



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:59 AM EDT

PDB ID : 2GJX / pdb_00002gjx
Title : Crystallographic structure of human beta-Hexosaminidase A
Authors : Lemieux, M.J.; Mark, B.L.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.;
James, M.N.G.
Deposited on : 2006-03-31
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

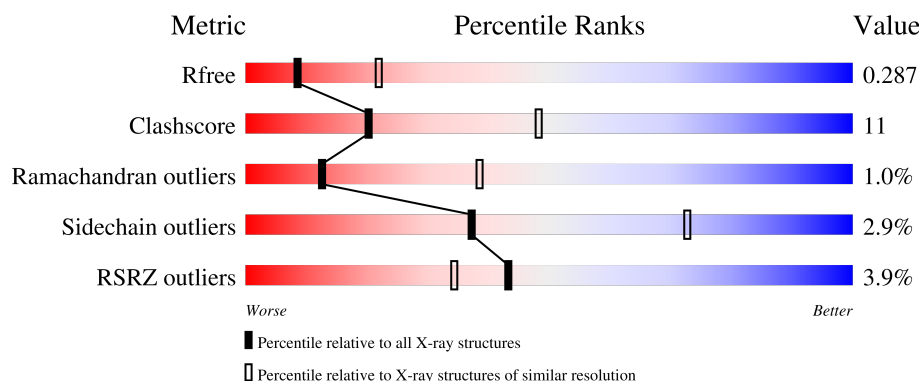
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	507	5% 78% 17% • •
1	D	507	2% 69% 25% • • •
1	E	507	10% 65% 28% • •
1	H	507	4% 66% 28% • •
2	B	507	2% 79% 15% • 5%

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Mol	Chain	Length	Quality of chain
2	C	507	
2	F	507	
2	G	507	
3	I	3	
3	J	3	
3	K	3	
3	M	3	
4	L	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	K	1	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32132 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.

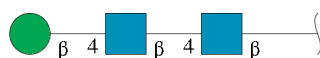
- Molecule 1 is a protein called Beta-hexosaminidase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			
1	D	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			
1	E	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			
1	H	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			

- Molecule 2 is a protein called Beta-hexosaminidase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			
2	C	481	Total	C	N	O	S	0	0	0
			3885	2511	644	717	13			
2	F	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			
2	G	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			

- Molecule 3 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
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



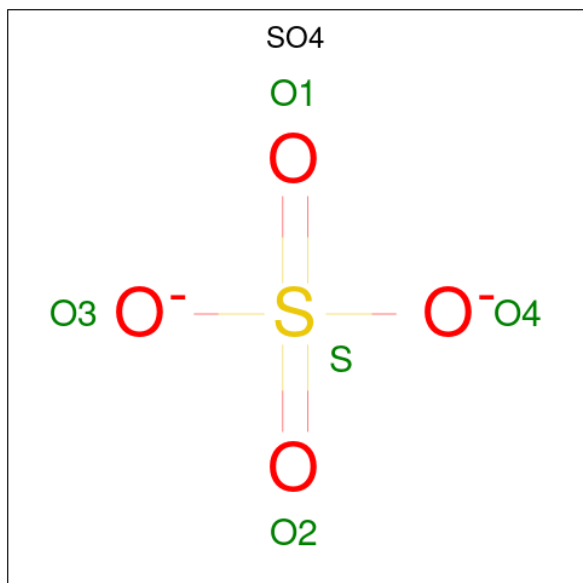
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0

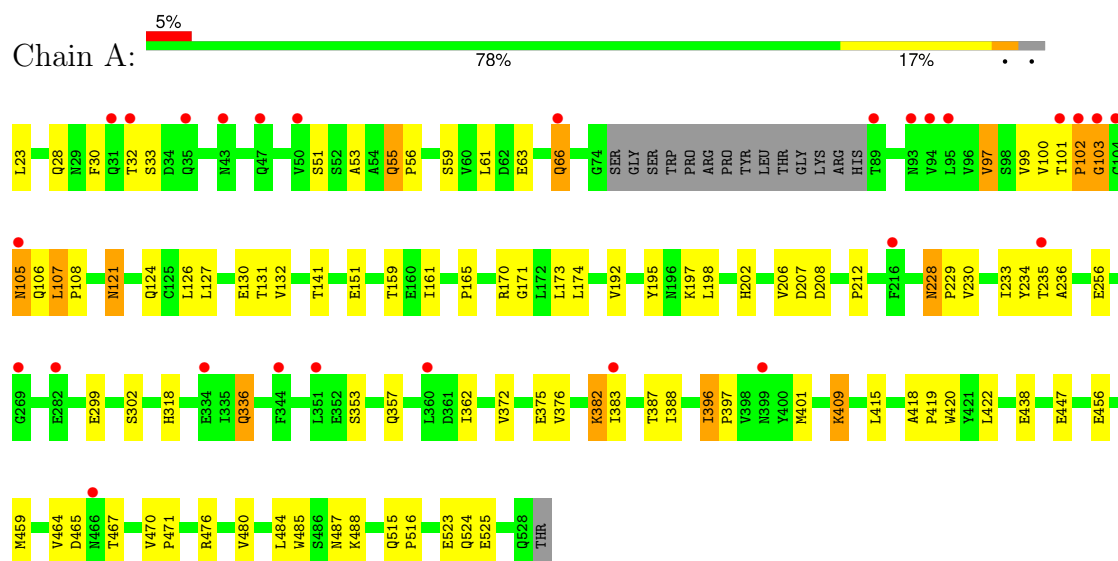
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	34	Total O 34 34	0	0
7	B	20	Total O 20 20	0	0
7	C	22	Total O 22 22	0	0
7	D	18	Total O 18 18	0	0
7	E	20	Total O 20 20	0	0
7	F	11	Total O 11 11	0	0
7	G	17	Total O 17 17	0	0
7	H	6	Total O 6 6	0	0

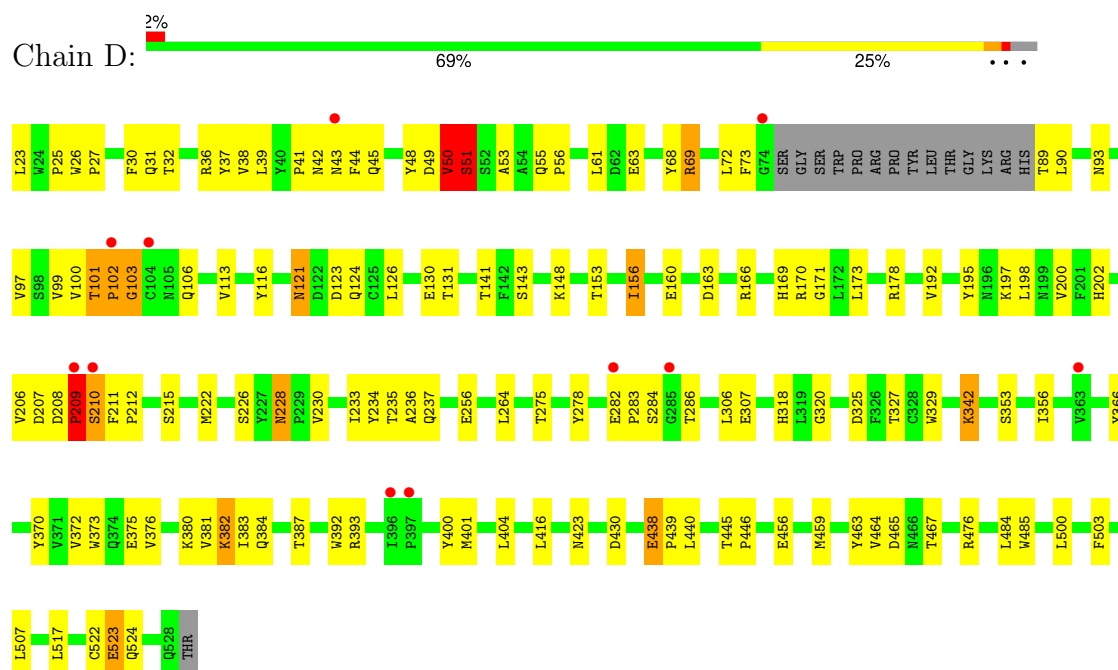
3 Residue-property plots

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

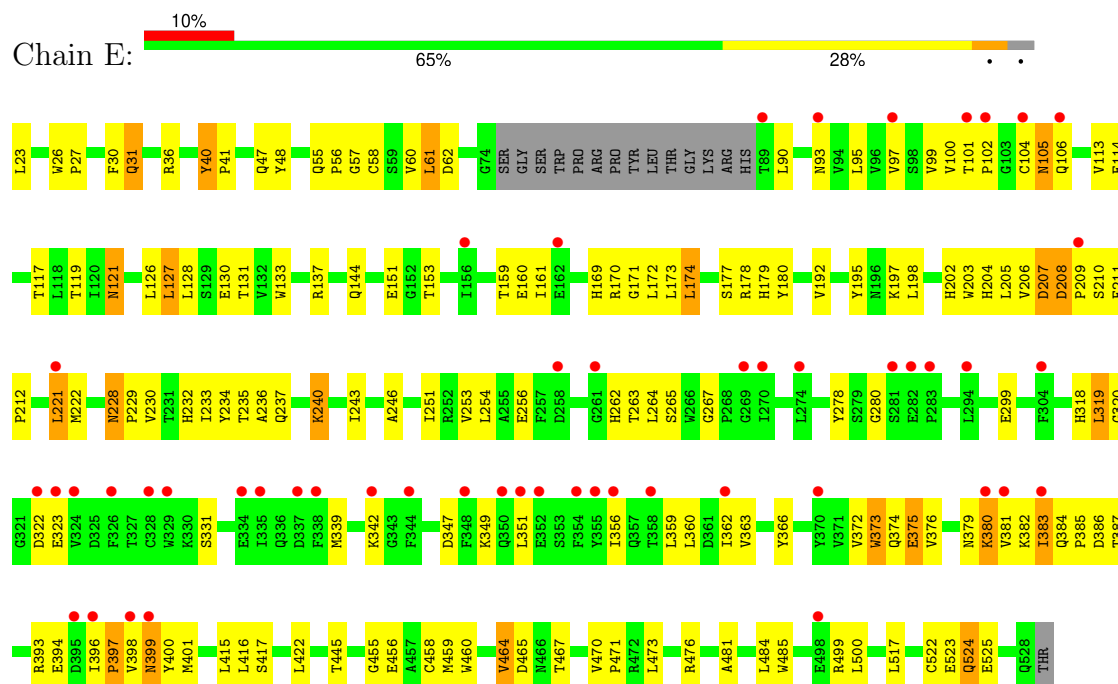
• Molecule 1: Beta-hexosaminidase alpha chain



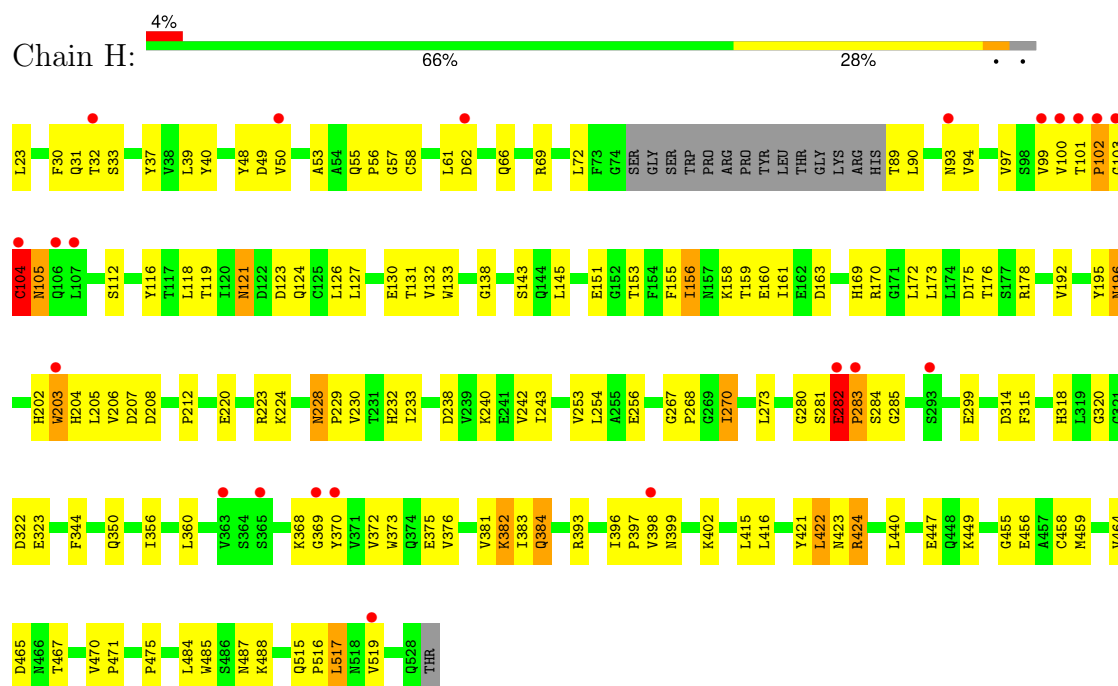
• Molecule 1: Beta-hexosaminidase alpha chain



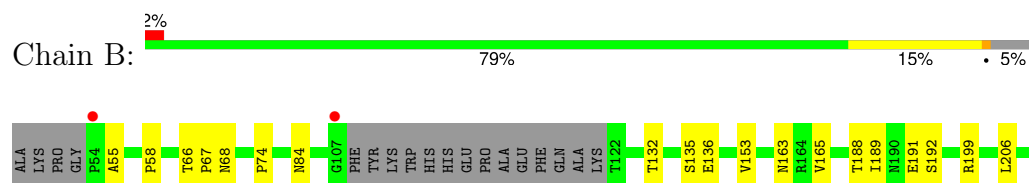
• Molecule 1: Beta-hexosaminidase alpha chain

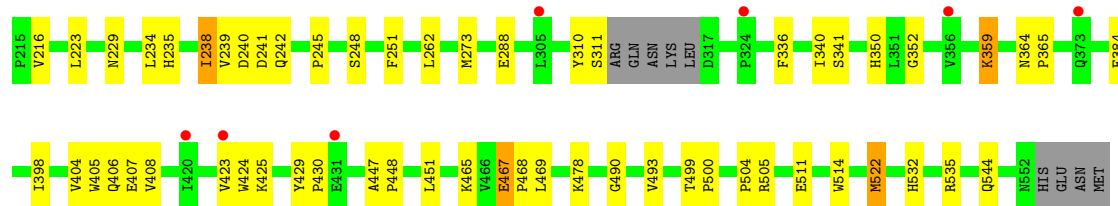


• Molecule 1: Beta-hexosaminidase alpha chain

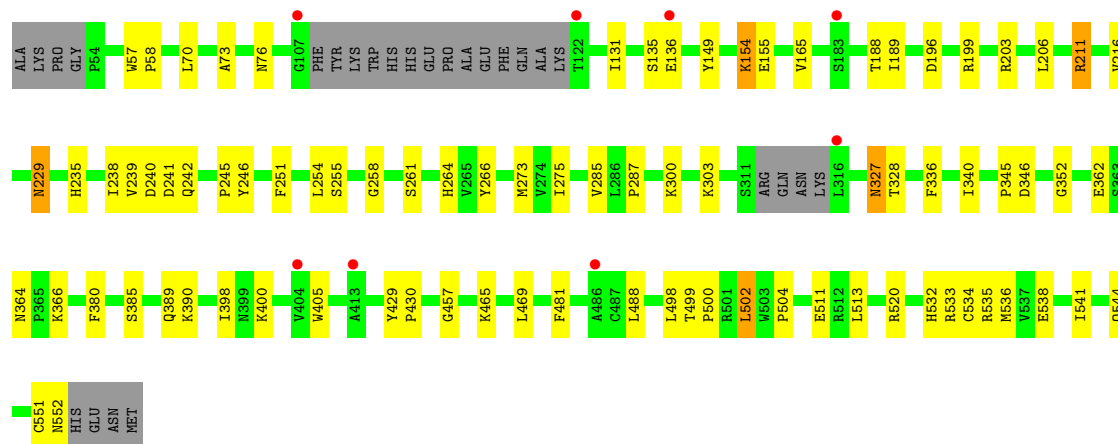
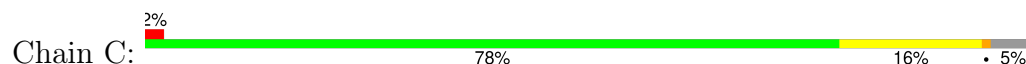


• Molecule 2: Beta-hexosaminidase beta chain

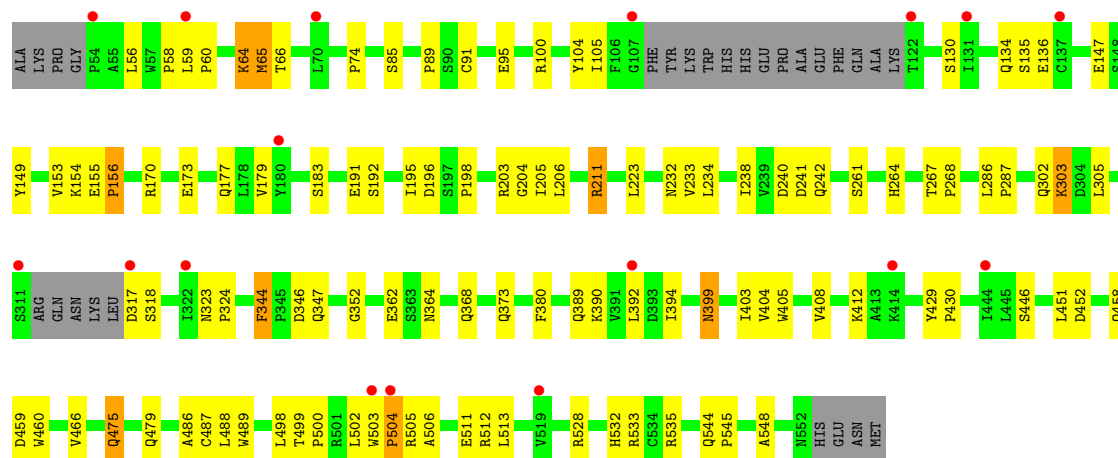




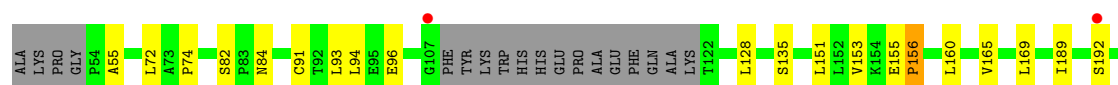
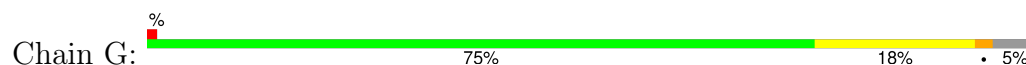
• Molecule 2: Beta-hexosaminidase beta chain

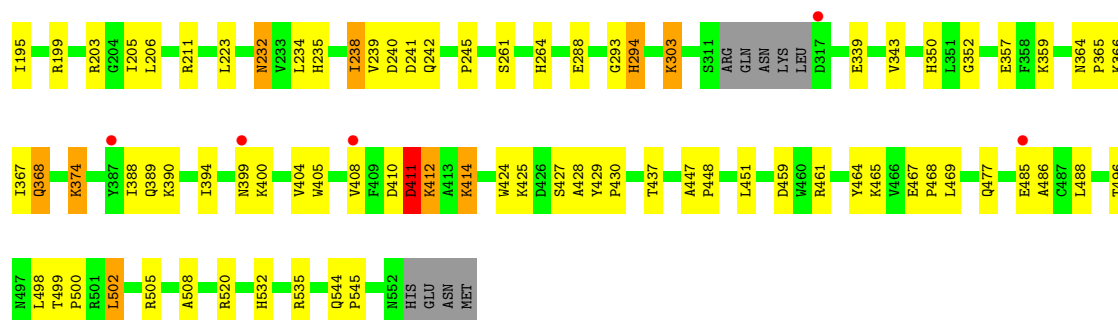


• Molecule 2: Beta-hexosaminidase beta chain



• Molecule 2: Beta-hexosaminidase beta chain





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

Chain I: 100%



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

Chain J: 100%



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

Chain K: 33% 67%



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

Chain M: 33% 33% 33%



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

Chain L: 100%



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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  50% 50%

