



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:24 AM UTC

PDB ID : 1ORV / pdb_00001orv
Title : Crystal Structure of Porcine Dipeptidyl Peptidase IV (CD26)
Authors : Engel, M.; Hoffmann, T.; Wagner, L.; Wermann, M.; Heiser, U.; Kiefersauer, R.; Huber, R.; Bode, W.; Demuth, H.U.; Brandstetter, H.
Deposited on : 2003-03-16
Resolution : 1.80 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

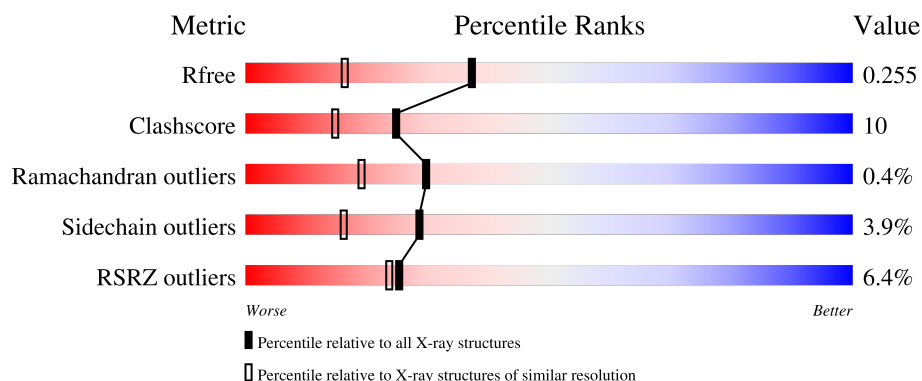
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	728	9% 77% 21% .
1	B	728	4% 76% 22% .
1	C	728	6% 76% 22% .
1	D	728	7% 74% 24% .
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	H	2	 100%
2	I	2	 50% 50%
2	K	2	 100%
2	L	2	 50% 50%
2	M	2	 50% 50%
3	G	3	 67% 33%
3	J	3	 33% 33% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25836 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 dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	80	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	83	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

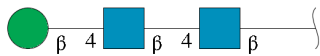
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

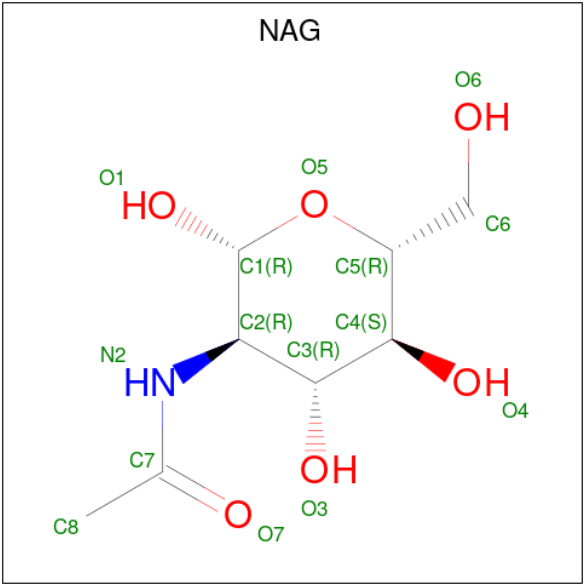
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	3	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

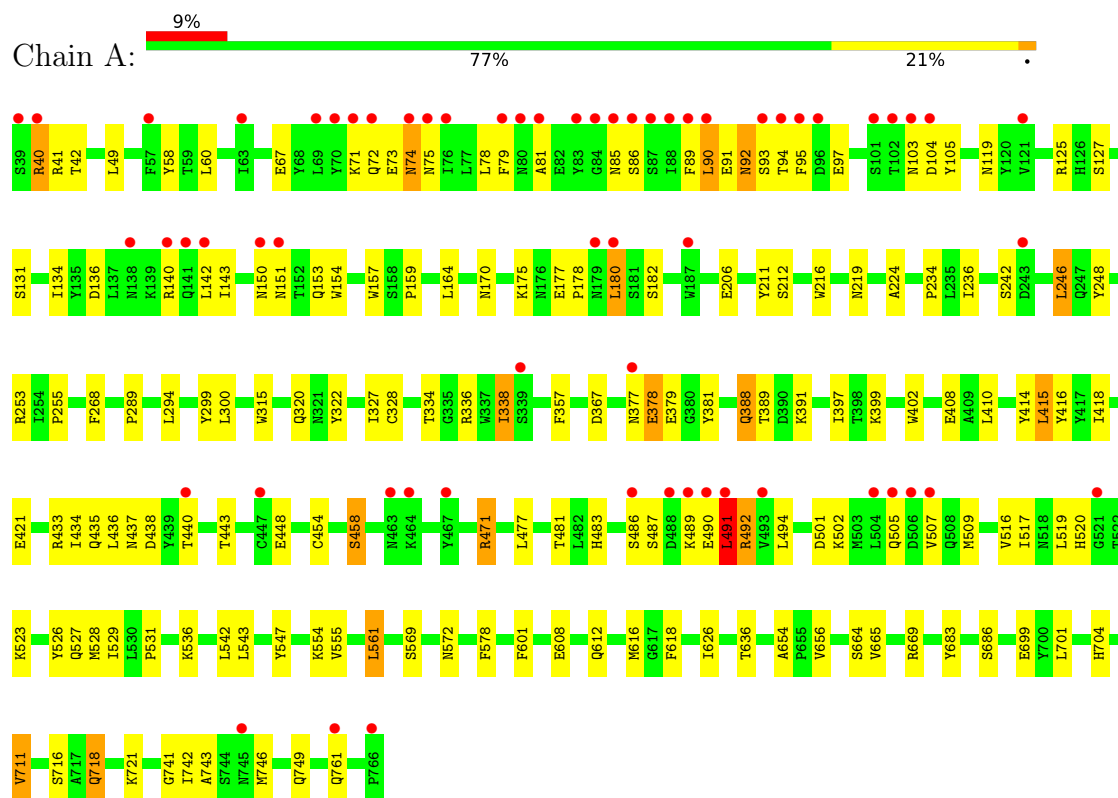
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	334	Total	O	0	0
			334	334		
6	B	431	Total	O	0	0
			431	431		
6	C	378	Total	O	0	0
			378	378		
6	D	325	Total	O	0	0
			325	325		

