Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 04:15 PM EST

PDB ID	:	8DPU
Title	:	The crystal structure of the IL-11 signalling complex
Authors	:	Metcalfe, R.D.; Aizel, K.; Griffin, M.D.W.
Deposited on	:	2022-07-17
Resolution	:	3.78 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:

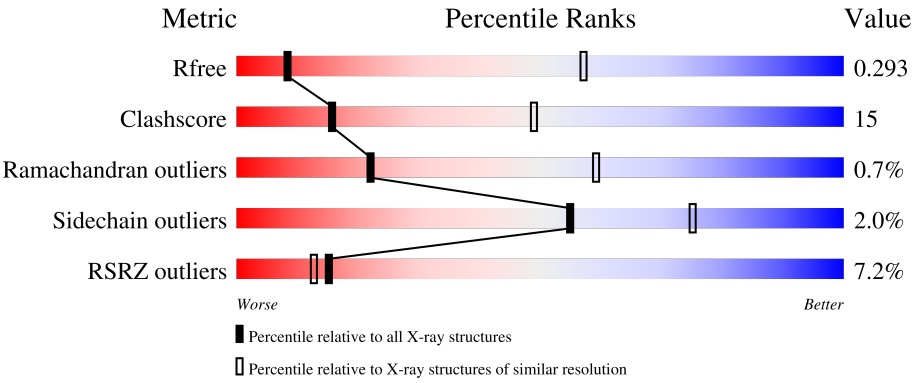
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.78 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	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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	303	6% 61% 35%
1	D	303	3% 61% 35%
1	G	303	6% 61% 36%
1	J	303	3% 61% 35%
1	M	303	% 61% 36%

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Mol	Chain	Length	Quality of chain
1	P	303	8% 61% 35%
2	B	179	2% 72% 20% 8%
2	E	179	74% 18% 8%
2	H	179	% 73% 18% 8%
2	K	179	3% 73% 19% 8%
2	N	179	3% 72% 20% 8%
2	Q	179	% 73% 18% 8%
3	C	348	9% 57% 23% 19%
3	F	348	16% 57% 23% 19%
3	I	348	9% 56% 24% 19%
3	L	348	12% 56% 24% 19%
3	O	348	10% 57% 23% 19%
3	R	348	8% 56% 24% 19%
4	S	2	100%
4	U	2	100%
4	W	2	100%
4	Y	2	100%
4	a	2	100%
4	c	2	100%
5	T	3	67% 33%
5	V	3	67% 33%
5	X	3	33% 67%
5	Z	3	67% 33%
5	b	3	67% 33%
5	d	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	Z	3	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35568 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 Interleukin-6 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2394	1527	393	462	12			
1	D	298	Total	C	N	O	S	0	0	0
			2394	1527	393	462	12			
1	G	298	Total	C	N	O	S	0	0	0
			2394	1527	393	462	12			
1	J	298	Total	C	N	O	S	0	0	0
			2394	1527	393	462	12			
1	M	298	Total	C	N	O	S	0	0	0
			2394	1527	393	462	12			
1	P	298	Total	C	N	O	S	0	0	0
			2394	1527	393	462	12			

- Molecule 2 is a protein called Interleukin-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1255	797	237	219	2			
2	E	164	Total	C	N	O	S	0	0	0
			1255	797	237	219	2			
2	H	164	Total	C	N	O	S	0	0	0
			1255	797	237	219	2			
2	K	164	Total	C	N	O	S	0	0	0
			1255	797	237	219	2			
2	N	164	Total	C	N	O	S	0	0	0
			1255	797	237	219	2			
2	Q	164	Total	C	N	O	S	0	0	0
			1255	797	237	219	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P20809

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P20809
H	0	GLY	-	expression tag	UNP P20809
K	0	GLY	-	expression tag	UNP P20809
N	0	GLY	-	expression tag	UNP P20809
Q	0	GLY	-	expression tag	UNP P20809

- Molecule 3 is a protein called Interleukin-11 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	283	Total	C	N	O	S	0	0	0
			2170	1380	379	403	8			
3	F	283	Total	C	N	O	S	0	0	0
			2170	1380	379	403	8			
3	I	283	Total	C	N	O	S	0	0	0
			2170	1380	379	403	8			
3	L	283	Total	C	N	O	S	0	0	0
			2170	1380	379	403	8			
3	O	283	Total	C	N	O	S	0	0	0
			2170	1380	379	403	8			
3	R	283	Total	C	N	O	S	0	0	0
			2170	1380	379	403	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	226	SER	CYS	engineered mutation	UNP Q14626
C	342	HIS	-	expression tag	UNP Q14626
C	343	HIS	-	expression tag	UNP Q14626
C	344	HIS	-	expression tag	UNP Q14626
C	345	HIS	-	expression tag	UNP Q14626
C	346	HIS	-	expression tag	UNP Q14626
C	347	HIS	-	expression tag	UNP Q14626
C	348	HIS	-	expression tag	UNP Q14626
F	226	SER	CYS	engineered mutation	UNP Q14626
F	342	HIS	-	expression tag	UNP Q14626
F	343	HIS	-	expression tag	UNP Q14626
F	344	HIS	-	expression tag	UNP Q14626
F	345	HIS	-	expression tag	UNP Q14626
F	346	HIS	-	expression tag	UNP Q14626
F	347	HIS	-	expression tag	UNP Q14626
F	348	HIS	-	expression tag	UNP Q14626
I	226	SER	CYS	engineered mutation	UNP Q14626

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Chain	Residue	Modelled	Actual	Comment	Reference
I	342	HIS	-	expression tag	UNP Q14626
I	343	HIS	-	expression tag	UNP Q14626
I	344	HIS	-	expression tag	UNP Q14626
I	345	HIS	-	expression tag	UNP Q14626
I	346	HIS	-	expression tag	UNP Q14626
I	347	HIS	-	expression tag	UNP Q14626
I	348	HIS	-	expression tag	UNP Q14626
L	226	SER	CYS	engineered mutation	UNP Q14626
L	342	HIS	-	expression tag	UNP Q14626
L	343	HIS	-	expression tag	UNP Q14626
L	344	HIS	-	expression tag	UNP Q14626
L	345	HIS	-	expression tag	UNP Q14626
L	346	HIS	-	expression tag	UNP Q14626
L	347	HIS	-	expression tag	UNP Q14626
L	348	HIS	-	expression tag	UNP Q14626
O	226	SER	CYS	engineered mutation	UNP Q14626
O	342	HIS	-	expression tag	UNP Q14626
O	343	HIS	-	expression tag	UNP Q14626
O	344	HIS	-	expression tag	UNP Q14626
O	345	HIS	-	expression tag	UNP Q14626
O	346	HIS	-	expression tag	UNP Q14626
O	347	HIS	-	expression tag	UNP Q14626
O	348	HIS	-	expression tag	UNP Q14626
R	226	SER	CYS	engineered mutation	UNP Q14626
R	342	HIS	-	expression tag	UNP Q14626
R	343	HIS	-	expression tag	UNP Q14626
R	344	HIS	-	expression tag	UNP Q14626
R	345	HIS	-	expression tag	UNP Q14626
R	346	HIS	-	expression tag	UNP Q14626
R	347	HIS	-	expression tag	UNP Q14626
R	348	HIS	-	expression tag	UNP Q14626

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

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

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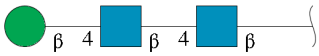
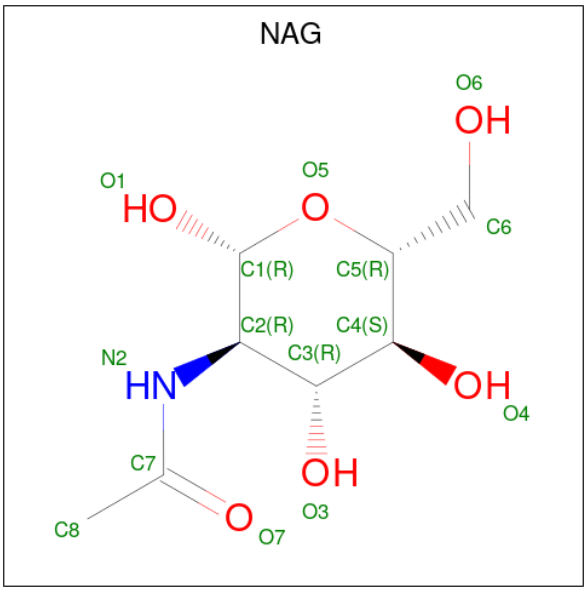
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	U	2	Total C N O 28 16 2 10	0	0	0
4	W	2	Total C N O 28 16 2 10	0	0	0
4	Y	2	Total C N O 28 16 2 10	0	0	0
4	a	2	Total C N O 28 16 2 10	0	0	0
4	c	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	T	3	Total C N O 39 22 2 15	0	0	0
5	V	3	Total C N O 39 22 2 15	0	0	0
5	X	3	Total C N O 39 22 2 15	0	0	0
5	Z	3	Total C N O 39 22 2 15	0	0	0
5	b	3	Total C N O 39 22 2 15	0	0	0
5	d	3	Total C N O 39 22 2 15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	I	1	Total C N O 14 8 1 5	0	0
6	J	1	Total C N O 14 8 1 5	0	0
6	J	1	Total C N O 14 8 1 5	0	0
6	L	1	Total C N O 14 8 1 5	0	0
6	M	1	Total C N O 14 8 1 5	0	0
6	M	1	Total C N O 14 8 1 5	0	0

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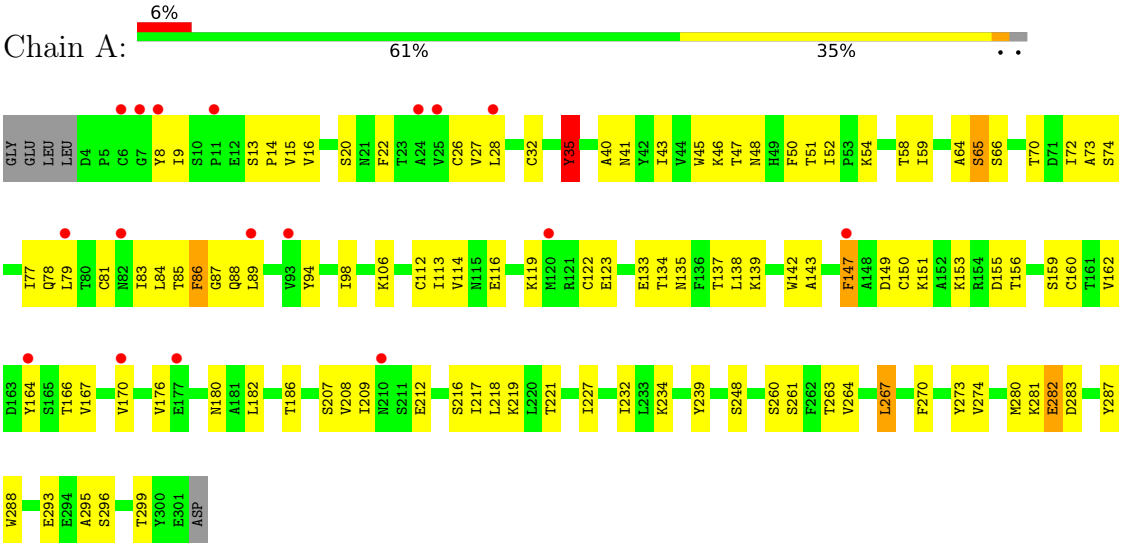
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	P	1	Total	C	N	O	0	0
			14	8	1	5		
6	P	1	Total	C	N	O	0	0
			14	8	1	5		
6	R	1	Total	C	N	O	0	0
			14	8	1	5		

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.

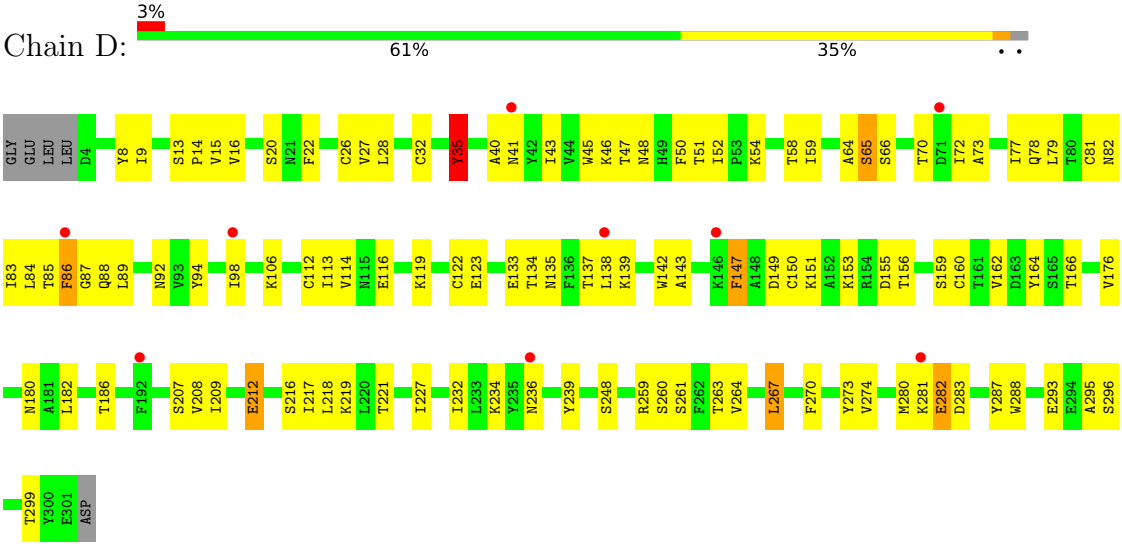
• Molecule 1: Interleukin-6 receptor subunit beta

Chain A:



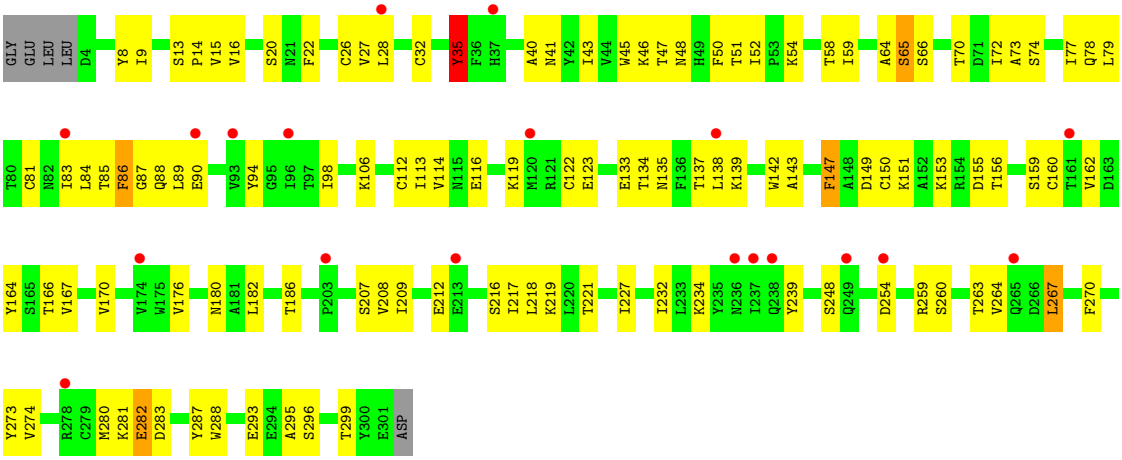
• Molecule 1: Interleukin-6 receptor subunit beta

Chain D:



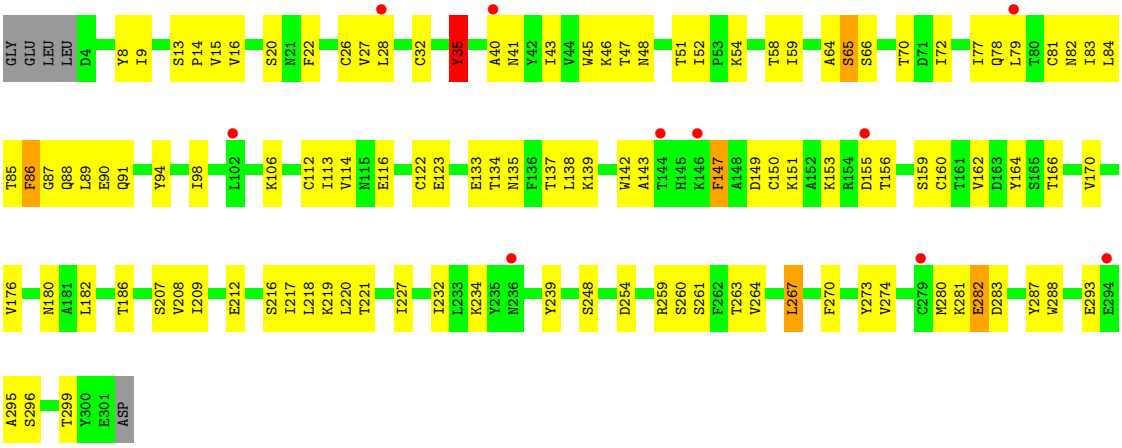
• Molecule 1: Interleukin-6 receptor subunit beta

Chain G:



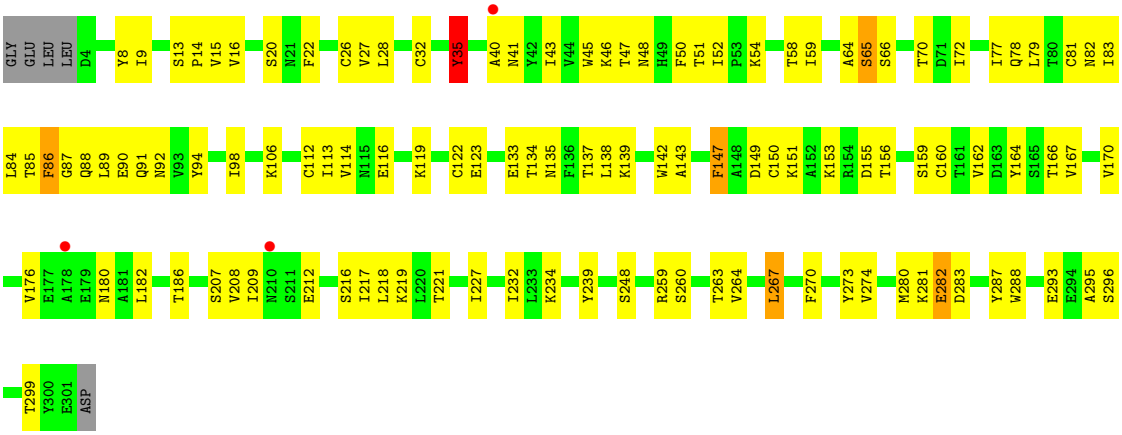
• Molecule 1: Interleukin-6 receptor subunit beta

Chain J:



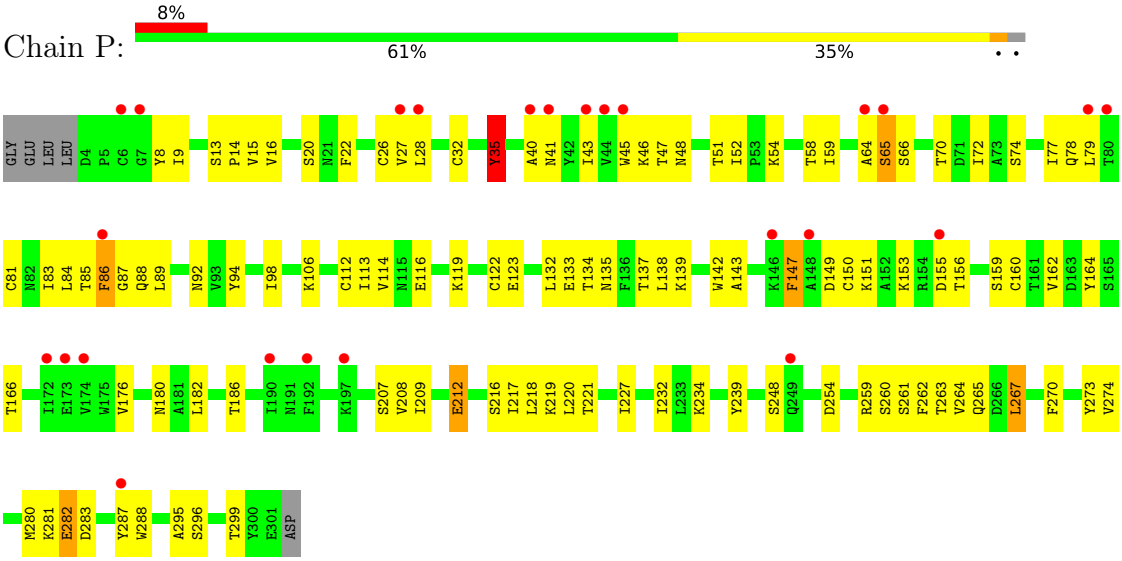
• Molecule 1: Interleukin-6 receptor subunit beta

Chain M:



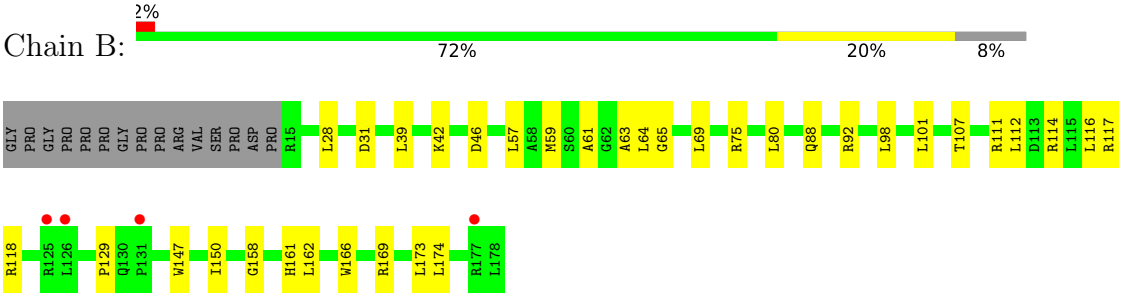
• Molecule 1: Interleukin-6 receptor subunit beta

Chain P:



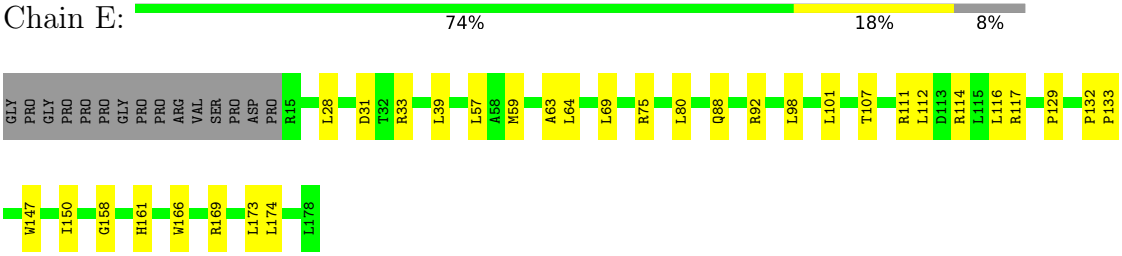
• Molecule 2: Interleukin-11

Chain B:



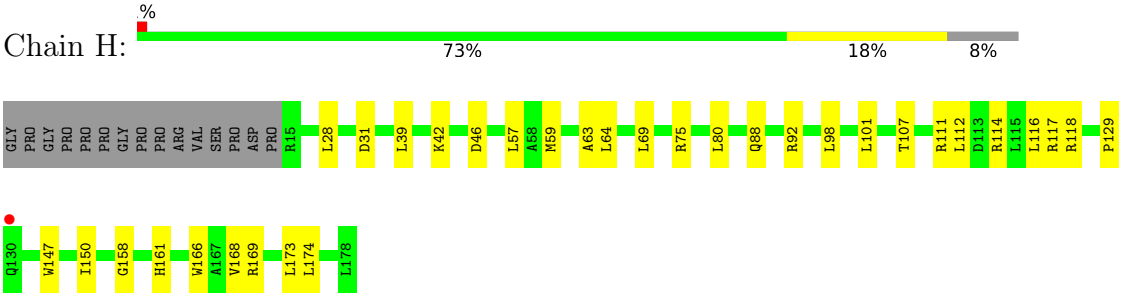
• Molecule 2: Interleukin-11

Chain E:



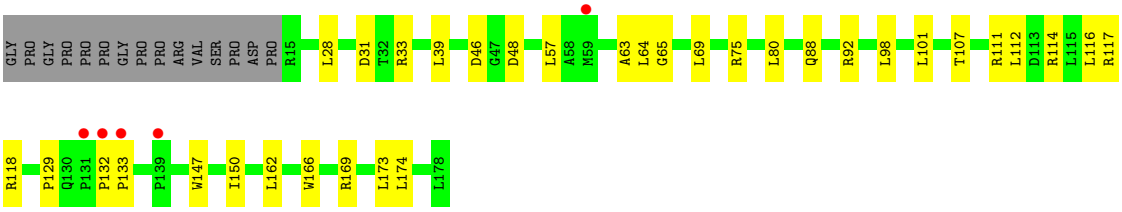
• Molecule 2: Interleukin-11

Chain H:



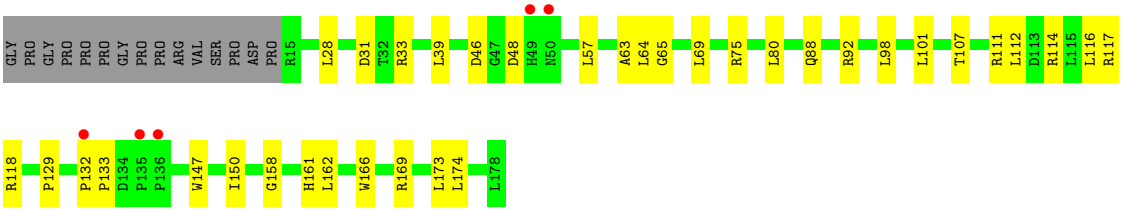
• Molecule 2: Interleukin-11

Chain K:



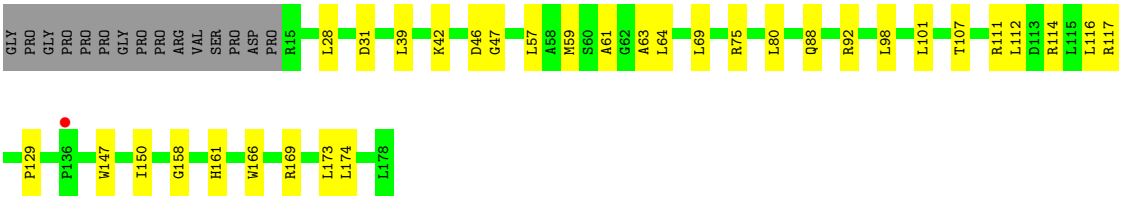
• Molecule 2: Interleukin-11

Chain N:



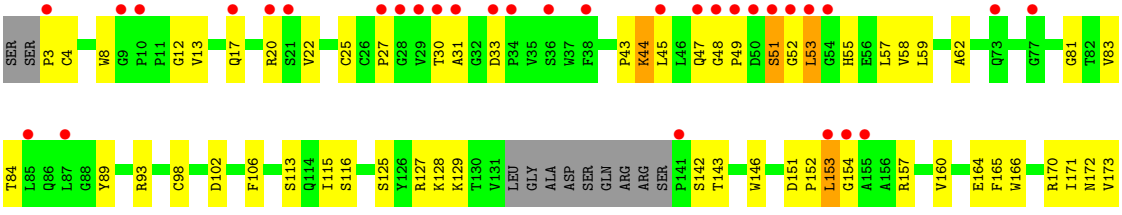
• Molecule 2: Interleukin-11

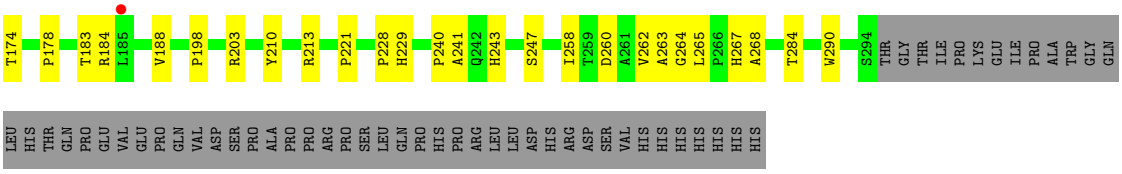
Chain Q:



• Molecule 3: Interleukin-11 receptor subunit alpha

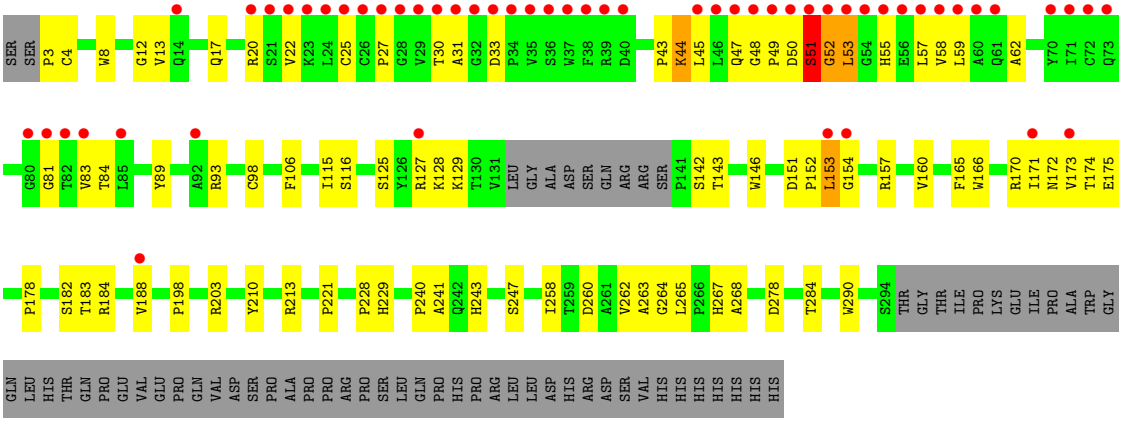
Chain C:





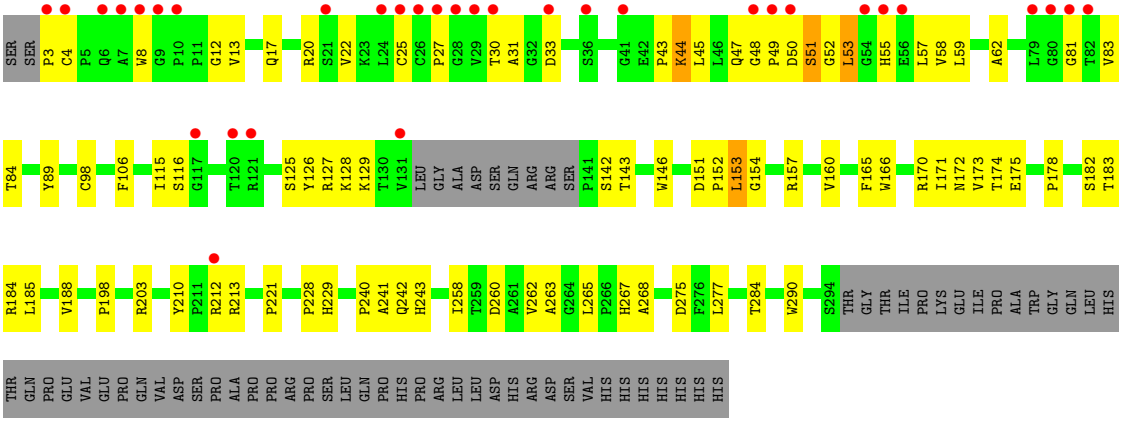
• Molecule 3: Interleukin-11 receptor subunit alpha

Chain F:



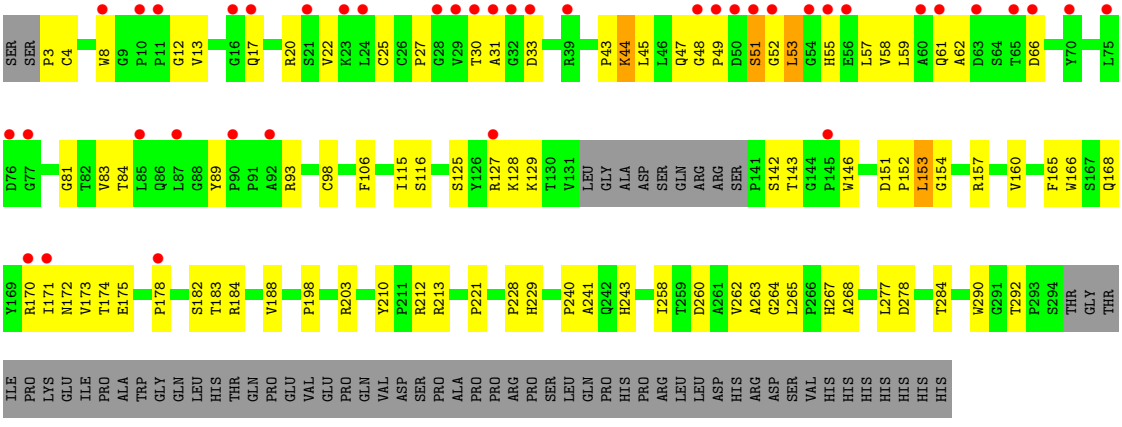
• Molecule 3: Interleukin-11 receptor subunit alpha

Chain I:



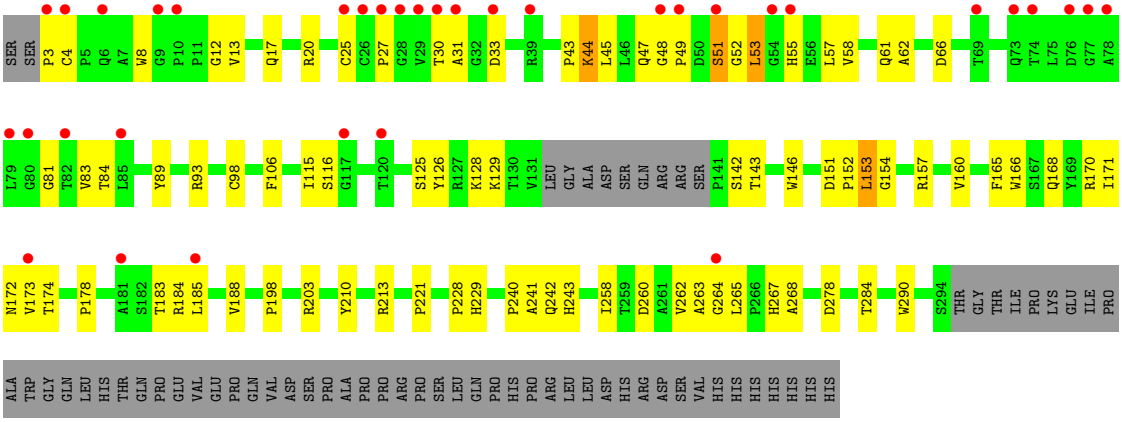
• Molecule 3: Interleukin-11 receptor subunit alpha

Chain L:



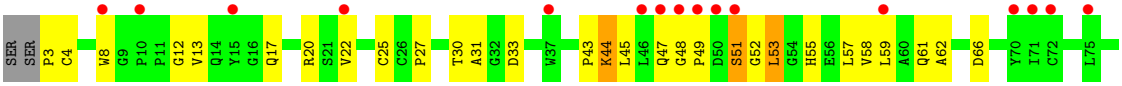
• Molecule 3: Interleukin-11 receptor subunit alpha

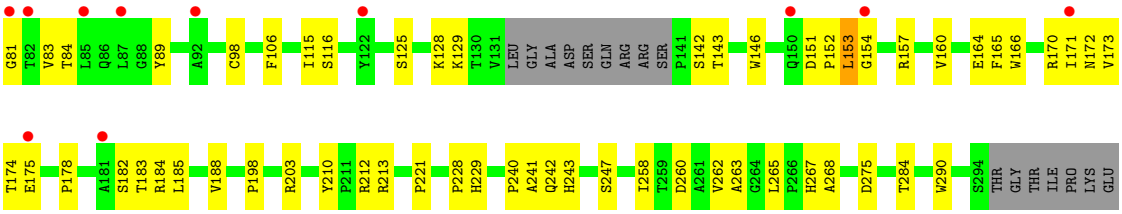
Chain O:

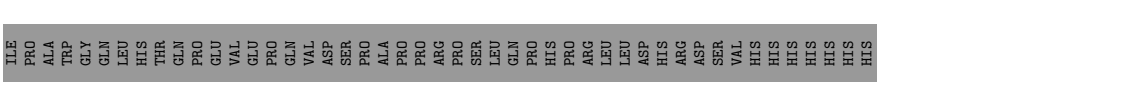


• Molecule 3: Interleukin-11 receptor subunit alpha

Chain R:

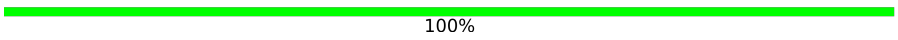






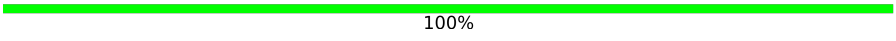
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



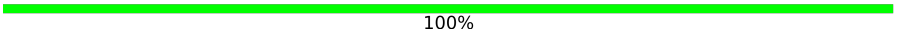
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



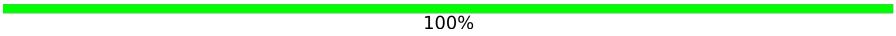
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



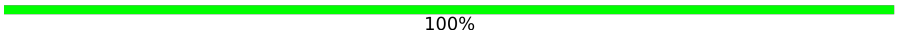
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



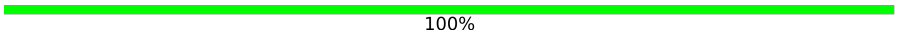
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



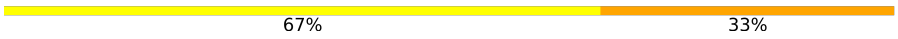
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



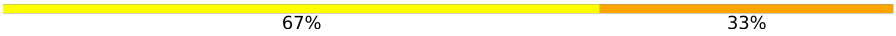
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	163.41Å 163.41Å 506.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.86 – 3.78 49.27 – 3.78	Depositor EDS
% Data completeness (in resolution range)	58.0 (40.86-3.78) 58.1 (49.27-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.29	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.276 , 0.295 0.274 , 0.293	Depositor DCC
R_{free} test set	2057 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å^2)	126.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 145.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.083 for -h,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	35568	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/2457	0.67	2/3348 (0.1%)
1	D	0.31	0/2457	0.67	2/3348 (0.1%)
1	G	0.31	0/2457	0.67	2/3348 (0.1%)
1	J	0.31	0/2457	0.67	2/3348 (0.1%)
1	M	0.31	0/2457	0.67	2/3348 (0.1%)
1	P	0.31	0/2457	0.67	2/3348 (0.1%)
2	B	0.28	0/1280	0.66	1/1743 (0.1%)
2	E	0.28	0/1280	0.66	1/1743 (0.1%)
2	H	0.28	0/1280	0.66	1/1743 (0.1%)
2	K	0.28	0/1280	0.66	1/1743 (0.1%)
2	N	0.28	0/1280	0.66	1/1743 (0.1%)
2	Q	0.28	0/1280	0.66	1/1743 (0.1%)
3	C	0.35	0/2245	0.72	5/3085 (0.2%)
3	F	0.35	0/2245	0.72	5/3085 (0.2%)
3	I	0.35	0/2245	0.72	5/3085 (0.2%)
3	L	0.35	0/2245	0.72	5/3085 (0.2%)
3	O	0.35	0/2245	0.72	5/3085 (0.2%)
3	R	0.35	0/2245	0.72	5/3085 (0.2%)
All	All	0.32	0/35892	0.69	48/49056 (0.1%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	267	LEU	CA-CB-CG	7.90	133.48	115.30
1	A	267	LEU	CA-CB-CG	7.90	133.46	115.30
1	G	267	LEU	CA-CB-CG	7.90	133.47	115.30
1	M	267	LEU	CA-CB-CG	7.89	133.44	115.30
1	P	267	LEU	CA-CB-CG	7.88	133.41	115.30
1	D	267	LEU	CA-CB-CG	7.87	133.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	51	SER	N-CA-C	7.18	130.38	111.00
3	F	51	SER	N-CA-C	7.18	130.38	111.00
3	C	51	SER	N-CA-C	7.17	130.37	111.00
3	L	51	SER	N-CA-C	7.17	130.37	111.00
3	R	51	SER	N-CA-C	7.17	130.36	111.00
3	I	51	SER	N-CA-C	7.17	130.35	111.00
3	C	53	LEU	CA-CB-CG	6.59	130.46	115.30
3	L	53	LEU	CA-CB-CG	6.59	130.46	115.30
3	O	53	LEU	CA-CB-CG	6.59	130.45	115.30
3	F	53	LEU	CA-CB-CG	6.58	130.44	115.30
3	R	53	LEU	CA-CB-CG	6.58	130.44	115.30
3	I	53	LEU	CA-CB-CG	6.57	130.41	115.30
3	C	52	GLY	N-CA-C	6.46	129.25	113.10
3	L	52	GLY	N-CA-C	6.45	129.23	113.10
3	R	52	GLY	N-CA-C	6.45	129.22	113.10
3	O	52	GLY	N-CA-C	6.44	129.19	113.10
3	F	52	GLY	N-CA-C	6.43	129.18	113.10
3	I	52	GLY	N-CA-C	6.43	129.19	113.10
2	Q	129	PRO	C-N-CA	-5.92	106.90	121.70
2	E	129	PRO	C-N-CA	-5.92	106.90	121.70
2	N	129	PRO	C-N-CA	-5.92	106.91	121.70
2	H	129	PRO	C-N-CA	-5.90	106.95	121.70
2	B	129	PRO	C-N-CA	-5.90	106.95	121.70
2	K	129	PRO	C-N-CA	-5.90	106.96	121.70
1	G	35	TYR	CA-CB-CG	5.75	124.32	113.40
1	J	35	TYR	CA-CB-CG	5.72	124.28	113.40
1	P	35	TYR	CA-CB-CG	5.72	124.27	113.40
3	L	153	LEU	CA-CB-CG	5.72	128.45	115.30
1	M	35	TYR	CA-CB-CG	5.71	124.26	113.40
1	A	35	TYR	CA-CB-CG	5.71	124.25	113.40
3	I	153	LEU	CA-CB-CG	5.71	128.43	115.30
3	O	153	LEU	CA-CB-CG	5.71	128.43	115.30
1	D	35	TYR	CA-CB-CG	5.70	124.24	113.40
3	C	153	LEU	CA-CB-CG	5.70	128.41	115.30
3	F	153	LEU	CA-CB-CG	5.70	128.41	115.30
3	R	153	LEU	CA-CB-CG	5.70	128.40	115.30
3	I	51	SER	CB-CA-C	-5.20	100.22	110.10
3	R	51	SER	CB-CA-C	-5.20	100.23	110.10
3	F	51	SER	CB-CA-C	-5.19	100.24	110.10
3	C	51	SER	CB-CA-C	-5.18	100.25	110.10
3	L	51	SER	CB-CA-C	-5.18	100.25	110.10
3	O	51	SER	CB-CA-C	-5.17	100.27	110.10

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	2394	0	2322	97	0
1	D	2394	0	2322	101	0
1	G	2394	0	2322	88	0
1	J	2394	0	2322	91	0
1	M	2394	0	2322	101	0
1	P	2394	0	2322	96	0
2	B	1255	0	1329	35	0
2	E	1255	0	1329	21	0
2	H	1255	0	1329	30	0
2	K	1255	0	1329	28	0
2	N	1255	0	1329	32	0
2	Q	1255	0	1329	30	0
3	C	2170	0	2082	66	0
3	F	2170	0	2082	69	9
3	I	2170	0	2082	69	1
3	L	2170	0	2082	68	0
3	O	2170	0	2082	70	0
3	R	2170	0	2082	69	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
4	W	28	0	25	0	0
4	Y	28	0	25	0	0
4	a	28	0	25	0	0
4	c	28	0	25	0	0
5	T	39	0	34	2	0
5	V	39	0	34	2	0
5	X	39	0	34	1	0
5	Z	39	0	34	2	0
5	b	39	0	34	0	0
5	d	39	0	34	0	0
6	A	28	0	26	4	0
6	C	14	0	13	1	0
6	D	28	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	14	0	13	0	0
6	G	28	0	26	4	0
6	I	14	0	13	0	0
6	J	28	0	26	4	0
6	L	14	0	13	0	0
6	M	28	0	26	4	0
6	O	14	0	13	0	0
6	P	28	0	26	4	0
6	R	14	0	13	0	0
All	All	35568	0	34986	1036	10

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 15.