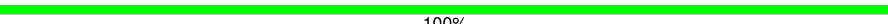


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	321.09Å 110.54Å 129.67Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	39.87 – 2.80 39.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.87-2.80) 99.7 (39.87-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.269 , 0.288 0.267 , 0.287	Depositor DCC
R_{free} test set	5525 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32132	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, SO4, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	1/4132 (0.0%)	0.77	0/5633
1	D	0.61	5/4132 (0.1%)	0.79	9/5633 (0.2%)
1	E	0.40	0/4132	0.74	6/5633 (0.1%)
1	H	0.48	1/4132 (0.0%)	0.78	7/5633 (0.1%)
2	B	0.36	0/3988	0.72	3/5423 (0.1%)
2	C	0.37	0/3996	0.73	4/5434 (0.1%)
2	F	0.38	0/3988	0.73	6/5423 (0.1%)
2	G	0.52	2/3988 (0.1%)	0.74	5/5423 (0.1%)
All	All	0.45	9/32488 (0.0%)	0.75	40/44235 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3
2	G	0	2
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	411	ASP	CA-C	20.17	1.85	1.52
1	D	210	SER	N-CA	19.79	1.70	1.46
1	H	422	LEU	C-O	13.55	1.42	1.24
1	D	209	PRO	CA-C	12.27	1.69	1.52
1	D	50	VAL	C-N	10.89	1.49	1.33
1	A	51	SER	CB-OG	7.34	1.56	1.42
1	D	209	PRO	CA-CB	7.32	1.64	1.53
1	D	209	PRO	C-O	-6.81	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	411	ASP	C-N	5.86	1.41	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	SER	N-CA-C	-10.59	88.24	110.80
2	G	411	ASP	CA-C-O	-8.68	110.69	121.89
1	H	282	GLU	C-N-CD	-8.15	102.66	120.60
1	H	422	LEU	O-C-N	-7.86	111.62	122.46
2	F	503	TRP	N-CA-C	7.30	125.94	109.81
1	H	282	GLU	CA-C-N	7.07	143.97	127.00
1	H	282	GLU	C-N-CA	7.07	143.97	127.00
2	C	303	LYS	N-CA-C	6.77	118.35	110.97
1	H	57	GLY	N-CA-C	-6.54	105.85	115.72
2	B	238	ILE	N-CA-C	6.38	116.53	110.53
2	G	238	ILE	N-CA-C	6.20	116.98	110.72
1	D	210	SER	N-CA-C	-6.00	97.80	108.13
1	H	40	TYR	CA-C-N	5.97	127.30	119.84
1	H	40	TYR	C-N-CA	5.97	127.30	119.84
2	G	411	ASP	N-CA-C	-5.83	103.44	110.44
2	F	344	PHE	CA-C-N	5.75	125.37	119.56
2	F	344	PHE	C-N-CA	5.75	125.37	119.56
2	F	238	ILE	N-CA-C	5.74	116.52	110.72
1	D	210	SER	CA-C-N	-5.67	115.80	123.46
1	D	210	SER	C-N-CA	-5.67	115.80	123.46
2	B	467	GLU	CA-C-N	5.54	124.73	118.97
2	B	467	GLU	C-N-CA	5.54	124.73	118.97
2	C	238	ILE	N-CA-C	5.47	116.25	110.72
1	E	57	GLY	N-CA-C	-5.47	106.98	114.64
1	E	171	GLY	N-CA-C	5.41	119.11	111.42
1	D	438	GLU	CA-C-N	5.35	125.02	119.56
1	D	438	GLU	C-N-CA	5.35	125.02	119.56
2	F	364	ASN	CA-C-N	5.33	124.51	118.97
2	F	364	ASN	C-N-CA	5.33	124.51	118.97
2	C	364	ASN	CA-C-N	5.29	124.74	119.24
2	C	364	ASN	C-N-CA	5.29	124.74	119.24
1	D	209	PRO	CA-C-O	-5.26	111.03	120.60
2	G	135	SER	N-CA-C	5.24	118.46	111.75
1	D	50	VAL	CA-C-N	-5.21	111.58	121.54
1	D	50	VAL	C-N-CA	-5.21	111.58	121.54
1	E	40	TYR	CA-C-N	5.18	126.32	119.84
1	E	40	TYR	C-N-CA	5.18	126.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	323	GLU	N-CA-C	5.14	116.55	109.15
2	G	399	ASN	N-CA-C	5.09	117.38	111.02
1	E	464	VAL	N-CA-C	5.03	115.51	108.17

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	209	PRO	Mainchain,Peptide
1	D	50	VAL	Peptide
2	G	411	ASP	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4010	0	3840	81	0
1	D	4010	0	3840	116	0
1	E	4010	0	3841	143	0
1	H	4010	0	3841	124	0
2	B	3877	0	3783	58	0
2	C	3885	0	3794	55	0
2	F	3877	0	3783	85	0
2	G	3877	0	3782	76	0
3	I	39	0	34	0	0
3	J	39	0	34	0	0
3	K	39	0	34	0	0
3	M	39	0	34	1	0
4	L	28	0	25	0	0
4	N	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	2	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	14	0	13	0	0
5	G	14	0	13	0	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
6	H	10	0	0	1	0
7	A	34	0	0	0	0
7	B	20	0	0	2	0
7	C	22	0	0	1	0
7	D	18	0	0	0	0
7	E	20	0	0	2	0
7	F	11	0	0	0	0
7	G	17	0	0	0	0
7	H	6	0	0	0	0
All	All	32132	0	30867	710	0