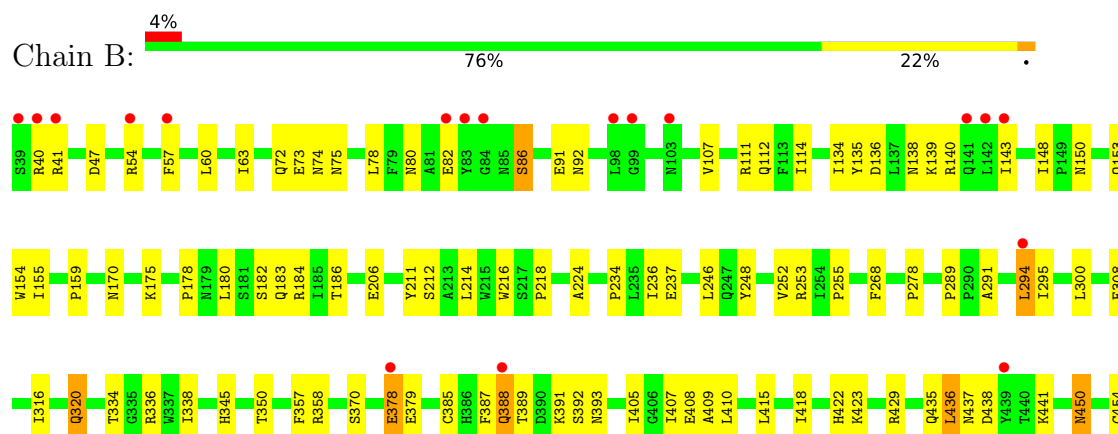
3 Residue-property plots

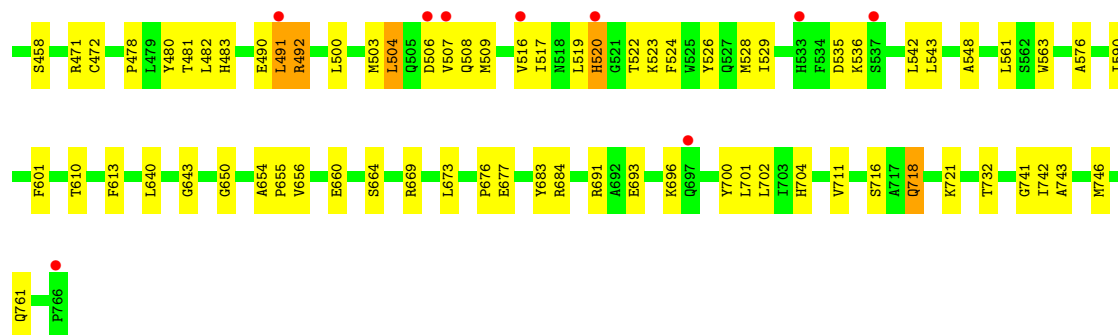
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