All (1036) 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:A:263:THR:HG22	3:C:260:ASP:HB2	1.39	1.04
3:C:93:ARG:HD2	1:D:88:GLN:HE21	1.23	1.02
3:C:93:ARG:HD2	1:D:88:GLN:NE2	1.78	0.98
2:B:46:ASP:HB3	1:D:92:ASN:HB2	1.51	0.91
1:A:170:VAL:HG12	2:B:118:ARG:HH21	1.34	0.90
1:A:167:VAL:HG21	2:B:114:ARG:CZ	2.06	0.86
1:A:88:GLN:HE21	3:F:93:ARG:HD2	1.40	0.85
3:L:3:PRO:HA	3:L:31:ALA:HB2	1.62	0.82
1:J:138:LEU:HB3	1:J:150:CYS:HB3	1.61	0.82
3:O:3:PRO:HA	3:O:31:ALA:HB2	1.62	0.82
1:G:138:LEU:HB3	1:G:150:CYS:HB3	1.61	0.81
1:M:138:LEU:HB3	1:M:150:CYS:HB3	1.61	0.81
1:D:138:LEU:HB3	1:D:150:CYS:HB3	1.61	0.81
1:A:138:LEU:HB3	1:A:150:CYS:HB3	1.61	0.81
1:P:138:LEU:HB3	1:P:150:CYS:HB3	1.61	0.81
3:I:3:PRO:HA	3:I:31:ALA:HB2	1.62	0.80
3:C:3:PRO:HA	3:C:31:ALA:HB2	1.62	0.80
3:R:3:PRO:HA	3:R:31:ALA:HB2	1.62	0.80
3:F:3:PRO:HA	3:F:31:ALA:HB2	1.62	0.79
1:M:88:GLN:NE2	3:R:183:THR:O	2.15	0.78
3:I:184:ARG:HA	1:J:88:GLN:NE2	1.99	0.78
1:P:254:ASP:OD2	3:R:212:ARG:NH2	2.17	0.77
2:H:42:LYS:NZ	3:R:242:GLN:OE1	2.17	0.76
2:Q:59:MET:SD	3:R:128:LYS:HE3	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:THR:O	2:K:111:ARG:NH1	2.18	0.76
1:D:263:THR:HG22	3:F:260:ASP:HB2	1.68	0.75
2:Q:92:ARG:HB2	2:Q:92:ARG:HH21	1.52	0.75
1:A:166:THR:O	2:B:111:ARG:NH1	2.20	0.75
2:N:92:ARG:HH21	2:N:92:ARG:HB2	1.52	0.74
2:H:92:ARG:HB2	2:H:92:ARG:HH21	1.52	0.74
1:G:123:GLU:OE1	1:G:159:SER:OG	2.06	0.74
1:P:123:GLU:OE1	1:P:159:SER:OG	2.06	0.74
2:K:92:ARG:HH21	2:K:92:ARG:HB2	1.52	0.74
3:O:174:THR:HA	3:O:183:THR:HA	1.70	0.74
3:L:174:THR:HA	3:L:183:THR:HA	1.70	0.73
1:J:123:GLU:OE1	1:J:159:SER:OG	2.06	0.73
1:A:123:GLU:OE1	1:A:159:SER:OG	2.06	0.73
2:K:57:LEU:HD11	2:K:75:ARG:HG3	1.70	0.73
2:B:92:ARG:HH21	2:B:92:ARG:HB2	1.52	0.73
3:C:174:THR:HA	3:C:183:THR:HA	1.70	0.73
2:E:92:ARG:HB2	2:E:92:ARG:HH21	1.52	0.73
2:B:57:LEU:HD11	2:B:75:ARG:HG3	1.71	0.73
2:E:57:LEU:HD11	2:E:75:ARG:HG3	1.71	0.73
3:F:174:THR:HA	3:F:183:THR:HA	1.70	0.72
3:I:174:THR:HA	3:I:183:THR:HA	1.70	0.72
3:R:174:THR:HA	3:R:183:THR:HA	1.70	0.72
1:D:123:GLU:OE1	1:D:159:SER:OG	2.06	0.72
1:M:167:VAL:HG21	2:N:114:ARG:CZ	2.19	0.72
1:P:262:PHE:CE1	3:R:260:ASP:HB3	2.24	0.72
2:N:57:LEU:HD11	2:N:75:ARG:HG3	1.71	0.72
1:P:261:SER:OG	3:R:247:SER:OG	2.07	0.72
1:M:88:GLN:OE1	3:R:185:LEU:HD12	1.89	0.72
1:M:123:GLU:OE1	1:M:159:SER:OG	2.06	0.72
1:P:259:ARG:NH2	3:R:260:ASP:OD2	2.23	0.72
2:H:57:LEU:HD11	2:H:75:ARG:HG3	1.71	0.72
2:Q:57:LEU:HD11	2:Q:75:ARG:HG3	1.71	0.71
1:A:88:GLN:NE2	3:F:93:ARG:HD2	2.07	0.70
1:A:27:VAL:HG12	1:A:64:ALA:HB2	1.74	0.70
2:B:46:ASP:OD1	1:D:82:ASN:ND2	2.24	0.70
1:P:27:VAL:HG12	1:P:64:ALA:HB2	1.74	0.70
1:M:91:GLN:HA	2:Q:46:ASP:O	1.92	0.69
1:M:27:VAL:HG12	1:M:64:ALA:HB2	1.74	0.69
3:I:185:LEU:HD12	1:J:88:GLN:OE1	1.93	0.69
1:J:27:VAL:HG12	1:J:64:ALA:HB2	1.74	0.69
2:E:59:MET:SD	3:F:128:LYS:HE3	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:VAL:HG12	1:G:64:ALA:HB2	1.74	0.69
1:D:27:VAL:HG12	1:D:64:ALA:HB2	1.74	0.68
3:F:129:LYS:HE2	3:F:170:ARG:HB2	1.76	0.68
3:I:129:LYS:HE2	3:I:170:ARG:HB2	1.76	0.68
1:P:265:GLN:OE1	3:R:262:VAL:HA	1.93	0.68
3:O:129:LYS:HE2	3:O:170:ARG:HB2	1.76	0.68
3:R:129:LYS:HE2	3:R:170:ARG:HB2	1.76	0.68
3:L:129:LYS:HE2	3:L:170:ARG:HB2	1.76	0.68
3:C:129:LYS:HE2	3:C:170:ARG:HB2	1.76	0.67
2:K:169:ARG:NH1	3:L:277:LEU:HD12	2.10	0.67
2:K:162:LEU:HD22	3:L:166:TRP:HD1	1.60	0.66
1:D:261:SER:OG	3:F:247:SER:OG	2.11	0.66
1:J:77:ILE:HB	1:J:98:ILE:HB	1.78	0.66
1:G:84:LEU:HD23	1:G:87:GLY:HA2	1.78	0.66
3:L:153:LEU:HD12	3:L:154:GLY:H	1.61	0.66
3:R:129:LYS:HZ2	3:R:170:ARG:HH21	1.41	0.66
1:A:84:LEU:HD23	1:A:87:GLY:HA2	1.78	0.66
2:B:59:MET:SD	3:C:128:LYS:HE3	2.35	0.66
3:I:153:LEU:HD12	3:I:154:GLY:H	1.61	0.66
1:P:84:LEU:HD23	1:P:87:GLY:HA2	1.78	0.66
1:D:77:ILE:HB	1:D:98:ILE:HB	1.78	0.66
3:C:153:LEU:HD12	3:C:154:GLY:H	1.61	0.65
1:P:77:ILE:HB	1:P:98:ILE:HB	1.78	0.65
1:D:84:LEU:HD23	1:D:87:GLY:HA2	1.78	0.65
1:D:134:THR:HG22	1:D:180:ASN:HB3	1.78	0.65
1:J:84:LEU:HD23	1:J:87:GLY:HA2	1.78	0.65
1:J:134:THR:HG22	1:J:180:ASN:HB3	1.78	0.65
3:F:153:LEU:HD12	3:F:154:GLY:H	1.61	0.65
3:O:153:LEU:HD12	3:O:154:GLY:H	1.61	0.65
1:P:134:THR:HG22	1:P:180:ASN:HB3	1.78	0.65
1:G:77:ILE:HB	1:G:98:ILE:HB	1.78	0.65
1:G:134:THR:HG22	1:G:180:ASN:HB3	1.78	0.65
1:M:84:LEU:HD23	1:M:87:GLY:HA2	1.78	0.65
3:R:153:LEU:HD12	3:R:154:GLY:H	1.61	0.65
1:A:77:ILE:HB	1:A:98:ILE:HB	1.78	0.65
1:D:106:LYS:NZ	1:D:186:THR:O	2.30	0.64
1:M:77:ILE:HB	1:M:98:ILE:HB	1.78	0.64
1:M:281:LYS:NZ	1:M:283:ASP:OD1	2.30	0.64
1:D:232:ILE:HB	1:D:282:GLU:HG2	1.80	0.64
1:A:134:THR:HG22	1:A:180:ASN:HB3	1.78	0.64
1:G:232:ILE:HB	1:G:282:GLU:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:THR:HG22	1:M:180:ASN:HB3	1.78	0.64
3:O:171:ILE:HD13	3:O:188:VAL:HB	1.79	0.64
1:G:106:LYS:NZ	1:G:186:THR:O	2.30	0.64
2:N:173:LEU:HG	3:O:229:HIS:CE1	2.33	0.64
1:D:281:LYS:NZ	1:D:283:ASP:OD1	2.29	0.63
3:F:171:ILE:HD13	3:F:188:VAL:HB	1.79	0.63
1:P:212:GLU:CD	3:R:243:HIS:HA	2.18	0.63
2:K:162:LEU:HD22	3:L:166:TRP:CD1	2.31	0.63
1:G:254:ASP:OD2	3:I:212:ARG:NH2	2.31	0.63
1:P:232:ILE:HB	1:P:282:GLU:HG2	1.80	0.63
1:J:281:LYS:NZ	1:J:283:ASP:OD1	2.29	0.63
1:A:281:LYS:NZ	1:A:283:ASP:OD1	2.29	0.63
1:G:166:THR:O	2:H:111:ARG:NH1	2.31	0.63
1:M:263:THR:HG22	3:O:260:ASP:HB2	1.81	0.63
1:A:106:LYS:NZ	1:A:186:THR:O	2.30	0.63
3:C:171:ILE:HD13	3:C:188:VAL:HB	1.79	0.63
1:G:281:LYS:NZ	1:G:283:ASP:OD1	2.29	0.63
1:M:9:ILE:HD11	1:M:81:CYS:HB2	1.80	0.62
3:I:171:ILE:HD13	3:I:188:VAL:HB	1.79	0.62
1:J:16:VAL:HG11	1:J:72:ILE:HD12	1.82	0.62
1:J:9:ILE:HD11	1:J:81:CYS:HB2	1.80	0.62
1:M:219:LYS:HE3	1:M:263:THR:HB	1.82	0.62
1:J:232:ILE:HB	1:J:282:GLU:HG2	1.80	0.62
1:A:16:VAL:HG11	1:A:72:ILE:HD12	1.82	0.62
1:G:234:LYS:HB2	1:G:282:GLU:HA	1.82	0.62
1:M:232:ILE:HB	1:M:282:GLU:HG2	1.80	0.62
1:P:106:LYS:NZ	1:P:186:THR:O	2.31	0.62
1:A:9:ILE:HD11	1:A:81:CYS:HB2	1.80	0.62
1:A:219:LYS:HE3	1:A:263:THR:HB	1.82	0.62
1:A:232:ILE:HB	1:A:282:GLU:HG2	1.80	0.62
1:D:16:VAL:HG11	1:D:72:ILE:HD12	1.82	0.62
3:L:171:ILE:HD13	3:L:188:VAL:HB	1.79	0.62
1:M:106:LYS:NZ	1:M:186:THR:O	2.31	0.62
1:P:9:ILE:HD11	1:P:81:CYS:HB2	1.80	0.62
1:D:9:ILE:HD11	1:D:81:CYS:HB2	1.80	0.62
1:J:106:LYS:NZ	1:J:186:THR:O	2.30	0.62
3:R:171:ILE:HD13	3:R:188:VAL:HB	1.79	0.62
1:M:16:VAL:HG11	1:M:72:ILE:HD12	1.82	0.62
1:G:167:VAL:HG21	2:H:114:ARG:CZ	2.31	0.61
1:G:219:LYS:HE3	1:G:263:THR:HB	1.82	0.61
1:J:219:LYS:HE3	1:J:263:THR:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:16:VAL:HG11	1:P:72:ILE:HD12	1.82	0.61
1:P:219:LYS:HE3	1:P:263:THR:HB	1.82	0.61
1:G:9:ILE:HD11	1:G:81:CYS:HB2	1.80	0.61
1:P:234:LYS:HB2	1:P:282:GLU:HA	1.82	0.61
1:D:219:LYS:HE3	1:D:263:THR:HB	1.82	0.61
1:G:90:GLU:HB2	2:K:46:ASP:OD1	2.00	0.61
1:M:234:LYS:HB2	1:M:282:GLU:HA	1.82	0.61
1:P:281:LYS:NZ	1:P:283:ASP:OD1	2.29	0.61
1:A:219:LYS:HA	1:A:263:THR:HA	1.83	0.60
3:O:93:ARG:HD2	1:P:88:GLN:HE21	1.66	0.60
1:A:234:LYS:HB2	1:A:282:GLU:HA	1.82	0.60
1:D:219:LYS:HA	1:D:263:THR:HA	1.83	0.60
1:D:142:TRP:HD1	1:D:143:ALA:H	1.50	0.60
1:D:234:LYS:HB2	1:D:282:GLU:HA	1.82	0.60
2:K:33:ARG:NH2	3:L:278:ASP:HB3	2.17	0.60
1:P:219:LYS:HA	1:P:263:THR:HA	1.83	0.60
1:M:45:TRP:HB3	1:M:52:ILE:HD12	1.84	0.60
1:G:16:VAL:HG11	1:G:72:ILE:HD12	1.82	0.60
1:J:234:LYS:HB2	1:J:282:GLU:HA	1.82	0.60
3:O:183:THR:O	1:P:88:GLN:OE1	2.20	0.60
1:A:32:CYS:HA	1:A:35:TYR:CZ	2.37	0.60
3:I:262:VAL:HG23	3:I:265:LEU:HB2	1.84	0.60
1:P:32:CYS:HA	1:P:35:TYR:CZ	2.37	0.60
1:G:45:TRP:HB3	1:G:52:ILE:HD12	1.84	0.60
1:J:45:TRP:HB3	1:J:52:ILE:HD12	1.84	0.60
1:J:58:THR:OG1	1:J:66:SER:OG	2.20	0.60
1:G:219:LYS:HA	1:G:263:THR:HA	1.83	0.59
1:J:32:CYS:HA	1:J:35:TYR:CZ	2.37	0.59
1:J:142:TRP:HD1	1:J:143:ALA:H	1.49	0.59
1:D:32:CYS:HA	1:D:35:TYR:CZ	2.37	0.59
1:G:58:THR:OG1	1:G:66:SER:OG	2.20	0.59
2:K:173:LEU:HG	3:L:229:HIS:CE1	2.37	0.59
1:P:45:TRP:HB3	1:P:52:ILE:HD12	1.84	0.59
1:G:32:CYS:HA	1:G:35:TYR:CZ	2.37	0.59
3:I:242:GLN:OE1	2:Q:42:LYS:NZ	2.35	0.59
1:M:32:CYS:HA	1:M:35:TYR:CZ	2.37	0.59
1:P:58:THR:OG1	1:P:66:SER:OG	2.20	0.59
3:R:262:VAL:HG23	3:R:265:LEU:HB2	1.83	0.59
1:A:45:TRP:HB3	1:A:52:ILE:HD12	1.84	0.59
1:A:142:TRP:HD1	1:A:143:ALA:H	1.49	0.59
3:O:262:VAL:HG23	3:O:265:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:PRO:HD2	3:C:58:VAL:HG23	1.85	0.59
1:J:219:LYS:HA	1:J:263:THR:HA	1.83	0.59
3:C:93:ARG:HH11	1:D:88:GLN:HG3	1.66	0.59
3:F:49:PRO:HD2	3:F:58:VAL:HG23	1.85	0.59
1:M:142:TRP:HD1	1:M:143:ALA:H	1.49	0.59
1:P:142:TRP:HD1	1:P:143:ALA:H	1.49	0.59
1:A:58:THR:OG1	1:A:66:SER:OG	2.20	0.59
3:F:262:VAL:HG23	3:F:265:LEU:HB2	1.83	0.59
3:F:127:ARG:HE	5:V:1:NAG:H81	1.68	0.58
3:I:127:ARG:HE	5:X:1:NAG:H81	1.68	0.58
3:C:262:VAL:HG23	3:C:265:LEU:HB2	1.84	0.58
3:C:129:LYS:HZ2	3:C:170:ARG:HH21	1.51	0.58
3:O:30:THR:HB	3:O:33:ASP:OD2	2.03	0.58
2:E:173:LEU:HG	3:F:229:HIS:CE1	2.38	0.58
3:C:30:THR:HB	3:C:33:ASP:OD2	2.03	0.58
3:F:30:THR:HB	3:F:33:ASP:OD2	2.03	0.58
1:D:45:TRP:HB3	1:D:52:ILE:HD12	1.84	0.58
1:M:91:GLN:CD	2:Q:47:GLY:HA3	2.23	0.58
2:H:46:ASP:OD1	1:J:90:GLU:HB2	2.03	0.58
1:M:219:LYS:HA	1:M:263:THR:HA	1.83	0.58
1:D:166:THR:O	2:E:111:ARG:NH1	2.37	0.58
3:L:262:VAL:HG23	3:L:265:LEU:HB2	1.83	0.58
3:L:30:THR:HB	3:L:33:ASP:OD2	2.03	0.58
3:L:49:PRO:HD2	3:L:58:VAL:HG23	1.85	0.58
1:G:142:TRP:HD1	1:G:143:ALA:H	1.49	0.58
3:I:49:PRO:HD2	3:I:58:VAL:HG23	1.85	0.58
1:M:58:THR:OG1	1:M:66:SER:OG	2.20	0.58
1:A:239:TYR:O	1:A:248:SER:OG	2.20	0.57
1:J:239:TYR:O	1:J:248:SER:OG	2.20	0.57
3:F:290:TRP:CD1	1:G:50:PHE:CD1	2.92	0.57
1:J:254:ASP:OD2	3:L:212:ARG:NH2	2.37	0.57
2:H:169:ARG:NH2	3:I:275:ASP:OD1	2.37	0.57
1:M:90:GLU:HB2	2:Q:46:ASP:OD1	2.05	0.57
3:O:129:LYS:HZ2	3:O:170:ARG:HH21	1.53	0.57
1:P:84:LEU:CD2	1:P:87:GLY:HA2	2.35	0.57
3:R:49:PRO:HD2	3:R:58:VAL:HG23	1.85	0.57
3:C:127:ARG:HE	5:T:1:NAG:H81	1.68	0.57
3:I:30:THR:HB	3:I:33:ASP:OD2	2.03	0.57
2:N:162:LEU:HD22	3:O:166:TRP:HB3	1.87	0.57
1:D:139:LYS:NZ	1:D:149:ASP:OD1	2.32	0.57
3:I:183:THR:O	1:J:88:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:OG1	1:D:66:SER:OG	2.20	0.57
1:D:84:LEU:CD2	1:D:87:GLY:HA2	2.35	0.57
1:G:84:LEU:CD2	1:G:87:GLY:HA2	2.35	0.57
3:L:127:ARG:HE	5:Z:1:NAG:H81	1.68	0.57
1:M:82:ASN:HD22	2:Q:46:ASP:CG	2.08	0.57
3:O:49:PRO:HD2	3:O:58:VAL:HG23	1.85	0.57
3:R:30:THR:HB	3:R:33:ASP:OD2	2.03	0.57
1:M:84:LEU:CD2	1:M:87:GLY:HA2	2.35	0.57
1:A:84:LEU:CD2	1:A:87:GLY:HA2	2.35	0.57
1:A:167:VAL:HG21	2:B:114:ARG:NH2	2.18	0.57
3:I:184:ARG:HA	1:J:88:GLN:CD	2.24	0.57
3:L:129:LYS:HZ2	3:L:170:ARG:HH21	1.51	0.57
1:A:167:VAL:HG21	2:B:114:ARG:NH1	2.19	0.56
1:G:8:TYR:HA	1:G:94:TYR:CG	2.41	0.56
1:G:137:THR:HG22	1:G:151:LYS:HG3	1.88	0.56
2:H:69:LEU:HD13	2:H:174:LEU:HD22	1.87	0.56
1:J:84:LEU:CD2	1:J:87:GLY:HA2	2.35	0.56
2:K:69:LEU:HD13	2:K:174:LEU:HD22	1.87	0.56
3:O:8:TRP:CG	3:O:178:PRO:HG3	2.41	0.56
1:P:137:THR:HG22	1:P:151:LYS:HG3	1.88	0.56
1:J:139:LYS:NZ	1:J:149:ASP:OD1	2.32	0.56
3:C:8:TRP:CG	3:C:178:PRO:HG3	2.41	0.56
3:F:89:TYR:OH	3:F:115:ILE:O	2.23	0.56
3:L:8:TRP:CG	3:L:178:PRO:HG3	2.41	0.56
1:D:239:TYR:O	1:D:248:SER:OG	2.20	0.56
3:F:173:VAL:O	3:F:184:ARG:N	2.38	0.56
3:F:210:TYR:HB3	3:F:213:ARG:HG3	1.88	0.56
3:L:89:TYR:OH	3:L:115:ILE:O	2.23	0.56
1:A:216:SER:O	1:A:267:LEU:HD23	2.06	0.56
3:C:210:TYR:HB3	3:C:213:ARG:HG3	1.88	0.56
1:D:8:TYR:HA	1:D:94:TYR:CG	2.41	0.56
1:G:216:SER:O	1:G:267:LEU:HD23	2.06	0.56
3:L:210:TYR:HB3	3:L:213:ARG:HG3	1.88	0.56
3:O:89:TYR:OH	3:O:115:ILE:O	2.23	0.56
1:P:58:THR:N	1:P:66:SER:O	2.38	0.56
2:Q:69:LEU:HD13	2:Q:174:LEU:HD22	1.88	0.56
1:D:216:SER:O	1:D:267:LEU:HD23	2.06	0.56
3:I:8:TRP:CG	3:I:178:PRO:HG3	2.41	0.56
1:J:8:TYR:HA	1:J:94:TYR:CG	2.41	0.56
1:M:216:SER:O	1:M:267:LEU:HD23	2.06	0.56
1:P:216:SER:O	1:P:267:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TYR:HA	1:A:94:TYR:CG	2.41	0.56
1:M:58:THR:N	1:M:66:SER:O	2.38	0.56
1:G:153:LYS:HB3	1:G:155:ASP:OD2	2.06	0.55
1:M:8:TYR:HA	1:M:94:TYR:CG	2.41	0.55
3:O:210:TYR:HB3	3:O:213:ARG:HG3	1.88	0.55
1:P:8:TYR:HA	1:P:94:TYR:CG	2.41	0.55
1:A:137:THR:HG22	1:A:151:LYS:HG3	1.88	0.55
3:R:89:TYR:OH	3:R:115:ILE:O	2.23	0.55
1:A:32:CYS:HA	1:A:35:TYR:CE1	2.42	0.55
1:J:216:SER:O	1:J:267:LEU:HD23	2.06	0.55
1:M:137:THR:HG22	1:M:151:LYS:HG3	1.88	0.55
3:O:173:VAL:O	3:O:184:ARG:N	2.38	0.55
3:F:8:TRP:CG	3:F:178:PRO:HG3	2.41	0.55
1:G:32:CYS:HA	1:G:35:TYR:CE1	2.42	0.55
3:I:4:CYS:HB3	3:I:55:HIS:NE2	2.22	0.55
1:M:153:LYS:HB3	1:M:155:ASP:OD2	2.06	0.55
2:Q:61:ALA:HA	3:R:164:GLU:HA	1.89	0.55
3:R:8:TRP:CG	3:R:178:PRO:HG3	2.41	0.55
1:A:73:ALA:O	3:L:264:GLY:HA2	2.06	0.55
1:A:167:VAL:HG11	2:B:114:ARG:HD3	1.87	0.55
1:D:58:THR:N	1:D:66:SER:O	2.38	0.55
3:C:173:VAL:O	3:C:184:ARG:N	2.38	0.55
3:I:129:LYS:HZ2	3:I:170:ARG:HH21	1.53	0.55
3:R:240:PRO:HA	3:R:267:HIS:HA	1.89	0.55
3:C:89:TYR:OH	3:C:115:ILE:O	2.23	0.55
3:F:4:CYS:HB3	3:F:55:HIS:NE2	2.22	0.55
3:F:290:TRP:CD1	1:G:50:PHE:HD1	2.25	0.55
3:I:173:VAL:O	3:I:184:ARG:N	2.38	0.55
3:I:240:PRO:HA	3:I:267:HIS:HA	1.89	0.55
3:L:4:CYS:HB3	3:L:55:HIS:NE2	2.22	0.55
1:P:32:CYS:HA	1:P:35:TYR:CE1	2.42	0.55
1:P:153:LYS:HB3	1:P:155:ASP:OD2	2.06	0.55
2:B:69:LEU:HD13	2:B:174:LEU:HD22	1.88	0.55
3:C:8:TRP:CD2	3:C:178:PRO:HG3	2.42	0.55
1:D:32:CYS:HA	1:D:35:TYR:CE1	2.42	0.55
3:F:129:LYS:HZ2	3:F:170:ARG:HH21	1.55	0.55
1:G:239:TYR:O	1:G:248:SER:OG	2.20	0.55
2:N:69:LEU:HD13	2:N:174:LEU:HD22	1.87	0.55
1:D:137:THR:HG22	1:D:151:LYS:HG3	1.88	0.54
1:J:137:THR:HG22	1:J:151:LYS:HG3	1.88	0.54
3:L:8:TRP:CD2	3:L:178:PRO:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:LYS:HB3	1:J:155:ASP:OD2	2.06	0.54
2:K:147:TRP:HA	2:K:150:ILE:HD12	1.89	0.54
3:O:8:TRP:CD2	3:O:178:PRO:HG3	2.42	0.54
3:R:8:TRP:CD2	3:R:178:PRO:HG3	2.43	0.54
1:M:239:TYR:O	1:M:248:SER:OG	2.20	0.54
1:P:139:LYS:NZ	1:P:149:ASP:OD1	2.32	0.54
3:R:210:TYR:HB3	3:R:213:ARG:HG3	1.88	0.54
2:E:69:LEU:HD13	2:E:174:LEU:HD22	1.87	0.54
3:I:89:TYR:OH	3:I:115:ILE:O	2.23	0.54
1:M:139:LYS:NZ	1:M:149:ASP:OD1	2.32	0.54
2:N:147:TRP:HA	2:N:150:ILE:HD12	1.89	0.54
1:A:153:LYS:HB3	1:A:155:ASP:OD2	2.06	0.54
1:D:153:LYS:HB3	1:D:155:ASP:OD2	2.06	0.54
3:F:240:PRO:HA	3:F:267:HIS:HA	1.89	0.54
2:H:147:TRP:HA	2:H:150:ILE:HD12	1.89	0.54
3:I:210:TYR:HB3	3:I:213:ARG:HG3	1.88	0.54
1:A:162:VAL:HB	1:A:164:TYR:CE1	2.43	0.54
1:D:162:VAL:HB	1:D:164:TYR:CE1	2.43	0.54
2:H:173:LEU:HG	3:I:229:HIS:CE1	2.42	0.54
3:L:240:PRO:HA	3:L:267:HIS:HA	1.89	0.54
1:M:32:CYS:HA	1:M:35:TYR:CE1	2.42	0.54
2:B:173:LEU:HG	3:C:229:HIS:CE1	2.43	0.54
3:O:4:CYS:HB3	3:O:55:HIS:NE2	2.22	0.54
1:P:162:VAL:HB	1:P:164:TYR:CE1	2.43	0.54
1:P:239:TYR:O	1:P:248:SER:OG	2.20	0.54
3:R:4:CYS:HB3	3:R:55:HIS:NE2	2.22	0.54
1:A:155:ASP:OD2	1:A:155:ASP:N	2.41	0.54
3:F:8:TRP:CD2	3:F:178:PRO:HG3	2.42	0.54
1:M:166:THR:O	2:N:111:ARG:NH1	2.41	0.54
1:G:58:THR:N	1:G:66:SER:O	2.38	0.54
1:G:155:ASP:OD2	1:G:155:ASP:N	2.41	0.54
1:A:74:SER:HA	3:L:264:GLY:O	2.08	0.53
3:F:264:GLY:HA2	1:G:73:ALA:O	2.08	0.53
2:H:173:LEU:HG	3:I:229:HIS:ND1	2.23	0.53
3:I:126:TYR:HH	3:I:146:TRP:HE3	1.54	0.53
1:J:32:CYS:HA	1:J:35:TYR:CE1	2.42	0.53
1:J:155:ASP:OD2	1:J:155:ASP:N	2.41	0.53
2:Q:147:TRP:HA	2:Q:150:ILE:HD12	1.89	0.53
1:M:162:VAL:HB	1:M:164:TYR:CE1	2.43	0.53
3:C:4:CYS:HB3	3:C:55:HIS:NE2	2.22	0.53
3:O:240:PRO:HA	3:O:267:HIS:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HG12	2:B:118:ARG:NH2	2.16	0.53
2:N:28:LEU:HD21	2:N:112:LEU:HD13	1.91	0.53
3:R:173:VAL:O	3:R:184:ARG:N	2.38	0.53
2:B:147:TRP:HA	2:B:150:ILE:HD12	1.89	0.53
3:C:240:PRO:HA	3:C:267:HIS:HA	1.89	0.53
1:G:139:LYS:NZ	1:G:149:ASP:OD1	2.32	0.53
2:E:147:TRP:HA	2:E:150:ILE:HD12	1.89	0.53
1:J:170:VAL:HG12	2:K:118:ARG:HH21	1.72	0.53
1:J:259:ARG:NH2	3:L:260:ASP:OD2	2.37	0.53
1:G:162:VAL:HB	1:G:164:TYR:CE1	2.43	0.53
3:I:8:TRP:CD2	3:I:178:PRO:HG3	2.42	0.53
2:K:28:LEU:HD21	2:K:112:LEU:HD13	1.91	0.53
2:K:48:ASP:HB3	3:L:168:GLN:OE1	2.09	0.53
2:Q:28:LEU:HD21	2:Q:112:LEU:HD13	1.91	0.53
2:H:46:ASP:CG	1:J:82:ASN:HD22	2.11	0.53
2:B:46:ASP:CG	1:D:82:ASN:ND2	2.63	0.53
2:H:28:LEU:HD21	2:H:112:LEU:HD13	1.91	0.53
1:J:162:VAL:HB	1:J:164:TYR:CE1	2.43	0.53
1:P:212:GLU:OE2	3:R:243:HIS:CG	2.62	0.53
2:H:88:GLN:HG2	2:H:92:ARG:NH1	2.24	0.53
1:A:28:LEU:HD21	1:A:83:ILE:HG21	1.92	0.52
2:E:88:GLN:HG2	2:E:92:ARG:NH1	2.24	0.52
1:M:155:ASP:OD2	1:M:155:ASP:N	2.41	0.52
2:N:48:ASP:HB3	3:O:168:GLN:OE1	2.09	0.52
1:P:28:LEU:HD21	1:P:83:ILE:HG21	1.91	0.52
1:D:28:LEU:HD21	1:D:83:ILE:HG21	1.92	0.52
1:D:155:ASP:OD2	1:D:155:ASP:N	2.41	0.52
3:L:173:VAL:O	3:L:184:ARG:N	2.38	0.52
1:M:28:LEU:HD21	1:M:83:ILE:HG21	1.92	0.52
1:A:58:THR:N	1:A:66:SER:O	2.38	0.52
1:A:167:VAL:HG11	2:B:114:ARG:CD	2.40	0.52
2:B:88:GLN:HG2	2:B:92:ARG:NH1	2.24	0.52
1:G:28:LEU:HD21	1:G:83:ILE:HG21	1.92	0.52
1:J:28:LEU:HD21	1:J:83:ILE:HG21	1.91	0.52
2:K:88:GLN:HG2	2:K:92:ARG:NH1	2.24	0.52
2:N:88:GLN:HG2	2:N:92:ARG:NH1	2.24	0.52
2:B:28:LEU:HD21	2:B:112:LEU:HD13	1.91	0.52
2:B:61:ALA:HA	3:C:164:GLU:HA	1.92	0.52
2:E:28:LEU:HD21	2:E:112:LEU:HD13	1.91	0.52
2:N:162:LEU:HD22	3:O:166:TRP:CD1	2.45	0.52
1:D:47:THR:HG21	1:D:79:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:41:ASN:OD1	1:J:59:ILE:HD13	2.10	0.52
1:J:47:THR:HG21	1:J:79:LEU:HD12	1.92	0.52
1:P:155:ASP:OD2	1:P:155:ASP:N	2.41	0.52
1:G:47:THR:HG21	1:G:79:LEU:HD12	1.92	0.51
1:A:73:ALA:HB3	3:L:292:THR:OG1	2.09	0.51
1:P:47:THR:HG21	1:P:79:LEU:HD12	1.92	0.51
1:D:41:ASN:OD1	1:D:59:ILE:HD13	2.10	0.51
1:M:167:VAL:HG11	2:N:114:ARG:CD	2.40	0.51
2:Q:88:GLN:HG2	2:Q:92:ARG:NH1	2.24	0.51
3:F:264:GLY:O	1:G:74:SER:HA	2.11	0.51
1:G:41:ASN:OD1	1:G:59:ILE:HD13	2.10	0.51
2:K:162:LEU:CD2	3:L:166:TRP:HD1	2.24	0.51
3:L:45:LEU:O	3:L:47:GLN:NE2	2.42	0.51
1:M:47:THR:HG21	1:M:79:LEU:HD12	1.92	0.51
1:P:216:SER:C	1:P:267:LEU:HD23	2.31	0.51
1:A:216:SER:C	1:A:267:LEU:HD23	2.31	0.51
3:L:128:LYS:NZ	3:L:129:LYS:O	2.44	0.51
1:A:41:ASN:OD1	1:A:59:ILE:HD13	2.10	0.51
3:C:93:ARG:CD	1:D:88:GLN:NE2	2.65	0.51
3:C:128:LYS:NZ	3:C:129:LYS:O	2.44	0.51
3:I:290:TRP:HB2	1:M:50:PHE:CD1	2.45	0.51
1:M:207:SER:HB2	1:M:221:THR:OG1	2.11	0.51
1:M:216:SER:C	1:M:267:LEU:HD23	2.31	0.51
1:P:41:ASN:OD1	1:P:59:ILE:HD13	2.10	0.51
1:A:47:THR:HG21	1:A:79:LEU:HD12	1.92	0.51
3:O:45:LEU:O	3:O:47:GLN:NE2	2.42	0.51
3:O:128:LYS:NZ	3:O:129:LYS:O	2.44	0.51
3:I:128:LYS:NZ	3:I:129:LYS:O	2.44	0.50
3:I:151:ASP:OD1	3:I:151:ASP:N	2.44	0.50
1:A:207:SER:HB2	1:A:221:THR:OG1	2.11	0.50
1:G:216:SER:C	1:G:267:LEU:HD23	2.31	0.50
1:J:216:SER:C	1:J:267:LEU:HD23	2.31	0.50
3:O:151:ASP:OD1	3:O:151:ASP:N	2.44	0.50
1:D:212:GLU:OE1	3:F:243:HIS:CD2	2.65	0.50
1:G:207:SER:HB2	1:G:221:THR:OG1	2.11	0.50
3:I:43:PRO:HD2	3:I:44:LYS:HZ2	1.77	0.50
1:M:41:ASN:OD1	1:M:59:ILE:HD13	2.10	0.50
1:P:212:GLU:OE1	3:R:243:HIS:HA	2.12	0.50
1:G:88:GLN:HE21	3:L:93:ARG:HD2	1.76	0.50
1:J:22:PHE:HB3	1:J:72:ILE:HD11	1.93	0.50
1:J:208:VAL:HG21	1:J:296:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:ASP:N	3:L:151:ASP:OD1	2.44	0.50
1:P:22:PHE:HB3	1:P:72:ILE:HD11	1.93	0.50
1:A:208:VAL:HG21	1:A:296:SER:O	2.11	0.50
3:F:151:ASP:OD1	3:F:151:ASP:N	2.44	0.50
1:J:207:SER:HB2	1:J:221:THR:OG1	2.11	0.50
2:B:46:ASP:CB	1:D:92:ASN:HB2	2.34	0.50
3:F:106:PHE:CZ	3:F:160:VAL:HG21	2.47	0.50
3:F:128:LYS:NZ	3:F:129:LYS:O	2.44	0.50
1:A:139:LYS:NZ	1:A:149:ASP:OD1	2.32	0.50
1:M:92:ASN:OD1	2:Q:147:TRP:HZ2	1.94	0.50
2:B:42:LYS:NZ	3:O:242:GLN:OE1	2.43	0.50
1:G:22:PHE:HB3	1:G:72:ILE:HD11	1.93	0.50
1:M:22:PHE:HB3	1:M:72:ILE:HD11	1.93	0.50
1:A:22:PHE:HB3	1:A:72:ILE:HD11	1.93	0.49
2:E:33:ARG:NH2	3:F:278:ASP:HB3	2.27	0.49
1:P:207:SER:HB2	1:P:221:THR:OG1	2.11	0.49
1:D:14:PRO:HG3	1:D:22:PHE:CZ	2.47	0.49
1:J:14:PRO:HG3	1:J:22:PHE:CZ	2.48	0.49
3:R:45:LEU:O	3:R:47:GLN:NE2	2.42	0.49
3:C:93:ARG:O	3:C:113:SER:OG	2.23	0.49
1:D:216:SER:C	1:D:267:LEU:HD23	2.31	0.49
3:I:106:PHE:CZ	3:I:160:VAL:HG21	2.47	0.49
3:R:128:LYS:NZ	3:R:129:LYS:O	2.44	0.49
3:L:268:ALA:HB2	3:L:290:TRP:CZ2	2.48	0.49
3:R:151:ASP:OD2	3:R:157:ARG:NH1	2.46	0.49
1:D:22:PHE:HB3	1:D:72:ILE:HD11	1.93	0.49
6:G:401:NAG:H83	6:G:401:NAG:H3	1.94	0.49
6:J:401:NAG:H3	6:J:401:NAG:H83	1.94	0.49
1:M:208:VAL:HG21	1:M:296:SER:O	2.11	0.49
3:O:106:PHE:CZ	3:O:160:VAL:HG21	2.47	0.49
3:O:268:ALA:HB2	3:O:290:TRP:CZ2	2.48	0.49
2:B:64:LEU:HD11	2:B:166:TRP:CD1	2.48	0.49
1:D:263:THR:HG22	3:F:260:ASP:O	2.13	0.49
3:I:151:ASP:OD2	3:I:157:ARG:NH1	2.46	0.49
2:K:64:LEU:HD11	2:K:166:TRP:CD1	2.48	0.49
1:P:14:PRO:HG3	1:P:22:PHE:CZ	2.48	0.49
1:D:207:SER:HB2	1:D:221:THR:OG1	2.12	0.49
3:F:268:ALA:HB2	3:F:290:TRP:CZ2	2.48	0.49
1:G:48:ASN:OD1	1:G:78:GLN:HB2	2.13	0.49
1:G:208:VAL:HG21	1:G:296:SER:O	2.12	0.49
2:H:64:LEU:HD11	2:H:166:TRP:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:14:PRO:HG3	1:M:22:PHE:CZ	2.48	0.49
1:M:170:VAL:HG12	2:N:118:ARG:HH21	1.77	0.49
3:O:240:PRO:HB2	3:O:243:HIS:CD2	2.48	0.49
1:P:48:ASN:OD1	1:P:78:GLN:HB2	2.13	0.49
1:P:208:VAL:HG21	1:P:296:SER:O	2.12	0.49
3:R:240:PRO:HB2	3:R:243:HIS:CD2	2.48	0.49
3:R:268:ALA:HB2	3:R:290:TRP:CZ2	2.48	0.49
3:C:268:ALA:HB2	3:C:290:TRP:CZ2	2.48	0.49
1:D:267:LEU:HD12	1:D:273:TYR:CD2	2.48	0.49
6:D:401:NAG:H83	6:D:401:NAG:H3	1.94	0.49
3:F:151:ASP:OD2	3:F:157:ARG:NH1	2.46	0.49
1:J:48:ASN:OD1	1:J:78:GLN:HB2	2.13	0.49
3:O:152:PRO:O	3:O:153:LEU:HG	2.13	0.49
2:Q:64:LEU:HD11	2:Q:166:TRP:CD1	2.48	0.49
3:C:151:ASP:OD2	3:C:157:ARG:NH1	2.46	0.49
3:I:268:ALA:HB2	3:I:290:TRP:CZ2	2.48	0.49
3:L:151:ASP:OD2	3:L:157:ARG:NH1	2.46	0.49
3:R:106:PHE:CZ	3:R:160:VAL:HG21	2.47	0.49
1:D:208:VAL:HG21	1:D:296:SER:O	2.11	0.48
3:I:240:PRO:HB2	3:I:243:HIS:CD2	2.48	0.48
6:M:401:NAG:H3	6:M:401:NAG:H83	1.94	0.48
1:A:14:PRO:HG3	1:A:22:PHE:CZ	2.48	0.48
3:C:93:ARG:HH11	1:D:88:GLN:CG	2.26	0.48
3:C:152:PRO:O	3:C:153:LEU:HG	2.13	0.48
2:E:64:LEU:HD11	2:E:166:TRP:CD1	2.48	0.48
2:N:64:LEU:HD11	2:N:166:TRP:CD1	2.48	0.48
1:P:267:LEU:HD12	1:P:273:TYR:CD2	2.48	0.48
1:A:261:SER:OG	3:C:247:SER:OG	2.29	0.48
3:F:240:PRO:HB2	3:F:243:HIS:CD2	2.48	0.48
1:J:267:LEU:HD12	1:J:273:TYR:CD2	2.48	0.48
3:L:106:PHE:CZ	3:L:160:VAL:HG21	2.47	0.48
1:M:48:ASN:OD1	1:M:78:GLN:HB2	2.13	0.48
1:A:26:CYS:HB2	1:A:45:TRP:CH2	2.48	0.48
1:A:218:LEU:O	1:A:264:VAL:N	2.46	0.48
2:E:107:THR:O	2:E:111:ARG:HG2	2.14	0.48
1:G:14:PRO:HG3	1:G:22:PHE:CZ	2.47	0.48
1:J:26:CYS:HB2	1:J:45:TRP:CH2	2.48	0.48
1:P:26:CYS:HB2	1:P:45:TRP:CH2	2.48	0.48
1:A:48:ASN:OD1	1:A:78:GLN:HB2	2.13	0.48
3:C:106:PHE:CZ	3:C:160:VAL:HG21	2.47	0.48
3:F:143:THR:HA	3:F:146:TRP:CZ2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:143:THR:HA	3:I:146:TRP:CZ2	2.49	0.48