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

All (710) 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:D:210:SER:N	1:D:210:SER:CA	1.70	1.53
2:G:411:ASP:C	2:G:411:ASP:CA	1.85	1.50
1:E:55:GLN:HG3	1:E:56:PRO:HD2	1.29	1.13
1:H:424:ARG:HH11	1:H:424:ARG:HG2	1.08	1.12
1:H:53:ALA:HB1	1:H:101:THR:HA	1.33	1.10
1:E:383:ILE:HD11	1:E:387:THR:HB	1.32	1.06
2:G:242:GLN:HG2	1:H:519:VAL:HG21	1.37	1.05
1:D:55:GLN:HG3	1:D:56:PRO:HD2	1.36	1.03
2:G:411:ASP:HA	2:G:412:LYS:HE3	1.39	1.02
1:A:66:GLN:HA	1:A:66:GLN:OE1	1.59	1.00
1:A:55:GLN:HG3	1:A:56:PRO:HD2	1.47	0.95
1:H:55:GLN:HG3	1:H:56:PRO:HD2	1.47	0.94
1:H:424:ARG:HG2	1:H:424:ARG:NH1	1.80	0.94
1:D:380:LYS:HE2	1:D:380:LYS:HA	1.48	0.93
2:F:504:PRO:HG3	2:F:544:GLN:HG2	1.49	0.92
2:C:131:ILE:HG21	2:C:135:SER:HB3	1.50	0.92
2:F:504:PRO:CG	2:F:544:GLN:HG2	2.01	0.91
1:D:100:VAL:HG12	1:D:102:PRO:HD2	1.52	0.90
1:E:222:MET:SD	7:E:734:HOH:O	2.30	0.90
1:A:382:LYS:HE3	1:A:382:LYS:HA	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LYS:HG3	7:B:574:HOH:O	1.71	0.89
1:D:89:THR:HG22	1:D:90:LEU:HD23	1.54	0.87
1:H:53:ALA:CB	1:H:101:THR:HA	2.05	0.86
1:H:360:LEU:HD13	1:H:383:ILE:HG12	1.59	0.84
2:C:532:HIS:HD2	2:C:535:ARG:HH21	1.21	0.84
1:A:467:THR:HG21	2:B:544:GLN:HA	1.57	0.84
1:D:170:ARG:HG2	1:D:484:LEU:HB3	1.59	0.84
2:G:303:LYS:HE2	2:G:303:LYS:H	1.42	0.84
1:D:465:ASP:OD2	1:D:467:THR:HG22	1.79	0.82
1:H:100:VAL:HG12	1:H:102:PRO:HD2	1.62	0.82
1:A:372:VAL:HG21	1:A:376:VAL:HG21	1.61	0.82
1:D:228:ASN:HD22	1:D:230:VAL:H	1.29	0.80
1:H:282:GLU:OE1	1:H:283:PRO:HD3	1.82	0.80
1:E:393:ARG:HD2	1:E:396:ILE:HB	1.63	0.79
1:E:393:ARG:HD2	1:E:397:PRO:HD3	1.63	0.79
1:A:170:ARG:HG2	1:A:484:LEU:HB3	1.65	0.79
1:D:209:PRO:C	1:D:210:SER:CA	2.55	0.79
2:C:532:HIS:CD2	2:C:535:ARG:HH21	2.00	0.78
2:F:352:GLY:HA2	2:F:405:TRP:CD1	2.18	0.78
1:E:26:TRP:HB2	1:E:499:ARG:HH21	1.47	0.78
1:D:210:SER:N	1:D:210:SER:C	2.42	0.78
2:G:94:LEU:HD21	2:G:165:VAL:HG23	1.66	0.78
1:A:396:ILE:HD12	1:A:397:PRO:HA	1.65	0.78
2:G:303:LYS:HE2	2:G:303:LYS:N	1.97	0.77
2:G:429:TYR:N	2:G:430:PRO:HD2	1.99	0.77
1:H:58:CYS:C	1:H:104:CYS:SG	2.67	0.77
1:A:228:ASN:HD22	1:A:230:VAL:H	1.31	0.77
2:G:368:GLN:HA	2:G:368:GLN:HE21	1.50	0.76
2:F:135:SER:O	2:F:136:GLU:HG2	1.86	0.76
1:E:342:LYS:HA	1:E:342:LYS:HE2	1.67	0.75
1:A:170:ARG:NH2	1:A:197:LYS:O	2.21	0.74
1:A:30:PHE:HD2	1:A:161:ILE:HG12	1.51	0.74
1:E:228:ASN:HD22	1:E:230:VAL:H	1.34	0.73
2:F:390:LYS:O	2:F:394:ILE:HG12	1.88	0.73
1:D:49:ASP:CG	1:D:51:SER:HB2	2.14	0.73
1:H:97:VAL:HG12	1:H:126:LEU:HD11	1.70	0.73
1:A:107:LEU:HD13	1:A:107:LEU:H	1.53	0.72
1:H:121:ASN:ND2	1:H:124:GLN:H	1.87	0.72
1:E:55:GLN:HG3	1:E:56:PRO:CD	2.15	0.72
1:E:170:ARG:NH2	1:E:197:LYS:O	2.23	0.72
1:A:465:ASP:OD2	1:A:467:THR:HG22	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASP:OD2	1:D:97:VAL:HB	1.90	0.70
1:E:254:LEU:HD21	1:E:318:HIS:HB2	1.72	0.70
2:F:532:HIS:HD2	2:F:535:ARG:HH21	1.37	0.70
1:H:240:LYS:HE2	1:H:240:LYS:HA	1.73	0.70
1:E:100:VAL:HG12	1:E:102:PRO:HD2	1.72	0.70
2:B:341:SER:OG	2:B:398:ILE:HD12	1.91	0.70
2:G:155:GLU:HG3	2:G:156:PRO:HD3	1.74	0.69
1:A:121:ASN:ND2	1:A:124:GLN:H	1.90	0.69
1:E:170:ARG:HG2	1:E:484:LEU:HB3	1.74	0.69
2:C:488:LEU:HD22	2:C:502:LEU:HG	1.74	0.68
1:A:101:THR:N	1:A:102:PRO:HD2	2.09	0.68
1:E:153:THR:HG23	1:H:151:GLU:HB3	1.76	0.67
1:H:205:LEU:HD12	1:H:205:LEU:H	1.58	0.67
2:G:91:CYS:SG	2:G:94:LEU:HD23	2.34	0.67
1:H:121:ASN:HD22	1:H:123:ASP:H	1.42	0.67
1:D:49:ASP:O	1:D:51:SER:N	2.27	0.67
1:E:113:VAL:O	1:E:131:THR:HG22	1.94	0.67
1:H:228:ASN:ND2	1:H:230:VAL:HG12	2.09	0.67
2:C:346:ASP:O	2:C:400:LYS:NZ	2.26	0.67
1:E:204:HIS:HD2	1:E:256:GLU:CD	2.02	0.67
2:F:147:GLU:HB2	2:F:198:PRO:HG3	1.77	0.67
2:G:411:ASP:HA	2:G:412:LYS:CE	2.21	0.67
1:A:100:VAL:HG12	1:A:102:PRO:HD2	1.77	0.66
1:A:131:THR:HG22	1:A:132:VAL:H	1.60	0.66
2:F:352:GLY:HA2	2:F:405:TRP:HD1	1.60	0.66
1:D:459:MET:HE2	1:D:464:VAL:HG21	1.78	0.66
1:H:424:ARG:HH11	1:H:424:ARG:CG	1.95	0.66
1:A:131:THR:HG22	1:A:132:VAL:N	2.11	0.66
1:H:383:ILE:HG13	1:H:384:GLN:NE2	2.11	0.66
1:D:209:PRO:HB2	1:D:210:SER:HB2	1.77	0.65
2:F:56:LEU:O	2:F:528:ARG:NH1	2.29	0.65
1:H:202:HIS:NE2	1:H:256:GLU:OE1	2.20	0.65
1:D:101:THR:O	1:D:102:PRO:C	2.40	0.65
2:G:451:LEU:O	2:G:505:ARG:NH2	2.29	0.65
2:C:534:CYS:O	2:C:538:GLU:HG2	1.96	0.65
1:E:100:VAL:HG12	1:E:102:PRO:HG2	1.77	0.65
1:H:228:ASN:HD21	1:H:230:VAL:HG12	1.61	0.65
1:D:383:ILE:HD11	1:D:387:THR:HG21	1.77	0.65
1:H:372:VAL:HG21	1:H:376:VAL:HG21	1.78	0.65
2:G:374:LYS:HZ2	2:G:374:LYS:HA	1.62	0.65
1:D:202:HIS:HE1	1:D:256:GLU:OE1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:LEU:HD13	1:H:132:VAL:HG13	1.80	0.64
2:F:459:ASP:OD2	2:F:505:ARG:NH1	2.29	0.64
1:E:525:GLU:HG2	2:F:264:HIS:HE1	1.62	0.64
1:D:192:VAL:HA	1:D:195:TYR:CD2	2.32	0.64
2:F:65:MET:O	2:F:65:MET:HE3	1.99	0.63
1:A:23:LEU:HD21	1:A:141:THR:HG23	1.81	0.63
1:H:421:TYR:OH	6:H:534:SO4:O1	2.15	0.63
1:D:121:ASN:HD22	1:D:123:ASP:H	1.47	0.63
1:E:318:HIS:C	1:E:320:GLY:H	2.05	0.63
1:E:278:TYR:O	1:E:331:SER:HB2	1.98	0.63
2:B:262:LEU:CD2	1:D:69:ARG:HH22	2.11	0.63
1:A:409:LYS:HZ2	1:A:409:LYS:HB2	1.64	0.63
1:D:282:GLU:HA	1:D:282:GLU:OE1	1.99	0.63
1:A:372:VAL:CG2	1:A:376:VAL:HG21	2.28	0.62
1:E:172:LEU:CD1	1:E:174:LEU:HD13	2.29	0.62
1:A:524:GLN:O	1:A:524:GLN:HG2	1.99	0.62
2:G:544:GLN:HA	1:H:467:THR:HG21	1.81	0.62
1:D:170:ARG:NH2	1:D:485:TRP:HE3	1.98	0.62
1:H:72:LEU:HD11	1:H:143:SER:HB2	1.82	0.62
2:C:240:ASP:OD2	2:C:241:ASP:N	2.26	0.61
2:C:551:CYS:O	2:C:552:ASN:HB2	1.99	0.61
2:F:451:LEU:O	2:F:505:ARG:NH2	2.32	0.61
1:A:192:VAL:HA	1:A:195:TYR:CD2	2.35	0.61
1:D:372:VAL:HG21	1:D:376:VAL:HG21	1.82	0.61
2:G:94:LEU:CD2	2:G:165:VAL:HG23	2.30	0.61
1:E:467:THR:HG21	2:F:544:GLN:HA	1.83	0.61
2:C:229:ASN:HD21	2:C:536:MET:HE2	1.64	0.61
1:E:318:HIS:HE1	1:E:373:TRP:NE1	1.99	0.61
1:D:380:LYS:HA	1:D:380:LYS:CE	2.25	0.61
2:G:223:LEU:HD21	2:G:234:LEU:HD22	1.81	0.61
2:C:216:VAL:HG11	2:C:273:MET:HE3	1.83	0.61
1:D:100:VAL:HG12	1:D:102:PRO:CD	2.26	0.61
1:H:360:LEU:CD1	1:H:383:ILE:HG12	2.29	0.61
1:E:383:ILE:CD1	1:E:387:THR:HB	2.22	0.61
2:F:100:ARG:HG2	2:F:104:TYR:HE2	1.65	0.61
2:F:135:SER:C	2:F:136:GLU:HG2	2.24	0.61
2:B:262:LEU:HD22	1:D:69:ARG:HH22	1.66	0.61
1:H:103:GLY:HA3	1:H:132:VAL:HG21	1.83	0.60
1:E:26:TRP:HB2	1:E:499:ARG:NH2	2.13	0.60
2:F:240:ASP:OD2	2:F:241:ASP:N	2.31	0.60
1:E:208:ASP:OD2	1:E:262:HIS:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:VAL:HA	1:E:195:TYR:CD2	2.36	0.60
2:F:85:SER:HB2	2:F:130:SER:HA	1.83	0.60
2:F:504:PRO:HG2	2:F:544:GLN:HG2	1.81	0.60
2:G:242:GLN:CG	1:H:519:VAL:HG21	2.25	0.60
1:E:372:VAL:HG11	1:E:376:VAL:HG21	1.83	0.60
1:E:393:ARG:CD	1:E:396:ILE:HB	2.32	0.60
1:H:176:THR:HG1	1:H:203:TRP:HZ3	1.50	0.60
1:E:211:PHE:CE1	1:E:221:LEU:HD13	2.37	0.60
1:E:318:HIS:HE1	1:E:373:TRP:CD1	2.20	0.59
2:B:58:PRO:HB3	2:B:511:GLU:HA	1.84	0.59
2:F:154:LYS:HB3	2:F:156:PRO:HD2	1.84	0.59
2:B:451:LEU:O	2:B:505:ARG:NH2	2.35	0.59
1:D:39:LEU:HG	1:D:156:ILE:HD11	1.85	0.59
1:A:170:ARG:HG2	1:A:484:LEU:CB	2.31	0.59
1:E:172:LEU:HD11	1:E:174:LEU:HD13	1.83	0.59
1:H:131:THR:HG22	1:H:132:VAL:H	1.66	0.59
1:D:31:GLN:HB2	1:D:160:GLU:HB3	1.84	0.59
2:B:499:THR:HB	2:B:500:PRO:HD3	1.85	0.59
2:F:58:PRO:HB3	2:F:511:GLU:HA	1.84	0.58
1:E:100:VAL:HG12	1:E:102:PRO:CD	2.33	0.58
1:A:459:MET:HE1	1:A:464:VAL:HG21	1.85	0.58
2:B:310:TYR:O	2:B:311:SER:HB3	2.02	0.58
2:F:134:GLN:HA	2:F:134:GLN:OE1	2.03	0.58
2:C:154:LYS:HE3	2:C:154:LYS:O	2.03	0.58
1:E:383:ILE:HD11	1:E:387:THR:CB	2.21	0.58
2:F:203:ARG:HG2	2:F:513:LEU:HB3	1.86	0.58
1:H:131:THR:HG22	1:H:132:VAL:N	2.16	0.58
2:F:173:GLU:O	2:F:177:GLN:HG3	2.03	0.58
2:F:532:HIS:CD2	2:F:535:ARG:HH21	2.19	0.58
1:H:196:ASN:N	1:H:196:ASN:HD22	2.01	0.58
1:E:100:VAL:CG1	1:E:102:PRO:HD2	2.33	0.58
1:E:459:MET:HE1	1:E:464:VAL:HG21	1.85	0.58
2:B:262:LEU:CD2	1:D:69:ARG:NH2	2.67	0.58
1:E:101:THR:N	1:E:102:PRO:HD2	2.18	0.58
1:A:61:LEU:CD1	1:A:132:VAL:HG23	2.34	0.58
1:A:383:ILE:HD11	1:A:387:THR:HB	1.85	0.58
1:E:384:GLN:OE1	1:E:384:GLN:N	2.31	0.58
2:F:488:LEU:HD22	2:F:502:LEU:HB2	1.86	0.58
2:G:240:ASP:OD2	2:G:241:ASP:N	2.27	0.57
1:H:243:ILE:HA	1:H:253:VAL:HG21	1.86	0.57
2:C:154:LYS:HE3	2:C:154:LYS:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:VAL:HG12	2:C:245:PRO:HD2	1.86	0.57
1:E:318:HIS:C	1:E:320:GLY:N	2.62	0.57
1:E:356:ILE:HD13	1:E:376:VAL:HG22	1.86	0.57
2:B:532:HIS:HD2	2:B:535:ARG:HH21	1.53	0.57
2:F:362:GLU:O	2:F:368:GLN:NE2	2.33	0.57
2:G:239:VAL:HG12	2:G:245:PRO:HD2	1.85	0.57
2:G:464:TYR:HB2	2:G:508:ALA:HB1	1.87	0.57
1:D:370:TYR:OH	1:D:384:GLN:HG3	2.03	0.57
1:E:30:PHE:CD2	1:E:161:ILE:HG12	2.39	0.57
1:E:205:LEU:H	1:E:205:LEU:HD12	1.70	0.57
1:E:235:THR:HG22	1:E:236:ALA:N	2.20	0.57
1:D:325:ASP:OD1	1:D:327:THR:HG22	2.04	0.57
2:G:374:LYS:HA	2:G:374:LYS:NZ	2.18	0.57
1:H:112:SER:HG	1:H:133:TRP:CD1	2.23	0.57
1:H:465:ASP:OD2	1:H:467:THR:HG22	2.04	0.57
1:A:66:GLN:OE1	1:A:66:GLN:CA	2.41	0.57
1:D:30:PHE:HE2	1:D:32:THR:HB	1.69	0.57
1:E:114:GLU:OE2	1:E:170:ARG:NH1	2.38	0.57
2:G:411:ASP:O	2:G:412:LYS:HB2	2.04	0.57
2:G:411:ASP:N	2:G:411:ASP:OD1	2.37	0.57
1:H:270:ILE:HG23	1:H:270:ILE:O	2.03	0.57
2:B:406:GLN:HE22	2:B:423:VAL:HG13	1.70	0.56
2:F:66:THR:HB	2:F:191:GLU:O	2.04	0.56
1:E:30:PHE:HD2	1:E:161:ILE:HG12	1.69	0.56
1:H:383:ILE:HG13	1:H:384:GLN:H	1.69	0.56
1:D:101:THR:N	1:D:102:PRO:HD2	2.21	0.56
2:B:429:TYR:N	2:B:430:PRO:CD	2.69	0.56
1:D:222:MET:CG	1:D:233:ILE:HD12	2.36	0.56
2:C:58:PRO:HB3	2:C:511:GLU:HA	1.86	0.56
1:E:58:CYS:SG	1:E:61:LEU:HB2	2.46	0.56
1:E:422:LEU:O	1:E:476:ARG:NH2	2.39	0.56
2:C:429:TYR:N	2:C:430:PRO:CD	2.68	0.56
2:F:153:VAL:HB	2:F:192:SER:H	1.70	0.56
1:H:282:GLU:CD	1:H:282:GLU:O	2.49	0.55
2:B:262:LEU:HD23	1:D:69:ARG:NH2	2.21	0.55
1:E:381:VAL:O	1:E:383:ILE:N	2.40	0.55
2:F:429:TYR:N	2:F:430:PRO:CD	2.69	0.55
1:E:100:VAL:HG12	1:E:102:PRO:CG	2.36	0.55
2:F:389:GLN:HA	2:F:392:LEU:CD2	2.37	0.55
1:H:475:PRO:HG2	1:H:517:LEU:CD1	2.37	0.55
1:E:36:ARG:HD2	4:P:1:NAG:H62	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:PRO:HD2	1:D:197:LYS:HD3	1.89	0.55
1:E:90:LEU:H	1:E:90:LEU:HD23	1.72	0.55
1:A:55:GLN:HG3	1:A:56:PRO:CD	2.30	0.55
1:A:105:ASN:OD1	1:A:105:ASN:N	2.39	0.55
1:H:173:LEU:HA	1:H:202:HIS:HB3	1.89	0.55
1:E:347:ASP:OD1	1:E:349:LYS:HG2	2.07	0.55
2:F:267:THR:CG2	1:H:66:GLN:HG3	2.37	0.55
1:H:196:ASN:HD22	1:H:196:ASN:H	1.53	0.55
1:H:229:PRO:HA	1:H:233:ILE:HD11	1.89	0.55
1:A:207:ASP:OD2	1:A:208:ASP:N	2.31	0.55
1:D:171:GLY:HA2	1:D:200:VAL:O	2.07	0.55
1:E:500:LEU:HG	1:E:517:LEU:HD11	1.89	0.55
1:H:99:VAL:HG22	1:H:130:GLU:HA	1.89	0.55
1:A:151:GLU:HG3	1:D:38:VAL:HG11	1.88	0.54
1:A:151:GLU:HB3	1:D:153:THR:HG23	1.88	0.54
2:B:364:ASN:HD22	2:B:365:PRO:HD2	1.72	0.54
1:E:263:THR:C	1:E:265:SER:H	2.16	0.54
1:H:459:MET:HE2	1:H:464:VAL:HG21	1.88	0.54
2:G:240:ASP:OD2	2:G:294:HIS:HB3	2.07	0.54
2:G:429:TYR:N	2:G:430:PRO:CD	2.69	0.54
1:H:202:HIS:ND1	1:H:456:GLU:OE1	2.41	0.54
1:H:487:ASN:OD1	1:H:488:LYS:N	2.41	0.54
2:C:327:ASN:HD22	2:C:328:THR:N	2.05	0.54
1:E:235:THR:HG22	1:E:237:GLN:H	1.73	0.54
2:F:91:CYS:O	2:F:95:GLU:HG2	2.07	0.54
1:E:254:LEU:CD2	1:E:318:HIS:HB2	2.38	0.54
1:H:356:ILE:HD13	1:H:376:VAL:HG22	1.88	0.54
1:H:459:MET:HE3	1:H:459:MET:HA	1.89	0.54
2:B:406:GLN:NE2	2:B:423:VAL:HG13	2.22	0.54
1:H:30:PHE:CE2	1:H:32:THR:HB	2.43	0.54
1:H:118:LEU:HD13	1:H:127:LEU:HD23	1.90	0.54
2:C:258:GLY:HA2	2:C:300:LYS:HE3	1.90	0.54
2:F:532:HIS:HD2	2:F:535:ARG:NH2	2.05	0.54
2:G:153:VAL:HB	2:G:192:SER:H	1.73	0.54
2:B:240:ASP:OD1	2:B:241:ASP:N	2.30	0.53
1:D:170:ARG:HG2	1:D:484:LEU:CB	2.34	0.53
2:B:239:VAL:HG12	2:B:245:PRO:HD2	1.90	0.53
1:A:61:LEU:HD13	1:A:132:VAL:HG23	1.90	0.53
2:C:211:ARG:HD2	2:C:242:GLN:OE1	2.08	0.53
1:A:447:GLU:CD	1:A:447:GLU:H	2.16	0.53
1:A:382:LYS:HA	1:A:382:LYS:CE	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PRO:HB3	1:D:73:PHE:CD1	2.44	0.53
1:E:384:GLN:O	1:E:386:ASP:N	2.36	0.53
1:D:170:ARG:NH2	1:D:485:TRP:CE3	2.77	0.53
1:E:222:MET:SD	1:E:233:ILE:HD12	2.49	0.53
2:B:216:VAL:HG11	2:B:273:MET:HE3	1.89	0.52
2:G:261:SER:OG	2:G:264:HIS:HD2	1.92	0.52
2:G:203:ARG:H	2:G:232:ASN:HD21	1.56	0.52
1:A:235:THR:HG22	1:A:236:ALA:H	1.73	0.52
2:C:390:LYS:NZ	2:C:390:LYS:HB3	2.24	0.52
1:E:237:GLN:HB3	2:G:96:GLU:OE2	2.10	0.52
1:A:418:ALA:HB3	1:A:419:PRO:HD3	1.92	0.52
1:E:206:VAL:HG12	1:E:211:PHE:HA	1.92	0.52
2:B:425:LYS:O	2:B:429:TYR:HB3	2.10	0.52
1:H:416:LEU:O	1:H:455:GLY:HA3	2.09	0.52
4:S:1:NAG:H62	4:S:2:NAG:HN2	1.75	0.52
1:E:137:ARG:HB3	1:E:197:LYS:HE3	1.92	0.52
1:E:467:THR:CG2	2:F:544:GLN:HA	2.40	0.52
1:H:31:GLN:HB2	1:H:160:GLU:HB3	1.92	0.52
1:D:206:VAL:HG12	1:D:212:PRO:HD2	1.91	0.52
1:E:47:GLN:CD	1:E:93:ASN:HD21	2.18	0.52
2:F:499:THR:HB	2:F:500:PRO:HD3	1.92	0.52
2:G:357:GLU:HB3	2:G:359:LYS:HG2	1.92	0.52
2:F:317:ASP:OD2	2:F:318:SER:N	2.43	0.52
2:F:475:GLN:O	2:F:479:GLN:HG3	2.10	0.51
2:F:502:LEU:HD23	2:F:506:ALA:HB2	1.92	0.51
2:B:135:SER:HB2	2:B:165:VAL:HG23	1.92	0.51
2:F:135:SER:O	2:F:136:GLU:CG	2.58	0.51
1:H:344:PHE:HA	1:H:350:GLN:HE21	1.75	0.51
1:A:235:THR:HG22	1:A:236:ALA:N	2.25	0.51
1:E:173:LEU:C	1:E:173:LEU:HD23	2.36	0.51
1:E:322:ASP:HB3	1:E:373:TRP:CD1	2.45	0.51
1:D:53:ALA:HB1	1:D:101:THR:CG2	2.41	0.51
1:D:235:THR:HG22	1:D:237:GLN:H	1.75	0.51
2:G:72:LEU:HD11	2:G:189:ILE:HG22	1.91	0.51
1:H:33:SER:HB3	1:H:158:LYS:HB3	1.92	0.51
1:A:256:GLU:HB2	1:A:318:HIS:HB3	1.93	0.51
1:D:522:CYS:O	1:D:523:GLU:C	2.53	0.51
2:G:410:ASP:O	2:G:412:LYS:HG3	2.10	0.51
1:H:228:ASN:C	1:H:228:ASN:HD22	2.18	0.51
1:E:105:ASN:OD1	1:E:105:ASN:N	2.44	0.51
1:E:465:ASP:OD1	1:E:467:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:404:VAL:HG11	2:F:408:VAL:HB	1.93	0.51
2:B:209:THR:HG22	2:B:214:LEU:HD12	1.92	0.51
2:B:532:HIS:CD2	2:B:535:ARG:HH21	2.28	0.51
1:D:45:GLN:HG3	1:D:93:ASN:HD22	1.76	0.51
1:H:170:ARG:HG2	1:H:484:LEU:HB3	1.93	0.51
1:E:525:GLU:CG	2:F:264:HIS:HE1	2.24	0.50
2:C:499:THR:HB	2:C:500:PRO:HD3	1.93	0.50
1:E:179:HIS:HB3	1:E:465:ASP:HB3	1.93	0.50
1:A:171:GLY:HA3	1:A:456:GLU:HG2	1.93	0.50
1:E:204:HIS:CD2	1:E:256:GLU:CD	2.88	0.50
2:G:411:ASP:C	2:G:411:ASP:N	2.61	0.50
1:A:202:HIS:ND1	1:A:456:GLU:OE1	2.45	0.50
1:D:524:GLN:O	1:D:524:GLN:HG2	2.10	0.50
2:G:368:GLN:HA	2:G:368:GLN:NE2	2.23	0.50
2:B:425:LYS:N	7:B:574:HOH:O	2.44	0.50
2:B:490:GLY:HA2	2:B:493:VAL:HB	1.94	0.50
2:C:135:SER:O	2:C:136:GLU:C	2.55	0.50
2:F:155:GLU:N	2:F:156:PRO:HD2	2.26	0.50
1:E:322:ASP:HB3	1:E:373:TRP:CG	2.47	0.50
2:F:64:LYS:O	2:F:192:SER:OG	2.23	0.50
1:H:254:LEU:CD2	1:H:318:HIS:HB2	2.41	0.50
2:C:362:GLU:HG2	2:C:380:PHE:CE2	2.46	0.49
1:D:72:LEU:HD11	1:D:143:SER:HB2	1.93	0.49
1:E:318:HIS:ND1	1:E:320:GLY:HA2	2.27	0.49
1:E:522:CYS:O	1:E:523:GLU:C	2.54	0.49
1:D:97:VAL:HG12	1:D:126:LEU:HD11	1.92	0.49
1:E:384:GLN:H	1:E:384:GLN:CD	2.20	0.49
1:E:131:THR:HG23	1:E:133:TRP:H	1.77	0.49
2:F:206:LEU:C	2:F:206:LEU:HD23	2.37	0.49
1:A:28:GLN:HE22	1:A:487:ASN:HD22	1.60	0.49
2:C:242:GLN:OE1	2:C:242:GLN:N	2.44	0.49
1:E:207:ASP:OD1	1:E:262:HIS:CD2	2.65	0.49
1:A:99:VAL:HG22	1:A:130:GLU:HA	1.94	0.49
2:F:211:ARG:HD2	2:F:242:GLN:OE1	2.13	0.49
2:G:411:ASP:C	2:G:411:ASP:CB	2.78	0.49
1:E:372:VAL:HG11	1:E:376:VAL:CG2	2.41	0.49
2:F:399:ASN:C	2:F:399:ASN:HD22	2.21	0.49
1:H:104:CYS:C	1:H:105:ASN:HD22	2.21	0.49
1:H:224:LYS:HB3	1:H:268:PRO:HB2	1.94	0.49
1:H:281:SER:O	1:H:282:GLU:HB2	2.12	0.49
2:C:135:SER:HB2	2:C:165:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:199:ARG:HH21	2:C:469:LEU:HD12	1.77	0.49
1:D:353:SER:HA	1:D:381:VAL:HG13	1.94	0.49
1:E:318:HIS:CE1	1:E:373:TRP:NE1	2.80	0.49
1:H:48:TYR:CD1	1:H:56:PRO:HD3	2.47	0.49
2:G:414:LYS:H	2:G:414:LYS:HD2	1.77	0.49
1:H:422:LEU:O	1:H:423:ASN:C	2.55	0.49
2:F:362:GLU:HG2	2:F:380:PHE:CE2	2.48	0.49
2:G:93:LEU:HD21	2:G:169:LEU:HD21	1.95	0.49
2:G:411:ASP:CA	2:G:412:LYS:N	2.66	0.49