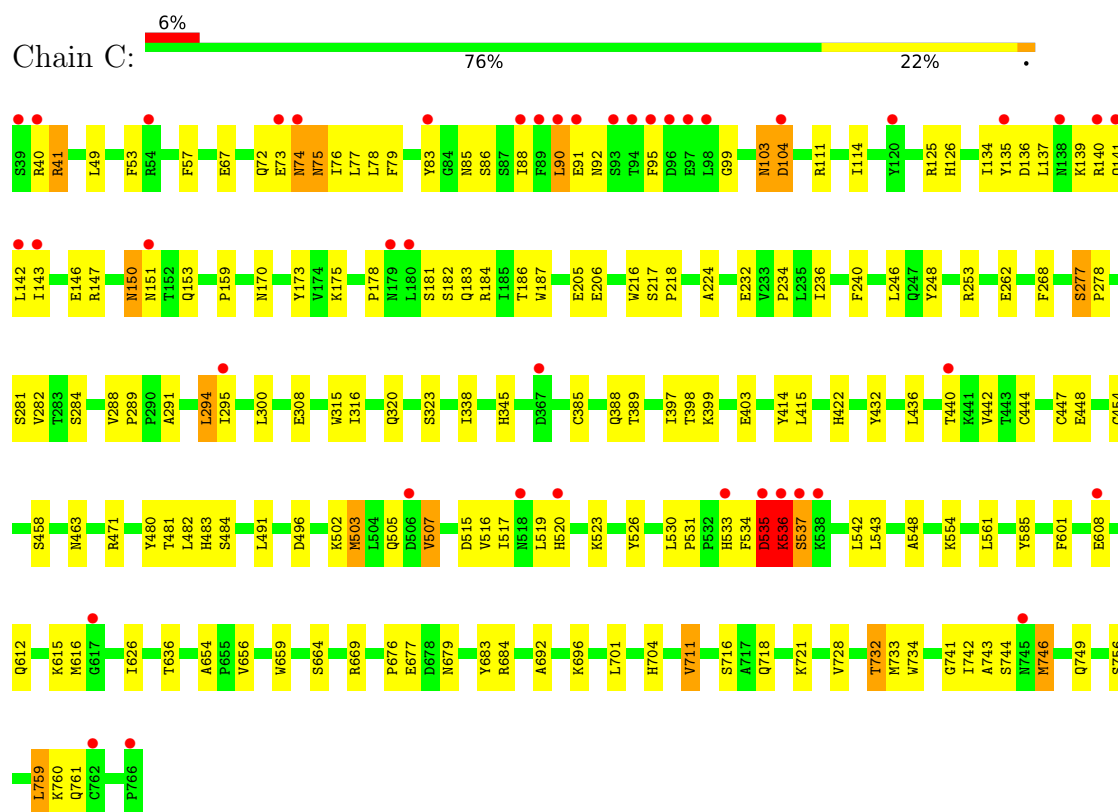


• Molecule 1: dipeptidyl peptidase IV

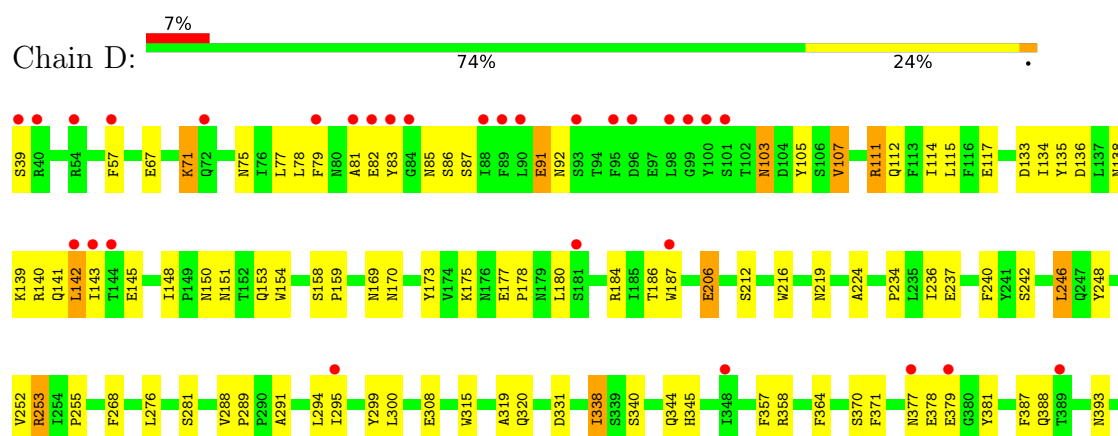


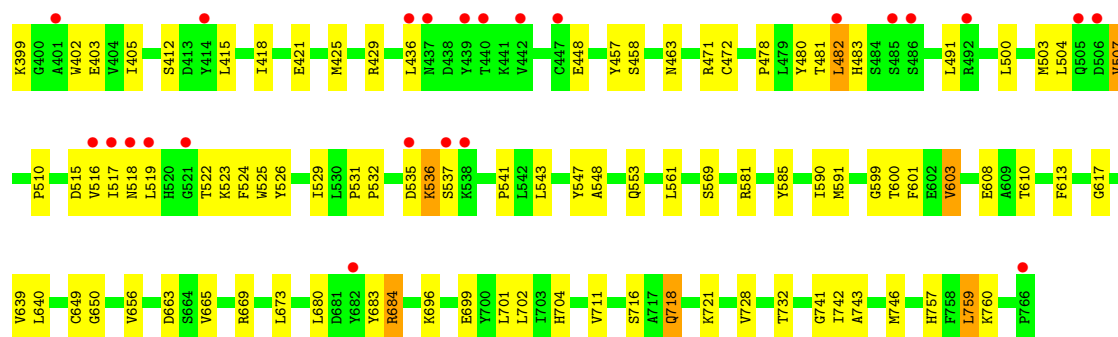


• Molecule 1: dipeptidyl peptidase IV

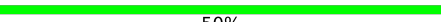
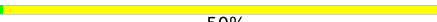


