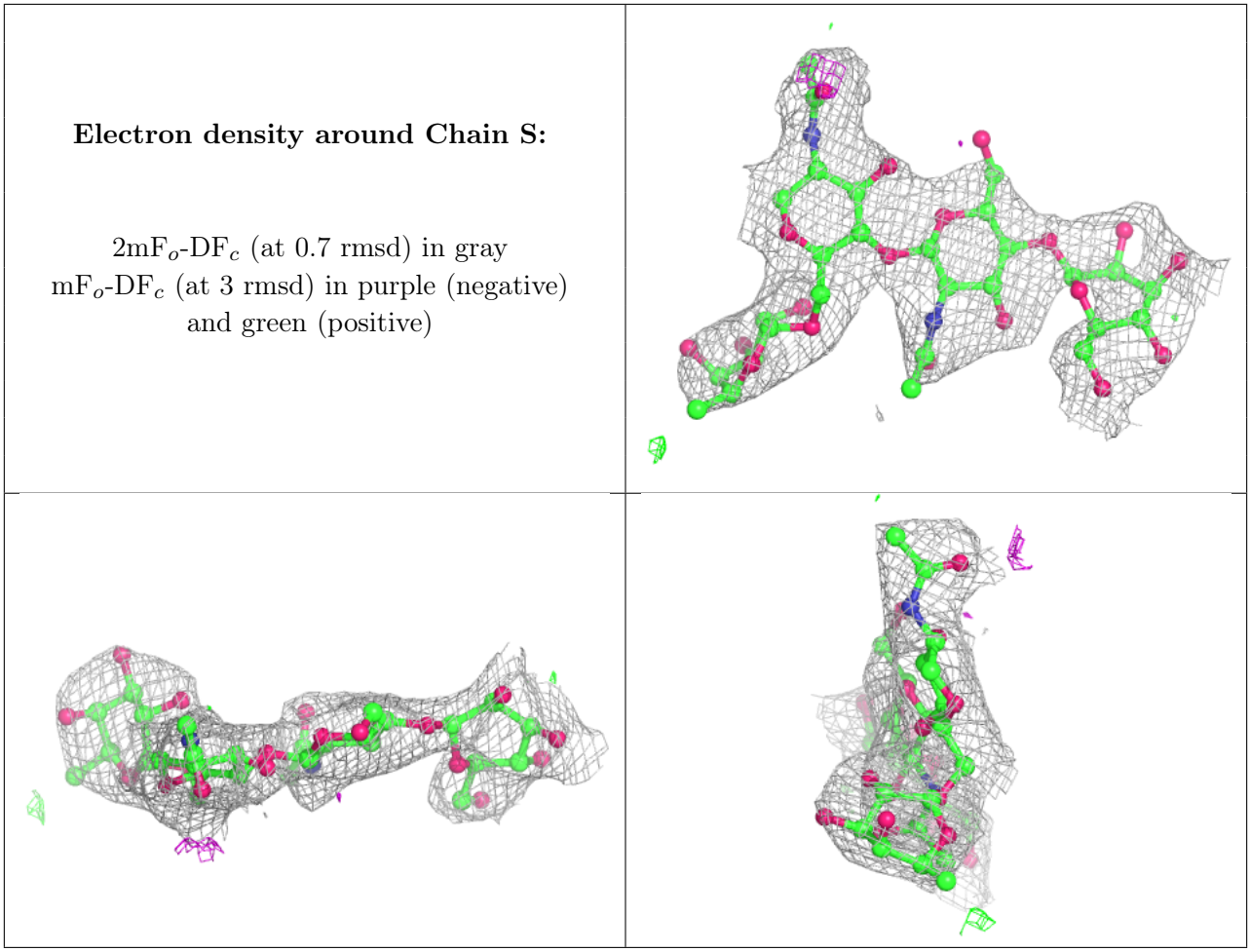
Electron density around Chain N:

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



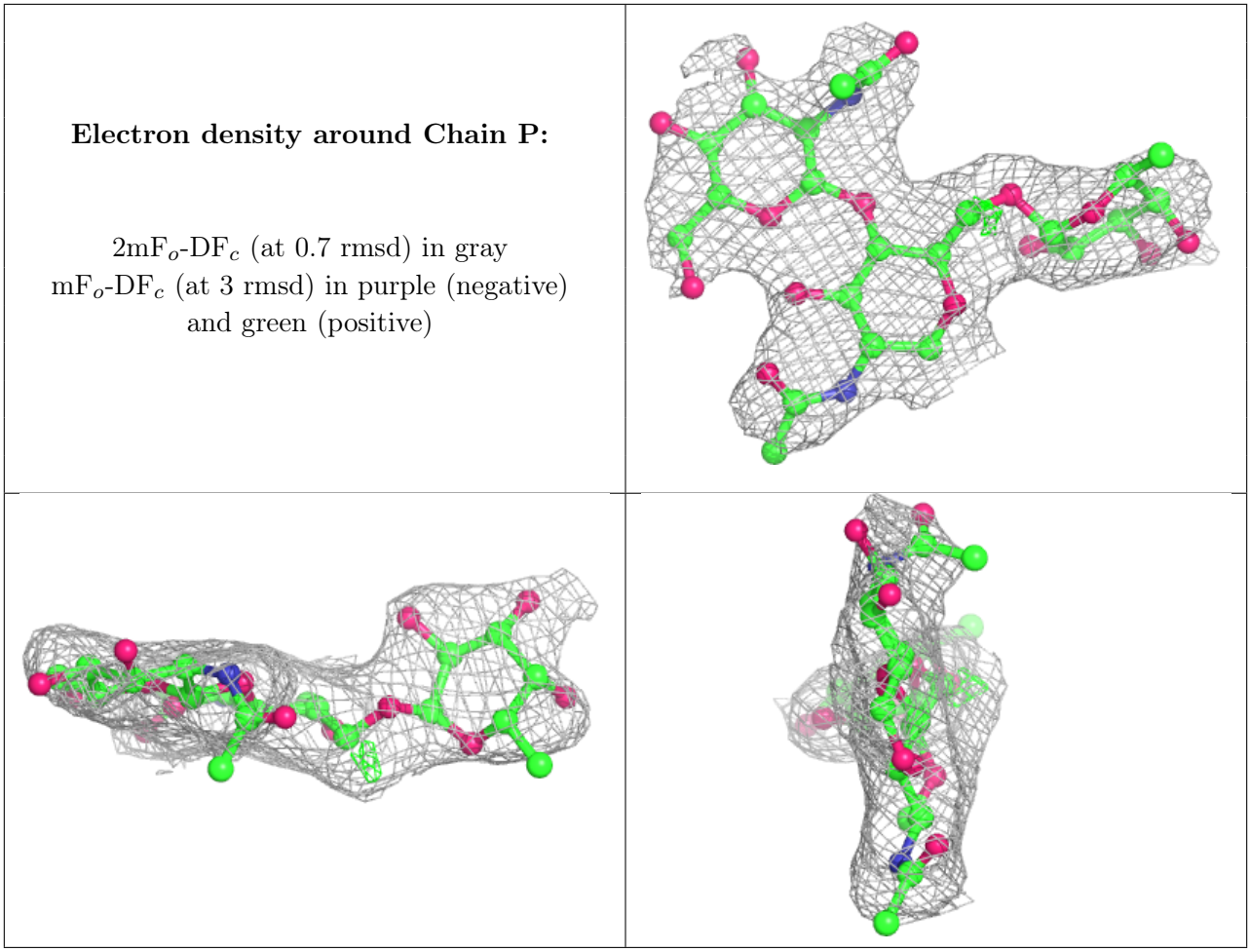
Electron density around Chain S:

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



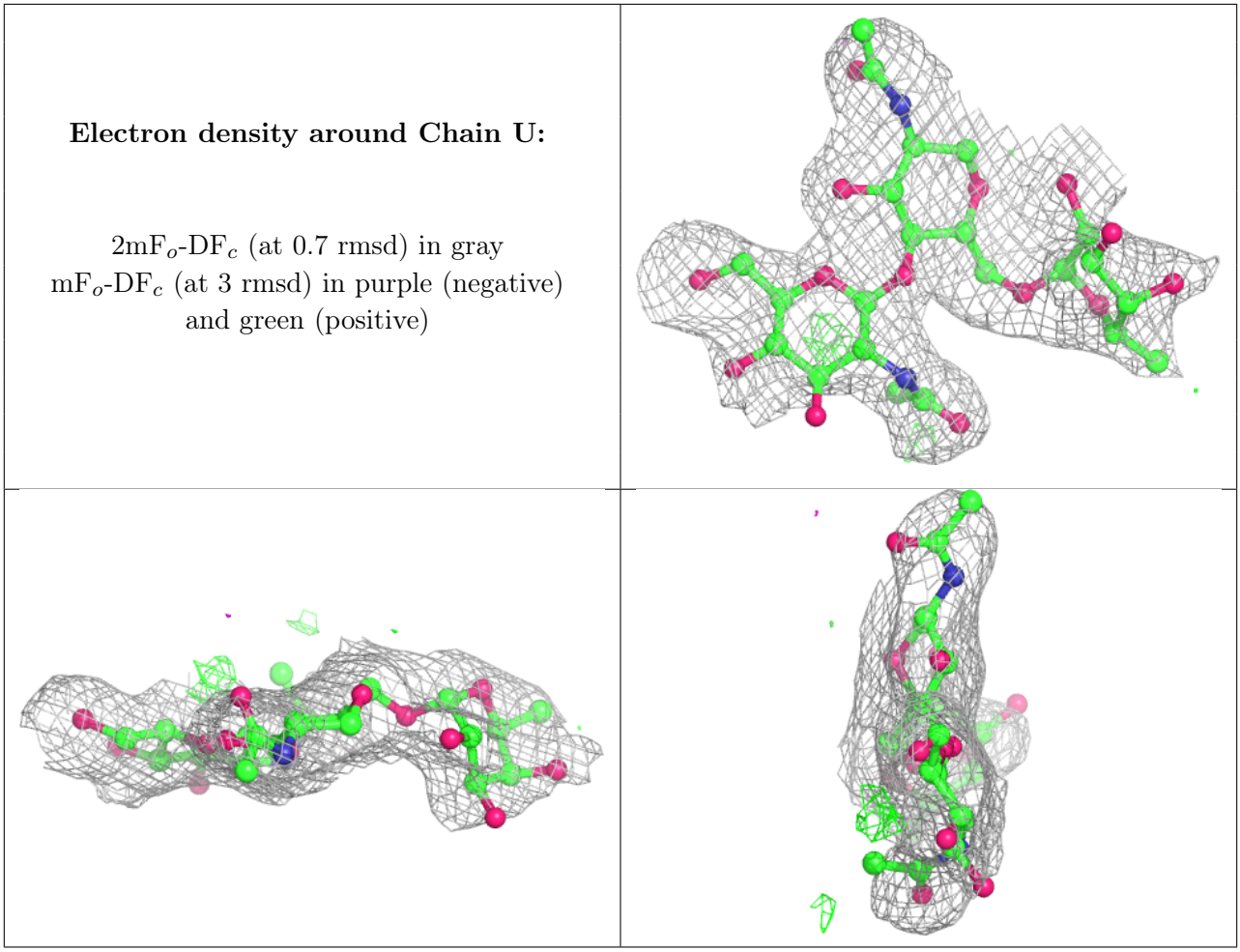
Electron density around Chain P:

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



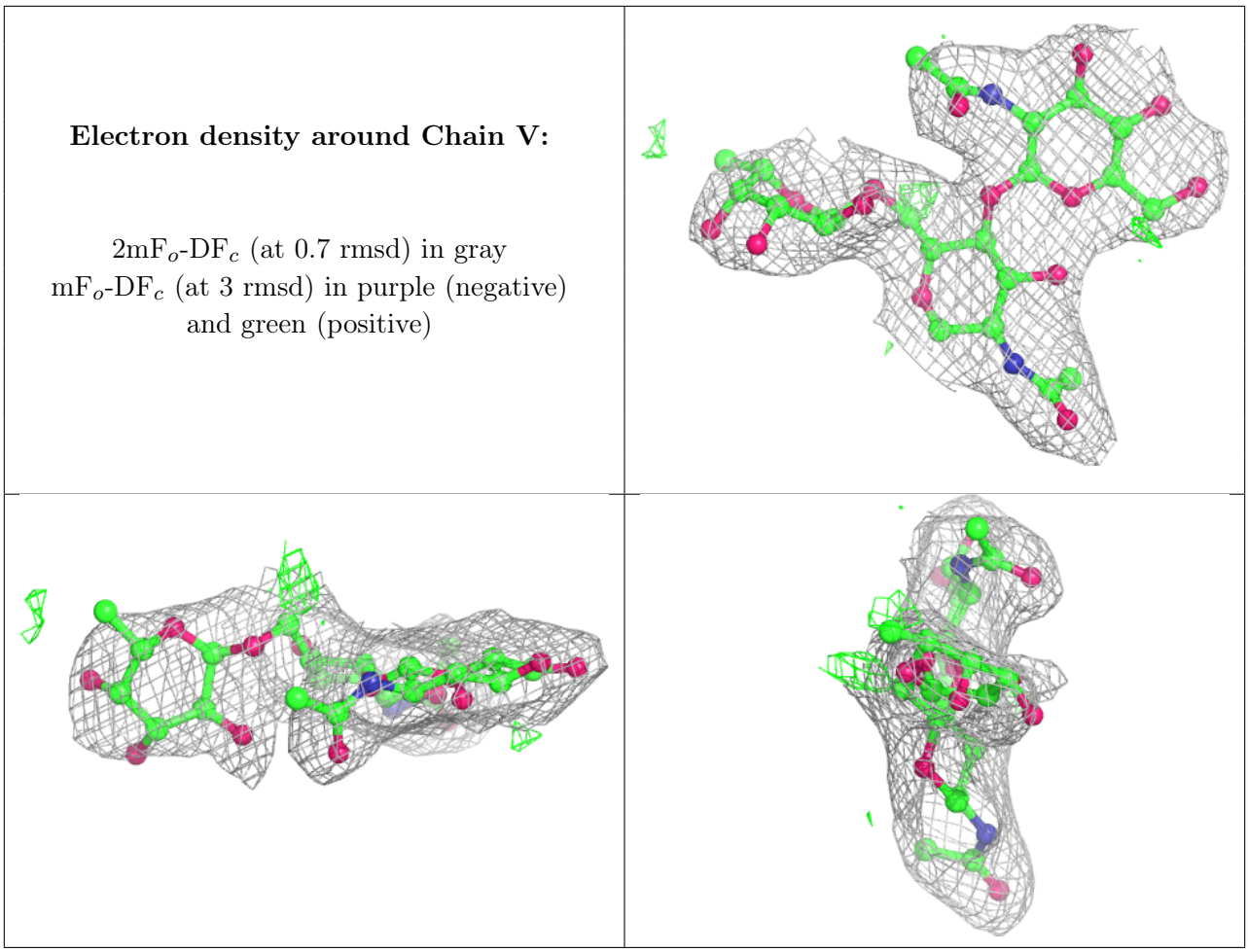
Electron density around Chain U:

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



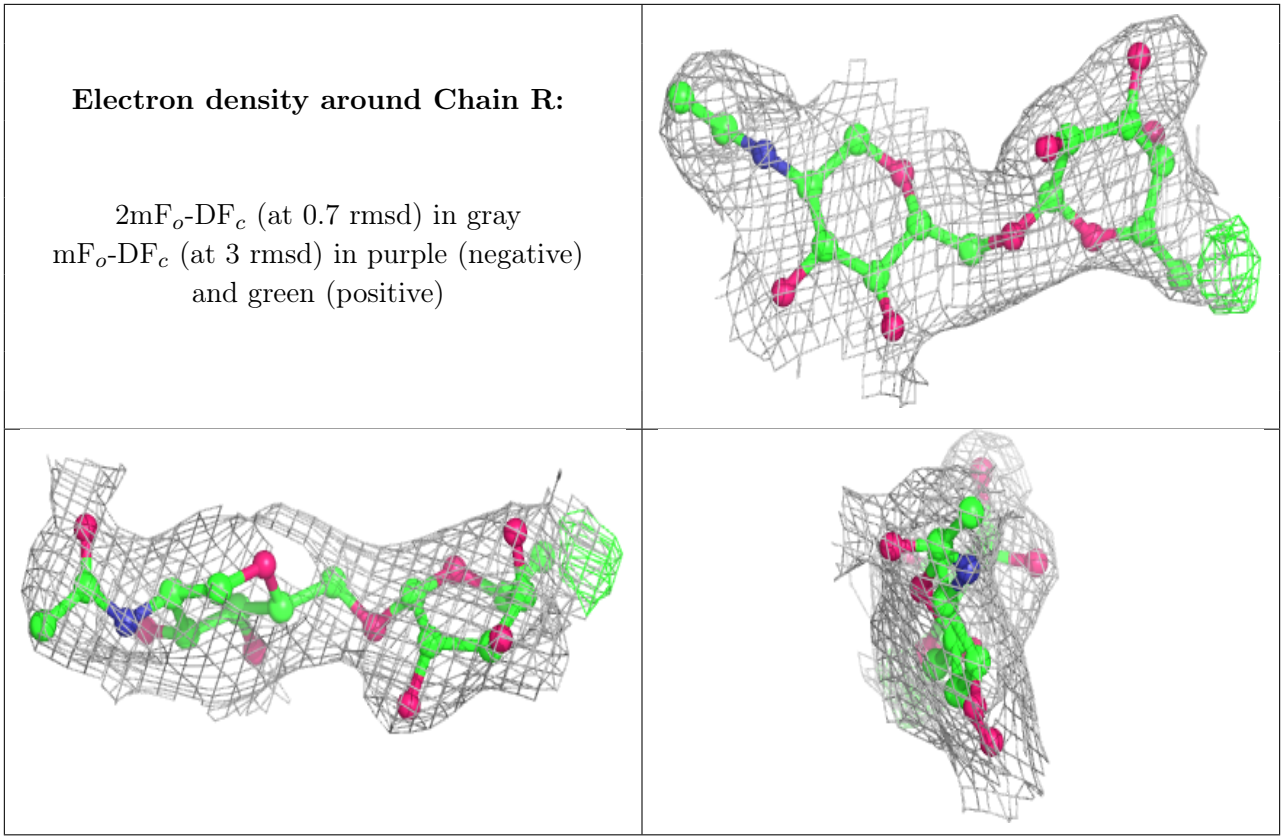
Electron density around Chain V:

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



Electron density around Chain R:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	E	802	1/1	0.79	0.07	41,41,41,41	0
7	CA	J	601	1/1	0.79	0.08	38,38,38,38	0
7	CA	G	803	1/1	0.83	0.12	33,33,33,33	0
8	NAG	L	602	14/15	0.84	0.31	61,67,73,77	0
8	NAG	H	602	14/15	0.86	0.19	59,62,69,72	0
7	CA	I	801	1/1	0.86	0.12	31,31,31,31	0
7	CA	C	802	1/1	0.87	0.08	45,45,45,45	0
7	CA	K	801	1/1	0.88	0.11	27,27,27,27	0
7	CA	A	801	1/1	0.88	0.13	27,27,27,27	0
7	CA	H	601	1/1	0.89	0.09	33,33,33,33	0
7	CA	C	801	1/1	0.90	0.07	27,27,27,27	0
7	CA	B	601	1/1	0.90	0.12	37,37,37,37	0
7	CA	I	802	1/1	0.90	0.07	37,37,37,37	0
7	CA	G	802	1/1	0.91	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	A	802	1/1	0.91	0.10	46,46,46,46	0
7	CA	I	803	1/1	0.91	0.07	37,37,37,37	0
7	CA	F	601	1/1	0.92	0.07	33,33,33,33	0
7	CA	A	803	1/1	0.94	0.04	29,29,29,29	0
7	CA	G	801	1/1	0.94	0.09	26,26,26,26	0
7	CA	K	802	1/1	0.94	0.11	45,45,45,45	0
7	CA	L	601	1/1	0.94	0.09	40,40,40,40	0
7	CA	E	801	1/1	0.94	0.10	28,28,28,28	0
7	CA	D	601	1/1	0.94	0.07	41,41,41,41	0
7	CA	K	803	1/1	0.95	0.09	32,32,32,32	0
7	CA	E	803	1/1	0.96	0.09	32,32,32,32	0
7	CA	C	803	1/1	0.99	0.08	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.