1:D:48:TYR:CD1	1:D:56:PRO:HD3	2.47	0.48
1:H:93:ASN:OD1	1:H:94:VAL:N	2.45	0.48
1:H:314:ASP:O	1:H:368:LYS:NZ	2.39	0.48
1:H:396:ILE:HA	1:H:397:PRO:C	2.37	0.48
1:H:423:ASN:HA	1:H:459:MET:HE1	1.95	0.48
1:A:206:VAL:HG12	1:A:212:PRO:HD2	1.94	0.48
2:B:352:GLY:HA2	2:B:405:TRP:CD1	2.48	0.48
1:E:101:THR:O	1:E:102:PRO:C	2.54	0.48
2:B:235:HIS:NE2	2:B:288:GLU:OE1	2.24	0.48
3:M:1:NAG:H61	3:M:2:NAG:H83	1.95	0.48
2:B:153:VAL:HB	2:B:192:SER:H	1.78	0.48
1:D:53:ALA:HB1	1:D:101:THR:HA	1.94	0.48
1:D:500:LEU:HG	1:D:517:LEU:HD11	1.95	0.48
1:E:467:THR:HG21	2:F:533:ARG:HH21	1.78	0.48
2:C:532:HIS:HD2	2:C:535:ARG:NH2	1.99	0.48
1:D:178:ARG:HA	1:D:209:PRO:HG3	1.95	0.48
1:D:423:ASN:HA	1:D:459:MET:HE1	1.95	0.48
1:E:246:ALA:HB1	1:E:251:ILE:HB	1.94	0.48
1:A:131:THR:CG2	1:A:132:VAL:H	2.27	0.48
2:B:238:ILE:HG23	2:B:239:VAL:HG13	1.95	0.48
2:C:206:LEU:HA	2:C:235:HIS:HB3	1.94	0.48
1:H:55:GLN:O	1:H:58:CYS:HB2	2.13	0.48
1:H:207:ASP:OD2	1:H:208:ASP:N	2.36	0.48
1:H:281:SER:O	1:H:282:GLU:CB	2.62	0.48
2:F:100:ARG:HG2	2:F:104:TYR:CE2	2.46	0.48
1:H:206:VAL:HG12	1:H:212:PRO:HD2	1.95	0.48
2:B:206:LEU:C	2:B:206:LEU:HD23	2.39	0.48
1:D:30:PHE:CE2	1:D:32:THR:HB	2.48	0.48
1:D:356:ILE:HD12	1:D:381:VAL:HG21	1.95	0.48
1:E:299:GLU:OE1	1:E:299:GLU:HA	2.14	0.48
2:F:89:PRO:HA	2:F:95:GLU:OE2	2.14	0.48
1:A:422:LEU:O	1:A:476:ARG:NH2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:GLY:HA3	1:H:132:VAL:CG2	2.44	0.47
1:A:375:GLU:N	1:A:375:GLU:OE1	2.45	0.47
1:D:459:MET:HE3	1:D:459:MET:HA	1.95	0.47
1:E:229:PRO:HA	7:E:734:HOH:O	2.15	0.47
2:F:502:LEU:HD23	2:F:502:LEU:C	2.39	0.47
2:C:188:THR:HG22	2:C:189:ILE:N	2.30	0.47
1:D:306:LEU:HG	1:D:366:TYR:CE2	2.49	0.47
1:D:382:LYS:HB2	1:D:382:LYS:NZ	2.29	0.47
2:F:206:LEU:HB3	2:F:487:CYS:HA	1.95	0.47
2:G:82:SER:HA	2:G:128:LEU:HD22	1.95	0.47
1:H:39:LEU:HG	1:H:156:ILE:HD11	1.96	0.47
2:G:499:THR:HB	2:G:500:PRO:HD3	1.96	0.47
1:D:210:SER:N	1:D:210:SER:CB	2.67	0.47
2:G:414:LYS:HD2	2:G:414:LYS:N	2.29	0.47
2:F:404:VAL:HG12	2:F:405:TRP:O	2.15	0.47
2:F:459:ASP:OD1	2:F:459:ASP:N	2.47	0.47
2:G:437:THR:HB	2:G:477:GLN:HB3	1.97	0.47
1:D:50:VAL:CG2	1:D:51:SER:OG	2.63	0.47
1:E:121:ASN:C	1:E:121:ASN:HD22	2.23	0.47
1:H:175:ASP:OD2	1:H:178:ARG:HD3	2.15	0.47
1:E:208:ASP:HB2	1:E:209:PRO:HD3	1.96	0.46
1:E:342:LYS:HA	1:E:342:LYS:CE	2.43	0.46
1:E:525:GLU:HG2	2:F:264:HIS:CE1	2.47	0.46
2:F:302:GLN:HG3	2:F:305:LEU:HB2	1.97	0.46
1:D:68:TYR:O	1:D:72:LEU:HD13	2.15	0.46
1:D:102:PRO:O	1:D:103:GLY:O	2.33	0.46
1:E:173:LEU:HB3	1:E:458:CYS:HA	1.96	0.46
2:F:223:LEU:HD21	2:F:234:LEU:HD22	1.98	0.46
1:H:192:VAL:HA	1:H:195:TYR:CD2	2.50	0.46
1:H:151:GLU:OE1	1:H:151:GLU:N	2.46	0.46
1:A:121:ASN:HD21	1:A:124:GLN:H	1.63	0.46
1:D:99:VAL:HG22	1:D:130:GLU:HA	1.98	0.46
2:F:352:GLY:CA	2:F:405:TRP:HD1	2.28	0.46
1:H:203:TRP:HE3	1:H:204:HIS:N	2.14	0.46
1:H:315:PHE:O	1:H:369:GLY:N	2.39	0.46
2:B:223:LEU:HD21	2:B:234:LEU:HD22	1.97	0.46
2:C:398:ILE:O	2:C:398:ILE:HG22	2.15	0.46
1:D:44:PHE:O	1:D:69:ARG:NH1	2.49	0.46
2:F:267:THR:HB	2:F:268:PRO:HD2	1.97	0.46
1:H:220:GLU:HA	1:H:223:ARG:HB2	1.98	0.46
1:H:515:GLN:HB2	1:H:516:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:536:MET:HB3	2:C:541:ILE:HB	1.98	0.46
1:E:278:TYR:HB2	1:E:331:SER:O	2.16	0.46
2:F:205:ILE:HD13	2:F:486:ALA:HB3	1.97	0.46
1:H:440:LEU:HD22	1:H:449:LYS:HB3	1.98	0.46
2:B:359:LYS:HB2	2:B:359:LYS:NZ	2.30	0.46
2:C:203:ARG:HG2	2:C:513:LEU:HB3	1.98	0.46
1:D:256:GLU:HB2	1:D:318:HIS:HB3	1.98	0.46
2:G:242:GLN:HG2	1:H:519:VAL:CG2	2.27	0.46
2:F:267:THR:HG21	1:H:66:GLN:HG3	1.98	0.46
2:C:366:LYS:H	2:C:366:LYS:HD2	1.81	0.46
1:E:207:ASP:OD1	1:E:262:HIS:HD2	1.99	0.46
1:E:100:VAL:CG1	1:E:102:PRO:HG2	2.42	0.46
1:H:53:ALA:HB1	1:H:101:THR:CA	2.23	0.46
2:G:195:ILE:HD12	2:G:195:ILE:N	2.32	0.45
1:D:215:SER:OG	1:D:307:GLU:OE2	2.33	0.45
1:E:221:LEU:HD12	1:E:222:MET:N	2.31	0.45
2:F:458:GLN:HB3	2:F:460:TRP:NE1	2.32	0.45
2:B:199:ARG:HH21	2:B:469:LEU:HD12	1.80	0.45
1:E:180:TYR:HB3	1:E:232:HIS:HD2	1.81	0.45
1:H:320:GLY:HA2	1:H:373:TRP:CD1	2.52	0.45
1:A:467:THR:CG2	2:B:544:GLN:HA	2.38	0.45
1:H:176:THR:OG1	1:H:203:TRP:HZ3	1.99	0.45
1:H:270:ILE:HD12	1:H:273:LEU:HB2	1.98	0.45
1:A:401:MET:HE1	1:A:438:GLU:O	2.15	0.45
2:C:206:LEU:C	2:C:206:LEU:HD23	2.42	0.45
1:D:23:LEU:HD11	1:D:141:THR:HG23	1.96	0.45
1:E:117:THR:OG1	1:E:128:LEU:HG	2.16	0.45
1:E:228:ASN:ND2	1:E:230:VAL:H	2.09	0.45
1:E:396:ILE:HD12	1:E:396:ILE:N	2.31	0.45
2:G:205:ILE:HD13	2:G:486:ALA:HB3	1.98	0.45
2:G:364:ASN:OD1	2:G:367:ILE:HG13	2.17	0.45
1:H:173:LEU:C	1:H:173:LEU:HD23	2.42	0.45
1:H:382:LYS:HD3	1:H:382:LYS:O	2.17	0.45
2:B:188:THR:HG22	2:B:189:ILE:N	2.31	0.45
1:D:72:LEU:HD11	1:D:143:SER:CB	2.46	0.45
1:E:524:GLN:NE2	1:E:524:GLN:O	2.50	0.45
1:A:131:THR:CG2	1:A:132:VAL:N	2.79	0.45
2:C:481:PHE:O	7:C:577:HOH:O	2.21	0.45
1:D:235:THR:HG22	1:D:236:ALA:N	2.30	0.45
1:E:318:HIS:CE1	1:E:320:GLY:HA2	2.52	0.45
2:G:151:LEU:HD13	2:G:160:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:GLU:CD	1:H:283:PRO:HD3	2.41	0.45
1:D:202:HIS:CE1	1:D:256:GLU:OE1	2.66	0.45
1:E:169:HIS:ND1	1:E:415:LEU:HD11	2.32	0.45
1:E:178:ARG:HH11	1:E:460:TRP:HE3	1.63	0.45
1:H:282:GLU:CD	1:H:282:GLU:C	2.85	0.45
1:A:470:VAL:N	1:A:471:PRO:HD2	2.32	0.45
2:G:388:ILE:HD12	2:G:389:GLN:N	2.32	0.45
1:A:302:SER:HA	1:A:362:ILE:HG21	1.99	0.44
2:B:229:ASN:OD1	2:B:532:HIS:HE1	1.99	0.44
2:F:544:GLN:HB2	2:F:545:PRO:HD2	1.99	0.44
1:H:103:GLY:O	1:H:105:ASN:N	2.50	0.44
1:H:173:LEU:HB3	1:H:458:CYS:HA	1.99	0.44
2:B:465:LYS:NZ	2:B:522:MET:HE2	2.33	0.44
2:F:105:ILE:HG23	2:F:179:VAL:HG21	1.99	0.44
2:F:155:GLU:N	2:F:156:PRO:CD	2.80	0.44
2:F:287:PRO:HG3	2:F:344:PHE:CG	2.53	0.44
1:D:169:HIS:CD2	1:D:200:VAL:HG21	2.53	0.44
1:E:26:TRP:HA	1:E:27:PRO:HD3	1.86	0.44
1:E:243:ILE:HA	1:E:253:VAL:HG21	2.00	0.44
2:G:199:ARG:HH21	2:G:469:LEU:HD12	1.81	0.44
1:H:196:ASN:N	1:H:196:ASN:ND2	2.66	0.44
1:D:503:PHE:O	1:D:507:LEU:HG	2.16	0.44
2:G:55:ALA:O	2:G:535:ARG:NH2	2.49	0.44
2:B:447:ALA:HB3	2:B:448:PRO:HD3	2.00	0.44
1:D:202:HIS:CD2	1:D:456:GLU:OE1	2.71	0.44
1:E:169:HIS:HE1	1:E:456:GLU:OE2	2.00	0.44
1:E:177:SER:O	1:E:210:SER:HB2	2.18	0.44
1:E:202:HIS:HE1	1:E:256:GLU:OE1	2.00	0.44
1:E:374:GLN:O	1:E:375:GLU:C	2.60	0.44
1:H:159:THR:HB	1:H:161:ILE:CD1	2.47	0.44
2:C:229:ASN:HD22	2:C:229:ASN:N	2.16	0.44
1:D:207:ASP:OD2	1:D:208:ASP:N	2.38	0.44
1:A:100:VAL:HG12	1:A:102:PRO:CD	2.46	0.44
1:A:173:LEU:C	1:A:173:LEU:HD23	2.43	0.44
2:B:248:SER:HB3	2:B:251:PHE:O	2.18	0.44
1:D:211:PHE:H	1:D:226:SER:HA	1.82	0.44
1:A:420:TRP:CD1	1:A:480:VAL:HG22	2.53	0.44
2:C:261:SER:OG	2:C:264:HIS:CD2	2.71	0.44
1:D:50:VAL:HG23	1:D:51:SER:OG	2.17	0.44
1:E:470:VAL:N	1:E:471:PRO:HD2	2.33	0.44
2:F:504:PRO:HG3	2:F:544:GLN:CG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ALA:O	2:B:535:ARG:NH2	2.44	0.43
2:B:504:PRO:HD3	2:B:544:GLN:O	2.18	0.43
2:G:155:GLU:N	2:G:156:PRO:CD	2.81	0.43
2:G:544:GLN:HA	1:H:467:THR:CG2	2.47	0.43
1:H:169:HIS:ND1	1:H:415:LEU:HD11	2.33	0.43
2:B:132:THR:HB	2:B:163:ASN:HA	2.00	0.43
2:B:153:VAL:O	2:B:191:GLU:HB2	2.18	0.43
1:D:430:ASP:OD2	1:D:476:ARG:NH1	2.51	0.43
2:F:452:ASP:OD1	2:F:489:TRP:HD1	2.01	0.43
1:A:165:PRO:HB3	1:A:485:TRP:CE3	2.53	0.43
2:C:352:GLY:HA2	2:C:405:TRP:CD1	2.54	0.43
1:E:48:TYR:OH	1:E:62:ASP:OD1	2.31	0.43
2:G:532:HIS:HD2	2:G:535:ARG:HE	1.66	0.43
1:H:89:THR:HG22	1:H:90:LEU:N	2.33	0.43
1:A:32:THR:OG1	1:A:33:SER:N	2.52	0.43
1:A:101:THR:N	1:A:102:PRO:CD	2.80	0.43
2:C:385:SER:O	2:C:389:GLN:HG3	2.18	0.43
1:E:198:LEU:HD11	1:E:481:ALA:CB	2.48	0.43
1:E:208:ASP:CB	1:E:209:PRO:HD3	2.49	0.43
2:C:504:PRO:HD3	2:C:544:GLN:O	2.18	0.43
1:E:212:PRO:HB2	1:E:234:TYR:CD1	2.53	0.43
1:E:359:LEU:HD23	1:E:359:LEU:O	2.18	0.43
2:B:469:LEU:HD22	2:B:478:LYS:HD2	2.00	0.43
1:D:275:THR:HG21	1:D:329:TRP:HD1	1.84	0.43
1:D:445:THR:HB	1:D:446:PRO:HD2	1.99	0.43
1:E:40:TYR:HA	1:E:41:PRO:HD2	1.73	0.43
1:A:228:ASN:HD22	1:A:228:ASN:C	2.26	0.43
1:A:336:GLN:HE21	1:A:336:GLN:HA	1.84	0.43
1:D:116:TYR:CE1	1:D:163:ASP:HB3	2.52	0.43
1:E:235:THR:CG2	1:E:236:ALA:N	2.81	0.43
2:F:466:VAL:O	2:F:512:ARG:HD3	2.18	0.43
2:G:352:GLY:HA2	2:G:405:TRP:CD1	2.53	0.43
1:H:232:HIS:O	1:H:233:ILE:HD13	2.18	0.43
1:A:97:VAL:CG1	1:A:126:LEU:HD21	2.49	0.43
1:D:166:ARG:HH21	1:D:440:LEU:HD12	1.84	0.43
1:E:60:VAL:HG23	1:E:104:CYS:O	2.18	0.43
2:G:459:ASP:OD2	2:G:505:ARG:NH1	2.51	0.43
1:H:103:GLY:O	1:H:105:ASN:ND2	2.52	0.43
1:H:393:ARG:HD3	1:H:396:ILE:O	2.18	0.43
2:B:406:GLN:HE21	2:B:423:VAL:HA	1.84	0.43
1:D:100:VAL:HG12	1:D:102:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:HG22	1:D:234:TYR:N	2.34	0.43
1:E:179:HIS:CE1	2:F:548:ALA:HA	2.54	0.43
1:E:384:GLN:C	1:E:386:ASP:H	2.22	0.43
2:G:390:LYS:O	2:G:394:ILE:HG13	2.19	0.43
2:G:428:ALA:C	2:G:430:PRO:HD2	2.44	0.43
1:H:254:LEU:HD21	1:H:318:HIS:HB2	2.00	0.43
1:H:375:GLU:OE1	1:H:375:GLU:N	2.50	0.43
1:A:121:ASN:HD21	1:A:124:GLN:HG2	1.83	0.43
1:A:121:ASN:C	1:A:121:ASN:HD22	2.27	0.43
2:B:68:ASN:HB3	2:B:191:GLU:HG2	2.01	0.43
2:B:262:LEU:HD23	1:D:69:ARG:HH22	1.83	0.43
2:F:195:ILE:N	2:F:195:ILE:HD12	2.34	0.43
2:G:447:ALA:HB3	2:G:448:PRO:HD3	2.00	0.43
2:B:350:HIS:CD2	2:B:352:GLY:H	2.37	0.42
2:C:498:LEU:C	2:C:498:LEU:HD23	2.44	0.42
2:G:206:LEU:HA	2:G:235:HIS:HB3	2.00	0.42
2:G:339:GLU:O	2:G:343:VAL:HG23	2.19	0.42
1:H:470:VAL:N	1:H:471:PRO:HD2	2.34	0.42
4:S:1:NAG:H62	4:S:2:NAG:N2	2.33	0.42
2:C:251:PHE:HB3	2:C:254:LEU:HD13	2.02	0.42
1:E:198:LEU:HD11	1:E:481:ALA:HB2	1.99	0.42
1:E:384:GLN:N	1:E:384:GLN:CD	2.77	0.42
2:G:404:VAL:HG21	2:G:408:VAL:HG21	2.01	0.42
1:E:151:GLU:HB3	1:H:153:THR:HG23	2.01	0.42
1:E:339:MET:SD	1:E:351:LEU:HD22	2.59	0.42
1:H:66:GLN:HA	1:H:69:ARG:HG2	2.02	0.42
1:H:90:LEU:N	1:H:90:LEU:HD23	2.34	0.42
1:A:100:VAL:HG12	1:A:102:PRO:HG2	2.00	0.42
1:E:256:GLU:HB2	1:E:318:HIS:HB3	2.00	0.42
2:G:488:LEU:HD22	2:G:502:LEU:HG	2.01	0.42
1:H:127:LEU:HD21	1:H:138:GLY:HA3	2.01	0.42
1:A:102:PRO:O	1:A:103:GLY:O	2.36	0.42
1:D:36:ARG:HD2	4:N:1:NAG:H62	2.02	0.42
1:D:55:GLN:O	1:D:56:PRO:C	2.63	0.42
1:D:208:ASP:OD1	1:D:264:LEU:HB2	2.19	0.42
1:D:228:ASN:HD22	1:D:228:ASN:C	2.28	0.42
1:D:284:SER:C	1:D:286:THR:H	2.27	0.42
1:A:101:THR:O	1:A:102:PRO:C	2.62	0.42
2:C:457:GLY:HA2	1:D:463:TYR:CZ	2.55	0.42
1:D:375:GLU:OE1	1:D:375:GLU:N	2.53	0.42
1:H:23:LEU:HD12	1:H:145:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD23	1:A:127:LEU:N	2.34	0.42
1:A:388:ILE:HG21	1:A:415:LEU:CD2	2.50	0.42
2:C:336:PHE:O	2:C:340:ILE:HG12	2.20	0.42
2:C:465:LYS:HA	2:C:520:ARG:NH1	2.35	0.42
2:G:544:GLN:HB2	2:G:545:PRO:HD2	2.00	0.42
2:B:404:VAL:HG21	2:B:408:VAL:HG21	2.02	0.42
2:C:551:CYS:O	2:C:552:ASN:CB	2.68	0.42
1:E:126:LEU:HD23	1:E:127:LEU:N	2.34	0.42
2:F:261:SER:OG	2:F:264:HIS:HD2	2.02	0.42
2:G:467:GLU:HA	2:G:468:PRO:HD2	1.92	0.42
1:H:238:ASP:O	1:H:242:VAL:HG23	2.20	0.42
1:A:55:GLN:O	1:A:56:PRO:C	2.63	0.42
1:A:151:GLU:HG3	1:D:38:VAL:CG1	2.49	0.42
2:B:135:SER:O	2:B:136:GLU:HB2	2.20	0.42
1:E:55:GLN:CG	1:E:56:PRO:HD2	2.22	0.42
1:E:172:LEU:HD11	1:E:174:LEU:CD1	2.49	0.42
2:G:424:TRP:CZ2	2:G:425:LYS:HE3	2.54	0.42
1:H:402:LYS:HE2	1:H:402:LYS:HA	2.02	0.42
2:C:245:PRO:HB2	2:C:266:TYR:CD2	2.55	0.42
1:E:416:LEU:O	1:E:455:GLY:CA	2.67	0.42
1:H:37:TYR:O	1:H:155:PHE:HA	2.20	0.42
1:H:270:ILE:C	1:H:270:ILE:HD13	2.45	0.42
2:B:211:ARG:HD2	2:B:242:GLN:OE1	2.20	0.41
2:B:514:TRP:CD1	2:B:514:TRP:C	2.97	0.41
1:D:26:TRP:HA	1:D:27:PRO:HD3	1.84	0.41
1:E:40:TYR:HE2	1:E:90:LEU:HB2	1.84	0.41
1:D:228:ASN:ND2	1:D:230:VAL:H	2.07	0.41
1:E:240:LYS:HB2	1:E:240:LYS:NZ	2.35	0.41
2:G:206:LEU:C	2:G:206:LEU:HD23	2.45	0.41
2:G:496:THR:OG1	1:H:515:GLN:HA	2.20	0.41
1:H:398:VAL:HG22	1:H:399:ASN:H	1.86	0.41
2:C:246:TYR:O	2:C:255:SER:HB3	2.20	0.41
1:D:163:ASP:CG	1:D:485:TRP:HE1	2.29	0.41
1:E:48:TYR:CD1	1:E:56:PRO:HD3	2.55	0.41
1:E:394:GLU:O	1:E:399:ASN:HA	2.19	0.41
2:G:288:GLU:HB2	2:G:350:HIS:HB3	2.03	0.41
2:G:366:LYS:HD2	2:G:366:LYS:N	2.35	0.41
1:A:228:ASN:ND2	1:A:230:VAL:H	2.09	0.41
1:D:121:ASN:ND2	1:D:124:GLN:H	2.18	0.41
1:E:372:VAL:HG12	1:E:373:TRP:N	2.35	0.41
2:F:498:LEU:C	2:F:498:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:235:HIS:HB2	2:G:485:GLU:OE2	2.20	0.41
1:H:55:GLN:O	1:H:56:PRO:C	2.63	0.41
1:A:515:GLN:HB2	1:A:516:PRO:HD2	2.01	0.41
1:D:53:ALA:HB1	1:D:101:THR:HG22	2.03	0.41
1:D:320:GLY:HA2	1:D:373:TRP:CD1	2.55	0.41
1:D:400:TYR:CE1	1:D:401:MET:HE2	2.55	0.41
2:C:57:TRP:HA	2:C:58:PRO:C	2.46	0.41
2:C:275:ILE:HD13	2:C:345:PRO:HD3	2.02	0.41
1:D:100:VAL:HG12	1:D:102:PRO:CG	2.51	0.41
1:D:404:LEU:HD11	1:D:416:LEU:HD13	2.03	0.41
1:E:485:TRP:CD1	1:E:485:TRP:C	2.98	0.41
2:F:204:GLY:HA2	2:F:233:VAL:O	2.21	0.41
2:F:286:LEU:HD21	2:F:403:ILE:HD12	2.02	0.41
1:H:322:ASP:HB3	1:H:373:TRP:CD1	2.55	0.41
1:H:383:ILE:HG13	1:H:384:GLN:N	2.35	0.41
2:C:285:VAL:O	2:C:287:PRO:HD3	2.21	0.41
2:F:346:ASP:OD2	2:F:347:GLN:N	2.53	0.41
2:G:364:ASN:HA	2:G:365:PRO:HD2	1.87	0.41
2:B:407:GLU:OE2	2:B:424:TRP:HZ2	2.04	0.41
1:E:318:HIS:O	1:E:320:GLY:N	2.53	0.41
1:A:53:ALA:HB1	1:A:101:THR:HA	2.01	0.41
1:A:59:SER:O	1:A:63:GLU:HG2	2.21	0.41
1:A:487:ASN:OD1	1:A:488:LYS:N	2.54	0.41
2:B:467:GLU:HA	2:B:468:PRO:HD2	1.87	0.41
2:C:533:ARG:HD3	2:C:533:ARG:C	2.46	0.41
1:D:25:PRO:CD	1:D:197:LYS:HD3	2.49	0.41
1:D:37:TYR:O	1:D:156:ILE:HD12	2.21	0.41
1:D:202:HIS:HD2	1:D:456:GLU:OE1	2.04	0.41
1:D:401:MET:HE1	1:D:438:GLU:O	2.20	0.41
1:E:95:LEU:HD12	1:E:95:LEU:N	2.36	0.41
1:E:362:ILE:HG22	1:E:366:TYR:CE1	2.56	0.41
1:E:393:ARG:HG2	1:E:396:ILE:HD13	2.03	0.41
2:F:323:ASN:HA	2:F:324:PRO:HD3	1.88	0.41
2:G:498:LEU:C	2:G:498:LEU:HD23	2.46	0.41
1:A:228:ASN:HA	1:A:229:PRO:HD3	1.82	0.41
1:A:524:GLN:H	1:A:524:GLN:CD	2.29	0.41
2:B:336:PHE:O	2:B:340:ILE:HG12	2.20	0.41
2:C:73:ALA:HB3	2:C:76:ASN:HB3	2.02	0.41
1:D:42:ASN:O	1:D:43:ASN:ND2	2.54	0.41
1:D:278:TYR:HA	1:D:283:PRO:HA	2.01	0.41
1:D:392:TRP:CE2	1:D:393:ARG:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:SER:O	2:G:74:PRO:HD2	2.21	0.41
2:F:458:GLN:HB3	2:F:460:TRP:CD1	2.56	0.41
2:B:364:ASN:HA	2:B:365:PRO:HD2	1.80	0.40
1:D:282:GLU:HB3	1:D:283:PRO:HD2	2.02	0.40
2:F:303:LYS:HB2	2:F:303:LYS:NZ	2.36	0.40
2:G:211:ARG:O	1:H:519:VAL:HG23	2.21	0.40
2:G:461:ARG:O	2:G:465:LYS:HB2	2.20	0.40
1:H:398:VAL:HG22	1:H:399:ASN:N	2.36	0.40
1:A:353:SER:O	1:A:357:GLN:HG3	2.21	0.40
2:B:66:THR:HA	2:B:67:PRO:HD3	1.87	0.40
2:B:398:ILE:H	2:B:398:ILE:HG12	1.77	0.40
2:C:149:TYR:CZ	2:C:196:ASP:HB3	2.56	0.40
2:C:327:ASN:HD22	2:C:327:ASN:C	2.29	0.40
1:E:203:TRP:CD1	1:E:205:LEU:HG	2.56	0.40
2:G:238:ILE:HG23	2:G:239:VAL:HG13	2.02	0.40
1:A:107:LEU:HB2	1:A:108:PRO:HD2	2.04	0.40
1:D:342:LYS:NZ	1:D:342:LYS:HB3	2.36	0.40
1:D:438:GLU:HA	1:D:439:PRO:HD3	1.83	0.40
1:E:23:LEU:HA	1:E:144:GLN:OE1	2.22	0.40
1:E:99:VAL:HG22	1:E:130:GLU:HA	2.03	0.40
1:E:319:LEU:HD21	1:E:363:VAL:HG11	2.03	0.40
2:F:390:LYS:HB3	2:F:390:LYS:NZ	2.36	0.40
2:C:70:LEU:HD11	2:C:154:LYS:HA	2.02	0.40
1:E:31:GLN:HB2	1:E:160:GLU:HB3	2.04	0.40
1:E:55:GLN:O	1:E:56:PRO:C	2.63	0.40
1:E:400:TYR:CE2	1:E:401:MET:HE2	2.56	0.40
2:F:170:ARG:HH21	2:F:232:ASN:HB3	1.85	0.40
1:H:49:ASP:OD1	1:H:50:VAL:N	2.55	0.40
1:H:116:TYR:CE1	1:H:163:ASP:HB3	2.56	0.40
1:H:485:TRP:CD1	1:H:485:TRP:C	3.00	0.40
1:A:233:ILE:HG22	1:A:234:TYR:N	2.35	0.40
1:D:113:VAL:O	1:D:131:THR:OG1	2.35	0.40
2:F:59:LEU:HA	2:F:60:PRO:HD3	1.89	0.40
2:F:149:TYR:CZ	2:F:196:ASP:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/507 (96%)	453 (93%)	33 (7%)	2 (0%)	30	60
1	D	488/507 (96%)	449 (92%)	36 (7%)	3 (1%)	21	51
1	E	488/507 (96%)	435 (89%)	39 (8%)	14 (3%)	3	13
1	H	488/507 (96%)	447 (92%)	31 (6%)	10 (2%)	6	21
2	B	474/507 (94%)	447 (94%)	26 (6%)	1 (0%)	43	72
2	C	475/507 (94%)	450 (95%)	25 (5%)	0	100	100
2	F	474/507 (94%)	434 (92%)	36 (8%)	4 (1%)	16	44
2	G	474/507 (94%)	442 (93%)	26 (6%)	6 (1%)	9	31
All	All	3849/4056 (95%)	3557 (92%)	252 (6%)	40 (1%)	12	38