3:L:143:THR:HA	3:L:146:TRP:CZ2	2.49	0.48
3:L:240:PRO:HB2	3:L:243:HIS:CD2	2.48	0.48
1:A:267:LEU:HD12	1:A:273:TYR:CD2	2.48	0.48
3:C:240:PRO:HB2	3:C:243:HIS:CD2	2.48	0.48
1:D:26:CYS:HB2	1:D:45:TRP:CH2	2.48	0.48
3:F:45:LEU:O	3:F:47:GLN:NE2	2.42	0.48
1:J:217:ILE:O	1:J:217:ILE:HD12	2.14	0.48
1:M:94:TYR:CZ	2:Q:147:TRP:HB3	2.49	0.48
1:M:267:LEU:HD12	1:M:273:TYR:CD2	2.48	0.48
6:A:401:NAG:H3	6:A:401:NAG:H83	1.94	0.48
2:B:107:THR:O	2:B:111:ARG:HG2	2.14	0.48
3:C:151:ASP:OD1	3:C:151:ASP:N	2.44	0.48
1:G:26:CYS:HB2	1:G:45:TRP:CH2	2.48	0.48
3:O:151:ASP:OD2	3:O:157:ARG:NH1	2.46	0.48
3:F:152:PRO:O	3:F:153:LEU:HG	2.13	0.48
1:G:217:ILE:HD12	1:G:217:ILE:O	2.14	0.48
1:G:267:LEU:HD12	1:G:273:TYR:CD2	2.48	0.48
2:H:107:THR:O	2:H:111:ARG:HG2	2.14	0.48
2:K:107:THR:O	2:K:111:ARG:HG2	2.14	0.48
3:L:152:PRO:O	3:L:153:LEU:HG	2.13	0.48
1:M:26:CYS:HB2	1:M:45:TRP:CH2	2.48	0.48
1:M:217:ILE:HD12	1:M:217:ILE:O	2.14	0.48
3:R:228:PRO:HG2	3:R:229:HIS:CE1	2.49	0.48
1:D:43:ILE:HD12	1:D:65:SER:HB3	1.96	0.48
1:D:48:ASN:OD1	1:D:78:GLN:HB2	2.13	0.48
1:G:43:ILE:HD12	1:G:65:SER:HB3	1.96	0.48
2:H:59:MET:SD	3:I:128:LYS:HE3	2.53	0.48
3:I:152:PRO:O	3:I:153:LEU:HG	2.13	0.48
3:L:213:ARG:HA	3:L:258:ILE:O	2.14	0.48
1:P:217:ILE:HD12	1:P:217:ILE:O	2.14	0.48
6:P:401:NAG:H83	6:P:401:NAG:H3	1.94	0.48
1:A:217:ILE:HD12	1:A:217:ILE:O	2.14	0.48
1:M:167:VAL:HG21	2:N:114:ARG:NH2	2.29	0.48
3:O:228:PRO:HG2	3:O:229:HIS:CE1	2.49	0.48
1:P:40:ALA:HA	1:P:43:ILE:HD12	1.96	0.48
1:D:40:ALA:HA	1:D:43:ILE:HD12	1.96	0.47
3:O:143:THR:HA	3:O:146:TRP:CZ2	2.49	0.47
3:O:213:ARG:HA	3:O:258:ILE:O	2.14	0.47
3:R:27:PRO:HG2	3:R:81:GLY:HA3	1.96	0.47
1:D:217:ILE:HD12	1:D:217:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:43:PRO:HD2	3:F:44:LYS:HZ2	1.79	0.47
3:I:213:ARG:HA	3:I:258:ILE:O	2.14	0.47
3:I:228:PRO:HG2	3:I:229:HIS:CE1	2.49	0.47
3:C:27:PRO:HG2	3:C:81:GLY:HA3	1.96	0.47
3:C:143:THR:HA	3:C:146:TRP:CZ2	2.49	0.47
1:D:50:PHE:CD1	3:O:290:TRP:CD1	3.03	0.47
1:D:218:LEU:O	1:D:264:VAL:N	2.46	0.47
1:D:219:LYS:NZ	3:F:247:SER:HB2	2.30	0.47
1:G:40:ALA:HA	1:G:43:ILE:HD12	1.96	0.47
1:J:58:THR:N	1:J:66:SER:O	2.38	0.47
2:N:33:ARG:NH2	3:O:278:ASP:O	2.48	0.47
3:R:152:PRO:O	3:R:153:LEU:HG	2.13	0.47
3:R:213:ARG:HA	3:R:258:ILE:O	2.14	0.47
3:C:143:THR:HA	3:C:146:TRP:HZ2	1.80	0.47
3:C:228:PRO:HG2	3:C:229:HIS:CE1	2.49	0.47
1:M:40:ALA:HA	1:M:43:ILE:HD12	1.96	0.47
2:Q:107:THR:O	2:Q:111:ARG:HG2	2.14	0.47
3:R:143:THR:HA	3:R:146:TRP:CZ2	2.49	0.47
3:C:213:ARG:HA	3:C:258:ILE:O	2.14	0.47
2:E:169:ARG:O	2:E:173:LEU:HD12	2.15	0.47
3:L:228:PRO:HG2	3:L:229:HIS:CE1	2.49	0.47
2:N:107:THR:O	2:N:111:ARG:HG2	2.14	0.47
1:A:40:ALA:HA	1:A:43:ILE:HD12	1.96	0.47
1:J:40:ALA:HA	1:J:43:ILE:HD12	1.96	0.47
3:O:185:LEU:HD13	1:P:86:PHE:CD1	2.50	0.47
1:A:28:LEU:HD11	1:A:43:ILE:HD11	1.97	0.47
1:A:43:ILE:HD12	1:A:65:SER:HB3	1.96	0.47
3:C:53:LEU:O	3:C:53:LEU:HG	2.15	0.47
3:F:213:ARG:HA	3:F:258:ILE:O	2.14	0.47
3:I:27:PRO:HG2	3:I:81:GLY:HA3	1.96	0.47
3:I:129:LYS:NZ	3:I:170:ARG:HH21	2.13	0.47
1:J:28:LEU:HD11	1:J:43:ILE:HD11	1.97	0.47
1:J:43:ILE:HD12	1:J:65:SER:HB3	1.96	0.47
3:L:53:LEU:HG	3:L:53:LEU:O	2.15	0.47
3:L:129:LYS:NZ	3:L:170:ARG:HH21	2.13	0.47
1:M:28:LEU:HD11	1:M:43:ILE:HD11	1.97	0.47
1:P:114:VAL:HG13	1:P:166:THR:HG21	1.97	0.47
2:B:46:ASP:HB3	1:D:92:ASN:CB	2.36	0.47
3:F:27:PRO:HG2	3:F:81:GLY:HA3	1.96	0.47
3:F:129:LYS:NZ	3:F:170:ARG:HH21	2.13	0.47
2:H:169:ARG:O	2:H:173:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:169:ARG:O	2:K:173:LEU:HD12	2.15	0.47
3:L:27:PRO:HG2	3:L:81:GLY:HA3	1.96	0.47
3:I:143:THR:HA	3:I:146:TRP:HZ2	1.79	0.47
1:M:43:ILE:HD12	1:M:65:SER:HB3	1.96	0.47
1:P:28:LEU:HD11	1:P:43:ILE:HD11	1.97	0.47
3:R:53:LEU:O	3:R:53:LEU:HG	2.15	0.47
1:A:114:VAL:HG13	1:A:166:THR:HG21	1.97	0.47
2:B:169:ARG:O	2:B:173:LEU:HD12	2.15	0.47
3:C:241:ALA:HB2	3:C:290:TRP:CZ3	2.50	0.47
3:F:228:PRO:HG2	3:F:229:HIS:CE1	2.49	0.47
3:I:53:LEU:HG	3:I:53:LEU:O	2.15	0.47
3:O:27:PRO:HG2	3:O:81:GLY:HA3	1.96	0.47
3:O:53:LEU:O	3:O:53:LEU:HG	2.15	0.47
1:P:112:CYS:HA	1:P:122:CYS:HA	1.97	0.47
2:Q:169:ARG:O	2:Q:173:LEU:HD12	2.15	0.47
3:F:143:THR:HA	3:F:146:TRP:HZ2	1.80	0.46
3:L:43:PRO:HD2	3:L:44:LYS:HZ2	1.79	0.46
1:M:112:CYS:HA	1:M:122:CYS:HA	1.97	0.46
1:P:43:ILE:HD12	1:P:65:SER:HB3	1.96	0.46
3:R:129:LYS:NZ	3:R:170:ARG:HH21	2.13	0.46
3:R:151:ASP:OD1	3:R:151:ASP:N	2.44	0.46
1:A:112:CYS:HA	1:A:122:CYS:HA	1.97	0.46
3:F:241:ALA:HB2	3:F:290:TRP:CZ3	2.50	0.46
1:G:114:VAL:HG13	1:G:166:THR:HG21	1.97	0.46
3:I:45:LEU:O	3:I:47:GLN:NE2	2.42	0.46
1:J:112:CYS:HA	1:J:122:CYS:HA	1.97	0.46
3:R:143:THR:HA	3:R:146:TRP:HZ2	1.80	0.46
1:M:114:VAL:HG13	1:M:166:THR:HG21	1.97	0.46
3:O:185:LEU:HD22	1:P:86:PHE:CE1	2.51	0.46
2:N:169:ARG:O	2:N:173:LEU:HD12	2.15	0.46
3:F:53:LEU:HG	3:F:53:LEU:O	2.15	0.46
1:G:28:LEU:HD11	1:G:43:ILE:HD11	1.97	0.46
3:L:143:THR:HA	3:L:146:TRP:HZ2	1.79	0.46
3:C:125:SER:O	3:C:172:ASN:HB3	2.16	0.46
3:C:129:LYS:NZ	3:C:170:ARG:HH21	2.13	0.46
1:D:114:VAL:HG13	1:D:166:THR:HG21	1.97	0.46
3:F:125:SER:O	3:F:172:ASN:HB3	2.16	0.46
1:G:112:CYS:HA	1:G:122:CYS:HA	1.98	0.46
3:O:125:SER:O	3:O:172:ASN:HB3	2.16	0.46
1:P:113:ILE:HG12	1:P:287:TYR:CE1	2.51	0.46
2:B:162:LEU:HD22	3:C:166:TRP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LYS:HB2	1:D:54:LYS:HE2	1.67	0.46
1:D:113:ILE:HG12	1:D:287:TYR:CE1	2.51	0.46
3:I:241:ALA:HB2	3:I:290:TRP:CZ3	2.50	0.46
1:J:114:VAL:HG13	1:J:166:THR:HG21	1.97	0.46
3:O:143:THR:HA	3:O:146:TRP:HZ2	1.79	0.46
1:P:116:GLU:OE1	1:P:227:ILE:HB	2.16	0.46
1:P:262:PHE:CD1	3:R:260:ASP:HB3	2.50	0.46
1:D:116:GLU:OE1	1:D:227:ILE:HB	2.16	0.46
1:M:54:LYS:HB2	1:M:54:LYS:HE2	1.67	0.46
3:O:129:LYS:NZ	3:O:170:ARG:HH21	2.13	0.46
3:R:241:ALA:HB2	3:R:290:TRP:CZ3	2.50	0.46
1:D:28:LEU:HD11	1:D:43:ILE:HD11	1.97	0.46
2:E:98:LEU:HD21	2:E:150:ILE:HG12	1.98	0.46
2:K:98:LEU:HD21	2:K:150:ILE:HG12	1.98	0.46
2:B:98:LEU:HD21	2:B:150:ILE:HG12	1.98	0.46
3:C:45:LEU:O	3:C:47:GLN:NE2	2.42	0.46
1:D:112:CYS:HA	1:D:122:CYS:HA	1.97	0.46
1:G:113:ILE:HG12	1:G:287:TYR:CE1	2.51	0.46
3:L:125:SER:O	3:L:172:ASN:HB3	2.16	0.46
3:L:241:ALA:HB2	3:L:290:TRP:CZ3	2.50	0.46
1:M:116:GLU:OE1	1:M:227:ILE:HB	2.16	0.46
2:N:98:LEU:HD21	2:N:150:ILE:HG12	1.98	0.46
3:O:241:ALA:HB2	3:O:290:TRP:CZ3	2.50	0.46
1:G:218:LEU:O	1:G:264:VAL:N	2.46	0.45
2:H:98:LEU:HD21	2:H:150:ILE:HG12	1.98	0.45
1:P:218:LEU:O	1:P:264:VAL:N	2.45	0.45
1:A:27:VAL:HG12	1:A:64:ALA:CB	2.45	0.45
1:J:134:THR:HG22	1:J:180:ASN:CB	2.47	0.45
1:A:116:GLU:OE1	1:A:227:ILE:HB	2.16	0.45
1:G:116:GLU:OE1	1:G:227:ILE:HB	2.16	0.45
2:Q:98:LEU:HD21	2:Q:150:ILE:HG12	1.98	0.45
1:G:134:THR:HG22	1:G:180:ASN:CB	2.46	0.45
1:M:94:TYR:CE1	2:Q:147:TRP:HB3	2.52	0.45
1:A:113:ILE:HG12	1:A:287:TYR:CE1	2.51	0.45
1:M:113:ILE:HG12	1:M:287:TYR:CE1	2.51	0.45
3:O:93:ARG:HD2	1:P:88:GLN:NE2	2.32	0.45
3:R:43:PRO:HD2	3:R:44:LYS:HZ2	1.82	0.45
1:D:73:ALA:O	3:O:264:GLY:HA2	2.16	0.45
3:I:125:SER:O	3:I:172:ASN:HB3	2.16	0.45
1:M:135:ASN:OD1	6:M:402:NAG:N2	2.50	0.45
1:J:135:ASN:OD1	6:J:402:NAG:N2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:263:THR:HG22	3:L:260:ASP:HB2	1.99	0.45
3:L:44:LYS:H	3:L:44:LYS:HD2	1.82	0.45
1:P:135:ASN:OD1	6:P:402:NAG:N2	2.50	0.45
1:D:135:ASN:OD1	6:D:402:NAG:N2	2.50	0.45
1:G:27:VAL:HG12	1:G:64:ALA:CB	2.45	0.45
3:I:151:ASP:CG	3:I:152:PRO:HD3	2.38	0.45
1:M:92:ASN:OD1	2:Q:147:TRP:CZ2	2.70	0.45
2:N:162:LEU:HD22	3:O:166:TRP:HD1	1.80	0.45
2:Q:80:LEU:HB2	2:Q:116:LEU:HD21	1.99	0.45
5:T:2:NAG:H4	5:T:3:BMA:H2	1.38	0.45
2:E:80:LEU:HB2	2:E:116:LEU:HD21	1.99	0.44
2:H:168:VAL:HG11	3:I:277:LEU:HD21	1.98	0.44
3:I:44:LYS:H	3:I:44:LYS:HD2	1.82	0.44
1:J:113:ILE:HG12	1:J:287:TYR:CE1	2.51	0.44
1:M:27:VAL:HG12	1:M:64:ALA:CB	2.45	0.44
1:M:92:ASN:N	2:Q:46:ASP:O	2.46	0.44
3:O:126:TYR:HH	3:O:146:TRP:HE3	1.64	0.44
1:P:87:GLY:O	1:P:88:GLN:HG3	2.17	0.44
3:R:125:SER:O	3:R:172:ASN:HB3	2.16	0.44
1:G:46:LYS:HE2	1:G:51:THR:HG22	1.99	0.44
3:L:48:GLY:HA3	3:L:58:VAL:HG22	1.99	0.44
1:M:88:GLN:NE2	3:R:184:ARG:HA	2.32	0.44
3:R:44:LYS:HD2	3:R:44:LYS:H	1.82	0.44
1:A:87:GLY:O	1:A:88:GLN:HG3	2.17	0.44
1:G:135:ASN:OD1	6:G:402:NAG:N2	2.50	0.44
2:H:80:LEU:HB2	2:H:116:LEU:HD21	1.99	0.44
2:H:169:ARG:NH1	3:I:277:LEU:HD12	2.33	0.44
1:J:46:LYS:HE2	1:J:51:THR:HG22	2.00	0.44
1:J:116:GLU:OE1	1:J:227:ILE:HB	2.16	0.44
3:L:151:ASP:CG	3:L:152:PRO:HD3	2.38	0.44
1:M:46:LYS:HE2	1:M:51:THR:HG22	2.00	0.44
2:N:80:LEU:HB2	2:N:116:LEU:HD21	1.99	0.44
3:O:48:GLY:HA3	3:O:58:VAL:HG22	1.99	0.44
5:V:2:NAG:H4	5:V:3:BMA:H2	1.38	0.44
1:D:87:GLY:O	1:D:88:GLN:HG3	2.17	0.44
3:F:48:GLY:HA3	3:F:58:VAL:HG22	1.99	0.44
1:M:218:LEU:O	1:M:264:VAL:N	2.46	0.44
1:A:46:LYS:HE2	1:A:51:THR:HG22	1.99	0.44
3:C:48:GLY:HA3	3:C:58:VAL:HG22	1.99	0.44
1:J:27:VAL:HG12	1:J:64:ALA:CB	2.45	0.44
1:J:54:LYS:HE2	1:J:54:LYS:HB2	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:GLU:OE2	6:M:402:NAG:H2	2.17	0.44
1:A:50:PHE:CD1	3:L:290:TRP:CD1	3.04	0.44
1:A:133:GLU:OE2	6:A:402:NAG:H2	2.18	0.44
3:C:44:LYS:H	3:C:44:LYS:HD2	1.82	0.44
3:C:151:ASP:CG	3:C:152:PRO:HD3	2.38	0.44
1:J:133:GLU:OE2	6:J:402:NAG:H2	2.18	0.44
1:M:87:GLY:O	1:M:88:GLN:HG3	2.17	0.44
1:P:46:LYS:HE2	1:P:51:THR:HG22	2.00	0.44
3:R:165:PHE:HB3	3:R:166:TRP:CE3	2.53	0.44
1:D:133:GLU:OE2	6:D:402:NAG:H2	2.18	0.44
2:B:80:LEU:HB2	2:B:116:LEU:HD21	1.99	0.44
3:C:198:PRO:HG3	3:C:284:THR:HG23	2.00	0.44
1:D:46:LYS:HE2	1:D:51:THR:HG22	2.00	0.44
1:D:259:ARG:NH2	3:F:260:ASP:OD2	2.50	0.44
3:F:44:LYS:H	3:F:44:LYS:HD2	1.82	0.44
1:G:28:LEU:CD1	1:G:43:ILE:HD11	2.48	0.44
2:H:39:LEU:HD13	2:H:101:LEU:HD11	2.00	0.44
1:J:87:GLY:O	1:J:88:GLN:HG3	2.17	0.44
3:O:184:ARG:HA	1:P:88:GLN:CD	2.38	0.44
1:P:28:LEU:CD1	1:P:43:ILE:HD11	2.48	0.44
1:A:135:ASN:OD1	6:A:402:NAG:N2	2.50	0.44
2:E:39:LEU:HD13	2:E:101:LEU:HD11	2.00	0.44
3:L:198:PRO:HG3	3:L:284:THR:HG23	2.00	0.44
1:M:259:ARG:NH2	3:O:260:ASP:OD2	2.48	0.44
3:O:151:ASP:CG	3:O:152:PRO:HD3	2.38	0.44
2:Q:158:GLY:O	2:Q:161:HIS:ND1	2.50	0.44
3:I:165:PHE:HB3	3:I:166:TRP:CE3	2.53	0.43
2:K:169:ARG:HG2	3:L:229:HIS:O	2.18	0.43
3:O:44:LYS:H	3:O:44:LYS:HD2	1.82	0.43
3:R:151:ASP:CG	3:R:152:PRO:HD3	2.38	0.43
1:G:167:VAL:HG11	2:H:114:ARG:CD	2.48	0.43
3:O:165:PHE:HB3	3:O:166:TRP:CE3	2.53	0.43
1:A:70:THR:HG23	6:A:401:NAG:HN2	1.83	0.43
1:D:263:THR:CG2	3:F:260:ASP:O	2.66	0.43
3:F:151:ASP:CG	3:F:152:PRO:HD3	2.38	0.43
1:G:54:LYS:HB2	1:G:54:LYS:HE2	1.67	0.43
1:J:28:LEU:CD1	1:J:43:ILE:HD11	2.48	0.43
1:M:15:VAL:HG12	1:M:182:LEU:HD21	2.00	0.43
2:N:39:LEU:HD13	2:N:101:LEU:HD11	2.00	0.43
3:O:43:PRO:HD2	3:O:44:LYS:HZ2	1.84	0.43
1:A:54:LYS:HB2	1:A:54:LYS:HE2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:HD12	1:D:176:VAL:HG12	2.01	0.43
2:E:114:ARG:HA	2:E:117:ARG:NH1	2.34	0.43
2:K:39:LEU:HD13	2:K:101:LEU:HD11	2.00	0.43
2:K:80:LEU:HB2	2:K:116:LEU:HD21	1.99	0.43
1:P:133:GLU:OE2	6:P:402:NAG:H2	2.17	0.43
3:R:13:VAL:HG12	3:R:84:THR:HB	2.01	0.43
2:B:114:ARG:HA	2:B:117:ARG:NH1	2.34	0.43
3:I:175:GLU:N	3:I:182:SER:O	2.50	0.43
1:J:15:VAL:HG12	1:J:182:LEU:HD21	2.00	0.43
1:J:147:PHE:CE1	1:J:164:TYR:CD1	3.07	0.43
1:M:134:THR:HG22	1:M:180:ASN:CB	2.46	0.43
2:N:114:ARG:HA	2:N:117:ARG:NH1	2.34	0.43
2:Q:39:LEU:HD13	2:Q:101:LEU:HD11	2.00	0.43
3:R:48:GLY:HA3	3:R:58:VAL:HG22	1.99	0.43
1:G:87:GLY:O	1:G:88:GLN:HG3	2.17	0.43
2:H:158:GLY:O	2:H:161:HIS:ND1	2.50	0.43
3:C:165:PHE:HB3	3:C:166:TRP:CE3	2.53	0.43
2:E:158:GLY:O	2:E:161:HIS:ND1	2.50	0.43
1:G:15:VAL:HG12	1:G:182:LEU:HD21	2.00	0.43
1:G:147:PHE:CE1	1:G:164:TYR:CD1	3.07	0.43
1:M:147:PHE:CE1	1:M:164:TYR:CD1	3.07	0.43
1:M:156:THR:OG1	1:M:159:SER:HB2	2.19	0.43
1:A:28:LEU:CD1	1:A:43:ILE:HD11	2.48	0.43
1:G:170:VAL:HG12	2:H:118:ARG:HH21	1.84	0.43
2:K:114:ARG:HA	2:K:117:ARG:NH1	2.34	0.43
3:O:240:PRO:HG2	3:O:243:HIS:CE1	2.54	0.43
3:R:198:PRO:HG3	3:R:284:THR:HG23	2.00	0.43
3:C:43:PRO:HD2	3:C:44:LYS:HZ2	1.84	0.43
1:D:15:VAL:HG12	1:D:182:LEU:HD21	2.00	0.43
1:D:270:PHE:N	1:D:299:THR:HB	2.34	0.43
3:F:165:PHE:HB3	3:F:166:TRP:CE3	2.53	0.43
1:G:259:ARG:NH2	3:I:260:ASP:OD2	2.41	0.43
1:J:70:THR:HG23	6:J:401:NAG:HN2	1.83	0.43
1:J:83:ILE:CD1	1:J:85:THR:HG23	2.49	0.43
1:P:147:PHE:CE1	1:P:164:TYR:CD1	3.07	0.43
2:Q:69:LEU:HB2	2:Q:174:LEU:HD11	2.01	0.43
1:A:15:VAL:HG12	1:A:182:LEU:HD21	2.00	0.43
1:D:156:THR:OG1	1:D:159:SER:HB2	2.19	0.43
3:F:198:PRO:HG3	3:F:284:THR:HG23	2.00	0.43
1:G:133:GLU:OE2	6:G:402:NAG:H2	2.18	0.43
3:I:48:GLY:HA3	3:I:58:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:240:PRO:HG2	3:I:243:HIS:CE1	2.54	0.43
3:L:165:PHE:HB3	3:L:166:TRP:CE3	2.53	0.43
3:L:175:GLU:N	3:L:182:SER:O	2.50	0.43
1:A:83:ILE:CD1	1:A:85:THR:HG23	2.49	0.42
1:A:270:PHE:N	1:A:299:THR:HB	2.34	0.42
2:B:69:LEU:HB2	2:B:174:LEU:HD11	2.01	0.42
3:C:240:PRO:HG2	3:C:243:HIS:CE1	2.54	0.42
1:D:28:LEU:CD1	1:D:43:ILE:HD11	2.48	0.42
3:F:129:LYS:HZ3	3:F:170:ARG:HE	1.67	0.42
1:G:280:MET:HG2	1:G:288:TRP:CZ3	2.54	0.42
3:L:240:PRO:HG2	3:L:243:HIS:CE1	2.54	0.42
1:M:83:ILE:CD1	1:M:85:THR:HG23	2.49	0.42
1:P:83:ILE:CD1	1:P:85:THR:HG23	2.49	0.42
1:P:156:THR:OG1	1:P:159:SER:HB2	2.19	0.42
3:R:142:SER:O	3:R:146:TRP:NE1	2.52	0.42
1:D:83:ILE:CD1	1:D:85:THR:HG23	2.49	0.42
1:D:280:MET:HG2	1:D:288:TRP:CZ3	2.54	0.42
3:F:175:GLU:N	3:F:182:SER:O	2.50	0.42
1:G:274:VAL:HA	1:G:295:ALA:O	2.19	0.42
1:M:170:VAL:HG21	2:N:114:ARG:HH12	1.84	0.42
1:M:293:GLU:H	1:M:293:GLU:CD	2.23	0.42
1:P:70:THR:HG23	6:P:401:NAG:HN2	1.83	0.42
1:P:138:LEU:HD12	1:P:176:VAL:HG12	2.01	0.42
1:A:280:MET:HG2	1:A:288:TRP:CZ3	2.54	0.42
1:D:70:THR:HG23	6:D:401:NAG:HN2	1.83	0.42
2:H:114:ARG:HA	2:H:117:ARG:NH1	2.34	0.42
1:J:280:MET:HG2	1:J:288:TRP:CZ3	2.54	0.42
3:L:142:SER:O	3:L:146:TRP:NE1	2.52	0.42
1:M:28:LEU:CD1	1:M:43:ILE:HD11	2.48	0.42
3:O:142:SER:O	3:O:146:TRP:NE1	2.52	0.42
1:P:85:THR:O	1:P:87:GLY:N	2.53	0.42
1:P:274:VAL:HA	1:P:295:ALA:O	2.20	0.42
3:R:240:PRO:HG2	3:R:243:HIS:CE1	2.54	0.42
1:A:83:ILE:HD12	1:A:85:THR:HG23	2.02	0.42
1:P:89:LEU:HD23	1:P:89:LEU:HA	1.95	0.42
2:B:39:LEU:HD13	2:B:101:LEU:HD11	2.00	0.42
1:D:79:LEU:HD22	1:D:98:ILE:HD11	2.02	0.42
3:F:142:SER:O	3:F:146:TRP:NE1	2.52	0.42
1:G:70:THR:HG23	6:G:401:NAG:HN2	1.83	0.42
1:G:83:ILE:CD1	1:G:85:THR:HG23	2.49	0.42
1:G:83:ILE:HD12	1:G:85:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:THR:O	1:J:87:GLY:N	2.53	0.42
1:J:138:LEU:HD12	1:J:176:VAL:HG12	2.01	0.42
1:J:156:THR:OG1	1:J:159:SER:HB2	2.19	0.42
1:M:70:THR:HG23	6:M:401:NAG:HN2	1.83	0.42
1:M:138:LEU:HD12	1:M:176:VAL:HG12	2.01	0.42
1:P:15:VAL:HG12	1:P:182:LEU:HD21	2.00	0.42
1:P:83:ILE:HD12	1:P:85:THR:HG23	2.02	0.42
2:Q:114:ARG:HA	2:Q:117:ARG:NH1	2.34	0.42
3:R:175:GLU:N	3:R:182:SER:O	2.50	0.42
1:A:138:LEU:HD12	1:A:176:VAL:HG12	2.01	0.42
2:H:46:ASP:O	1:J:91:GLN:HA	2.19	0.42
1:M:280:MET:HG2	1:M:288:TRP:CZ3	2.54	0.42
3:O:13:VAL:HG12	3:O:84:THR:HB	2.01	0.42
3:R:3:PRO:HA	3:R:31:ALA:CB	2.43	0.42
1:A:134:THR:HG22	1:A:180:ASN:CB	2.47	0.42
1:A:147:PHE:CE1	1:A:164:TYR:CD1	3.07	0.42
3:C:13:VAL:HG12	3:C:84:THR:HB	2.01	0.42
1:D:134:THR:HG22	1:D:180:ASN:CB	2.46	0.42
3:F:22:VAL:HG22	3:F:59:LEU:HB2	2.02	0.42
2:H:69:LEU:HB2	2:H:174:LEU:HD11	2.01	0.42
3:I:13:VAL:HG12	3:I:84:THR:HB	2.01	0.42
2:K:69:LEU:HB2	2:K:174:LEU:HD11	2.01	0.42
1:M:270:PHE:N	1:M:299:THR:HB	2.34	0.42
3:O:12:GLY:O	3:O:83:VAL:HA	2.20	0.42
3:O:198:PRO:HG3	3:O:284:THR:HG23	2.00	0.42
1:P:280:MET:HG2	1:P:288:TRP:CZ3	2.54	0.42
1:A:274:VAL:HA	1:A:295:ALA:O	2.20	0.42
3:C:22:VAL:HG22	3:C:59:LEU:HB2	2.02	0.42
1:D:147:PHE:CE1	1:D:164:TYR:CD1	3.07	0.42
3:F:240:PRO:HG2	3:F:243:HIS:CE1	2.54	0.42
1:G:138:LEU:HD12	1:G:176:VAL:HG12	2.01	0.42
1:G:270:PHE:N	1:G:299:THR:HB	2.34	0.42
3:I:198:PRO:HG3	3:I:284:THR:HG23	2.00	0.42
1:M:274:VAL:HA	1:M:295:ALA:O	2.20	0.42
1:A:79:LEU:HD22	1:A:98:ILE:HD11	2.02	0.42
3:C:263:ALA:O	3:C:265:LEU:HD23	2.20	0.42
1:D:274:VAL:HA	1:D:295:ALA:O	2.20	0.42
3:F:13:VAL:HG12	3:F:84:THR:HB	2.01	0.42
3:L:13:VAL:HG12	3:L:84:THR:HB	2.01	0.42
1:P:79:LEU:HD22	1:P:98:ILE:HD11	2.02	0.42
1:P:212:GLU:OE1	3:R:243:HIS:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:LEU:HB2	2:E:174:LEU:HD11	2.01	0.42
1:G:156:THR:OG1	1:G:159:SER:HB2	2.19	0.42
3:I:22:VAL:HG22	3:I:59:LEU:HB2	2.02	0.42
1:J:270:PHE:N	1:J:299:THR:HB	2.34	0.42
1:A:156:THR:OG1	1:A:159:SER:HB2	2.19	0.41
1:A:293:GLU:H	1:A:293:GLU:CD	2.23	0.41
1:D:85:THR:O	1:D:87:GLY:N	2.53	0.41
1:M:85:THR:O	1:M:87:GLY:N	2.53	0.41
2:N:69:LEU:HB2	2:N:174:LEU:HD11	2.01	0.41
3:R:22:VAL:HG22	3:R:59:LEU:HB2	2.02	0.41
1:A:293:GLU:OE1	1:A:293:GLU:N	2.45	0.41
3:C:17:GLN:HB3	3:C:20:ARG:HG3	2.02	0.41
3:F:17:GLN:HB3	3:F:20:ARG:HG3	2.02	0.41
3:I:198:PRO:O	3:I:221:PRO:HB3	2.20	0.41
3:I:263:ALA:O	3:I:265:LEU:HD23	2.20	0.41
1:P:134:THR:HG22	1:P:180:ASN:CB	2.47	0.41
5:Z:2:NAG:H4	5:Z:3:BMA:H2	1.38	0.41
3:C:142:SER:O	3:C:146:TRP:NE1	2.52	0.41
3:C:198:PRO:O	3:C:221:PRO:HB3	2.20	0.41
1:D:236:ASN:HD22	1:D:236:ASN:HA	1.65	0.41
3:F:263:ALA:O	3:F:265:LEU:HD23	2.20	0.41
1:G:138:LEU:CD1	1:G:176:VAL:HG12	2.50	0.41
1:G:293:GLU:H	1:G:293:GLU:CD	2.22	0.41
1:J:218:LEU:O	1:J:264:VAL:N	2.46	0.41
2:K:132:PRO:HA	2:K:133:PRO:HD3	1.96	0.41
1:P:270:PHE:N	1:P:299:THR:HB	2.34	0.41
3:R:12:GLY:O	3:R:83:VAL:HA	2.20	0.41
2:B:57:LEU:HD21	2:B:75:ARG:HG2	2.02	0.41
2:E:57:LEU:HD21	2:E:75:ARG:HG2	2.02	0.41
1:J:274:VAL:HA	1:J:295:ALA:O	2.20	0.41
3:O:17:GLN:HB3	3:O:20:ARG:HG3	2.03	0.41
1:P:27:VAL:HG12	1:P:64:ALA:CB	2.45	0.41
3:R:198:PRO:O	3:R:221:PRO:HB3	2.20	0.41
1:A:267:LEU:HB2	1:A:273:TYR:CZ	2.56	0.41
3:C:12:GLY:O	3:C:83:VAL:HA	2.20	0.41
1:D:83:ILE:HD12	1:D:85:THR:HG23	2.02	0.41
1:D:138:LEU:CD1	1:D:176:VAL:HG12	2.51	0.41
1:D:293:GLU:H	1:D:293:GLU:CD	2.23	0.41
3:I:142:SER:O	3:I:146:TRP:NE1	2.52	0.41
1:J:83:ILE:HD12	1:J:85:THR:HG23	2.02	0.41
3:L:12:GLY:O	3:L:83:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:65:GLY:HA3	2:N:173:LEU:HD22	2.03	0.41
1:P:119:LYS:HD2	1:P:164:TYR:O	2.21	0.41
1:P:138:LEU:CD1	1:P:176:VAL:HG12	2.50	0.41
2:Q:92:ARG:HB2	2:Q:92:ARG:NH2	2.29	0.41
3:C:89:TYR:CZ	3:C:116:SER:HA	2.56	0.41
1:D:27:VAL:HG12	1:D:64:ALA:CB	2.45	0.41
1:G:85:THR:O	1:G:87:GLY:N	2.53	0.41
3:I:89:TYR:CZ	3:I:116:SER:HA	2.56	0.41
1:M:79:LEU:HD22	1:M:98:ILE:HD11	2.02	0.41
1:M:139:LYS:HE3	1:M:139:LYS:HB3	1.89	0.41
2:B:65:GLY:HA3	2:B:173:LEU:HD22	2.03	0.41
1:D:119:LYS:HD2	1:D:164:TYR:O	2.21	0.41
3:F:57:LEU:HD12	3:F:58:VAL:H	1.86	0.41
3:F:198:PRO:O	3:F:221:PRO:HB3	2.20	0.41
1:J:267:LEU:HB2	1:J:273:TYR:CZ	2.56	0.41
2:K:57:LEU:HD21	2:K:75:ARG:HG2	2.02	0.41
1:M:138:LEU:CD1	1:M:176:VAL:HG12	2.50	0.41
2:N:46:ASP:HB3	1:P:92:ASN:HB2	2.03	0.41
2:Q:169:ARG:NH2	3:R:275:ASP:OD1	2.54	0.41
3:C:3:PRO:HA	3:C:31:ALA:CB	2.43	0.41
3:C:264:GLY:O	1:P:74:SER:HA	2.20	0.41
1:G:86:PHE:HZ	1:G:89:LEU:HD12	1.86	0.41
1:G:119:LYS:HD2	1:G:164:TYR:O	2.21	0.41
2:H:57:LEU:HD21	2:H:75:ARG:HG2	2.02	0.41
3:I:185:LEU:HD22	1:J:86:PHE:CE1	2.55	0.41
1:J:79:LEU:HD22	1:J:98:ILE:HD11	2.02	0.41
1:J:86:PHE:HZ	1:J:89:LEU:HD12	1.86	0.41
3:L:22:VAL:HG22	3:L:59:LEU:HB2	2.02	0.41
2:N:57:LEU:HD21	2:N:75:ARG:HG2	2.02	0.41
2:N:158:GLY:O	2:N:161:HIS:ND1	2.50	0.41
1:P:86:PHE:HZ	1:P:89:LEU:HD12	1.86	0.41
1:A:138:LEU:CD1	1:A:176:VAL:HG12	2.51	0.41
1:A:147:PHE:HE1	1:A:164:TYR:CD1	2.39	0.41
3:C:129:LYS:HZ3	3:C:170:ARG:HE	1.69	0.41
1:D:86:PHE:HZ	1:D:89:LEU:HD12	1.86	0.41
1:D:123:GLU:CD	1:D:159:SER:OG	2.60	0.41
1:D:293:GLU:OE1	1:D:293:GLU:N	2.45	0.41
3:F:12:GLY:O	3:F:83:VAL:HA	2.20	0.41
1:G:267:LEU:HB2	1:G:273:TYR:CZ	2.56	0.41
3:I:17:GLN:HB3	3:I:20:ARG:HG3	2.02	0.41
1:J:138:LEU:CD1	1:J:176:VAL:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:17:GLN:HB3	3:L:20:ARG:HG3	2.03	0.41
3:L:263:ALA:O	3:L:265:LEU:HD23	2.20	0.41
1:M:47:THR:HG23	1:M:52:ILE:HD11	2.03	0.41
1:M:83:ILE:HD12	1:M:85:THR:HG23	2.02	0.41
1:M:267:LEU:HB2	1:M:273:TYR:CZ	2.56	0.41
2:N:33:ARG:NH2	3:O:278:ASP:HB3	2.36	0.41
2:N:132:PRO:HA	2:N:133:PRO:HD3	1.96	0.41
3:O:57:LEU:HD12	3:O:58:VAL:H	1.86	0.41
3:O:61:GLN:HG2	3:O:66:ASP:OD2	2.21	0.41
3:O:198:PRO:O	3:O:221:PRO:HB3	2.20	0.41
3:O:263:ALA:O	3:O:265:LEU:HD23	2.20	0.41
3:R:61:GLN:HG2	3:R:66:ASP:OD2	2.21	0.41
3:R:263:ALA:O	3:R:265:LEU:HD23	2.20	0.41
1:A:16:VAL:HG22	1:A:20:SER:OG	2.21	0.41
1:A:85:THR:O	1:A:87:GLY:N	2.53	0.41
1:D:43:ILE:CD1	1:D:65:SER:HB3	2.51	0.41
2:E:132:PRO:HA	2:E:133:PRO:HD3	1.96	0.41
1:G:79:LEU:HD22	1:G:98:ILE:HD11	2.02	0.41
3:L:198:PRO:O	3:L:221:PRO:HB3	2.20	0.41
1:M:86:PHE:HZ	1:M:89:LEU:HD12	1.86	0.41
3:O:55:HIS:O	3:O:55:HIS:CG	2.74	0.41
3:O:146:TRP:CD1	3:O:146:TRP:N	2.89	0.41
1:P:47:THR:HG23	1:P:52:ILE:HD11	2.03	0.41
1:A:123:GLU:CD	1:A:159:SER:OG	2.60	0.40
3:F:89:TYR:CZ	3:F:116:SER:HA	2.56	0.40
3:L:57:LEU:HD12	3:L:58:VAL:H	1.86	0.40
1:M:119:LYS:HD2	1:M:164:TYR:O	2.21	0.40
1:P:16:VAL:HG22	1:P:20:SER:OG	2.21	0.40
1:A:43:ILE:CD1	1:A:65:SER:HB3	2.51	0.40
3:C:57:LEU:HD12	3:C:58:VAL:H	1.86	0.40
1:D:47:THR:HG23	1:D:52:ILE:HD11	2.03	0.40
3:F:3:PRO:HA	3:F:31:ALA:CB	2.43	0.40
1:M:16:VAL:HG22	1:M:20:SER:OG	2.21	0.40
1:M:123:GLU:CD	1:M:159:SER:OG	2.60	0.40
3:R:89:TYR:CZ	3:R:116:SER:HA	2.56	0.40
1:A:47:THR:HG23	1:A:52:ILE:HD11	2.03	0.40
1:D:147:PHE:HE1	1:D:164:TYR:CD1	2.39	0.40
1:G:16:VAL:HG22	1:G:20:SER:OG	2.21	0.40
3:I:55:HIS:O	3:I:55:HIS:CG	2.75	0.40
3:I:57:LEU:HD12	3:I:58:VAL:H	1.86	0.40
1:J:123:GLU:CD	1:J:159:SER:OG	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:293:GLU:H	1:J:293:GLU:CD	2.23	0.40
2:K:65:GLY:HA3	2:K:173:LEU:HD22	2.03	0.40
3:O:89:TYR:CZ	3:O:116:SER:HA	2.56	0.40
1:P:220:LEU:O	1:P:261:SER:HA	2.22	0.40
2:Q:57:LEU:HD21	2:Q:75:ARG:HG2	2.02	0.40
3:R:57:LEU:HD12	3:R:58:VAL:H	1.86	0.40
1:A:40:ALA:HA	1:A:43:ILE:CD1	2.52	0.40
1:A:86:PHE:HZ	1:A:89:LEU:HD12	1.86	0.40
1:A:119:LYS:HD2	1:A:164:TYR:O	2.21	0.40
2:B:158:GLY:O	2:B:161:HIS:ND1	2.50	0.40
1:J:16:VAL:HG22	1:J:20:SER:OG	2.21	0.40
1:J:40:ALA:HA	1:J:43:ILE:CD1	2.52	0.40
1:J:220:LEU:O	1:J:261:SER:HA	2.22	0.40
1:J:293:GLU:OE1	1:J:293:GLU:N	2.45	0.40
3:L:61:GLN:HG2	3:L:66:ASP:OD2	2.21	0.40
1:M:43:ILE:CD1	1:M:65:SER:HB3	2.51	0.40
1:P:267:LEU:HB2	1:P:273:TYR:CZ	2.56	0.40
3:R:17:GLN:HB3	3:R:20:ARG:HG3	2.03	0.40
3:C:102:ASP:OD2	6:C:401:NAG:H82	2.22	0.40
1:D:16:VAL:HG22	1:D:20:SER:OG	2.21	0.40
1:D:267:LEU:HB2	1:D:273:TYR:CZ	2.56	0.40
1:G:47:THR:HG23	1:G:52:ILE:HD11	2.03	0.40
3:I:12:GLY:O	3:I:83:VAL:HA	2.20	0.40
3:I:129:LYS:HZ3	3:I:170:ARG:HE	1.69	0.40
3:L:89:TYR:CZ	3:L:116:SER:HA	2.56	0.40
1:M:40:ALA:HA	1:M:43:ILE:CD1	2.52	0.40
1:P:54:LYS:HE2	1:P:54:LYS:HB2	1.67	0.40
1:P:132:LEU:O	1:P:134:THR:HG23	2.22	0.40