• Molecule 1: dipeptidyl peptidase IV



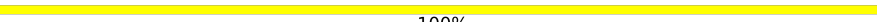


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 



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

Chain F:  100%

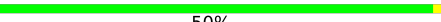
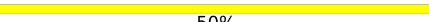


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

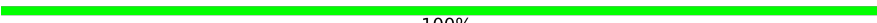


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 



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

Chain K:  100%



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

Chain L:  50% 50%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

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

Chain G:  67% 33%

MAG1
MAG2
BMA3

- 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:  33% 33% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.00Å 118.18Å 133.59Å 112.76° 94.93° 91.14°	Depositor
Resolution (Å)	19.25 – 1.80 19.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.25-1.80) 96.1 (19.25-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.252 0.222 , 0.255	Depositor DCC
R_{free} test set	15446 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25836	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/6141	0.96	23/8353 (0.3%)
1	B	0.56	0/6141	0.99	27/8353 (0.3%)
1	C	0.54	0/6141	1.01	30/8353 (0.4%)
1	D	0.51	1/6141 (0.0%)	0.97	26/8353 (0.3%)
All	All	0.53	1/24564 (0.0%)	0.98	106/33412 (0.3%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	531	PRO	CA-C	5.59	1.54	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ASN	N-CA-C	8.98	129.93	110.80
1	D	378	GLU	N-CA-C	-8.51	102.88	113.18
1	A	656	VAL	N-CA-C	-8.46	97.71	109.21
1	C	104	ASP	N-CA-C	-8.45	92.79	110.80
1	C	656	VAL	N-CA-C	-8.24	98.01	109.21
1	A	378	GLU	N-CA-C	-7.98	102.80	112.54
1	B	656	VAL	N-CA-C	-7.93	98.43	109.21
1	D	656	VAL	N-CA-C	-7.93	98.43	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	ALA	N-CA-C	7.64	122.78	113.38
1	D	458	SER	N-CA-C	-7.40	98.16	109.41
1	A	458	SER	N-CA-C	-7.22	98.34	109.24
1	C	743	ALA	N-CA-C	7.09	122.10	113.17
1	D	743	ALA	N-CA-C	7.03	122.02	113.17
1	B	300	LEU	N-CA-C	-6.91	97.98	109.24
1	D	319	ALA	N-CA-C	-6.80	96.03	107.99
1	C	458	SER	N-CA-C	-6.75	99.05	109.24
1	D	357	PHE	N-CA-C	-6.73	105.69	114.04
1	C	537	SER	N-CA-C	-6.61	105.12	113.72
1	B	458	SER	N-CA-C	-6.54	99.48	109.41
1	C	91	GLU	N-CA-C	6.47	119.07	110.53
1	B	548	ALA	N-CA-C	6.41	120.68	112.86
1	A	236	ILE	N-CA-C	-6.41	99.13	108.87
1	A	743	ALA	N-CA-C	6.38	121.21	113.17
1	D	158	SER	N-CA-C	-6.37	101.02	110.20
1	D	463	ASN	N-CA-C	6.22	121.63	111.37
1	D	206	GLU	N-CA-C	6.15	121.06	113.50
1	D	148	ILE	N-CA-C	-6.09	103.36	109.02
1	B	454	CYS	N-CA-C	6.05	118.61	108.02
1	D	541	PRO	N-CA-C	-6.05	102.34	111.41
1	D	255	PRO	N-CA-C	-5.98	101.11	110.50
1	D	236	ILE	N-CA-C	-5.96	99.80	108.87
1	B	388	GLN	N-CA-C	-5.95	99.54	109.24
1	D	684	ARG	N-CA-C	5.95	117.43	111.07
1	B	338	ILE	N-CA-C	5.94	117.13	108.58