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	103	GLY
1	D	50	VAL
1	D	103	GLY
1	E	382	LYS
2	G	412	LYS
1	H	104	CYS
1	H	105	ASN
1	H	283	PRO
1	H	284	SER
1	H	102	PRO
1	D	102	PRO
1	E	380	LYS
1	E	417	SER
2	F	446	SER
2	G	156	PRO
2	G	427	SER

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Mol	Chain	Res	Type
1	H	280	GLY
1	H	282	GLU
1	H	323	GLU
1	E	208	ASP
1	E	373	TRP
1	E	375	GLU
2	F	156	PRO
2	G	294	HIS
1	E	207	ASP
1	E	385	PRO
2	F	504	PRO
1	E	264	LEU
1	E	267	GLY
1	E	319	LEU
2	F	74	PRO
2	G	520	ARG
1	E	280	GLY
2	G	293	GLY
1	H	267	GLY
2	B	74	PRO
1	E	397	PRO
1	H	285	GLY
1	E	398	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	441/454 (97%)	423 (96%)	18 (4%)	27	62
1	D	441/454 (97%)	426 (97%)	15 (3%)	32	68
1	E	441/454 (97%)	420 (95%)	21 (5%)	23	56
1	H	441/454 (97%)	423 (96%)	18 (4%)	27	62
2	B	426/449 (95%)	421 (99%)	5 (1%)	63	87
2	C	427/449 (95%)	421 (99%)	6 (1%)	59	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	426/449 (95%)	418 (98%)	8 (2%)	50 81
2	G	426/449 (95%)	417 (98%)	9 (2%)	47 79
All	All	3469/3612 (96%)	3369 (97%)	100 (3%)	37 73

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	66	GLN
1	A	97	VAL
1	A	105	ASN
1	A	106	GLN
1	A	107	LEU
1	A	121	ASN
1	A	159	THR
1	A	174	LEU
1	A	198	LEU
1	A	228	ASN
1	A	299	GLU
1	A	336	GLN
1	A	382	LYS
1	A	396	ILE
1	A	409	LYS
1	A	523	GLU
1	A	525	GLU
2	B	84	ASN
2	B	211	ARG
2	B	359	LYS
2	B	384	GLU
2	B	522	MET
2	C	154	LYS
2	C	155	GLU
2	C	211	ARG
2	C	229	ASN
2	C	327	ASN
2	C	502	LEU
1	D	51	SER
1	D	61	LEU
1	D	63	GLU
1	D	69	ARG
1	D	101	THR

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Mol	Chain	Res	Type
1	D	106	GLN
1	D	121	ASN
1	D	148	LYS
1	D	156	ILE
1	D	173	LEU
1	D	198	LEU
1	D	228	ASN
1	D	342	LYS
1	D	382	LYS
1	D	523	GLU
1	E	31	GLN
1	E	61	LEU
1	E	97	VAL
1	E	105	ASN
1	E	106	GLN
1	E	119	THR
1	E	121	ASN
1	E	127	LEU
1	E	159	THR
1	E	174	LEU
1	E	221	LEU
1	E	228	ASN
1	E	240	LYS
1	E	360	LEU
1	E	379	ASN
1	E	380	LYS
1	E	383	ILE
1	E	399	ASN
1	E	445	THR
1	E	473	LEU
1	E	524	GLN
2	F	64	LYS
2	F	65	MET
2	F	211	ARG
2	F	303	LYS
2	F	373	GLN
2	F	399	ASN
2	F	412	LYS
2	F	475	GLN
2	G	84	ASN
2	G	232	ASN
2	G	303	LYS

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Mol	Chain	Res	Type
2	G	368	GLN
2	G	374	LYS
2	G	400	LYS
2	G	411	ASP
2	G	414	LYS
2	G	502	LEU
1	H	62	ASP
1	H	104	CYS
1	H	119	THR
1	H	121	ASN
1	H	156	ILE
1	H	172	LEU
1	H	196	ASN
1	H	203	TRP
1	H	228	ASN
1	H	270	ILE
1	H	299	GLU
1	H	370	TYR
1	H	381	VAL
1	H	382	LYS
1	H	384	GLN
1	H	424	ARG
1	H	447	GLU
1	H	517	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	47	GLN
1	A	55	GLN
1	A	106	GLN
1	A	121	ASN
1	A	124	GLN
1	A	204	HIS
1	A	228	ASN
1	A	336	GLN
1	A	350	GLN
1	A	357	GLN
1	A	399	ASN
1	A	448	GLN
1	A	466	ASN

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Mol	Chain	Res	Type
1	A	513	GLN
2	B	76	ASN
2	B	81	HIS
2	B	84	ASN
2	B	123	GLN
2	B	126	GLN
2	B	134	GLN
2	B	237	HIS
2	B	264	HIS
2	B	302	GLN
2	B	364	ASN
2	B	406	GLN
2	B	532	HIS
2	C	68	ASN
2	C	123	GLN
2	C	126	GLN
2	C	134	GLN
2	C	237	HIS
2	C	264	HIS
2	C	269	ASN
2	C	327	ASN
2	C	350	HIS
2	C	368	GLN
2	C	475	GLN
2	C	479	GLN
2	C	532	HIS
1	D	28	GLN
1	D	29	ASN
1	D	43	ASN
1	D	47	GLN
1	D	66	GLN
1	D	106	GLN
1	D	121	ASN
1	D	202	HIS
1	D	228	ASN
1	D	296	ASN
1	D	399	ASN
1	D	487	ASN
1	D	513	GLN
1	E	28	GLN
1	E	31	GLN
1	E	55	GLN

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Mol	Chain	Res	Type
1	E	121	ASN
1	E	196	ASN
1	E	204	HIS
1	E	228	ASN
1	E	262	HIS
1	E	296	ASN
1	E	318	HIS
1	E	336	GLN
1	E	357	GLN
1	E	379	ASN
1	E	513	GLN
1	E	524	GLN
2	F	68	ASN
2	F	76	ASN
2	F	81	HIS
2	F	84	ASN
2	F	123	GLN
2	F	177	GLN
2	F	202	HIS
2	F	264	HIS
2	F	323	ASN
2	F	373	GLN
2	F	399	ASN
2	F	475	GLN
2	F	477	GLN
2	F	532	HIS
2	G	76	ASN
2	G	123	GLN
2	G	126	GLN
2	G	232	ASN
2	G	264	HIS
2	G	269	ASN
2	G	294	HIS
2	G	368	GLN
2	G	475	GLN
2	G	477	GLN
2	G	479	GLN
2	G	532	HIS
1	H	28	GLN
1	H	31	GLN
1	H	42	ASN
1	H	45	GLN

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Mol	Chain	Res	Type
1	H	47	GLN
1	H	55	GLN
1	H	105	ASN
1	H	106	GLN
1	H	121	ASN
1	H	196	ASN
1	H	204	HIS
1	H	228	ASN
1	H	295	ASN
1	H	296	ASN
1	H	350	GLN
1	H	357	GLN
1	H	384	GLN
1	H	466	ASN
1	H	513	GLN
1	H	524	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

26 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.62	0	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.53	0	17,19,21	0.66	0
3	BMA	I	3	3	11,11,12	0.56	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	1	1,3	14,14,15	0.59	0	17,19,21	0.91	1 (5%)
3	NAG	J	2	3	14,14,15	0.66	0	17,19,21	0.85	1 (5%)
3	BMA	J	3	3	11,11,12	0.51	0	15,15,17	1.20	2 (13%)
3	NAG	K	1	2,3	14,14,15	0.76	0	17,19,21	0.98	1 (5%)
3	NAG	K	2	3	14,14,15	0.62	0	17,19,21	0.70	0
3	BMA	K	3	3	11,11,12	0.59	0	15,15,17	0.81	1 (6%)
4	NAG	L	1	4,2	14,14,15	0.47	0	17,19,21	0.70	0
4	NAG	L	2	4	14,14,15	0.47	0	17,19,21	0.71	0
3	NAG	M	1	1,3	14,14,15	0.83	0	17,19,21	1.10	2 (11%)
3	NAG	M	2	3	14,14,15	0.61	0	17,19,21	0.76	0
3	BMA	M	3	3	11,11,12	0.57	0	15,15,17	0.59	0
4	NAG	N	1	1,4	14,14,15	0.68	0	17,19,21	1.06	1 (5%)
4	NAG	N	2	4	14,14,15	0.49	0	17,19,21	0.73	0
4	NAG	O	1	1,4	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
4	NAG	O	2	4	14,14,15	0.57	0	17,19,21	0.53	0
4	NAG	P	1	1,4	14,14,15	0.63	0	17,19,21	0.77	0
4	NAG	P	2	4	14,14,15	0.52	0	17,19,21	0.63	0
4	NAG	Q	1	4,2	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
4	NAG	Q	2	4	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	R	1	1,4	14,14,15	0.55	0	17,19,21	0.67	0
4	NAG	R	2	4	14,14,15	0.48	0	17,19,21	0.63	0
4	NAG	S	1	1,4	14,14,15	0.63	0	17,19,21	0.99	2 (11%)
4	NAG	S	2	4	14,14,15	0.47	0	17,19,21	0.60	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
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	5/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	2,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C4-C3-C2	3.22	115.74	111.02
3	J	3	BMA	C1-C2-C3	3.20	114.31	109.64
4	N	1	NAG	C4-C3-C2	2.75	115.05	111.02
4	Q	1	NAG	O5-C1-C2	-2.44	107.52	111.29
3	J	3	BMA	C1-O5-C5	2.34	115.32	112.19
3	J	2	NAG	C4-C3-C2	2.33	114.43	111.02
3	K	3	BMA	C1-C2-C3	2.33	113.03	109.64
3	M	1	NAG	C1-O5-C5	2.23	115.17	112.19
3	J	1	NAG	O5-C1-C2	-2.15	107.96	111.29
4	O	1	NAG	O5-C1-C2	-2.10	108.04	111.29
4	S	1	NAG	O5-C1-C2	-2.09	108.05	111.29
3	M	1	NAG	C4-C3-C2	2.08	114.06	111.02
4	S	1	NAG	C4-C3-C2	2.00	113.95	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	1	NAG	C1

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C1-C2-N2-C7
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C3-C2-N2-C7
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C1-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	Q	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
3	J	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
3	J	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O7-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
3	I	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
3	I	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7
4	Q	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	Q	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C8-C7-N2-C2
3	M	3	BMA	C4-C5-C6-O6
4	S	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C4-C5-C6-O6

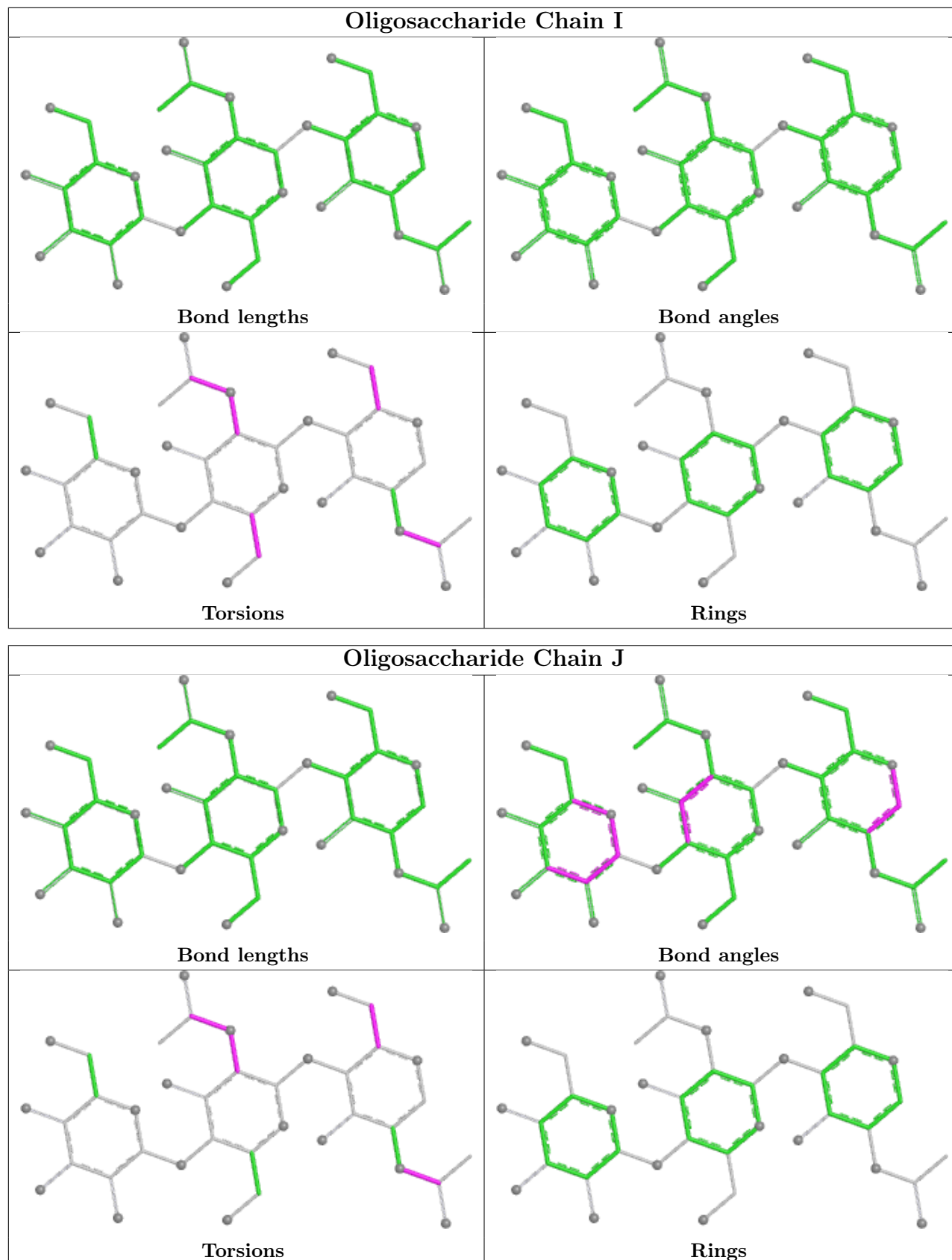
There are no ring outliers.