All (10) 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)
3:F:49:PRO:O	3:F:52:GLY:N[5_655]	1.26	0.94
3:F:50:ASP:N	3:F:50:ASP:O[5_655]	1.39	0.81
3:F:48:GLY:O	3:F:51:SER:N[5_655]	1.62	0.58
3:F:49:PRO:C	3:F:50:ASP:O[5_655]	1.64	0.56
3:F:48:GLY:O	3:F:50:ASP:C[5_655]	1.77	0.43
3:F:48:GLY:O	3:F:50:ASP:O[5_655]	2.08	0.12
3:I:20:ARG:NH2	3:I:50:ASP:OD2[4_664]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:49:PRO:O	3:F:52:GLY:CA[5_655]	2.10	0.10
3:F:50:ASP:N	3:F:50:ASP:C[5_655]	2.10	0.10
3:F:48:GLY:C	3:F:50:ASP:O[5_655]	2.14	0.06

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	296/303 (98%)	278 (94%)	15 (5%)	3 (1%)	15	52
1	D	296/303 (98%)	279 (94%)	14 (5%)	3 (1%)	15	52
1	G	296/303 (98%)	278 (94%)	15 (5%)	3 (1%)	15	52
1	J	296/303 (98%)	278 (94%)	15 (5%)	3 (1%)	15	52
1	M	296/303 (98%)	279 (94%)	14 (5%)	3 (1%)	15	52
1	P	296/303 (98%)	278 (94%)	15 (5%)	3 (1%)	15	52
2	B	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	61
2	E	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	61
2	H	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	61
2	K	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	61
2	N	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	61
2	Q	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	61
3	C	279/348 (80%)	260 (93%)	18 (6%)	1 (0%)	34	69
3	F	279/348 (80%)	260 (93%)	18 (6%)	1 (0%)	34	69
3	I	279/348 (80%)	260 (93%)	18 (6%)	1 (0%)	34	69
3	L	279/348 (80%)	260 (93%)	18 (6%)	1 (0%)	34	69
3	O	279/348 (80%)	260 (93%)	18 (6%)	1 (0%)	34	69
3	R	279/348 (80%)	260 (93%)	18 (6%)	1 (0%)	34	69
All	All	4422/4980 (89%)	4172 (94%)	220 (5%)	30 (1%)	22	59

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PHE
1	D	86	PHE
1	G	86	PHE
1	J	86	PHE
1	M	86	PHE
1	P	86	PHE
1	A	209	ILE
1	D	209	ILE
1	G	209	ILE
1	J	209	ILE
1	M	209	ILE
1	P	209	ILE
1	A	212	GLU
1	D	212	GLU
1	G	212	GLU
1	J	212	GLU
1	M	212	GLU
1	P	212	GLU
2	B	63	ALA
3	C	62	ALA
2	E	63	ALA
3	F	62	ALA
2	H	63	ALA
3	I	62	ALA
2	K	63	ALA
3	L	62	ALA
2	N	63	ALA
3	O	62	ALA
2	Q	63	ALA
3	R	62	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/279 (99%)	268 (98%)	7 (2%)	47	70
1	D	275/279 (99%)	268 (98%)	7 (2%)	47	70
1	G	275/279 (99%)	268 (98%)	7 (2%)	47	70
1	J	275/279 (99%)	268 (98%)	7 (2%)	47	70
1	M	275/279 (99%)	268 (98%)	7 (2%)	47	70
1	P	275/279 (99%)	268 (98%)	7 (2%)	47	70
2	B	132/144 (92%)	131 (99%)	1 (1%)	81	89
2	E	132/144 (92%)	131 (99%)	1 (1%)	81	89
2	H	132/144 (92%)	131 (99%)	1 (1%)	81	89
2	K	132/144 (92%)	131 (99%)	1 (1%)	81	89
2	N	132/144 (92%)	131 (99%)	1 (1%)	81	89
2	Q	132/144 (92%)	131 (99%)	1 (1%)	81	89
3	C	234/293 (80%)	229 (98%)	5 (2%)	53	74
3	F	234/293 (80%)	229 (98%)	5 (2%)	53	74
3	I	234/293 (80%)	229 (98%)	5 (2%)	53	74
3	L	234/293 (80%)	229 (98%)	5 (2%)	53	74
3	O	234/293 (80%)	229 (98%)	5 (2%)	53	74
3	R	234/293 (80%)	229 (98%)	5 (2%)	53	74
All	All	3846/4296 (90%)	3768 (98%)	78 (2%)	55	75

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	35	TYR
1	A	65	SER
1	A	147	PHE
1	A	160	CYS
1	A	260	SER
1	A	282	GLU
2	B	31	ASP
3	C	25	CYS
3	C	44	LYS
3	C	51	SER

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Mol	Chain	Res	Type
3	C	98	CYS
3	C	203	ARG
1	D	13	SER
1	D	35	TYR
1	D	65	SER
1	D	147	PHE
1	D	160	CYS
1	D	260	SER
1	D	282	GLU
2	E	31	ASP
3	F	25	CYS
3	F	44	LYS
3	F	51	SER
3	F	98	CYS
3	F	203	ARG
1	G	13	SER
1	G	35	TYR
1	G	65	SER
1	G	147	PHE
1	G	160	CYS
1	G	260	SER
1	G	282	GLU
2	H	31	ASP
3	I	25	CYS
3	I	44	LYS
3	I	51	SER
3	I	98	CYS
3	I	203	ARG
1	J	13	SER
1	J	35	TYR
1	J	65	SER
1	J	147	PHE
1	J	160	CYS
1	J	260	SER
1	J	282	GLU
2	K	31	ASP
3	L	25	CYS
3	L	44	LYS
3	L	51	SER
3	L	98	CYS
3	L	203	ARG
1	M	13	SER

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Mol	Chain	Res	Type
1	M	35	TYR
1	M	65	SER
1	M	147	PHE
1	M	160	CYS
1	M	260	SER
1	M	282	GLU
2	N	31	ASP
3	O	25	CYS
3	O	44	LYS
3	O	51	SER
3	O	98	CYS
3	O	203	ARG
1	P	13	SER
1	P	35	TYR
1	P	65	SER
1	P	147	PHE
1	P	160	CYS
1	P	260	SER
1	P	282	GLU
2	Q	31	ASP
3	R	25	CYS
3	R	44	LYS
3	R	51	SER
3	R	98	CYS
3	R	203	ARG

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

Mol	Chain	Res	Type
1	A	265	GLN
1	D	88	GLN
1	D	265	GLN
3	F	243	HIS
1	G	265	GLN
3	I	243	HIS
1	J	265	GLN
3	L	243	HIS
1	M	92	ASN
1	M	265	GLN
3	O	243	HIS
3	R	243	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

30 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	$\#\|Z\| > 2$
4	NAG	S	1	1,4	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	S	2	4	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	T	1	5,3	14,14,15	0.51	0	17,19,21	0.78	0
5	NAG	T	2	5	14,14,15	0.34	0	17,19,21	0.53	0
5	BMA	T	3	5	11,11,12	1.65	3 (27%)	15,15,17	1.05	0
4	NAG	U	1	1,4	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	U	2	4	14,14,15	0.39	0	17,19,21	0.43	0
5	NAG	V	1	5,3	14,14,15	0.50	0	17,19,21	0.78	0
5	NAG	V	2	5	14,14,15	0.34	0	17,19,21	0.54	0
5	BMA	V	3	5	11,11,12	1.65	3 (27%)	15,15,17	1.05	0
4	NAG	W	1	1,4	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	W	2	4	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	X	1	5,3	14,14,15	0.51	0	17,19,21	0.78	0
5	NAG	X	2	5	14,14,15	0.34	0	17,19,21	0.54	0
5	BMA	X	3	5	11,11,12	1.65	3 (27%)	15,15,17	1.05	0
4	NAG	Y	1	1,4	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	Y	2	4	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	Z	1	5,3	14,14,15	0.51	0	17,19,21	0.78	0
5	NAG	Z	2	5	14,14,15	0.34	0	17,19,21	0.54	0
5	BMA	Z	3	5	11,11,12	1.65	3 (27%)	15,15,17	1.05	0
4	NAG	a	1	1,4	14,14,15	0.35	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	a	2	4	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	b	1	5,3	14,14,15	0.50	0	17,19,21	0.78	0
5	NAG	b	2	5	14,14,15	0.34	0	17,19,21	0.54	0
5	BMA	b	3	5	11,11,12	1.65	3 (27%)	15,15,17	1.05	0
4	NAG	c	1	1,4	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	c	2	4	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	d	1	5,3	14,14,15	0.51	0	17,19,21	0.78	0
5	NAG	d	2	5	14,14,15	0.34	0	17,19,21	0.54	0
5	BMA	d	3	5	11,11,12	1.65	3 (27%)	15,15,17	1.05	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
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
5	NAG	T	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
5	NAG	V	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	BMA	V	3	5	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
5	NAG	X	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
5	NAG	Z	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
4	NAG	c	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
5	NAG	d	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
5	BMA	d	3	5	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	d	3	BMA	C4-C5	3.28	1.59	1.53
5	X	3	BMA	C4-C5	3.28	1.59	1.53
5	Z	3	BMA	C4-C5	3.28	1.59	1.53
5	T	3	BMA	C4-C5	3.28	1.59	1.53
5	V	3	BMA	C4-C5	3.28	1.59	1.53
5	b	3	BMA	C4-C5	3.27	1.59	1.53
5	X	3	BMA	C1-C2	3.26	1.59	1.52
5	T	3	BMA	C1-C2	3.26	1.59	1.52
5	V	3	BMA	C1-C2	3.26	1.59	1.52
5	Z	3	BMA	C1-C2	3.26	1.59	1.52
5	d	3	BMA	C1-C2	3.26	1.59	1.52
5	b	3	BMA	C1-C2	3.26	1.59	1.52
5	X	3	BMA	C4-C3	2.34	1.58	1.52
5	d	3	BMA	C4-C3	2.34	1.58	1.52
5	T	3	BMA	C4-C3	2.34	1.58	1.52
5	b	3	BMA	C4-C3	2.34	1.58	1.52
5	V	3	BMA	C4-C3	2.34	1.58	1.52
5	Z	3	BMA	C4-C3	2.34	1.58	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	c	2	NAG	O5-C5-C6-O6
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
5	d	1	NAG	C8-C7-N2-C2
5	d	1	NAG	O7-C7-N2-C2
4	S	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2	NAG	1	0
5	Z	1	NAG	1	0
5	X	1	NAG	1	0
5	V	1	NAG	1	0
5	V	3	BMA	1	0
5	Z	2	NAG	1	0

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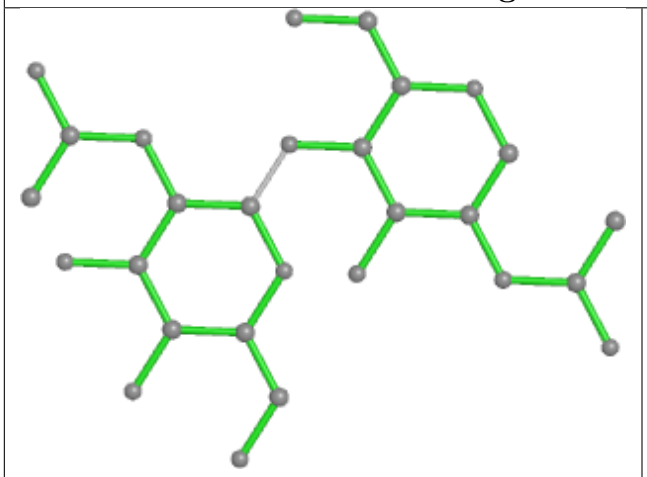
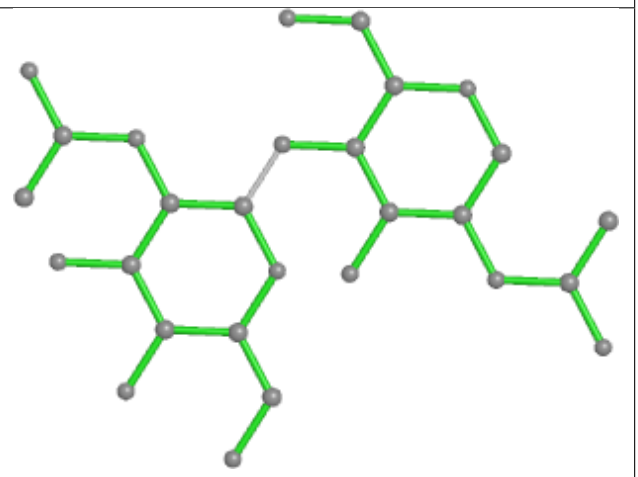
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Z	3	BMA	1	0
5	V	2	NAG	1	0
5	T	1	NAG	1	0
5	T	3	BMA	1	0