1	A	143	ILE	N-CA-C	-5.92	101.07	108.89
1	A	388	GLN	N-CA-C	-5.91	99.66	109.46
1	D	601	PHE	N-CA-C	5.91	117.72	111.28
1	D	338	ILE	N-CA-C	5.90	117.84	108.87
1	D	300	LEU	N-CA-C	-5.89	99.60	108.96
1	B	683	TYR	N-CA-C	-5.88	104.23	111.40
1	C	683	TYR	N-CA-C	-5.87	104.96	111.36
1	D	548	ALA	N-CA-C	5.85	120.00	112.86
1	A	448	GLU	N-CA-C	5.82	120.51	113.17
1	D	591	MET	N-CA-C	5.78	117.25	111.07
1	A	206	GLU	N-CA-C	5.72	120.54	113.50
1	B	150	ASN	N-CA-C	-5.71	103.39	110.41
1	C	659	TRP	N-CA-C	5.70	118.26	111.71
1	A	529	ILE	N-CA-C	-5.66	99.07	107.51
1	C	338	ILE	N-CA-C	5.66	116.46	108.36
1	C	300	LEU	N-CA-C	-5.65	99.98	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	ALA	N-CA-C	5.58	119.66	112.86
1	C	206	GLU	N-CA-C	5.58	121.11	113.97
1	B	236	ILE	N-CA-C	-5.53	100.46	108.87
1	A	454	CYS	N-CA-C	5.53	117.86	108.02
1	B	206	GLU	N-CA-C	5.51	121.03	113.97
1	B	357	PHE	N-CA-C	-5.51	107.20	114.31
1	C	205	GLU	N-CA-C	5.50	117.08	111.14
1	C	447	CYS	N-CA-C	5.50	117.71	111.11
1	C	103	ASN	CA-C-N	5.49	132.03	121.54
1	C	103	ASN	C-N-CA	5.49	132.03	121.54
1	D	529	ILE	N-CA-C	-5.49	99.34	107.51
1	C	236	ILE	N-CA-C	-5.48	100.54	108.87
1	B	255	PRO	N-CA-C	-5.47	101.91	110.50
1	B	358	ARG	N-CA-C	-5.47	103.30	108.22
1	B	450	ASN	CA-C-N	5.46	125.55	119.32
1	B	450	ASN	C-N-CA	5.46	125.55	119.32
1	C	40	ARG	N-CA-C	5.46	122.43	110.80
1	D	388	GLN	N-CA-C	-5.46	100.34	109.24
1	C	692	ALA	N-CA-C	5.45	117.64	111.11
1	D	617	GLY	N-CA-C	5.43	119.25	112.73
1	B	529	ILE	N-CA-C	-5.42	99.43	107.51
1	D	683	TYR	N-CA-C	-5.38	105.50	111.36
1	A	255	PRO	N-CA-C	-5.37	102.07	110.50
1	A	561	LEU	N-CA-C	-5.35	97.79	107.75
1	C	454	CYS	N-CA-C	5.31	117.47	108.02
1	A	92	ASN	N-CA-C	-5.30	101.49	109.60
1	A	300	LEU	N-CA-C	-5.30	100.66	109.46
1	B	601	PHE	N-CA-C	5.29	117.04	111.28
1	D	281	SER	N-CA-C	-5.26	103.74	110.53
1	C	150	ASN	N-CA-C	-5.25	102.70	110.48
1	C	388	GLN	N-CA-C	-5.25	101.15	109.76
1	B	492	ARG	N-CA-C	5.25	116.50	108.42
1	A	89	PHE	N-CA-C	-5.23	107.45	113.88
1	C	601	PHE	N-CA-C	5.22	116.97	111.28
1	A	664	SER	N-CA-C	5.21	116.65	111.07
1	B	320	GLN	N-CA-C	5.21	119.58	113.23
1	A	338	ILE	N-CA-C	5.19	116.44	108.71
1	C	281	SER	N-CA-C	-5.19	103.84	110.53
1	B	392	SER	N-CA-C	5.18	118.76	112.23
1	C	664	SER	N-CA-C	5.17	116.61	111.07
1	A	711	VAL	N-CA-C	-5.16	99.82	107.51
1	B	54	ARG	N-CA-C	5.15	117.14	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	SER	N-CA-C	5.14	116.57	111.07
1	C	422	HIS	N-CA-C	5.11	117.75	110.24
1	B	563	TRP	N-CA-C	-5.11	105.71	111.28
1	C	711	VAL	N-CA-C	-5.08	99.15	106.88
1	A	683	TYR	N-CA-C	-5.08	105.44	111.69
1	D	240	PHE	N-CA-C	-5.08	100.18	108.76
1	D	547	TYR	N-CA-C	-5.08	99.98	110.80
1	B	504	LEU	N-CA-C	5.08	118.73	112.54
1	A	357	PHE	N-CA-C	-5.07	107.77	114.31
1	A	601	PHE	N-CA-C	5.05	116.79	111.28
1	C	684	ARG	N-CA-C	5.05	116.79	111.28
1	C	240	PHE	N-CA-C	-5.02	100.11	108.34
1	B	684	ARG	N-CA-C	5.00	116.73	111.28
1	A	699	GLU	N-CA-C	-5.00	101.09	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	B	700	TYR	Sidechain