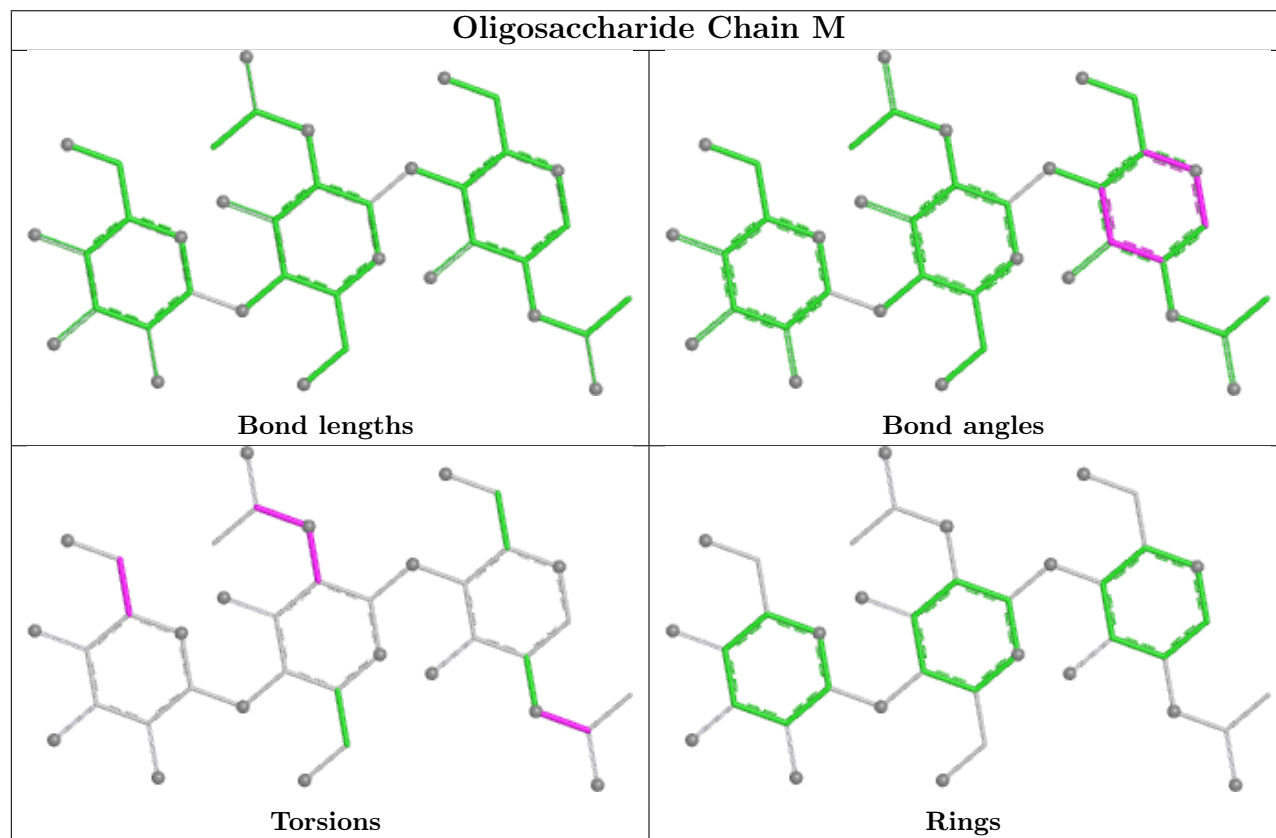
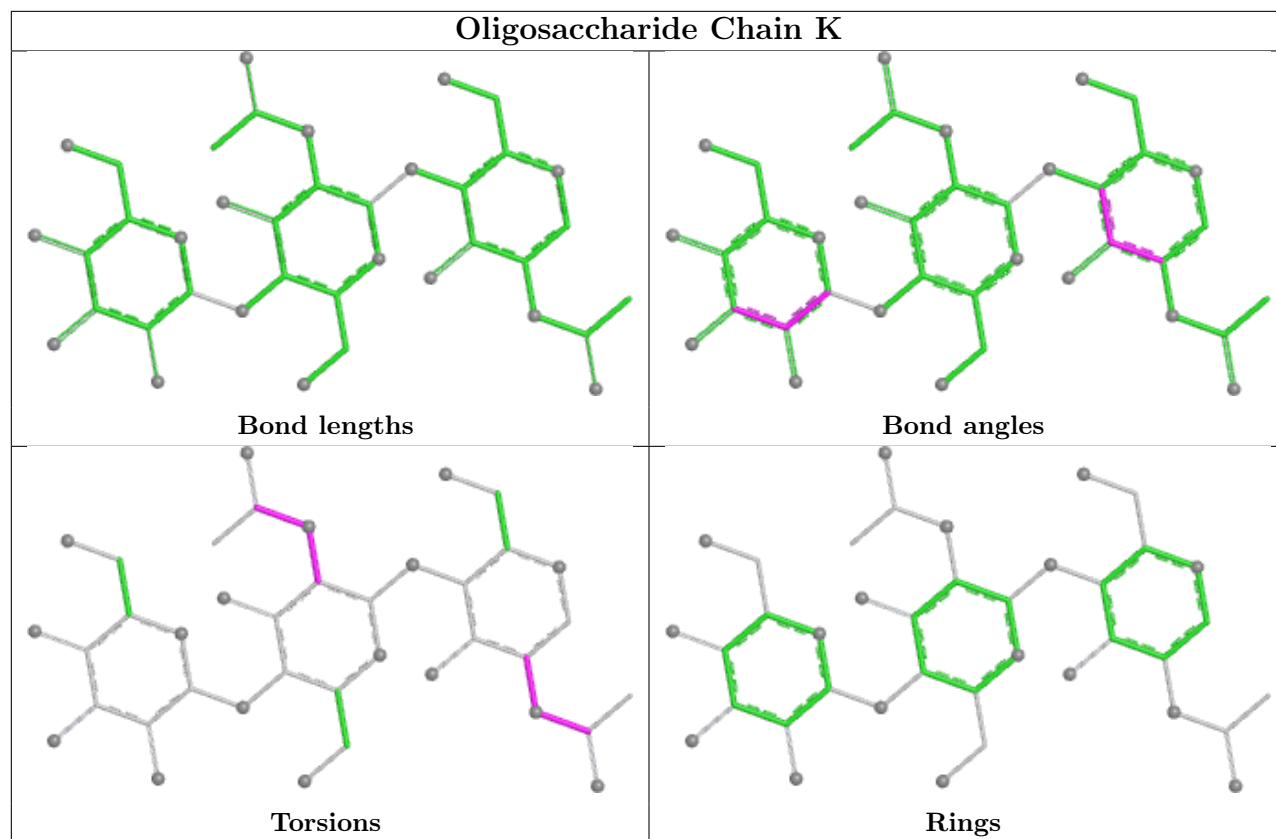
6 monomers are involved in 5 short contacts:

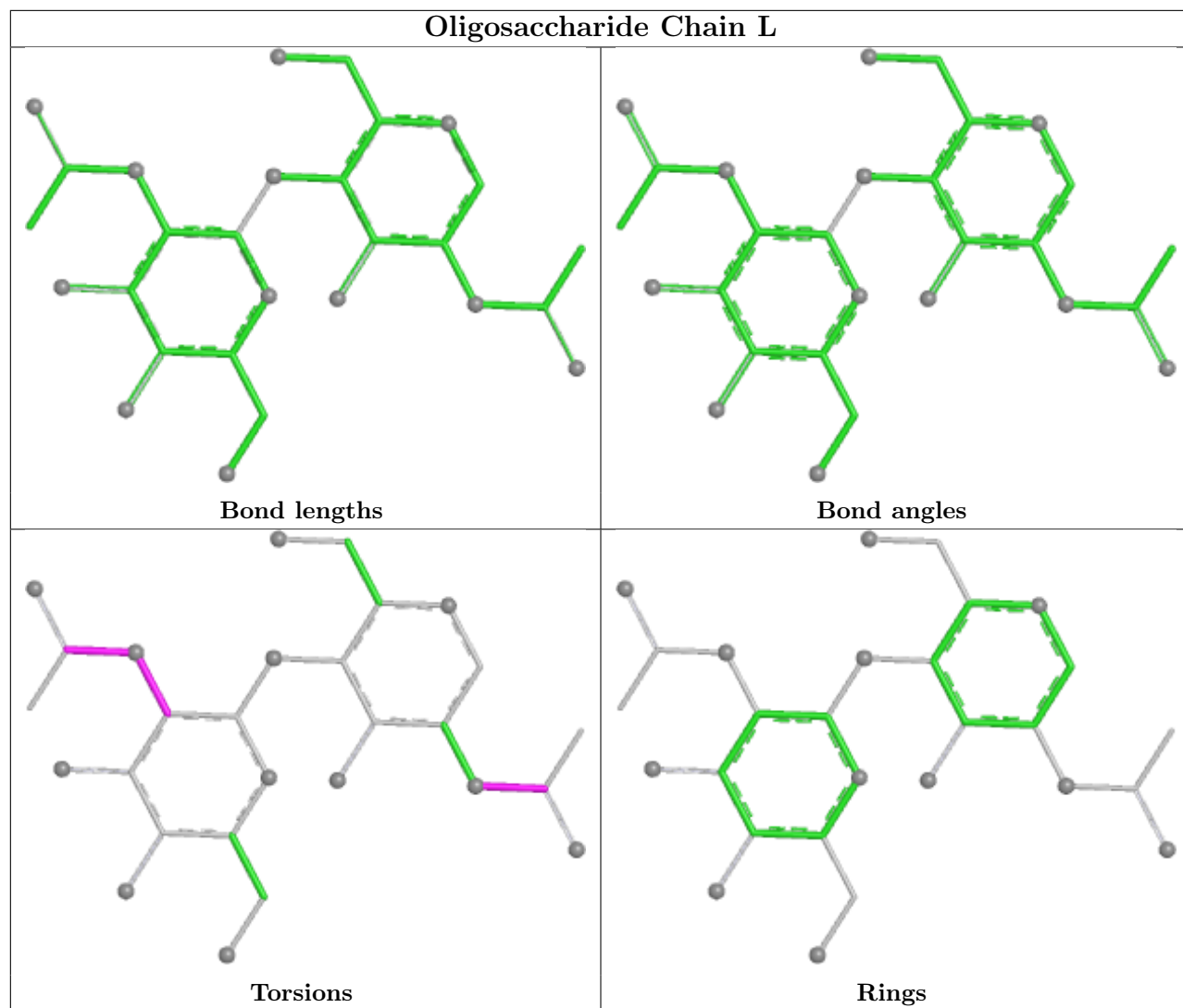
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	NAG	1	0
4	S	1	NAG	2	0
3	M	2	NAG	1	0
4	P	1	NAG	1	0
4	S	2	NAG	2	0
3	M	1	NAG	1	0

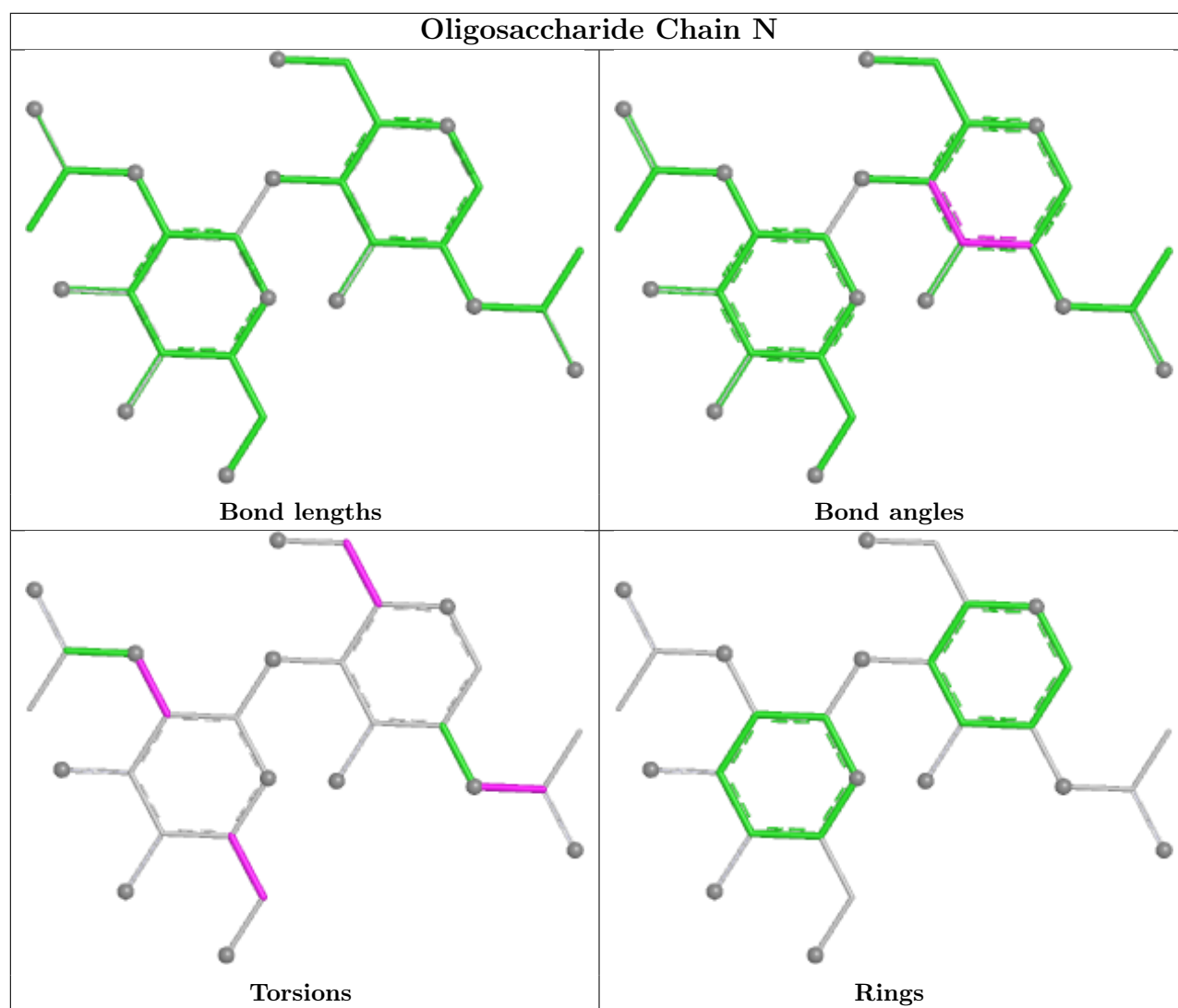
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

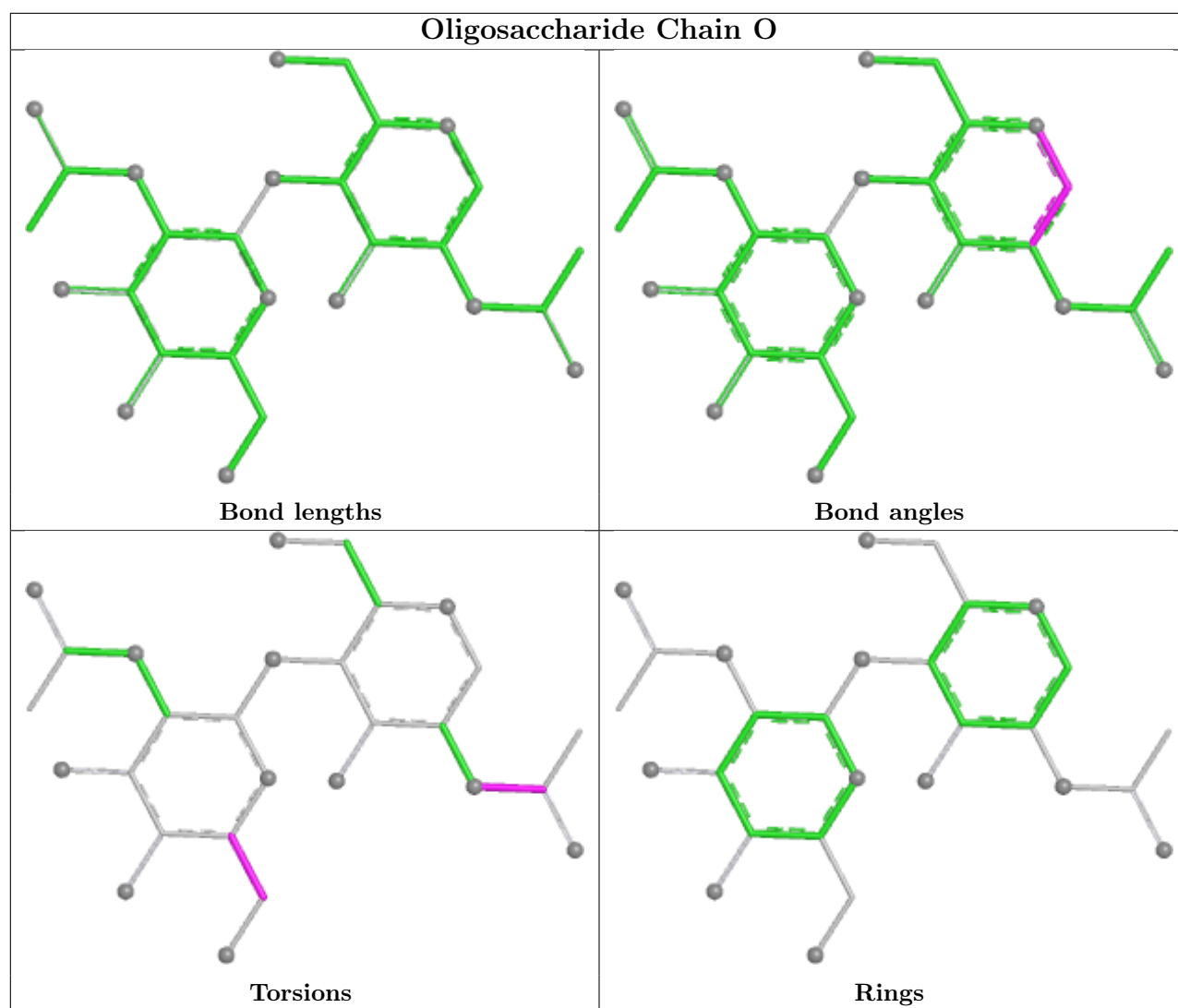
bond angles, torsion angles, and ring geometry for oligosaccharide.