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

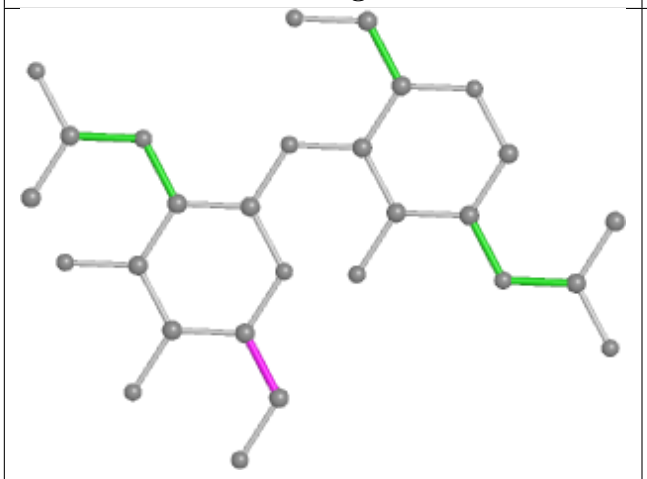
Oligosaccharide Chain S



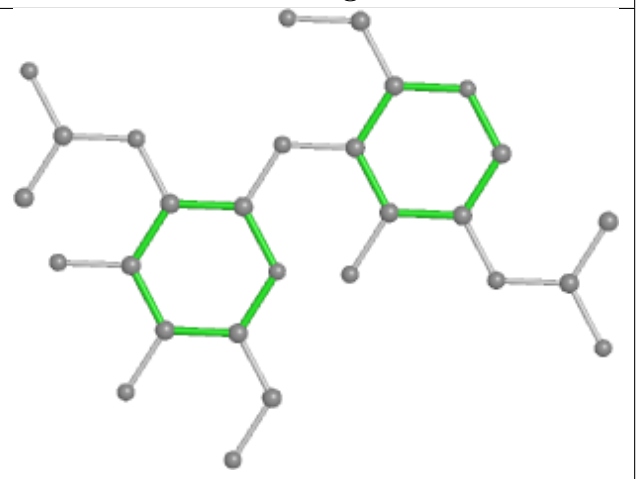
Bond lengths



Bond angles

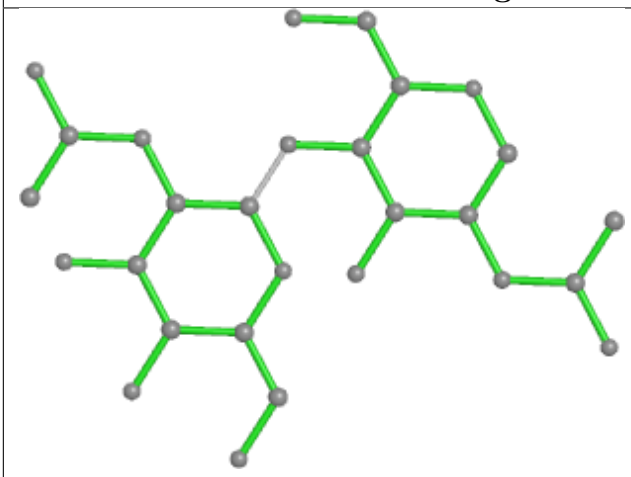


Torsions

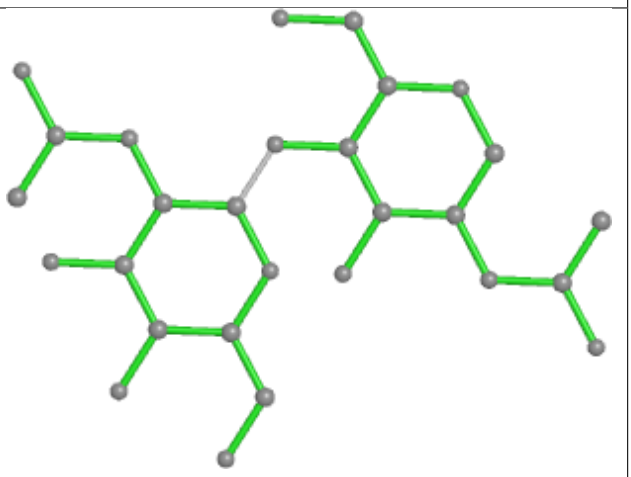


Rings

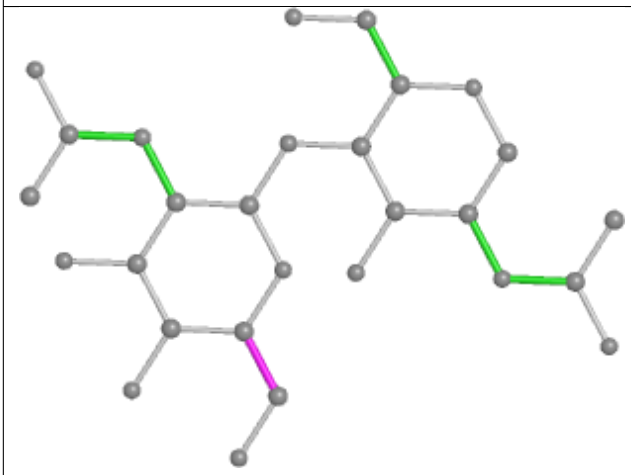
Oligosaccharide Chain U



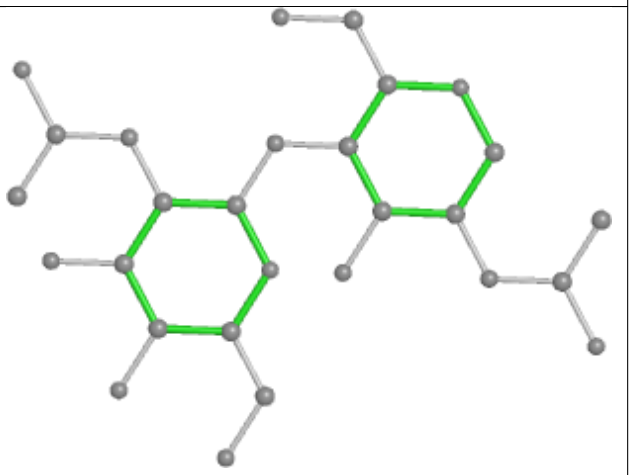
Bond lengths



Bond angles

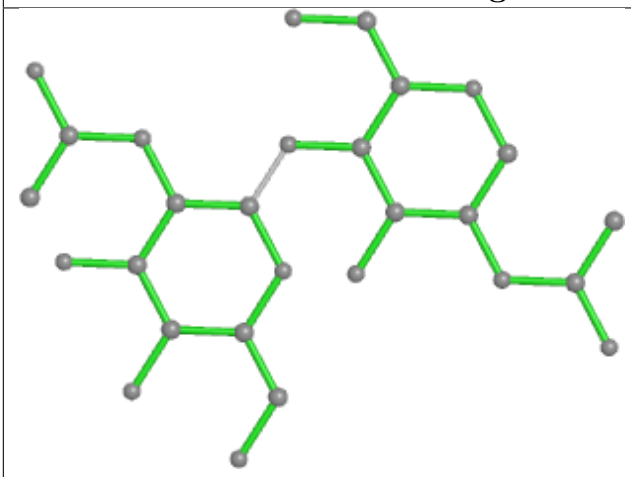


Torsions

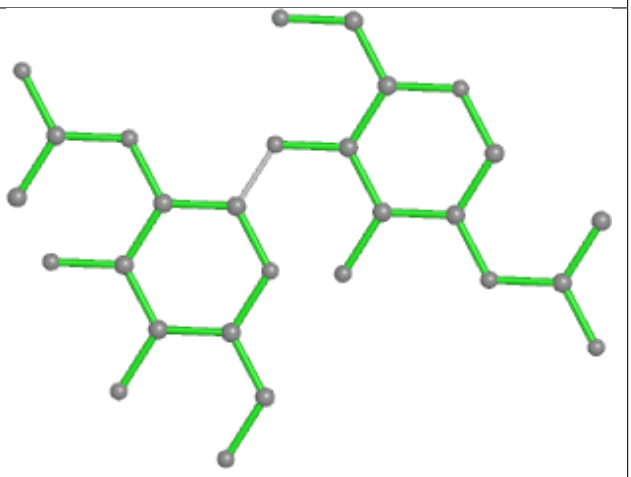


Rings

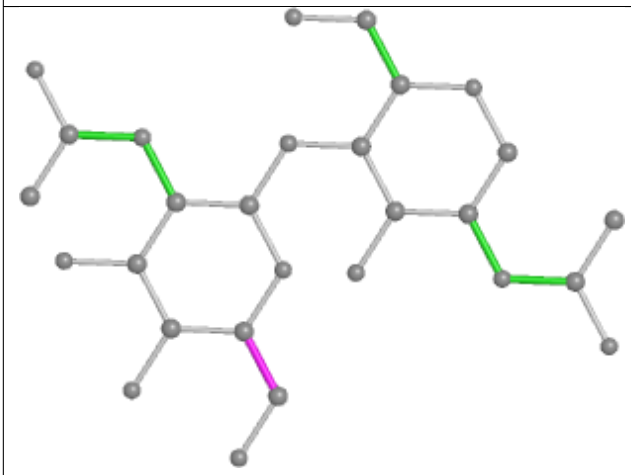
Oligosaccharide Chain W



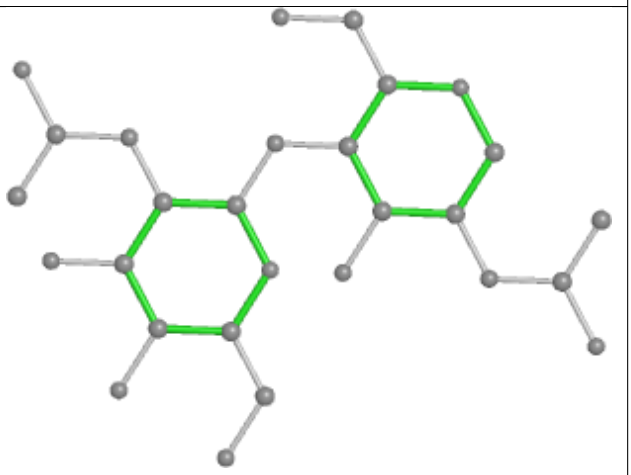
Bond lengths



Bond angles

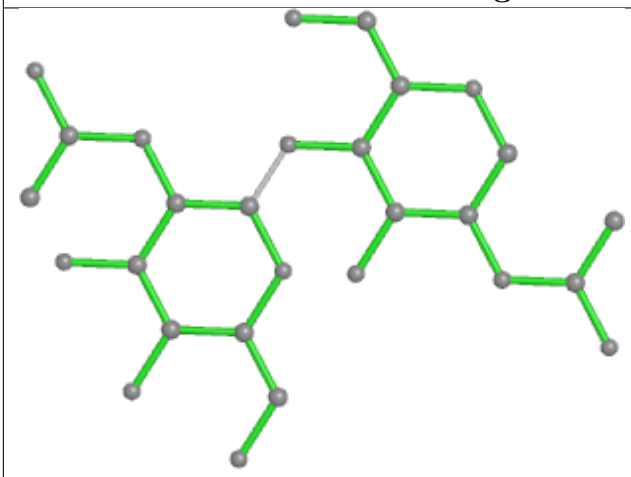


Torsions

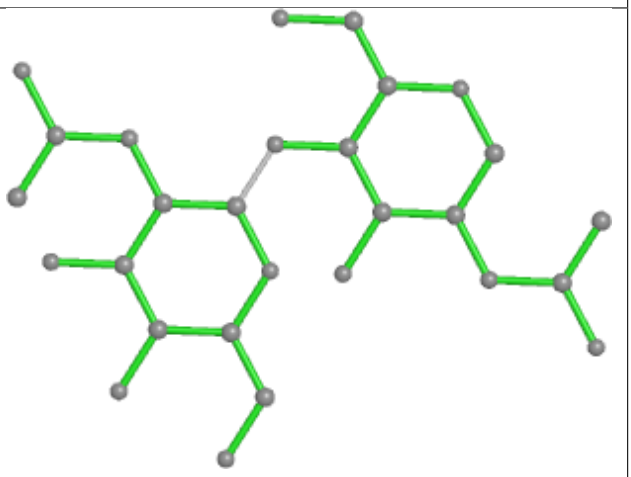


Rings

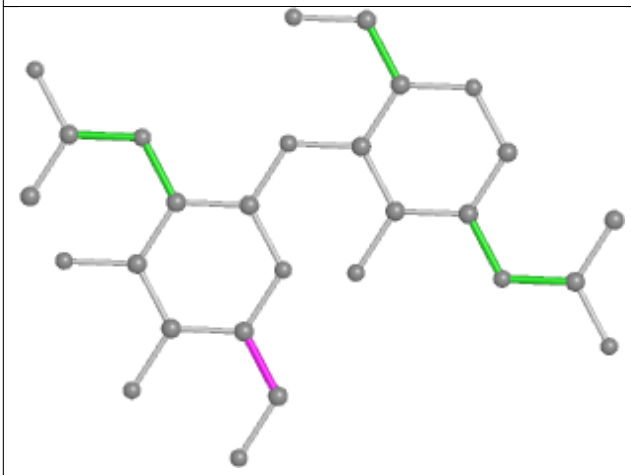
Oligosaccharide Chain Y



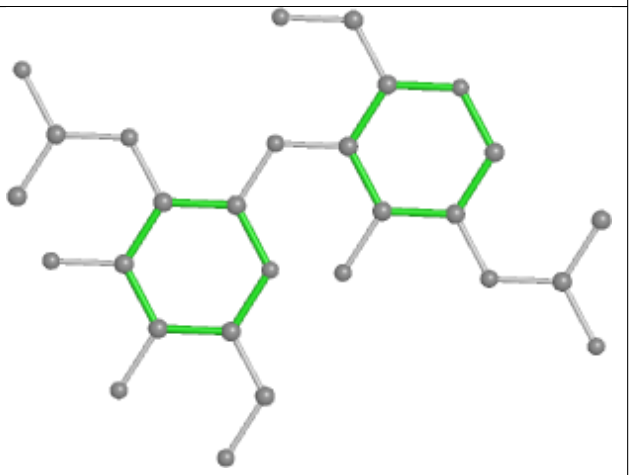
Bond lengths



Bond angles

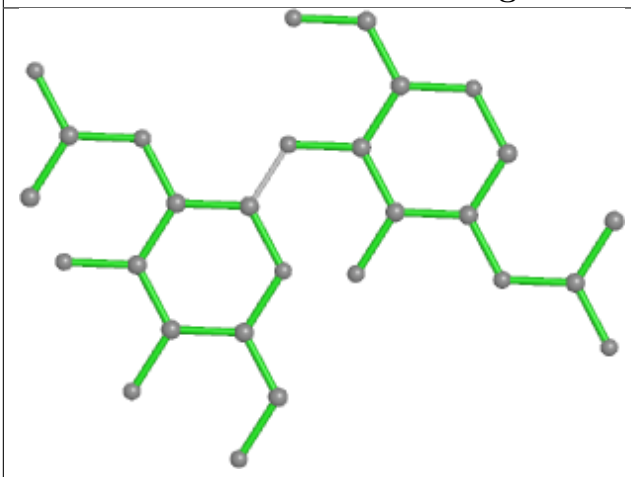


Torsions

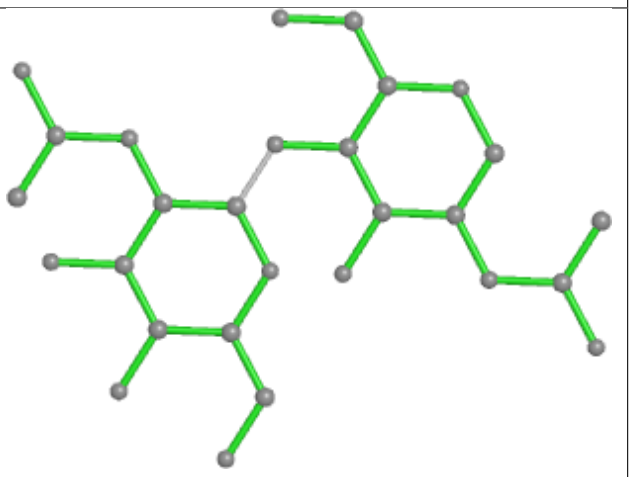


Rings

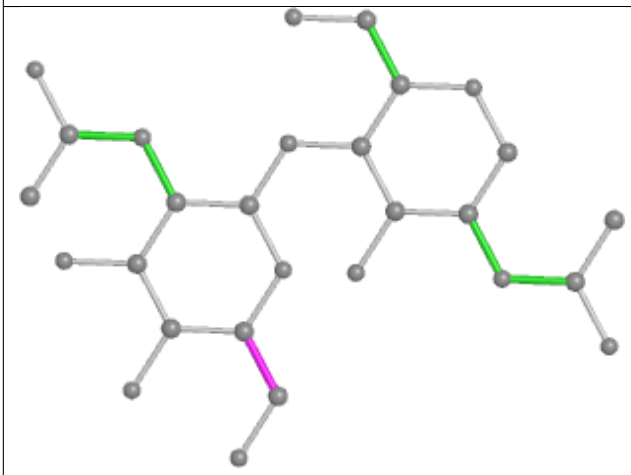
Oligosaccharide Chain a



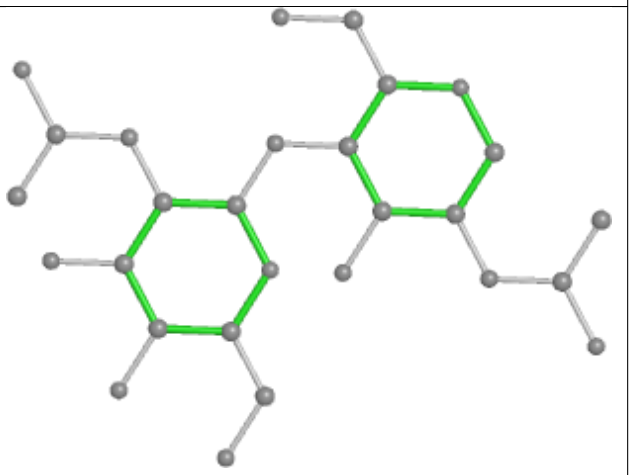
Bond lengths



Bond angles

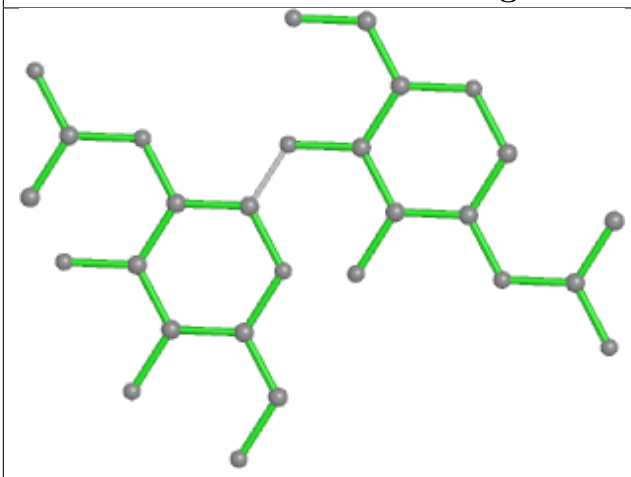


Torsions

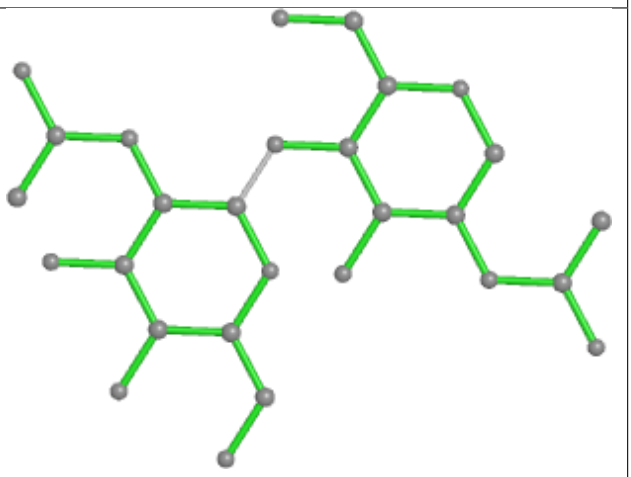


Rings

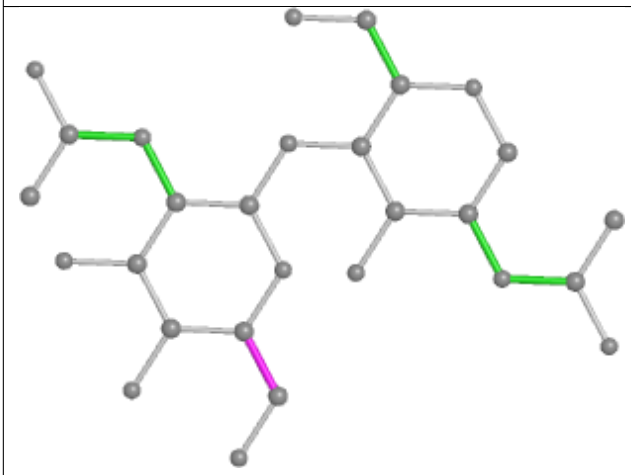
Oligosaccharide Chain c



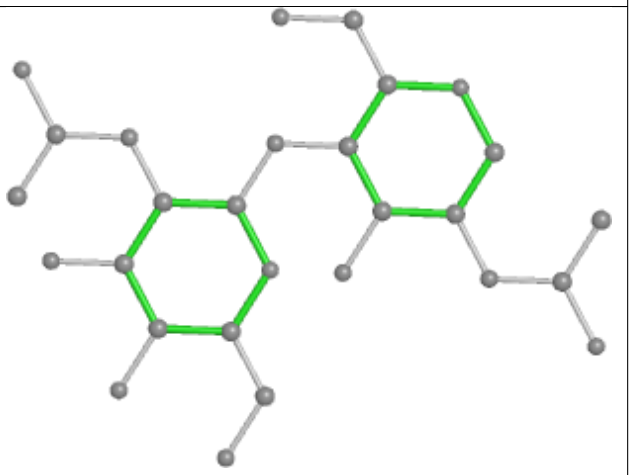
Bond lengths



Bond angles

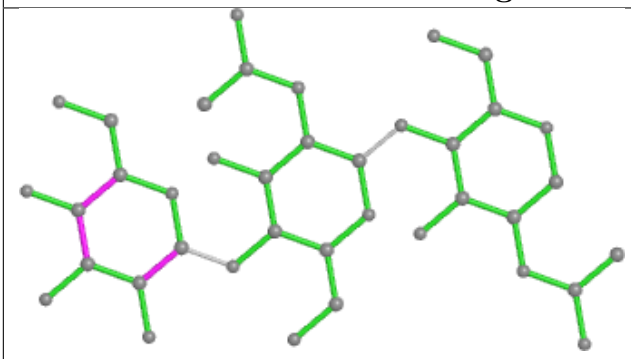


Torsions

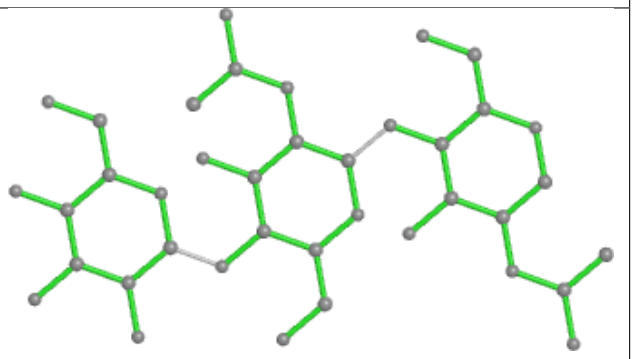


Rings

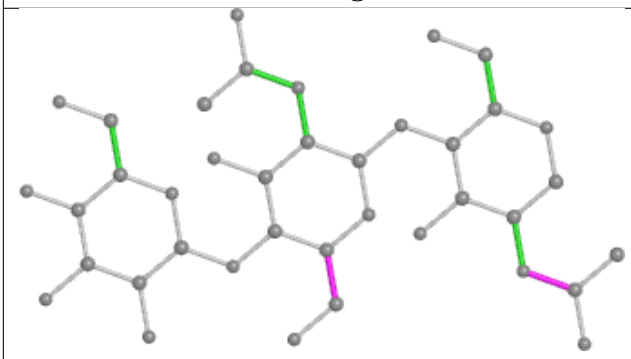
Oligosaccharide Chain T



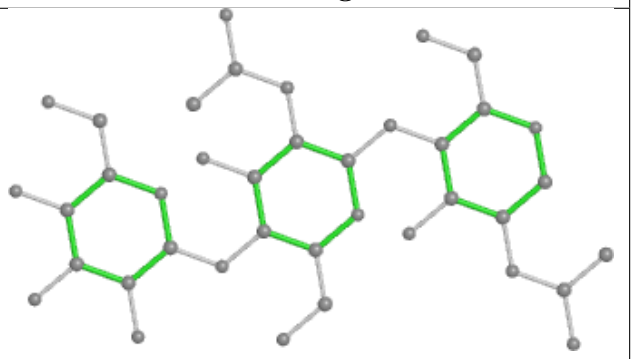
Bond lengths



Bond angles

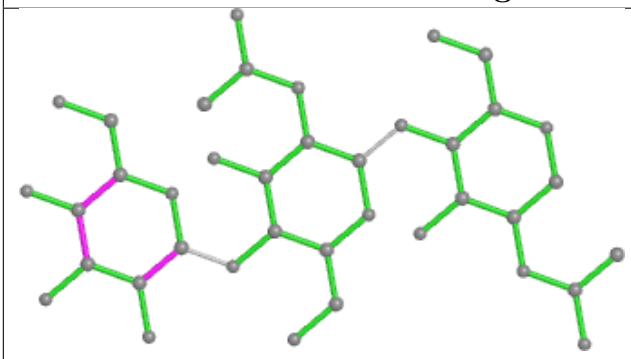


Torsions

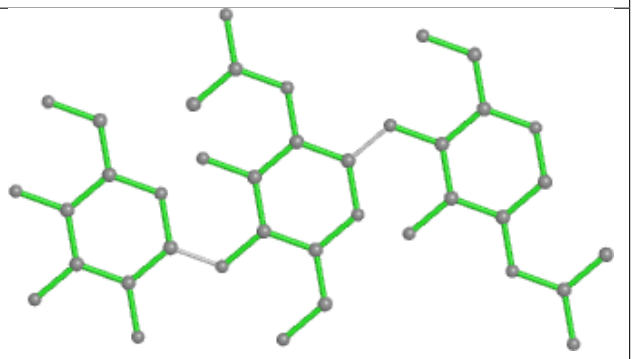


Rings

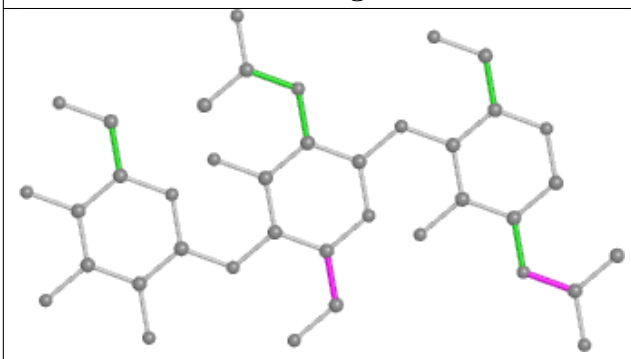
Oligosaccharide Chain V



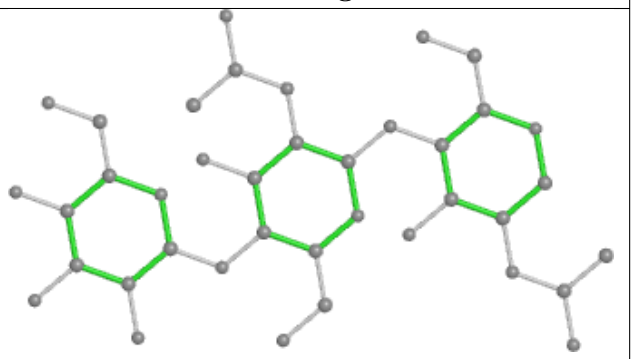
Bond lengths



Bond angles

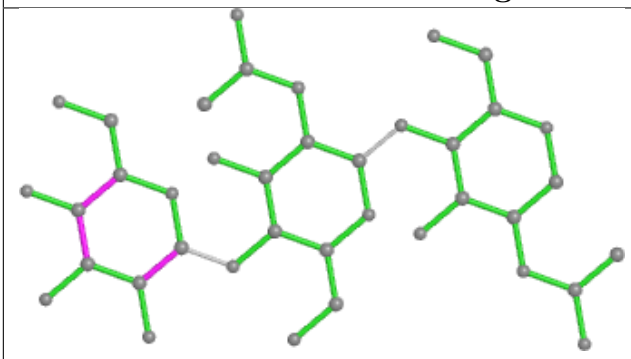


Torsions

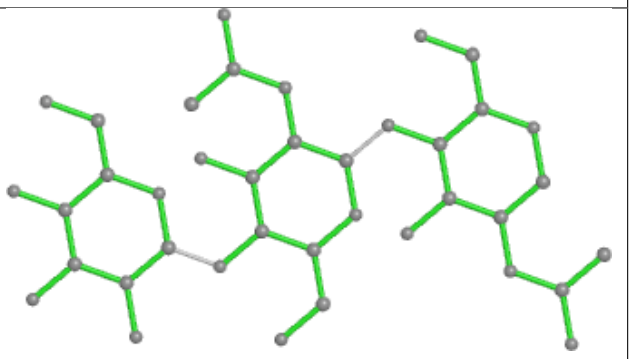


Rings

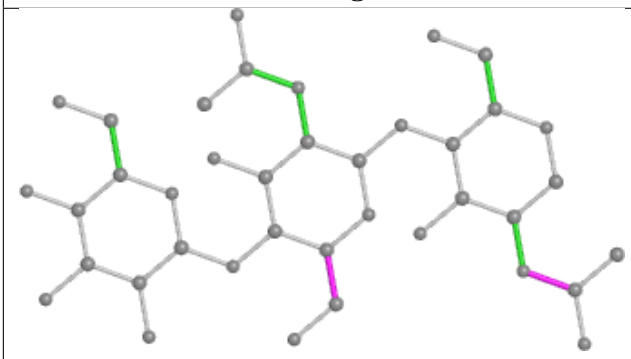
Oligosaccharide Chain X



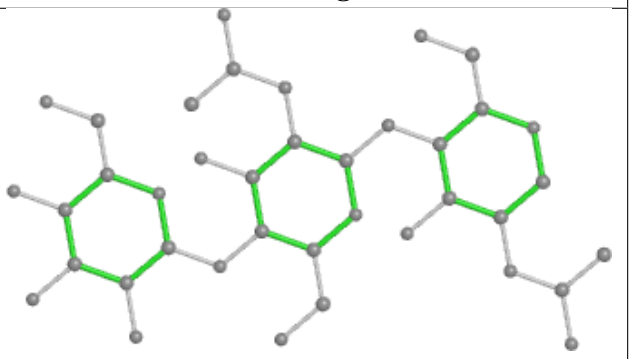
Bond lengths



Bond angles

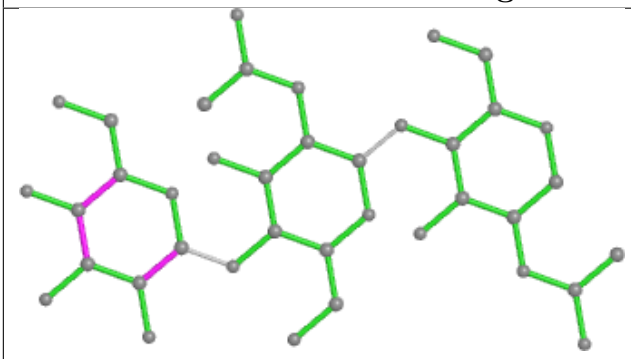


Torsions

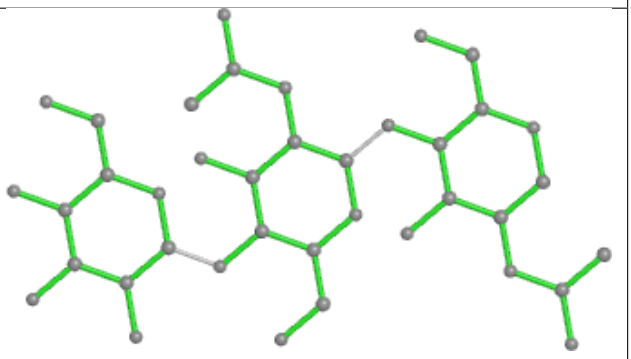


Rings

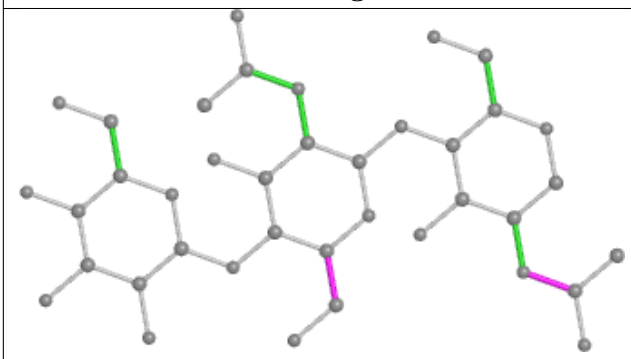
Oligosaccharide Chain Z



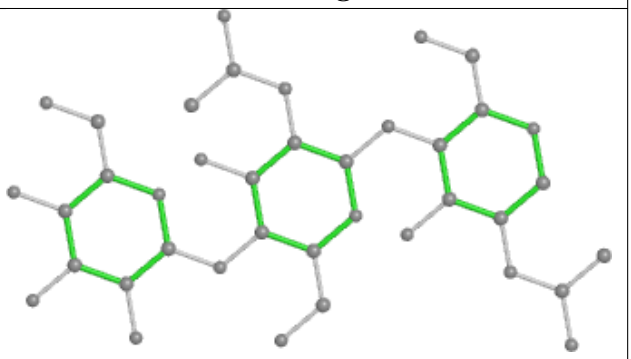
Bond lengths



Bond angles

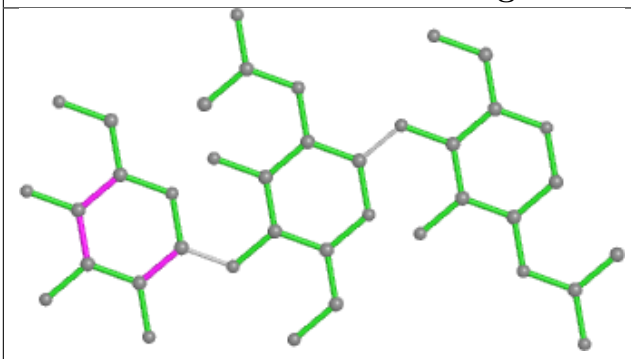


Torsions

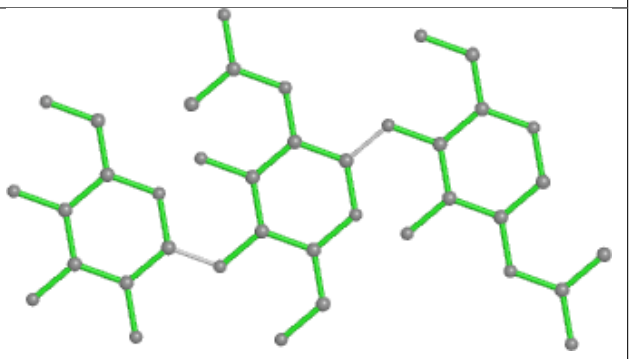


Rings

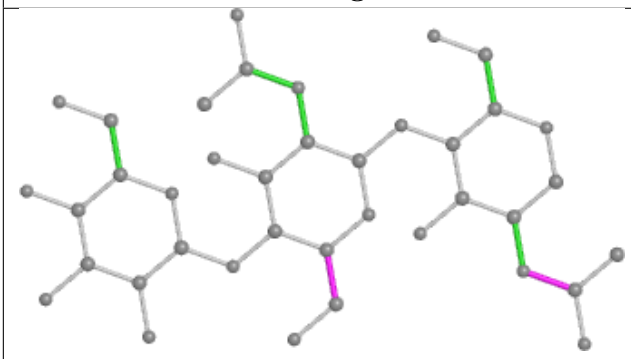
Oligosaccharide Chain b



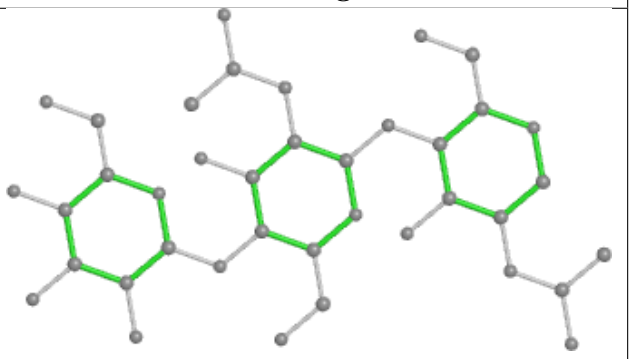
Bond lengths



Bond angles

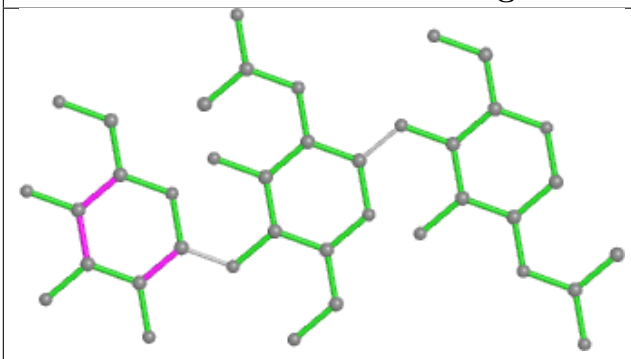


Torsions

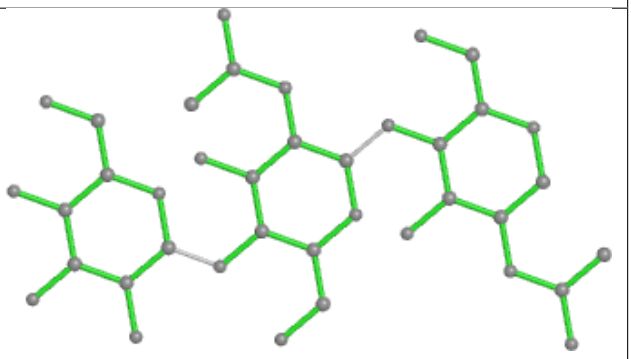


Rings

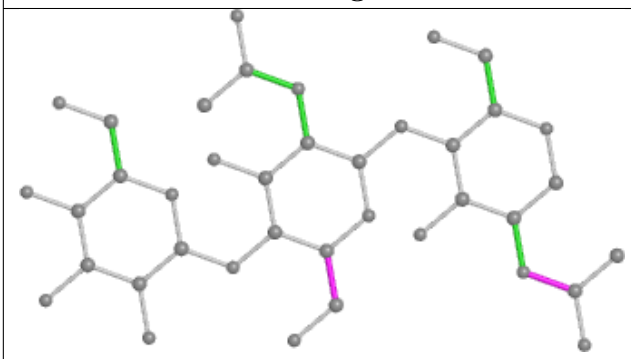
Oligosaccharide Chain d



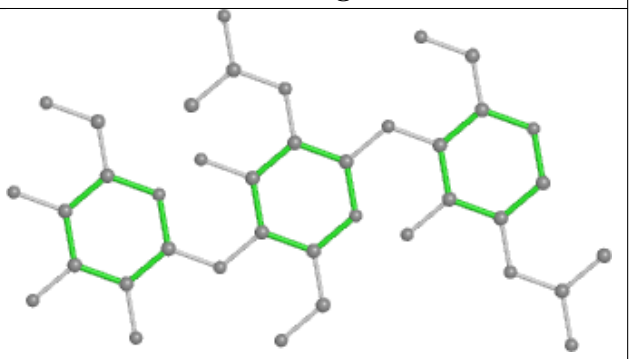
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	P	401	1	14,14,15	0.55	0	17,19,21	1.34	2 (11%)
6	NAG	J	402	1	14,14,15	0.65	0	17,19,21	0.58	0
6	NAG	G	402	1	14,14,15	0.65	0	17,19,21	0.58	0
6	NAG	O	401	3	14,14,15	0.45	0	17,19,21	0.48	0
6	NAG	G	401	1	14,14,15	0.54	0	17,19,21	1.34	2 (11%)
6	NAG	F	401	3	14,14,15	0.45	0	17,19,21	0.48	0
6	NAG	I	401	3	14,14,15	0.45	0	17,19,21	0.48	0
6	NAG	P	402	1	14,14,15	0.65	0	17,19,21	0.58	0
6	NAG	L	401	3	14,14,15	0.44	0	17,19,21	0.48	0
6	NAG	M	401	1	14,14,15	0.55	0	17,19,21	1.34	2 (11%)
6	NAG	J	401	1	14,14,15	0.55	0	17,19,21	1.34	2 (11%)
6	NAG	C	401	3	14,14,15	0.44	0	17,19,21	0.48	0
6	NAG	M	402	1	14,14,15	0.65	0	17,19,21	0.58	0
6	NAG	A	402	1	14,14,15	0.65	0	17,19,21	0.58	0
6	NAG	R	401	3	14,14,15	0.44	0	17,19,21	0.48	0
6	NAG	A	401	1	14,14,15	0.54	0	17,19,21	1.33	2 (11%)
6	NAG	D	402	1	14,14,15	0.65	0	17,19,21	0.58	0
6	NAG	D	401	1	14,14,15	0.55	0	17,19,21	1.34	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	401	1	-	5/6/23/26	0/1/1/1
6	NAG	J	402	1	-	3/6/23/26	0/1/1/1
6	NAG	G	402	1	-	3/6/23/26	0/1/1/1
6	NAG	O	401	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	401	1	-	5/6/23/26	0/1/1/1
6	NAG	F	401	3	-	2/6/23/26	0/1/1/1
6	NAG	I	401	3	-	2/6/23/26	0/1/1/1
6	NAG	P	402	1	-	3/6/23/26	0/1/1/1
6	NAG	L	401	3	-	2/6/23/26	0/1/1/1
6	NAG	M	401	1	-	5/6/23/26	0/1/1/1
6	NAG	J	401	1	-	5/6/23/26	0/1/1/1
6	NAG	C	401	3	-	2/6/23/26	0/1/1/1
6	NAG	M	402	1	-	3/6/23/26	0/1/1/1
6	NAG	A	402	1	-	3/6/23/26	0/1/1/1
6	NAG	R	401	3	-	2/6/23/26	0/1/1/1
6	NAG	A	401	1	-	5/6/23/26	0/1/1/1
6	NAG	D	402	1	-	3/6/23/26	0/1/1/1
6	NAG	D	401	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	401	NAG	C2-N2-C7	4.41	129.19	122.90
6	D	401	NAG	C2-N2-C7	4.41	129.18	122.90
6	P	401	NAG	C2-N2-C7	4.41	129.18	122.90
6	J	401	NAG	C2-N2-C7	4.41	129.18	122.90
6	G	401	NAG	C2-N2-C7	4.41	129.18	122.90
6	A	401	NAG	C2-N2-C7	4.41	129.18	122.90
6	J	401	NAG	C1-C2-N2	2.16	114.18	110.49
6	G	401	NAG	C1-C2-N2	2.16	114.17	110.49
6	D	401	NAG	C1-C2-N2	2.16	114.17	110.49
6	P	401	NAG	C1-C2-N2	2.16	114.17	110.49
6	A	401	NAG	C1-C2-N2	2.15	114.17	110.49
6	M	401	NAG	C1-C2-N2	2.15	114.17	110.49

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	NAG	C4-C5-C6-O6
6	F	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	I	401	NAG	C4-C5-C6-O6
6	L	401	NAG	C4-C5-C6-O6
6	O	401	NAG	C4-C5-C6-O6
6	R	401	NAG	C4-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	F	401	NAG	O5-C5-C6-O6
6	I	401	NAG	O5-C5-C6-O6
6	L	401	NAG	O5-C5-C6-O6
6	O	401	NAG	O5-C5-C6-O6
6	R	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C8-C7-N2-C2
6	A	401	NAG	O7-C7-N2-C2
6	D	401	NAG	C8-C7-N2-C2
6	D	401	NAG	O7-C7-N2-C2
6	G	401	NAG	C8-C7-N2-C2
6	G	401	NAG	O7-C7-N2-C2
6	J	401	NAG	C8-C7-N2-C2
6	J	401	NAG	O7-C7-N2-C2
6	M	401	NAG	C8-C7-N2-C2
6	M	401	NAG	O7-C7-N2-C2
6	P	401	NAG	C8-C7-N2-C2
6	P	401	NAG	O7-C7-N2-C2
6	A	401	NAG	O5-C5-C6-O6
6	D	401	NAG	O5-C5-C6-O6
6	G	401	NAG	O5-C5-C6-O6
6	J	401	NAG	O5-C5-C6-O6
6	M	401	NAG	O5-C5-C6-O6
6	P	401	NAG	O5-C5-C6-O6
6	A	402	NAG	O5-C5-C6-O6
6	D	402	NAG	O5-C5-C6-O6
6	G	402	NAG	O5-C5-C6-O6
6	J	402	NAG	O5-C5-C6-O6
6	M	402	NAG	O5-C5-C6-O6
6	P	402	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	D	401	NAG	C4-C5-C6-O6
6	G	401	NAG	C4-C5-C6-O6
6	J	401	NAG	C4-C5-C6-O6
6	M	401	NAG	C4-C5-C6-O6
6	P	401	NAG	C4-C5-C6-O6
6	A	401	NAG	C3-C2-N2-C7
6	A	402	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	D	401	NAG	C3-C2-N2-C7
6	D	402	NAG	C3-C2-N2-C7
6	G	401	NAG	C3-C2-N2-C7
6	G	402	NAG	C3-C2-N2-C7
6	J	401	NAG	C3-C2-N2-C7
6	J	402	NAG	C3-C2-N2-C7
6	M	401	NAG	C3-C2-N2-C7
6	M	402	NAG	C3-C2-N2-C7
6	P	401	NAG	C3-C2-N2-C7
6	P	402	NAG	C3-C2-N2-C7
6	A	402	NAG	C4-C5-C6-O6
6	D	402	NAG	C4-C5-C6-O6
6	G	402	NAG	C4-C5-C6-O6
6	J	402	NAG	C4-C5-C6-O6
6	M	402	NAG	C4-C5-C6-O6
6	P	402	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	401	NAG	2	0
6	J	402	NAG	2	0
6	G	402	NAG	2	0
6	G	401	NAG	2	0
6	P	402	NAG	2	0
6	M	401	NAG	2	0
6	J	401	NAG	2	0
6	C	401	NAG	1	0
6	M	402	NAG	2	0