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	5966	0	5663	106	0
1	B	5966	0	5663	110	0
1	C	5966	0	5662	126	0
1	D	5966	0	5662	130	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	39	0	34	1	0
3	J	39	0	34	1	0
4	A	56	0	52	2	0
4	B	56	0	52	2	0
4	C	70	0	65	1	0
4	D	28	0	26	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	334	0	0	7	0
6	B	431	0	0	11	0
6	C	378	0	0	6	0
6	D	325	0	0	10	0
All	All	25836	0	23088	460	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 10.

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ASP:C	1:C:536:LYS:HD3	1.83	1.02
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.40	1.01
1:C:746:MET:HE2	1:C:746:MET:H	1.28	0.98
1:C:536:LYS:HG2	1:C:537:SER:H	1.31	0.95
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.36	0.87
1:B:378:GLU:CD	1:B:378:GLU:H	1.83	0.87
1:C:746:MET:H	1:C:746:MET:CE	1.89	0.86
1:D:75:ASN:ND2	1:D:92:ASN:H	1.78	0.81
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.78	0.81
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.80	0.79
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.81	0.78
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.64	0.78
1:C:253:ARG:HH21	1:D:253:ARG:HH22	1.33	0.77
1:D:746:MET:HE1	6:D:1816:HOH:O	1.84	0.77
1:B:693:GLU:OE1	1:B:696:LYS:HE3	1.84	0.77
1:D:680:LEU:HD11	1:D:684:ARG:HE	1.49	0.77
1:D:291:ALA:O	1:D:295:ILE:HG13	1.85	0.77
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.83	0.76
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:MET:HE2	1:C:746:MET:N	2.01	0.75
1:B:75:ASN:ND2	1:B:92:ASN:H	1.85	0.75
1:A:492:ARG:HB3	1:A:492:ARG:NH2	2.02	0.74
1:A:75:ASN:HD22	1:A:92:ASN:ND2	1.85	0.73
1:B:490:GLU:O	1:B:492:ARG:N	2.21	0.73
1:B:175:LYS:HZ1	1:B:178:PRO:HA	1.53	0.73
1:D:184:ARG:HD3	1:D:186:THR:O	1.89	0.72
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.72	0.72
1:B:516:VAL:HG13	1:B:524:PHE:O	1.90	0.72
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.87	0.72
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.89	0.71
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.88	0.71
1:B:111:ARG:HD2	6:B:1806:HOH:O	1.89	0.71
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.71	0.71
1:C:184:ARG:HD3	1:C:186:THR:O	1.90	0.71
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.16	0.71
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.06	0.71
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.72	0.70
1:A:507:VAL:HG13	1:A:509:MET:HG2	1.73	0.70
1:C:519:LEU:HD22	1:C:608:GLU:OE1	1.92	0.70
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.88	0.69
1:C:733:MET:HA	1:D:732:THR:CG2	2.23	0.69
1:D:536:LYS:O	1:D:537:SER:HB2	1.91	0.69
1:D:83:TYR:HB3	1:D:85:ASN:OD1	1.93	0.68
1:D:704:HIS:HD2	1:D:716:SER:OG	1.77	0.68
1:C:75:ASN:HD22	1:C:92:ASN:HB2	1.58	0.68
1:A:75:ASN:HB3	1:A:92:ASN:N	2.08	0.68
1:B:526:TYR:HE1	1:B:528:MET:HE2	1.60	0.67
1:C:440:THR:HG21	6:C:1719:HOH:O	1.95	0.67
1:C:734:TRP:CZ3	1:D:732:THR:OG1	2.48	0.66
1:A:93:SER:C	1:A:95:PHE:H	2.03	0.66
1:D:87:SER:HB3	4:D:767(A):NAG:O6	1.95	0.66
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.79	0.66
1:B:490:GLU:O	1:B:490:GLU:HG2	1.95	0.66
1:B:704:HIS:HD2	1:B:716:SER:OG	1.78	0.66
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.79	0.65
1:B:691:ARG:HG3	1:B:691:ARG:HH11	1.62	0.64
1:C:90:LEU:HD13	1:C:90:LEU:O	1.98	0.64
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.28	0.64
1:A:418:ILE:HD12	6:A:1739:HOH:O	1.98	0.63
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:HIS:HD2	1:C:716:SER:OG	1.80	0.63
1:A:433:ARG:NH1	1:A:443:THR:HG21	2.14	0.63
1:C:612:GLN:O	1:C:615:LYS:HG2	1.98	0.63
1:C:536:LYS:HG2	1:C:537:SER:N	2.10	0.62
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.24	0.62
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.80	0.62
1:A:408:GLU:HG2	6:A:1624:HOH:O	1.98	0.62
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.97	0.62
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.82	0.61
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.83	0.61
1:B:516:VAL:HG11	1:B:523:LYS:HB2	1.82	0.61