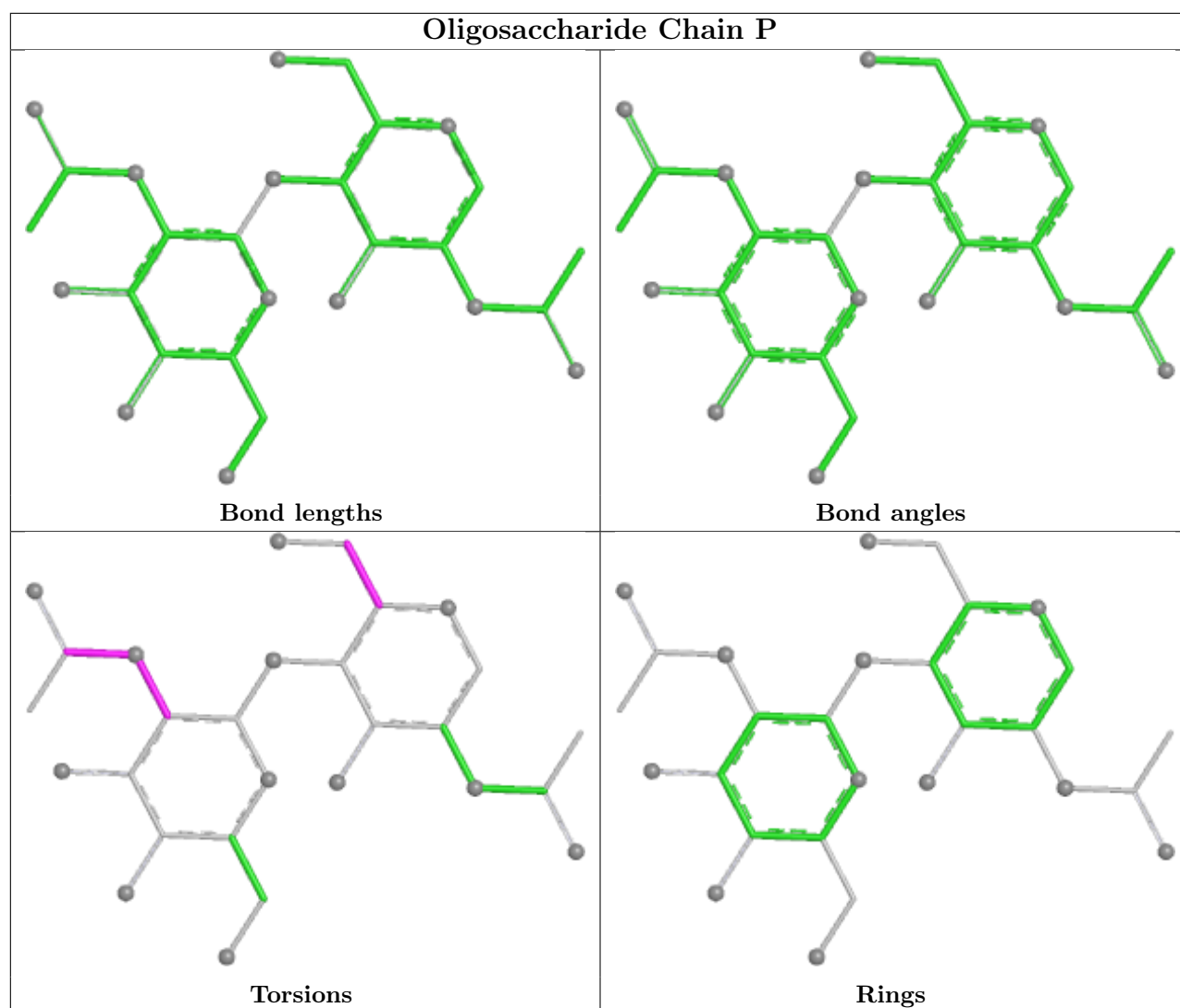


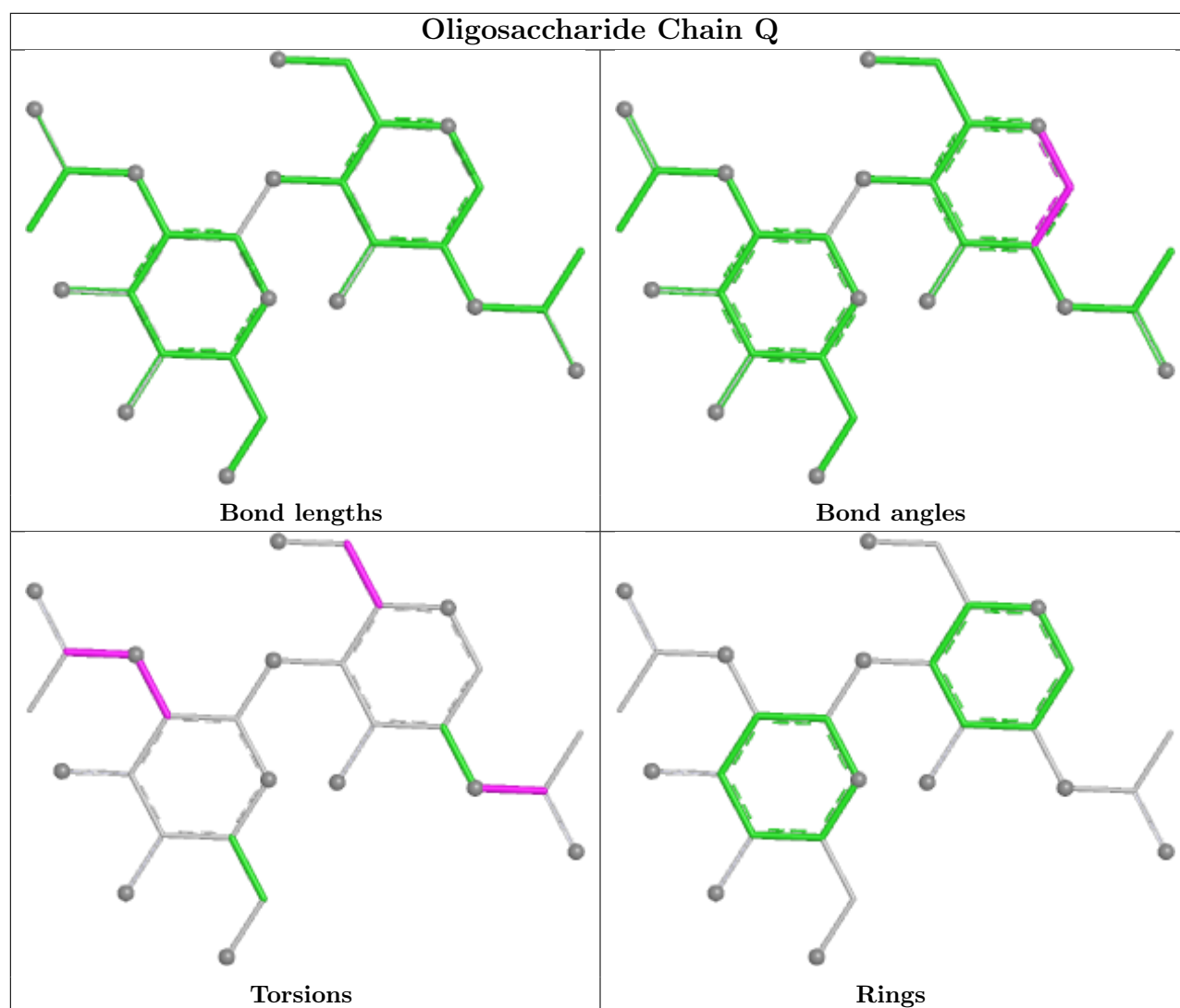


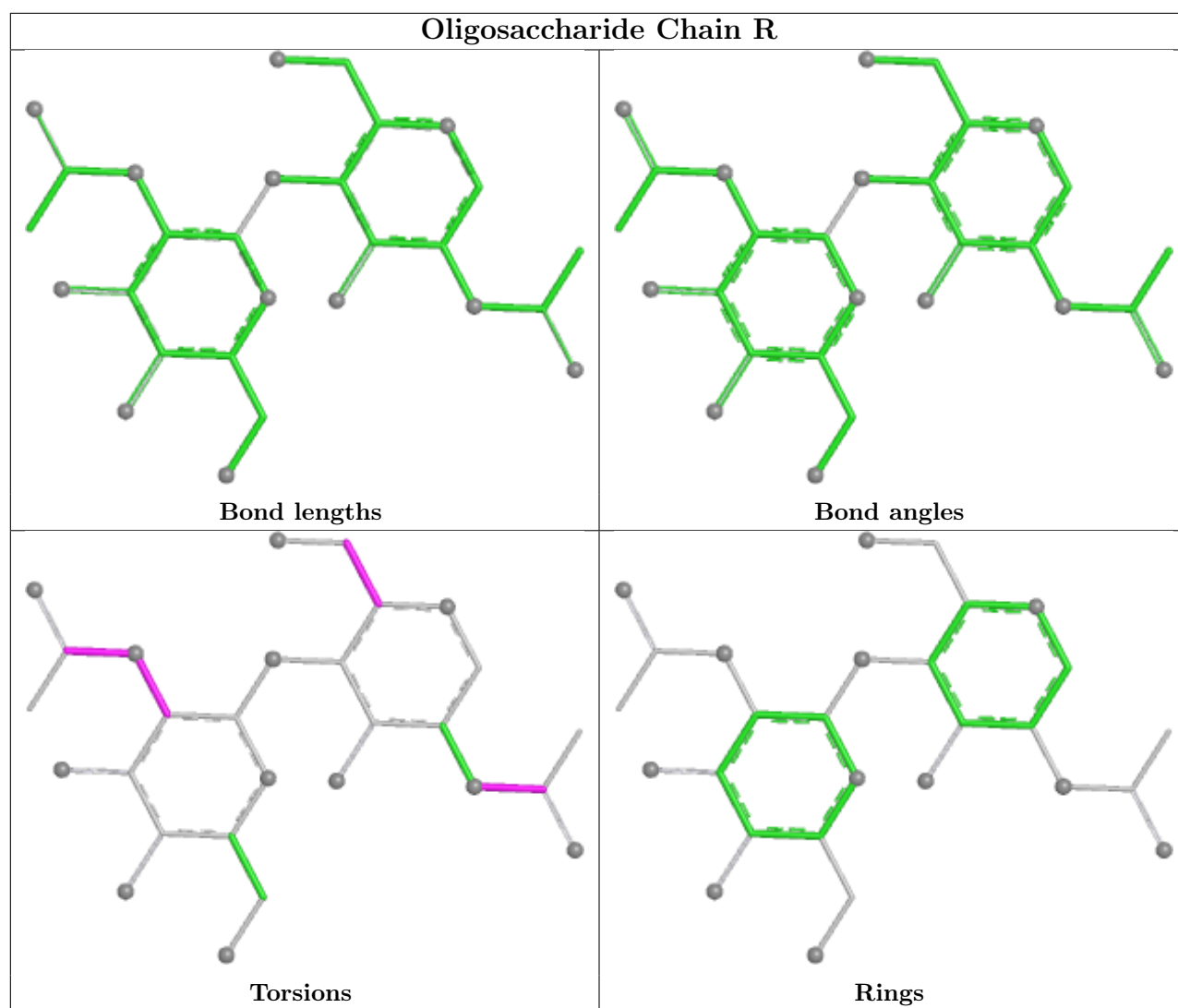


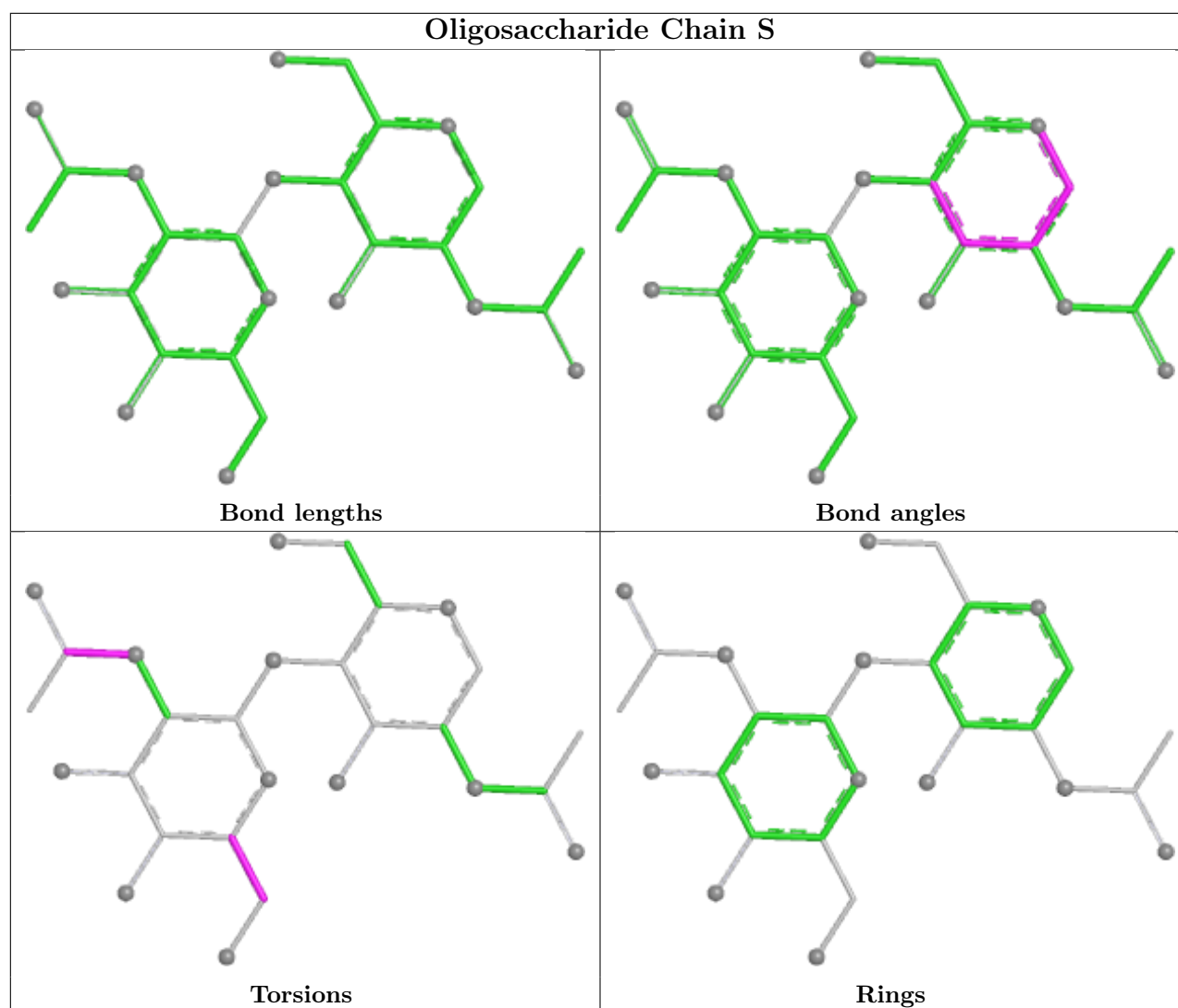












5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	G	726	2	14,14,15	0.52	0	17,19,21	0.57	0
5	NAG	D	716	1	14,14,15	0.56	0	17,19,21	0.76	0
5	NAG	A	707	1	14,14,15	0.48	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	H	535	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	D	717	-	4,4,4	0.25	0	6,6,6	0.05	0
5	NAG	E	723	2	14,14,15	0.46	0	17,19,21	0.71	0
6	SO4	H	534	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	A	708	-	4,4,4	0.25	0	6,6,6	0.05	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
5	NAG	A	707	1	-	4/6/23/26	0/1/1/1
5	NAG	G	726	2	-	4/6/23/26	0/1/1/1
5	NAG	E	723	2	-	2/6/23/26	0/1/1/1
5	NAG	D	716	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	707	NAG	C8-C7-N2-C2
5	A	707	NAG	O7-C7-N2-C2
5	D	716	NAG	C8-C7-N2-C2
5	D	716	NAG	O7-C7-N2-C2
5	G	726	NAG	C8-C7-N2-C2
5	G	726	NAG	O7-C7-N2-C2
5	G	726	NAG	O5-C5-C6-O6
5	G	726	NAG	C4-C5-C6-O6
5	A	707	NAG	C4-C5-C6-O6
5	D	716	NAG	O5-C5-C6-O6
5	A	707	NAG	O5-C5-C6-O6
5	E	723	NAG	C8-C7-N2-C2
5	E	723	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	534	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	492/507 (97%)	0.72	27 (5%) 30 23	17, 59, 80, 87	0
1	D	492/507 (97%)	0.57	11 (2%) 62 52	21, 61, 81, 89	0
1	E	492/507 (97%)	0.86	51 (10%) 11 8	17, 61, 82, 90	0
1	H	492/507 (97%)	0.60	22 (4%) 38 30	17, 61, 81, 88	0
2	B	480/507 (94%)	0.55	9 (1%) 66 57	26, 63, 76, 84	0
2	C	481/507 (94%)	0.60	8 (1%) 69 60	26, 61, 75, 85	0
2	F	480/507 (94%)	0.69	17 (3%) 47 38	27, 64, 76, 83	0
2	G	480/507 (94%)	0.52	7 (1%) 72 63	17, 62, 77, 82	0
All	All	3889/4056 (95%)	0.64	152 (3%) 43 34	17, 62, 78, 90	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	102	PRO	7.5
1	H	101	THR	5.8
1	D	102	PRO	5.6
2	G	317	ASP	5.6
1	A	101	THR	5.3
1	A	104	CYS	5.3
1	A	102	PRO	5.2
1	E	396	ILE	4.6
1	E	101	THR	4.6
1	H	104	CYS	4.4
2	G	399	ASN	4.0
1	E	104	CYS	3.9
1	H	106	GLN	3.8
1	E	355	TYR	3.7
1	E	399	ASN	3.7
1	A	95	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	282	GLU	3.7
1	E	351	LEU	3.6
1	H	62	ASP	3.6
1	E	322	ASP	3.6
2	B	107	GLY	3.5
1	H	365	SER	3.5
2	F	54	PRO	3.5
1	A	282	GLU	3.4
1	H	102	PRO	3.3
1	D	209	PRO	3.2
1	H	283	PRO	3.2
1	D	285	GLY	3.2
1	E	334	GLU	3.2
1	E	344	PHE	3.1
1	E	282	GLU	3.1
2	F	317	ASP	3.1
2	C	413	ALA	3.1
2	C	136	GLU	3.1
2	C	316	LEU	3.0
2	F	122	THR	3.0
1	A	103	GLY	3.0
1	H	370	TYR	2.9
1	D	282	GLU	2.9
2	B	373	GLN	2.9
1	A	89	THR	2.9
1	A	383	ILE	2.9
1	E	156	ILE	2.9
1	A	93	ASN	2.9
1	E	93	ASN	2.8
1	E	338	PHE	2.8
2	F	504	PRO	2.8
2	F	503	TRP	2.8
1	E	398	VAL	2.8
1	E	348	PHE	2.8
1	E	258	ASP	2.8
1	E	283	PRO	2.8
1	E	270	ILE	2.8
1	E	269	GLY	2.8
1	E	323	GLU	2.7
1	H	100	VAL	2.7
2	B	420	ILE	2.7
1	D	74	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	360	LEU	2.7
1	E	383	ILE	2.7
1	H	93	ASN	2.7
2	F	70	LEU	2.7
1	H	203	TRP	2.6
1	A	399	ASN	2.6
2	F	180	TYR	2.6
2	C	404	VAL	2.6
2	G	485	GLU	2.6
1	A	94	VAL	2.6
1	E	350	GLN	2.6
1	A	105	ASN	2.6
1	H	107	LEU	2.5
1	E	328	CYS	2.5
1	H	293	SER	2.5
2	F	311	SER	2.5
1	H	103	GLY	2.5
1	E	381	VAL	2.5
1	A	334	GLU	2.5
2	C	122	THR	2.5
1	H	99	VAL	2.5
1	A	32	THR	2.5
1	E	324	VAL	2.4
2	C	107	GLY	2.4
1	E	370	TYR	2.4
2	G	387	TYR	2.4
1	E	358	THR	2.4
1	D	363	VAL	2.4
2	F	414	LYS	2.4
1	A	43	ASN	2.4
1	E	209	PRO	2.4
2	F	137	CYS	2.4
1	H	369	GLY	2.4
1	A	216	PHE	2.4
1	E	326	PHE	2.4
1	E	221	LEU	2.4
1	E	274	LEU	2.4
2	F	444	ILE	2.4
2	B	324	PRO	2.4
1	H	363	VAL	2.4
1	D	104	CYS	2.4
2	B	423	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	261	GLY	2.3
2	G	107	GLY	2.3
1	E	162	GLU	2.3
1	A	47	GLN	2.3
1	E	106	GLN	2.3
2	G	192	SER	2.3
1	H	32	THR	2.3
2	F	131	ILE	2.3
1	E	354	PHE	2.3
2	B	305	LEU	2.3
1	H	519	VAL	2.3
1	E	89	THR	2.3
2	B	54	PRO	2.3
1	E	329	TRP	2.2
2	B	356	VAL	2.2
2	F	59	LEU	2.2
1	E	395	ASP	2.2
2	F	519	VAL	2.2
1	A	269	GLY	2.2
1	E	304	PHE	2.2
1	A	35	GLN	2.2
1	A	50	VAL	2.2
1	E	337	ASP	2.2
1	E	380	LYS	2.2
1	A	344	PHE	2.2
2	B	431	GLU	2.2
2	G	408	VAL	2.1
1	E	356	ILE	2.1
1	E	97	VAL	2.1
1	A	235	THR	2.1
1	A	351	LEU	2.1
1	E	352	GLU	2.1
2	C	183	SER	2.1
1	A	466	ASN	2.1
1	H	398	VAL	2.1
1	E	294	LEU	2.1
1	E	498	GLU	2.1
1	H	50	VAL	2.1
1	D	397	PRO	2.1
2	C	486	ALA	2.1
1	A	31	GLN	2.0
1	D	43	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	392	LEU	2.0
2	F	107	GLY	2.0
1	D	396	ILE	2.0
1	E	362	ILE	2.0
1	A	66	GLN	2.0
1	D	210	SER	2.0
1	E	281	SER	2.0
1	E	335	ILE	2.0
2	F	322	ILE	2.0
1	E	342	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

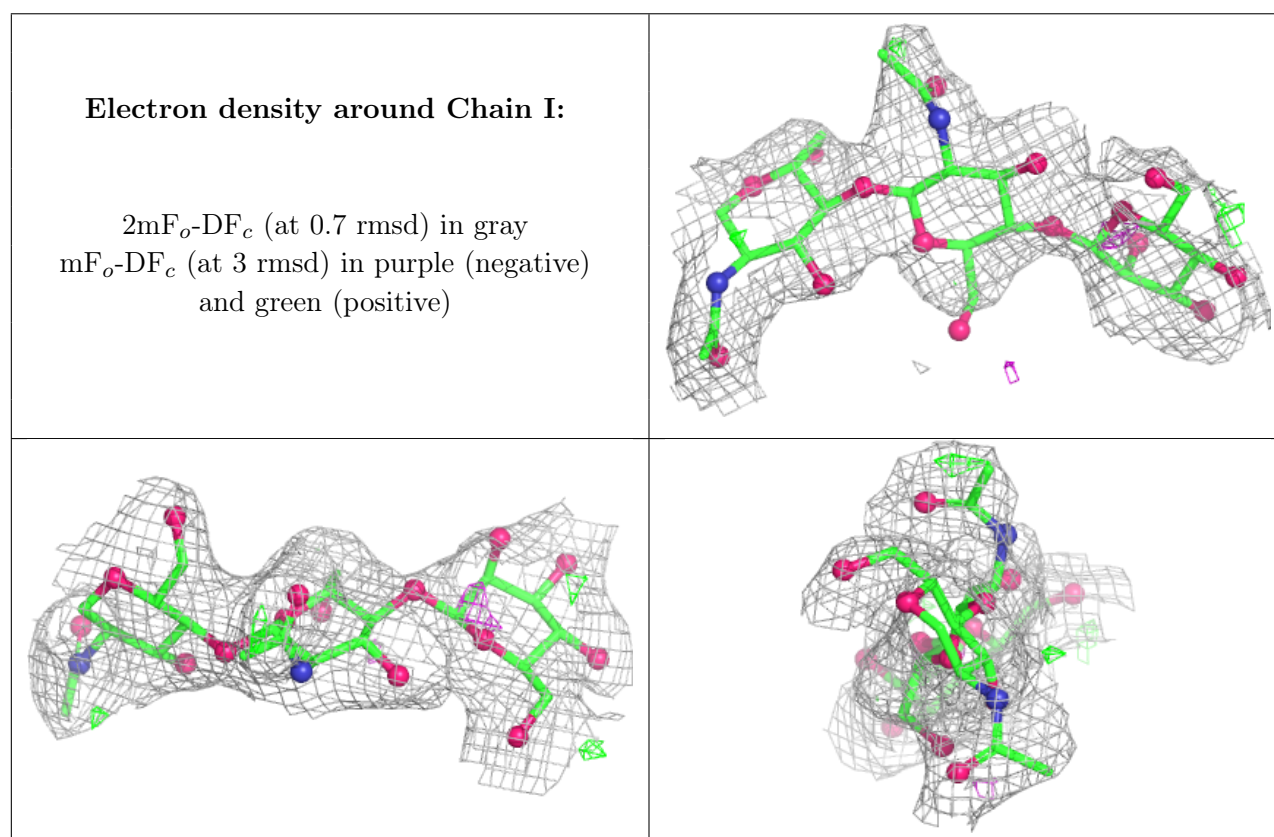
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	K	2	14/15	0.39	0.19	110,117,118,119	0
3	BMA	K	3	11/12	0.44	0.16	55,58,64,65	0
4	NAG	R	2	14/15	0.45	0.16	110,117,118,119	0
3	BMA	J	3	11/12	0.46	0.16	55,58,64,65	0
3	BMA	M	3	11/12	0.47	0.17	55,58,64,65	0
4	NAG	Q	2	14/15	0.54	0.15	110,117,118,119	0
3	NAG	I	2	14/15	0.58	0.19	110,117,118,119	0
3	NAG	J	2	14/15	0.59	0.17	110,117,118,119	0
3	BMA	I	3	11/12	0.61	0.13	55,58,64,65	0
4	NAG	S	2	14/15	0.61	0.14	91,94,95,96	0
3	NAG	K	1	14/15	0.62	0.17	70,74,80,89	0
4	NAG	P	2	14/15	0.63	0.17	110,117,118,119	0
4	NAG	O	2	14/15	0.68	0.14	110,117,118,119	0
4	NAG	N	2	14/15	0.69	0.20	110,117,118,119	0
4	NAG	L	2	14/15	0.69	0.14	110,117,118,119	0
3	NAG	M	2	14/15	0.74	0.17	110,117,118,119	0
4	NAG	N	1	14/15	0.78	0.14	70,74,80,89	0
4	NAG	R	1	14/15	0.78	0.15	70,74,80,89	0