6	A	402	NAG	2	0
6	A	401	NAG	2	0
6	D	402	NAG	2	0
6	D	401	NAG	2	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	298/303 (98%)	0.37	17 (5%) 23 21	101, 159, 225, 294	0
1	D	298/303 (98%)	0.37	9 (3%) 50 43	101, 159, 225, 294	0
1	G	298/303 (98%)	0.43	19 (6%) 19 16	101, 159, 225, 294	0
1	J	298/303 (98%)	0.35	10 (3%) 45 40	101, 159, 225, 294	0
1	M	298/303 (98%)	0.23	3 (1%) 82 80	101, 159, 225, 294	0
1	P	298/303 (98%)	0.50	25 (8%) 11 10	101, 159, 225, 294	0
2	B	164/179 (91%)	0.14	4 (2%) 59 54	85, 164, 253, 314	0
2	E	164/179 (91%)	0.13	0 100 100	85, 164, 253, 314	0
2	H	164/179 (91%)	0.26	1 (0%) 89 88	85, 164, 253, 314	0
2	K	164/179 (91%)	0.23	5 (3%) 50 43	85, 164, 253, 314	0
2	N	164/179 (91%)	0.28	5 (3%) 50 43	85, 164, 253, 314	0
2	Q	164/179 (91%)	0.08	1 (0%) 89 88	85, 164, 253, 314	0
3	C	283/348 (81%)	0.67	33 (11%) 4 5	89, 171, 334, 433	0
3	F	283/348 (81%)	1.14	55 (19%) 1 1	89, 171, 334, 433	0
3	I	283/348 (81%)	0.77	33 (11%) 4 5	89, 171, 334, 433	0
3	L	283/348 (81%)	0.78	41 (14%) 2 2	89, 171, 334, 433	0
3	O	283/348 (81%)	0.67	35 (12%) 4 4	89, 171, 334, 433	0
3	R	283/348 (81%)	0.49	27 (9%) 8 7	89, 171, 334, 433	0
All	All	4470/4980 (89%)	0.48	323 (7%) 15 13	85, 163, 281, 433	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	49	PRO	19.0
3	I	49	PRO	13.7
3	C	54	GLY	11.6

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Mol	Chain	Res	Type	RSRZ
3	C	48	GLY	11.2
3	F	33	ASP	11.1
3	I	27	PRO	10.7
3	C	33	ASP	10.5
3	L	49	PRO	10.5
3	R	48	GLY	10.4
3	C	49	PRO	10.2
3	F	54	GLY	9.9
3	L	31	ALA	9.8
3	F	21	SER	9.2
3	F	51	SER	8.8
3	F	30	THR	8.8
3	F	48	GLY	8.6
3	I	29	VAL	8.6
3	F	27	PRO	8.6
3	O	3	PRO	8.5
3	I	48	GLY	8.5
3	C	30	THR	8.4
3	O	27	PRO	7.7
3	I	28	GLY	7.6
3	I	3	PRO	7.6
3	L	55	HIS	7.5
3	F	82	THR	7.4
3	F	34	PRO	7.3
3	O	49	PRO	7.1
3	L	76	ASP	7.1
3	F	31	ALA	7.0
3	I	33	ASP	6.9
3	O	48	GLY	6.8
3	F	49	PRO	6.8
3	L	51	SER	6.8
3	I	4	CYS	6.7
3	F	35	VAL	6.5
3	F	47	GLN	6.5
3	F	85	LEU	6.4
3	R	50	ASP	6.4
3	L	30	THR	6.3
3	R	47	GLN	6.3
3	C	50	ASP	6.1
3	F	29	VAL	6.1
3	F	53	LEU	5.9
3	I	6	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
3	L	66	ASP	5.7
3	F	73	GLN	5.7
3	L	70	TYR	5.5
3	O	30	THR	5.5
3	F	70	TYR	5.4
3	C	154	GLY	5.4
3	C	27	PRO	5.2
2	K	132	PRO	5.2
3	C	34	PRO	5.2
3	O	79	LEU	5.1
3	F	23	LYS	5.1
3	I	55	HIS	5.0
3	O	55	HIS	5.0
3	I	79	LEU	5.0
3	R	51	SER	5.0
3	I	50	ASP	4.9
3	F	154	GLY	4.9
3	F	52	GLY	4.9
3	I	30	THR	4.9
3	O	31	ALA	4.8
3	C	3	PRO	4.7
3	L	50	ASP	4.6
3	O	9	GLY	4.6
3	F	28	GLY	4.5
3	L	178	PRO	4.5
3	F	36	SER	4.5
3	F	58	VAL	4.5
3	F	25	CYS	4.4
3	R	70	TYR	4.4
3	F	60	ALA	4.4
3	L	52	GLY	4.4
1	P	43	ILE	4.3
3	I	25	CYS	4.3
3	F	38	PHE	4.3
3	C	28	GLY	4.2
1	P	65	SER	4.2
3	C	73	GLN	4.2
3	I	80	GLY	4.2
3	F	37	TRP	4.1
2	B	177	ARG	4.1
3	O	33	ASP	4.1
3	L	29	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
3	F	20	ARG	4.0
3	L	17	GLN	4.0
3	C	31	ALA	4.0
3	O	76	ASP	3.9
3	L	8	TRP	3.9
3	F	71	ILE	3.9
3	C	9	GLY	3.8
3	F	80	GLY	3.8
3	C	17	GLN	3.7
3	O	25	CYS	3.7
3	L	145	PRO	3.7
3	F	81	GLY	3.6
3	F	83	VAL	3.6
3	O	29	VAL	3.5
3	O	78	ALA	3.5
3	C	45	LEU	3.5
3	F	127	ARG	3.5
1	P	7	GLY	3.5
3	C	153	LEU	3.4
3	R	150	GLN	3.4
3	C	47	GLN	3.4
3	F	32	GLY	3.4
3	F	72	CYS	3.4
3	F	22	VAL	3.4
1	P	79	LEU	3.4
3	O	173	VAL	3.4
1	P	155	ASP	3.4
1	D	146	LYS	3.4
3	L	28	GLY	3.4
3	O	73	GLN	3.4
3	R	175	GLU	3.4
3	I	7	ALA	3.3
3	C	29	VAL	3.3
3	L	63	ASP	3.3
3	O	69	THR	3.3
3	C	87	LEU	3.3
3	O	28	GLY	3.3
3	L	16	GLY	3.3
3	L	21	SER	3.3
1	P	146	LYS	3.3
3	L	87	LEU	3.3
1	P	197	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	49	HIS	3.2
3	F	39	ARG	3.2
2	K	59	MET	3.2
3	I	56	GLU	3.2
3	L	127	ARG	3.2
3	L	11	PRO	3.2
3	L	85	LEU	3.2
3	L	60	ALA	3.2
1	M	40	ALA	3.2
1	P	28	LEU	3.2
2	N	136	PRO	3.2
3	O	51	SER	3.2
3	O	85	LEU	3.2
3	I	9	GLY	3.2
3	I	212	ARG	3.1
3	I	21	SER	3.1
3	L	56	GLU	3.1
3	F	153	LEU	3.1
3	I	121	ARG	3.1
3	C	53	LEU	3.1
3	F	59	LEU	3.1
3	O	117	GLY	3.1
1	A	170	VAL	3.1
3	O	80	GLY	3.1
1	A	7	GLY	3.1
1	G	265	GLN	3.0
2	N	135	PRO	3.0
3	R	10	PRO	3.0
1	A	82	ASN	3.0
3	O	120	THR	3.0
1	J	79	LEU	3.0
3	F	56	GLU	3.0
1	P	190	ILE	3.0
1	P	27	VAL	3.0
3	L	170	ARG	3.0
1	P	80	THR	2.9
1	J	144	THR	2.9
1	P	64	ALA	2.9
3	R	15	TYR	2.9
3	L	48	GLY	2.9
3	L	54	GLY	2.9
1	P	45	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	85	LEU	2.9
3	F	50	ASP	2.9
3	L	32	GLY	2.9
1	D	86	PHE	2.8
1	G	161	THR	2.8
1	A	25	VAL	2.8
3	C	51	SER	2.8
3	O	26	CYS	2.8
2	Q	136	PRO	2.8
1	P	287	TYR	2.8
1	G	37	HIS	2.8
1	A	89	LEU	2.8
1	G	278	ARG	2.7
3	C	36	SER	2.7
3	F	173	VAL	2.7
1	G	249	GLN	2.7
1	J	155	ASP	2.7
1	P	174	VAL	2.7
3	L	33	ASP	2.7
1	J	236	ASN	2.7
1	A	164	TYR	2.7
1	G	120	MET	2.7
1	M	210	ASN	2.7
3	L	75	LEU	2.7
3	R	75	LEU	2.7
3	L	61	GLN	2.7
1	J	40	ALA	2.7
3	F	57	LEU	2.7
3	F	40	ASP	2.7
3	R	37	TRP	2.7
3	R	8	TRP	2.7
3	C	20	ARG	2.7
3	I	120	THR	2.6
3	L	77	GLY	2.6
3	R	72	CYS	2.6
2	B	126	LEU	2.6
3	R	85	LEU	2.6
1	G	174	VAL	2.6
3	F	55	HIS	2.6
3	I	41	GLY	2.6
1	A	28	LEU	2.6
3	F	24	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	45	LEU	2.6
2	K	131	PRO	2.6
3	L	24	LEU	2.6
3	I	36	SER	2.6
3	R	154	GLY	2.6
1	J	294	GLU	2.6
1	G	28	LEU	2.6
1	G	138	LEU	2.6
3	I	26	CYS	2.5
1	P	148	ALA	2.5
3	C	185	LEU	2.5
1	D	41	ASN	2.5
1	P	173	GLU	2.5
1	A	120	MET	2.5
3	C	77	GLY	2.5
3	I	54	GLY	2.5
3	L	10	PRO	2.5
1	A	93	VAL	2.5
3	R	181	ALA	2.5
2	H	130	GLN	2.5
1	P	192	PHE	2.5
1	G	254	ASP	2.5
1	A	6	CYS	2.5
3	O	82	THR	2.5
3	O	54	GLY	2.5
3	I	117	GLY	2.4
3	O	39	ARG	2.4
1	P	40	ALA	2.4
3	F	92	ALA	2.4
3	L	65	THR	2.4
3	I	24	LEU	2.4
3	I	81	GLY	2.4
3	O	4	CYS	2.4
1	A	210	ASN	2.4
1	G	93	VAL	2.4
3	L	23	LYS	2.4
3	O	77	GLY	2.4
1	G	236	ASN	2.4
2	K	133	PRO	2.3
3	L	90	PRO	2.3
3	I	131	VAL	2.3
3	R	22	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	44	VAL	2.3
1	D	236	ASN	2.3
3	C	52	GLY	2.3
1	G	237	ILE	2.3
2	K	139	PRO	2.3
3	L	171	ILE	2.3
3	F	188	VAL	2.3
3	O	185	LEU	2.3
3	C	38	PHE	2.3
3	F	46	LEU	2.3
3	O	10	PRO	2.3
1	D	192	PHE	2.3
1	A	79	LEU	2.3
1	G	238	GLN	2.3
3	C	141	PRO	2.3
3	I	82	THR	2.3
3	R	87	LEU	2.3
1	J	279	CYS	2.2
3	F	26	CYS	2.2
3	O	6	GLN	2.2
1	P	6	CYS	2.2
1	G	83	ILE	2.2
3	C	21	SER	2.2
3	C	10	PRO	2.2
2	N	132	PRO	2.2
1	A	11	PRO	2.2
1	J	146	LYS	2.2
1	P	41	ASN	2.2
3	R	82	THR	2.2
1	D	281	LYS	2.2
3	R	81	GLY	2.1
1	P	172	ILE	2.1
3	F	61	GLN	2.1
3	R	71	ILE	2.1
3	L	39	ARG	2.1
1	A	147	PHE	2.1
1	J	28	LEU	2.1
2	B	125	ARG	2.1
1	P	249	GLN	2.1
1	D	98	ILE	2.1
3	F	171	ILE	2.1
1	A	177	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	10	PRO	2.1
3	O	74	THR	2.1
3	R	59	LEU	2.1
3	C	155	ALA	2.1
3	R	46	LEU	2.1
1	P	86	PHE	2.1
1	A	8	TYR	2.1
1	G	203	PRO	2.1
2	B	131	PRO	2.1
2	N	50	ASN	2.1
3	R	122	TYR	2.1
1	G	213	GLU	2.1
3	O	264	GLY	2.1
3	I	8	TRP	2.0
3	F	14	GLN	2.0
1	A	24	ALA	2.0
3	R	92	ALA	2.0
3	O	181	ALA	2.0
1	D	71	ASP	2.0
1	G	90	GLU	2.0
1	M	178	ALA	2.0
1	G	96	ILE	2.0
1	J	102	LEU	2.0
3	L	92	ALA	2.0
3	R	171	ILE	2.0
1	D	138	LEU	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
5	BMA	b	3	11/12	0.32	0.39	93,93,93,93	0
4	NAG	c	2	14/15	0.60	0.33	155,211,229,230	0