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.45	0.61
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.80	0.61
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.47	0.60
1:C:218:PRO:HD2	1:C:308:GLU:OE2	2.01	0.60
1:A:458:SER:OG	1:A:471:ARG:HD3	2.02	0.60
1:B:516:VAL:HG12	1:B:517:ILE:N	2.16	0.60
1:C:718:GLN:HE22	1:C:721:LYS:NZ	1.99	0.60
1:C:733:MET:HA	1:D:732:THR:HG22	1.84	0.60
1:D:111:ARG:HD2	6:D:1812:HOH:O	2.00	0.60
1:D:482:LEU:HD22	1:D:491:LEU:HD12	1.84	0.60
1:D:377:ASN:HB3	1:D:379:GLU:H	1.66	0.59
1:A:92:ASN:C	1:A:94:THR:H	2.09	0.59
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.32	0.59
1:B:218:PRO:HD2	1:B:308:GLU:OE2	2.02	0.59
1:B:75:ASN:HD22	1:B:92:ASN:H	1.51	0.59
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.37	0.59
6:A:1518:HOH:O	1:B:746:MET:HE3	2.03	0.59
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.38	0.59
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.84	0.59
1:A:93:SER:C	1:A:95:PHE:N	2.58	0.58
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.85	0.58
1:C:291:ALA:O	1:C:295:ILE:HG13	2.03	0.58
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.84	0.58
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.85	0.58
1:B:522:THR:HG21	1:B:590:ILE:HD11	1.85	0.58
1:C:414:TYR:HA	1:C:436:LEU:HD13	1.85	0.58
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.03	0.58
1:B:334:THR:OG1	1:B:336:ARG:HG2	2.04	0.58
1:B:418:ILE:HD12	6:B:1782:HOH:O	2.04	0.58
1:C:536:LYS:HD3	1:C:536:LYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:LYS:O	1:C:505:GLN:HG2	2.05	0.57
1:B:415:LEU:HD13	1:B:415:LEU:C	2.29	0.57
1:A:519:LEU:HD22	1:A:608:GLU:OE2	2.03	0.57
1:A:746:MET:HE3	6:A:1566:HOH:O	2.04	0.57
1:A:502:LYS:O	1:A:505:GLN:HG2	2.05	0.57
1:C:536:LYS:CG	1:C:537:SER:H	2.06	0.57
1:D:718:GLN:HE22	1:D:721:LYS:NZ	2.02	0.56
1:A:58:TYR:CD2	1:A:494:LEU:HB3	2.40	0.56
1:B:80:ASN:OD1	1:B:82:GLU:HB2	2.05	0.56
1:B:500:LEU:HA	1:B:503:MET:HE3	1.86	0.56
1:B:408:GLU:HG2	6:B:1696:HOH:O	2.05	0.56
1:A:704:HIS:HD2	1:A:716:SER:OG	1.88	0.56
1:B:704:HIS:HE1	1:B:711:VAL:O	1.89	0.56
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.31	0.56
1:D:522:THR:HB	1:D:524:PHE:CE1	2.41	0.56
1:A:72:GLN:HG2	1:A:73:GLU:HG3	1.87	0.55
1:A:415:LEU:C	1:A:415:LEU:HD13	2.31	0.55
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.58	0.55
1:B:291:ALA:O	1:B:295:ILE:HG23	2.07	0.55
1:C:74:ASN:HB2	1:C:92:ASN:ND2	2.22	0.55
1:A:41:ARG:HB2	6:A:1780:HOH:O	2.05	0.55
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.06	0.55
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.55
1:B:57:PHE:HA	1:B:480:TYR:CE1	2.42	0.55
1:D:746:MET:CE	6:D:1816:HOH:O	2.46	0.55
1:B:175:LYS:NZ	1:B:178:PRO:HA	2.21	0.55
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.89	0.55
1:C:142:LEU:C	1:C:142:LEU:HD23	2.32	0.55
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.07	0.55
1:A:377:ASN:HB2	1:A:381:TYR:O	2.07	0.55
1:B:350:THR:HG22	4:B:773(A):NAG:H81	1.89	0.55
1:C:483:HIS:HA	1:C:491:LEU:HD23	1.89	0.55
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.37	0.55
1:D:134:ILE:HG21	1:D:178:PRO:HB3	1.89	0.54
1:B:507:VAL:HG13	1:B:509:MET:HG2	1.90	0.54
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.54
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.89	0.54
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.89	0.54
1:A:75:ASN:HD22	1:A:92:ASN:HD22	1.55	0.54
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.89	0.54
1:D:77:LEU:HB2	1:D:79:PHE:HE2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:SER:HB2	1:C:746:MET:HE3	1.90	0.54
1:D:393:ASN:H	1:D:393:ASN:HD22	1.53	0.54
1:A:492:ARG:HH21	1:A:492:ARG:CB	2.15	0.54
1:C:535:ASP:CA	1:C:536:LYS:HD3	2.38	0.54
1:D:518:ASN:O	1:D:519:LEU:HD23	2.08	0.53
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.56	0.53
1:A:75:ASN:ND2	1:A:92:ASN:ND2	2.56	0.53
1:A:75:ASN:ND2	1:A:92:ASN:HD22	2.07	0.53
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.44	0.53
1:B:378:GLU:CD	1:B:378:GLU:N	2.61	0.53
1:B:409:ALA:O	1:B:415:LEU:HD22	2.09	0.53
1:A:74:ASN:O	1:A:95:PHE:HE2	1.92	0.53