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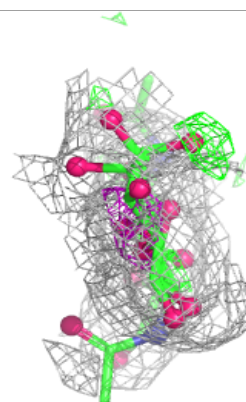
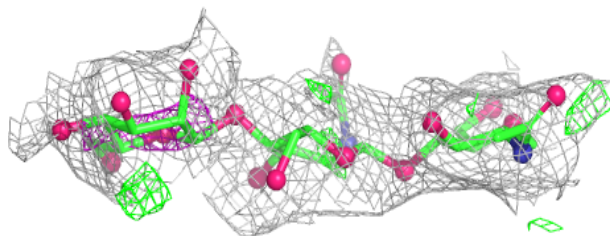
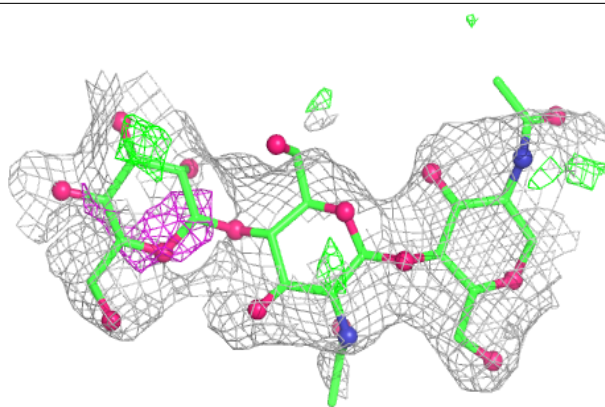
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	O	1	14/15	0.80	0.13	70,74,80,89	0
3	NAG	J	1	14/15	0.81	0.13	70,74,80,89	0
3	NAG	M	1	14/15	0.83	0.10	70,74,80,89	0
4	NAG	P	1	14/15	0.84	0.15	70,74,80,89	0
4	NAG	L	1	14/15	0.84	0.10	70,74,80,89	0
3	NAG	I	1	14/15	0.86	0.11	70,74,80,89	0
4	NAG	Q	1	14/15	0.86	0.10	70,74,80,89	0
4	NAG	S	1	14/15	0.88	0.11	66,71,74,79	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.

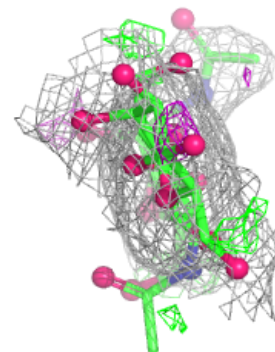
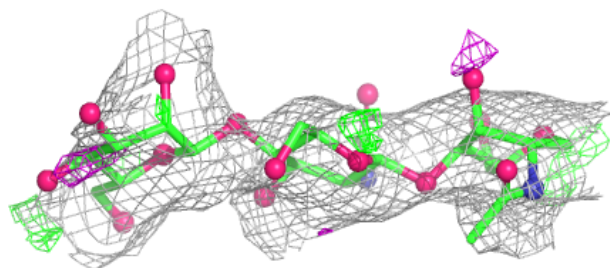
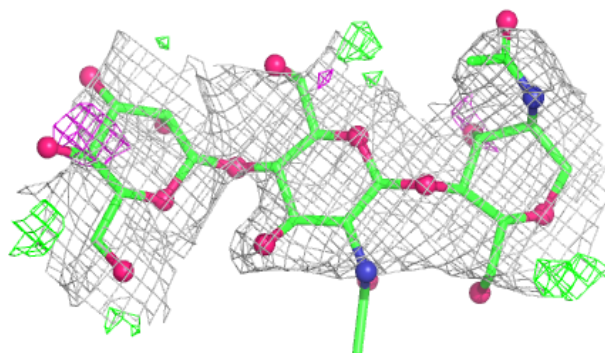


Electron density around Chain J:

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

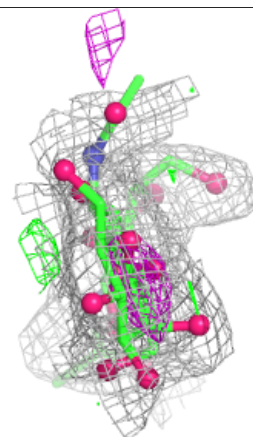
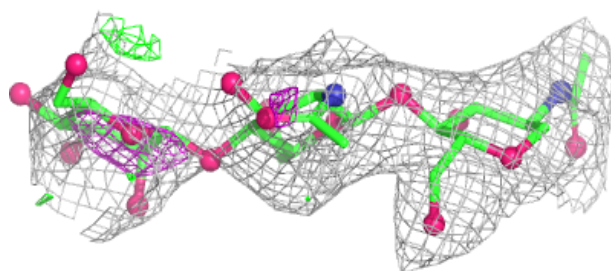
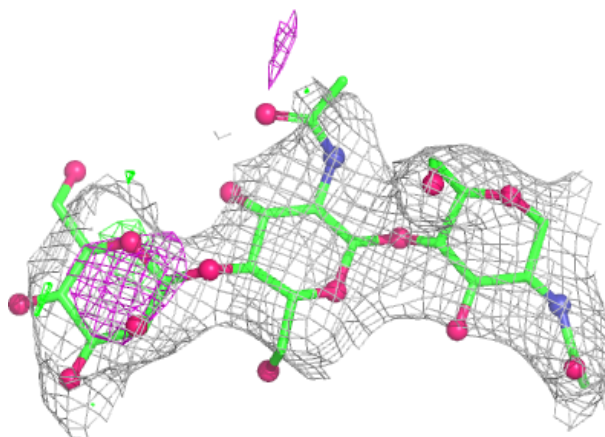
**Electron density around Chain K:**

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



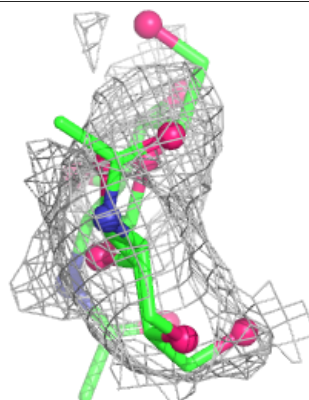
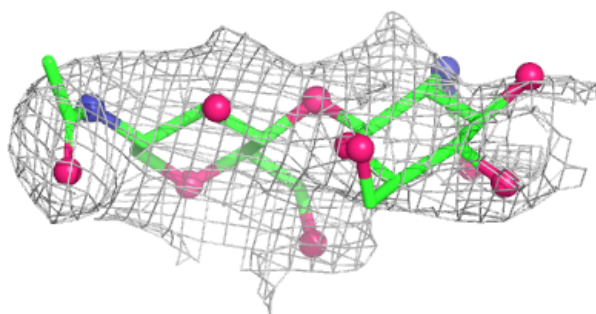
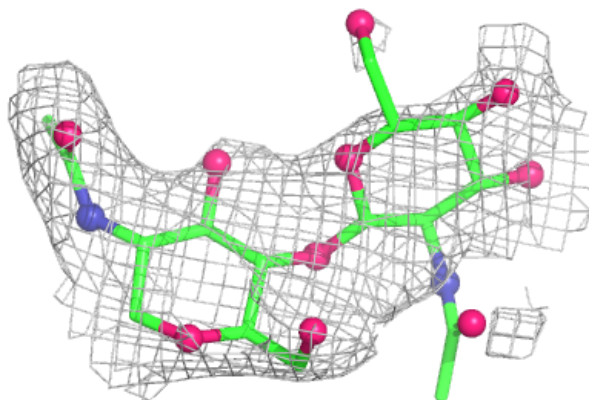
Electron density around Chain M:

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

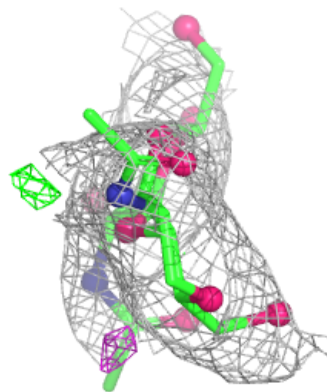
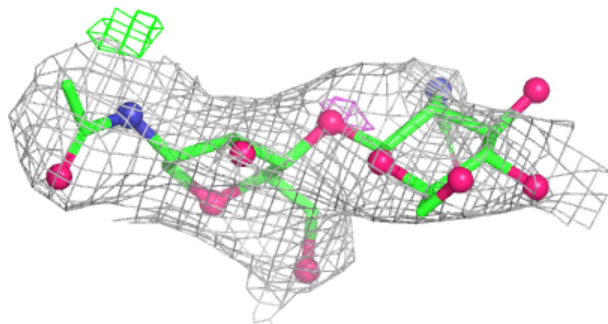
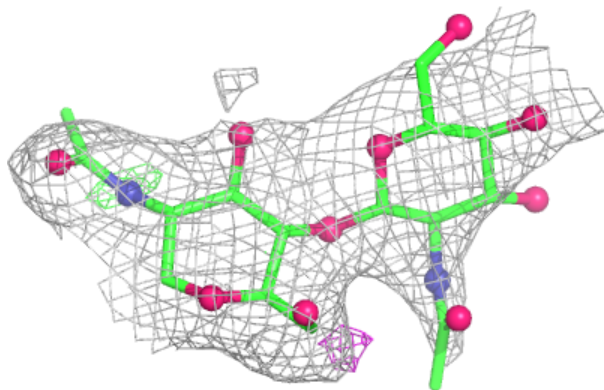


Electron density around Chain L:

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

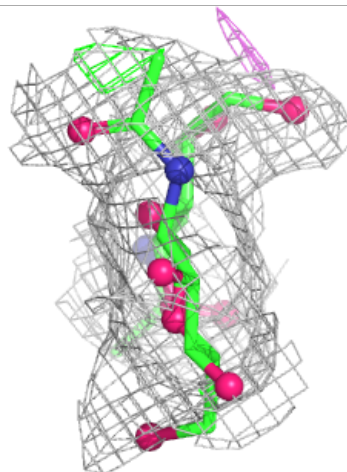
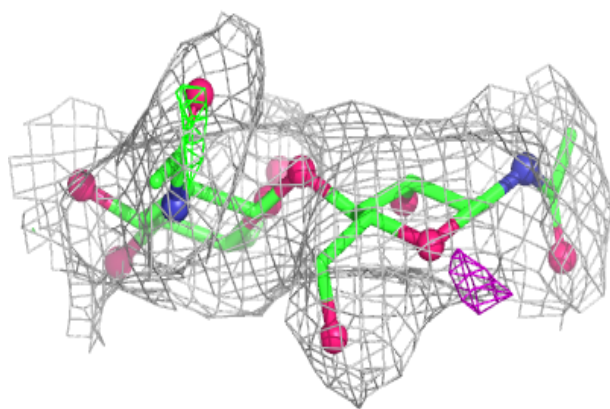
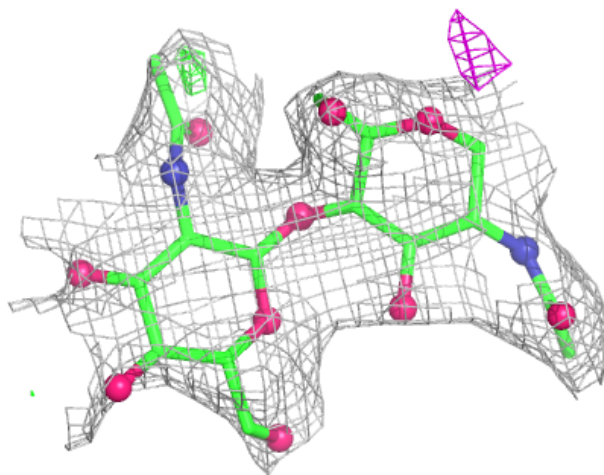
**Electron density around Chain N:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



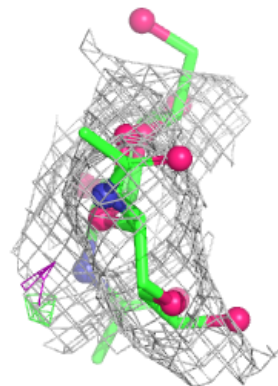
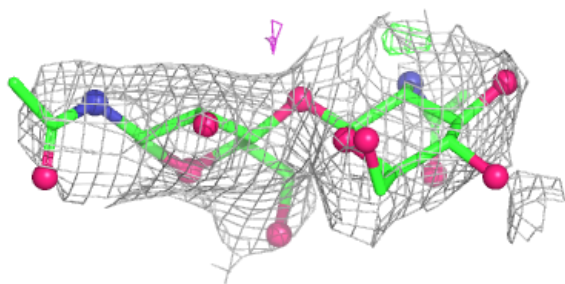
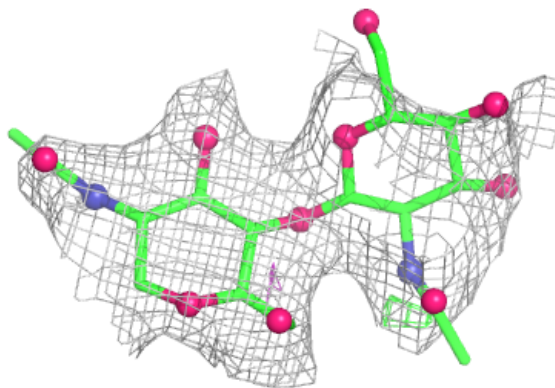
Electron density around Chain O:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



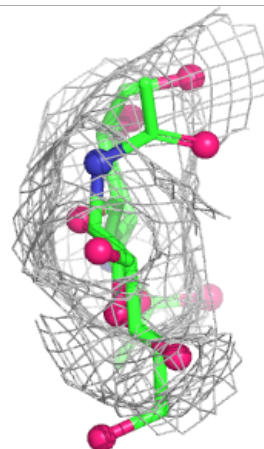
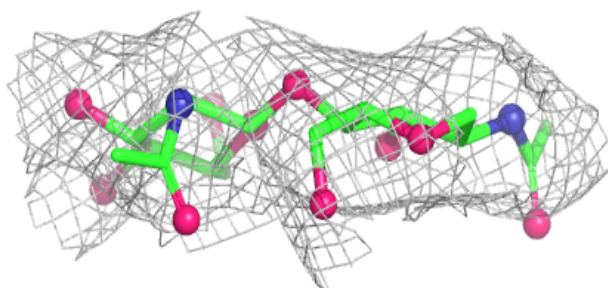
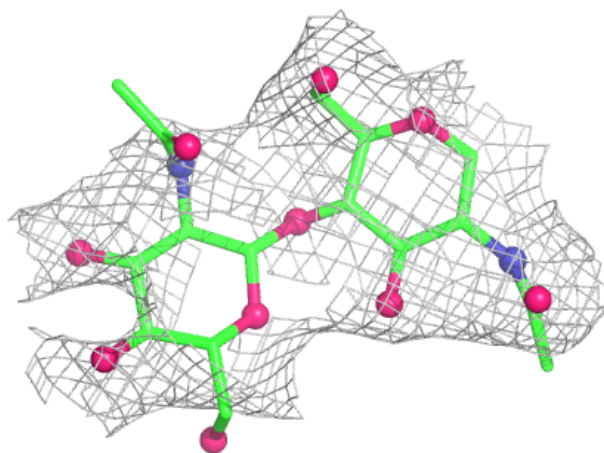
Electron density around Chain P:

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



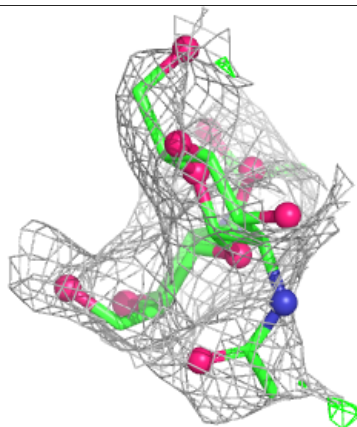
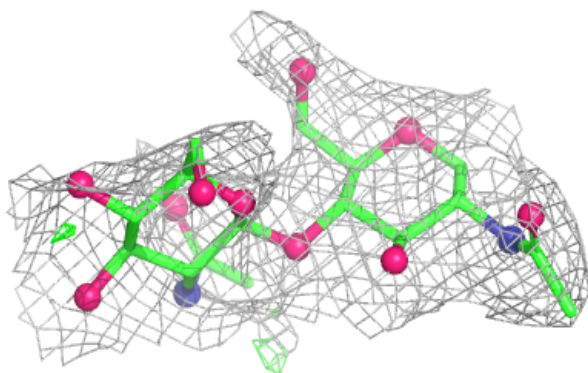
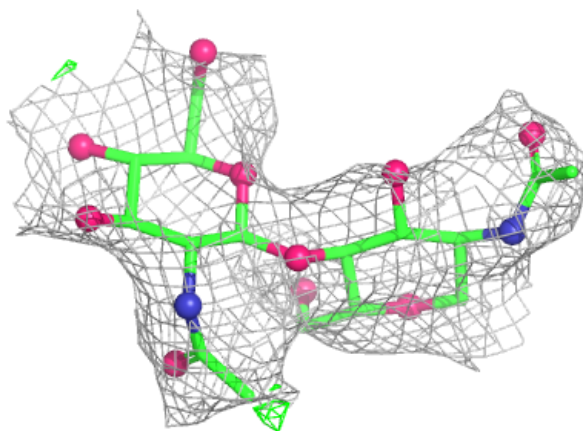
Electron density around Chain Q:

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and green (positive)

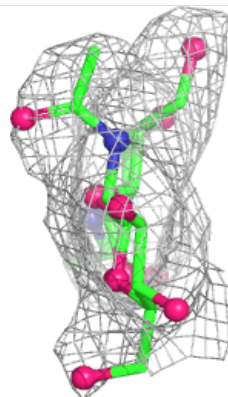
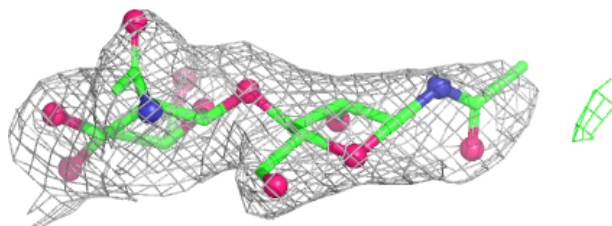
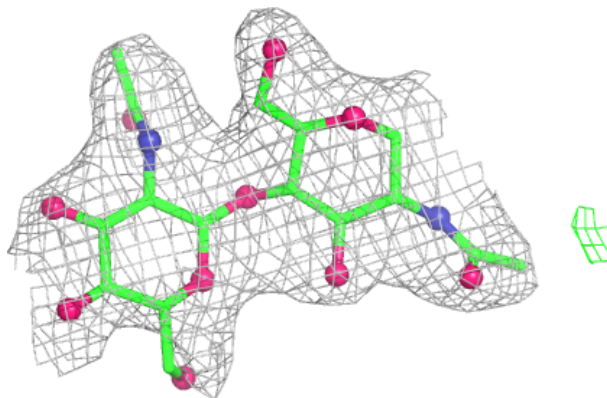


Electron density around Chain R:

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

**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)



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	D	716	14/15	0.22	0.17	120,122,122,122	0
5	NAG	A	707	14/15	0.41	0.16	90,94,95,95	0
5	NAG	G	726	14/15	0.57	0.16	70,74,80,89	0
6	SO4	H	535	5/5	0.70	0.26	104,104,105,106	0
5	NAG	E	723	14/15	0.79	0.12	70,74,80,89	0
6	SO4	D	717	5/5	0.84	0.29	104,104,105,106	0
6	SO4	A	708	5/5	0.85	0.31	104,104,105,106	0
6	SO4	H	534	5/5	0.88	0.28	104,104,105,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.