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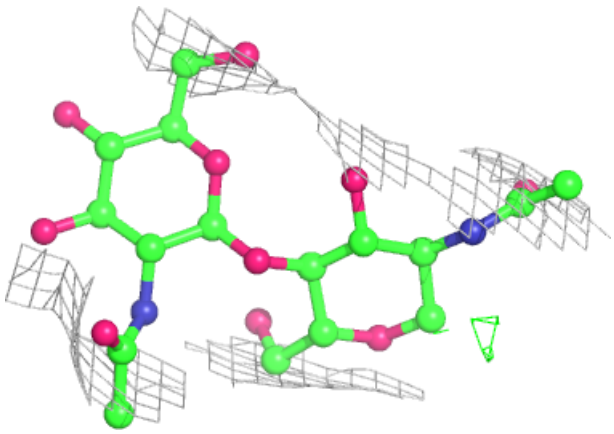
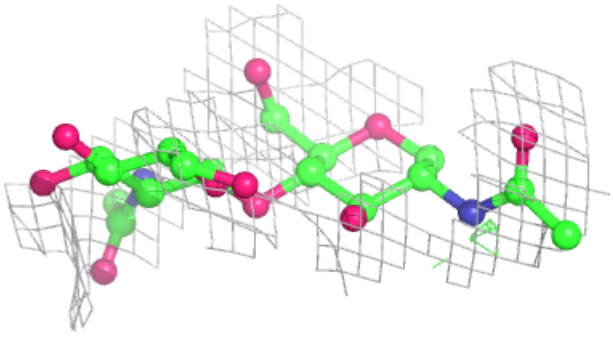
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	Z	3	11/12	0.61	0.43	93,93,93,93	0
4	NAG	U	2	14/15	0.62	0.29	155,211,229,230	0
4	NAG	S	2	14/15	0.66	0.22	155,211,229,230	0
4	NAG	W	2	14/15	0.73	0.28	155,211,229,230	0
4	NAG	Y	2	14/15	0.74	0.22	155,211,229,230	0
4	NAG	a	2	14/15	0.78	0.20	155,211,229,230	0
5	BMA	X	3	11/12	0.82	0.21	93,93,93,93	0
5	BMA	T	3	11/12	0.83	0.28	93,93,93,93	0
5	NAG	Z	2	14/15	0.83	0.45	81,81,81,81	0
5	NAG	b	2	14/15	0.85	0.39	81,81,81,81	0
4	NAG	a	1	14/15	0.85	0.14	174,186,199,206	0
5	NAG	T	1	14/15	0.86	0.35	67,67,67,67	0
5	NAG	b	1	14/15	0.86	0.39	67,67,67,67	0
5	NAG	d	2	14/15	0.86	0.27	81,81,81,81	0
5	NAG	V	2	14/15	0.87	0.23	81,81,81,81	0
5	BMA	V	3	11/12	0.87	0.25	93,93,93,93	0
4	NAG	U	1	14/15	0.87	0.18	174,186,199,206	0
4	NAG	c	1	14/15	0.88	0.30	174,186,199,206	0
5	NAG	T	2	14/15	0.88	0.32	81,81,81,81	0
4	NAG	W	1	14/15	0.88	0.25	174,186,199,206	0
5	NAG	Z	1	14/15	0.88	0.33	67,67,67,67	0
5	NAG	V	1	14/15	0.88	0.32	67,67,67,67	0
4	NAG	S	1	14/15	0.89	0.20	174,186,199,206	0
4	NAG	Y	1	14/15	0.90	0.17	174,186,199,206	0
5	NAG	d	1	14/15	0.91	0.27	67,67,67,67	0
5	BMA	d	3	11/12	0.91	0.17	93,93,93,93	0
5	NAG	X	2	14/15	0.92	0.25	81,81,81,81	0
5	NAG	X	1	14/15	0.93	0.22	67,67,67,67	0

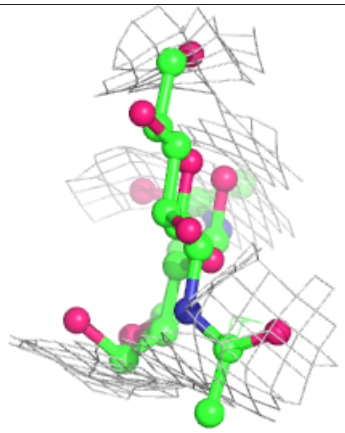
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

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

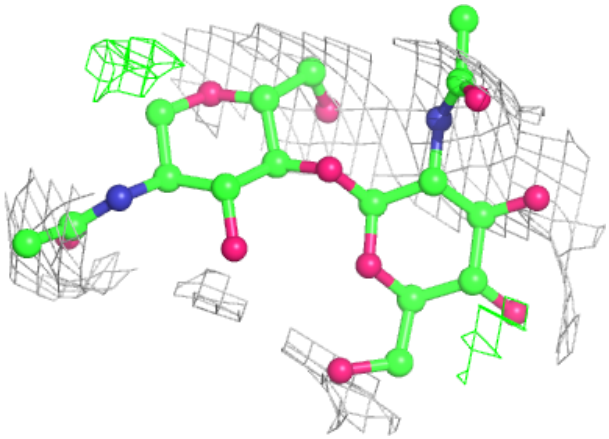


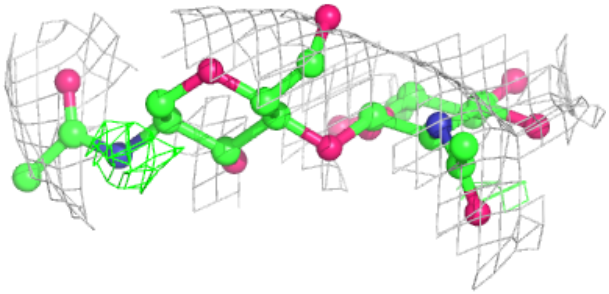


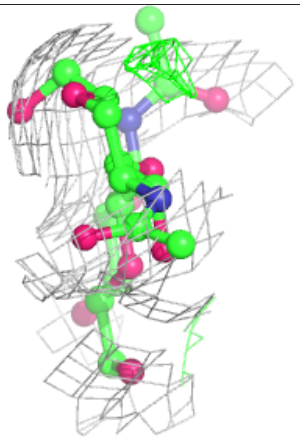


Electron density around Chain U:

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

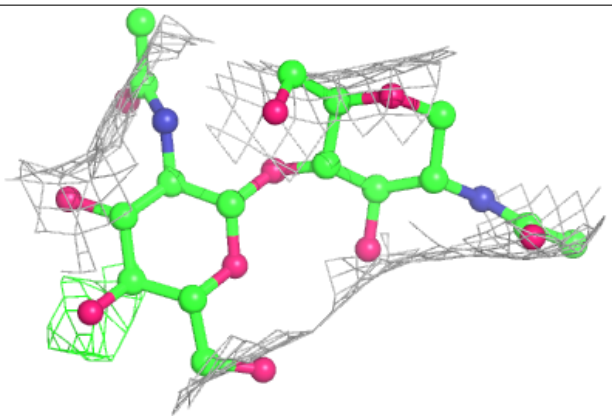


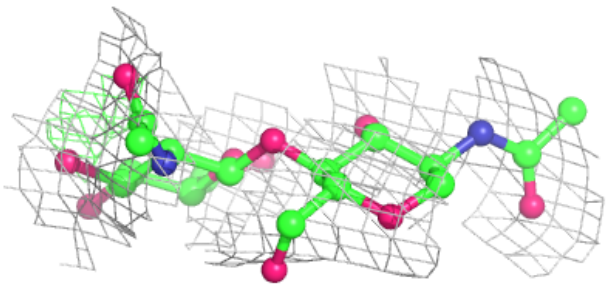


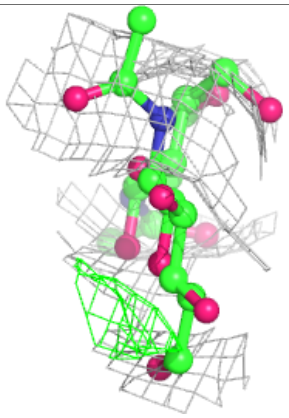


Electron density around Chain W:

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

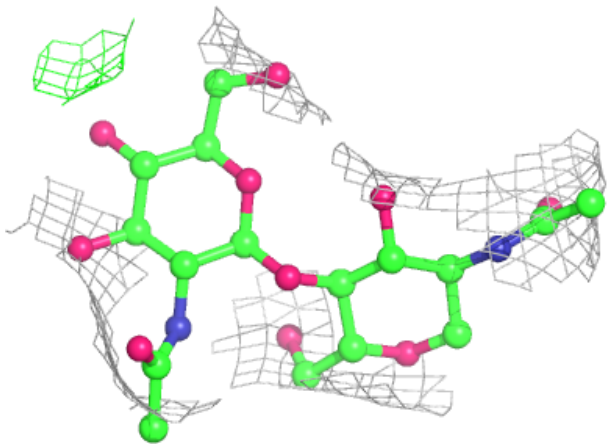


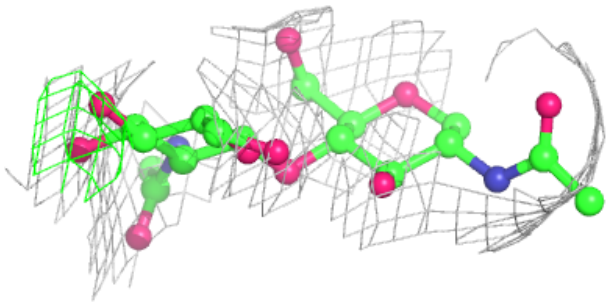


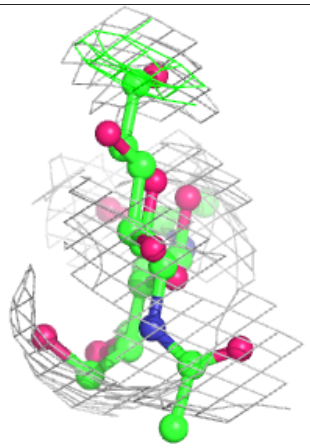


Electron density around Chain Y:

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

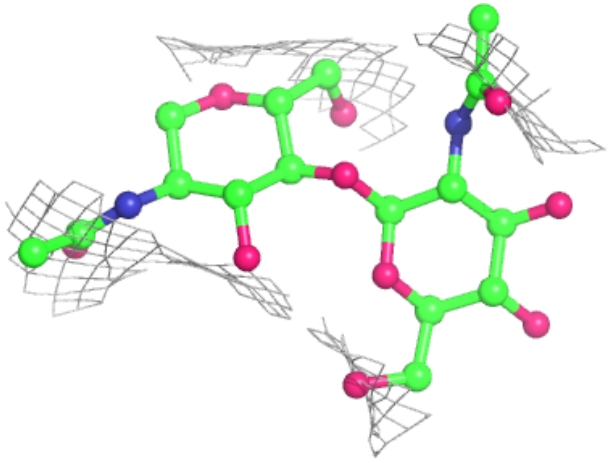


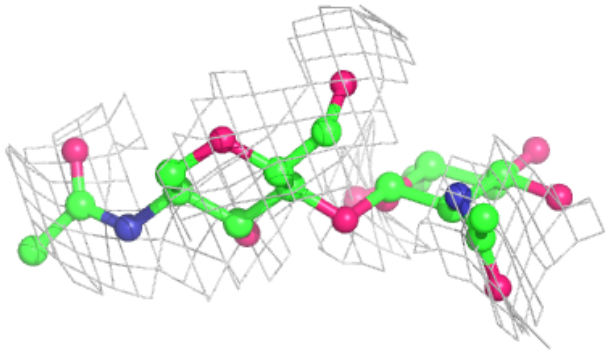


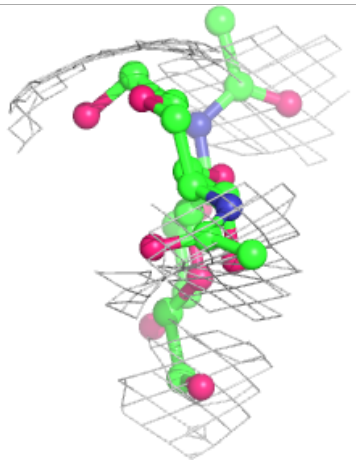


Electron density around Chain a:

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

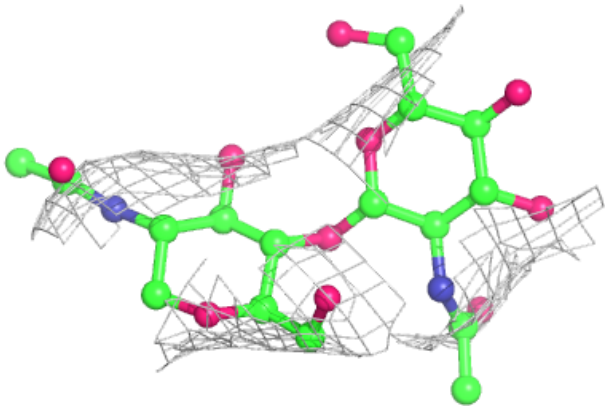


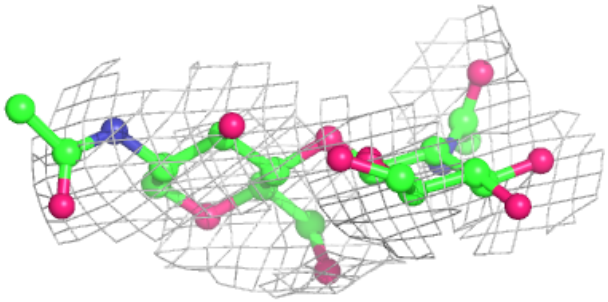


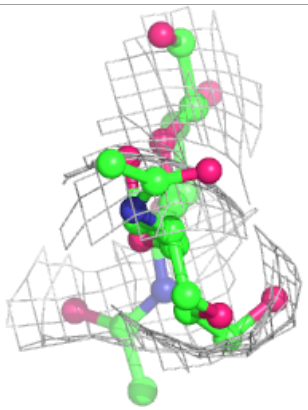


Electron density around Chain c:

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

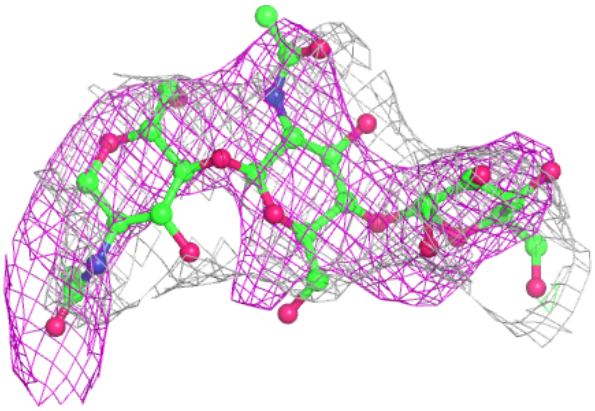


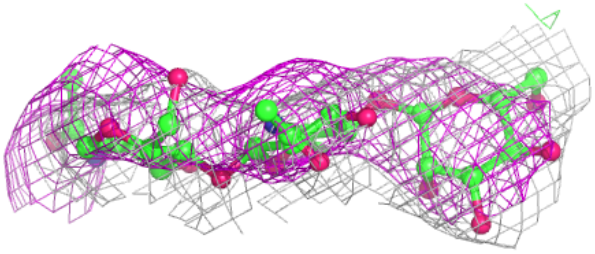


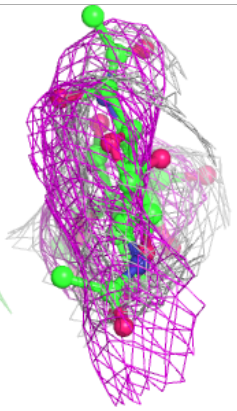


Electron density around Chain T:

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

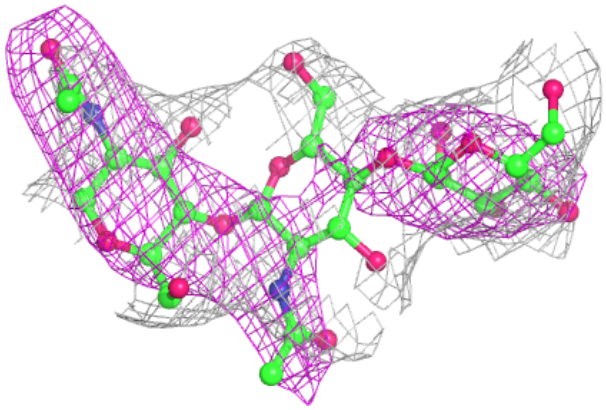


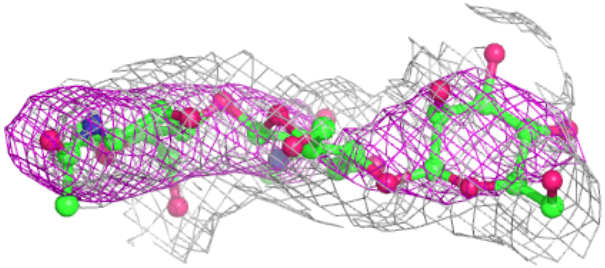


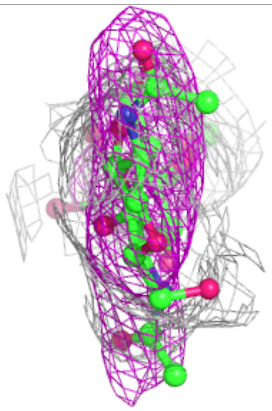


Electron density around Chain V:

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

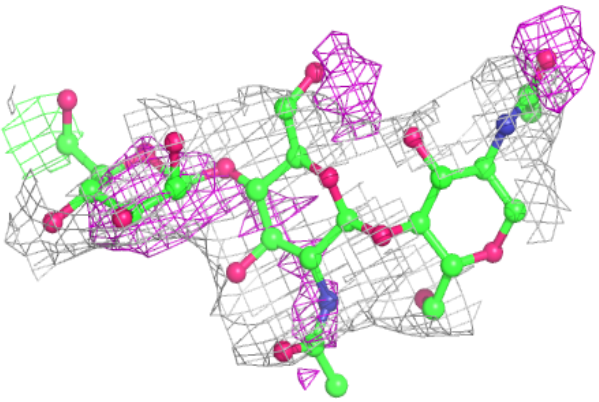


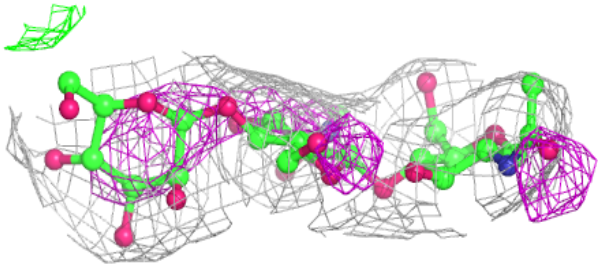


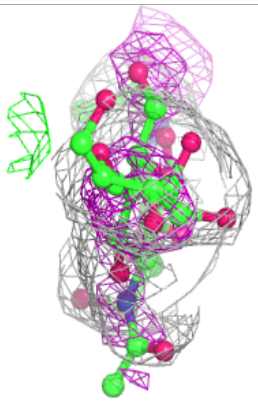


Electron density around Chain X:

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

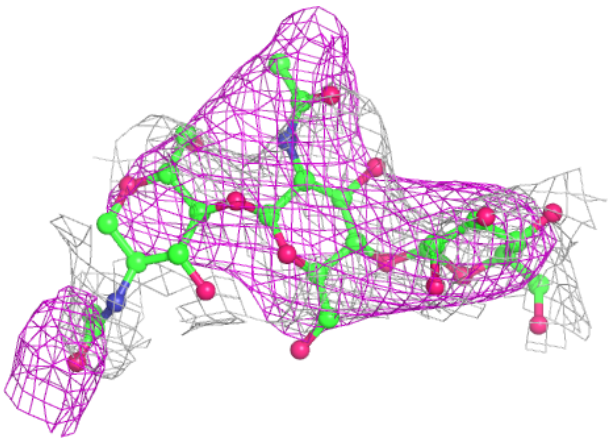


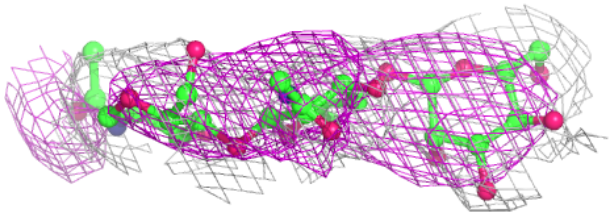


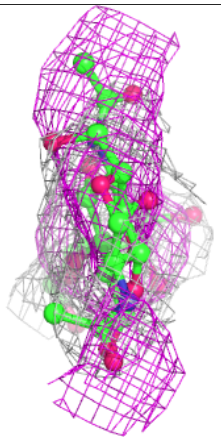


Electron density around Chain Z:

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

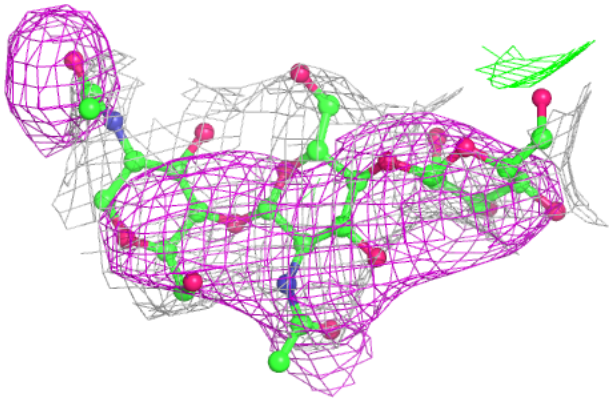


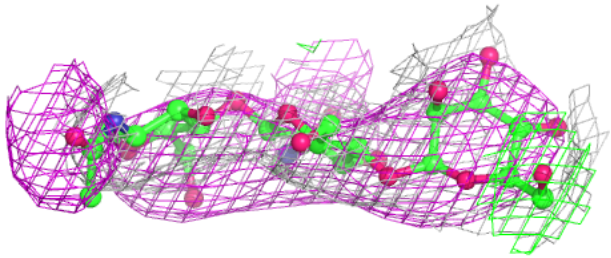


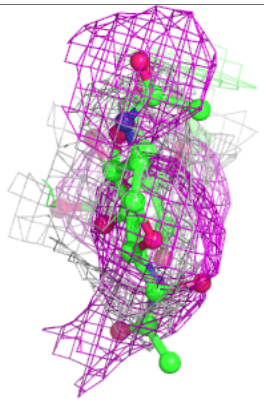


Electron density around Chain b:

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

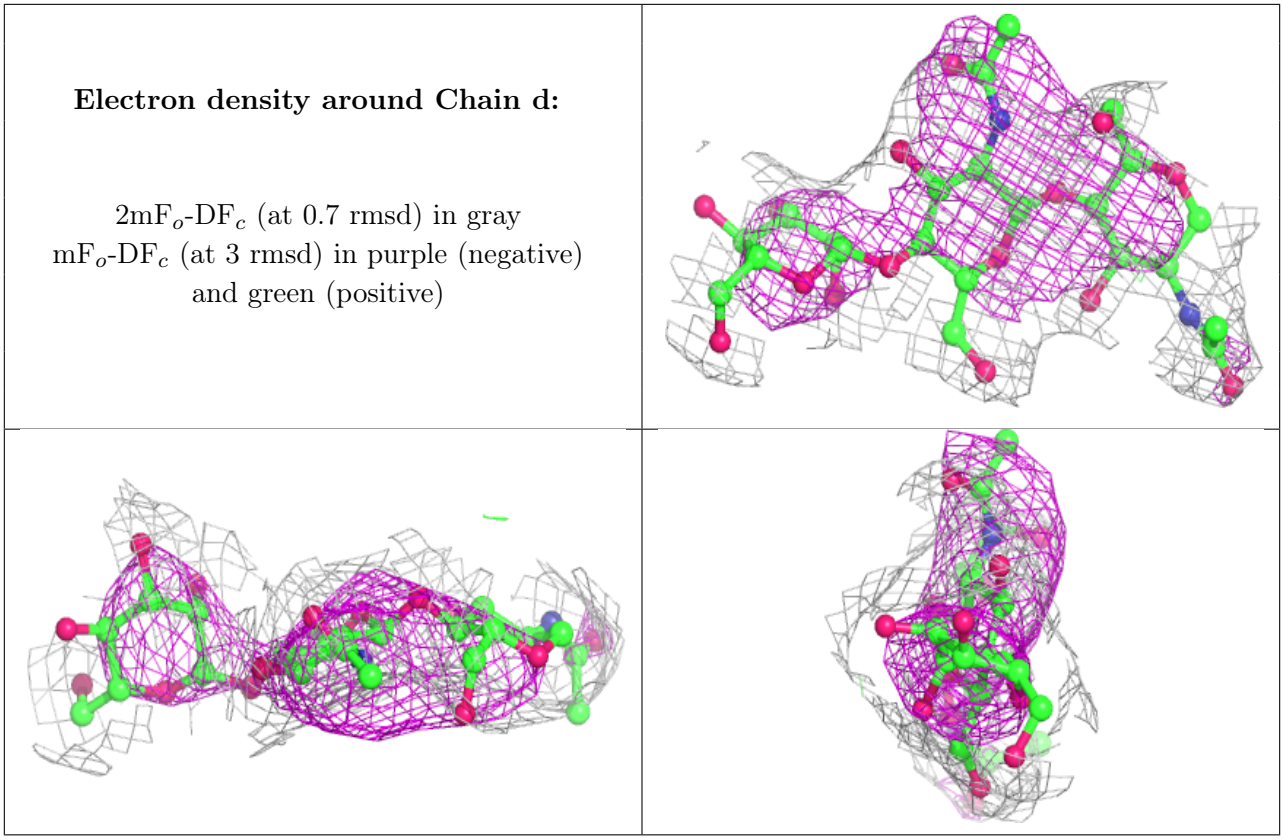






Electron density around Chain d:

$2mF_o$-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
6	NAG	P	402	14/15	0.49	0.34	149,179,207,213	0
6	NAG	C	401	14/15	0.58	0.22	77,183,262,267	0
6	NAG	J	402	14/15	0.61	0.31	149,179,207,213	0
6	NAG	L	401	14/15	0.64	0.23	77,183,262,267	0
6	NAG	R	401	14/15	0.66	0.33	77,183,262,267	0
6	NAG	I	401	14/15	0.68	0.25	77,183,262,267	0
6	NAG	D	401	14/15	0.71	0.29	78,78,78,78	0
6	NAG	D	402	14/15	0.75	0.31	149,179,207,213	0
6	NAG	G	402	14/15	0.76	0.28	149,179,207,213	0
6	NAG	O	401	14/15	0.76	0.25	77,183,262,267	0
6	NAG	P	401	14/15	0.77	0.24	78,78,78,78	0
6	NAG	M	402	14/15	0.79	0.18	149,179,207,213	0
6	NAG	F	401	14/15	0.80	0.34	77,183,262,267	0
6	NAG	A	402	14/15	0.80	0.20	149,179,207,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	G	401	14/15	0.81	0.27	78,78,78,78	0
6	NAG	J	401	14/15	0.83	0.25	78,78,78,78	0
6	NAG	A	401	14/15	0.85	0.21	78,78,78,78	0
6	NAG	M	401	14/15	0.86	0.16	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.