1:A:334:THR:OG1	1:A:336:ARG:HG3	2.09	0.53
1:A:489:LYS:HG3	1:A:491:LEU:H	1.74	0.53
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.06	0.53
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.44	0.52
1:D:532:PRO:HD3	1:D:569:SER:HA	1.91	0.52
1:B:148:ILE:HD13	1:B:155:ILE:CD1	2.39	0.52
1:B:490:GLU:O	1:B:490:GLU:CG	2.56	0.52
1:D:67:GLU:HB3	1:D:78:LEU:HD11	1.90	0.52
1:D:429:ARG:NH2	6:D:1663:HOH:O	2.42	0.52
1:D:553:GLN:NE2	6:D:1663:HOH:O	2.42	0.52
1:C:111:ARG:HD2	6:C:1865:HOH:O	2.09	0.52
1:B:669:ARG:HD2	6:B:1838:HOH:O	2.08	0.52
1:C:704:HIS:HE1	1:C:711:VAL:O	1.93	0.52
1:C:496:ASP:HB2	6:C:1655:HOH:O	2.08	0.52
1:D:288:VAL:HG12	1:D:289:PRO:HD2	1.92	0.52
1:C:183:GLN:NE2	1:C:277:SER:C	2.68	0.52
1:B:41:ARG:NH1	1:B:47:ASP:OD1	2.43	0.51
1:C:153:GLN:HE22	1:C:170:ASN:HD22	1.54	0.51
1:C:484:SER:HB2	1:C:491:LEU:HD21	1.91	0.51
1:D:418:ILE:HD12	6:D:1706:HOH:O	2.10	0.51
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.91	0.51
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.46	0.51
1:D:482:LEU:HD23	1:D:483:HIS:N	2.26	0.51
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.92	0.51
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.92	0.51
1:C:484:SER:CB	1:C:491:LEU:HD21	2.40	0.51
1:A:71:LYS:HE3	1:A:105:TYR:CD2	2.45	0.51
1:B:526:TYR:CE1	1:B:528:MET:HE2	2.44	0.51
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.46	0.51
1:D:331:ASP:HB2	1:D:338:ILE:HD12	1.93	0.51
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.46	0.51
1:C:718:GLN:HE22	1:C:721:LYS:HZ1	1.57	0.50
1:D:75:ASN:HD22	1:D:92:ASN:H	1.57	0.50
1:D:472:CYS:O	1:D:478:PRO:HA	2.11	0.50
1:B:86:SER:C	4:B:767(A):NAG:H81	2.36	0.50
1:B:112:GLN:HB3	1:B:138:ASN:HD21	1.76	0.50
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.41	0.50
1:A:94:THR:HG22	1:A:94:THR:O	2.11	0.50
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.93	0.50
1:A:438:ASP:OD1	1:A:440:THR:HB	2.11	0.50
1:A:131:SER:OG	1:A:150:ASN:ND2	2.45	0.50
1:B:422:HIS:CD2	1:B:423:LYS:HD3	2.46	0.50
1:B:73:GLU:OE2	1:B:73:GLU:HA	2.10	0.50
1:B:741:GLY:O	1:B:742:ILE:C	2.54	0.50
1:D:139:LYS:O	1:D:141:GLN:HG3	2.11	0.50
1:D:393:ASN:H	1:D:393:ASN:ND2	2.09	0.50
1:D:680:LEU:HD11	1:D:684:ARG:NE	2.23	0.50
1:B:175:LYS:NZ	1:B:175:LYS:HB3	2.27	0.50
1:A:103:ASN:O	1:A:104:ASP:HB2	2.12	0.49
1:D:103:ASN:OD1	1:D:117:GLU:OE2	2.29	0.49
1:D:177:GLU:HB2	1:D:180:LEU:HD23	1.93	0.49
1:B:471:ARG:NH2	6:B:1757:HOH:O	2.44	0.49
1:A:414:TYR:HA	1:A:436:LEU:HD13	1.95	0.49
1:C:90:LEU:C	1:C:90:LEU:HD22	2.38	0.49
1:A:526:TYR:CE1	1:A:528:MET:HE2	2.47	0.49
1:B:370:SER:HB2	1:B:387:PHE:O	2.12	0.49
1:B:214:LEU:HD12	6:B:1630:HOH:O	2.12	0.49
1:B:407:ILE:CG2	1:B:415:LEU:HD21	2.37	0.49
1:C:72:GLN:O	1:C:74:ASN:N	2.46	0.49
1:D:133:ASP:HB3	1:D:142:LEU:HD21	1.94	0.49
1:A:327:ILE:HD13	1:A:389:THR:HG23	1.95	0.49
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.78	0.49
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.78	0.48
1:C:615:LYS:HG2	1:C:616:MET:N	2.28	0.48
1:B:63:ILE:HD11	1:B:78:LEU:CD1	2.43	0.48
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.96	0.48
1:D:718:GLN:HE22	1:D:721:LYS:HZ1	1.61	0.48
1:C:253:ARG:NH2	1:D:253:ARG:NH2	2.62	0.48
1:C:463:ASN:N	1:C:463:ASN:HD22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.48	0.48
1:D:741:GLY:O	1:D:742:ILE:C	2.57	0.48
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.49	0.48
1:C:288:VAL:HG11	1:C:294:LEU:HD11	1.96	0.48
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.49	0.48
1:D:415:LEU:C	1:D:415:LEU:HD23	2.38	0.48
1:A:92:ASN:O	1:A:94:THR:N	2.43	0.48
1:C:83:TYR:HB2	1:C:85:ASN:OD1	2.13	0.48
1:D:82:GLU:H	1:D:491:LEU:HD13	1.78	0.48
1:C:135:TYR:HD2	1:C:137:LEU:HD23	1.78	0.48
1:C:146:GLU:OE1	1:C:181:SER:HA	2.13	0.48
1:D:57:PHE:HA	1:D:480:TYR:CE1	2.49	0.48
1:A:547:TYR:HB2	1:A:554:LYS:HD3	1.96	0.47
1:D:340:SER:O	1:D:344:GLN:HG3	2.14	0.47
1:C:741:GLY:O	1:C:742:ILE:C	2.56	0.47
1:A:378:GLU:CD	1:A:378:GLU:H	2.22	0.47
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.44	0.47
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.49	0.47
1:D:600:THR:O	1:D:603:VAL:CG1	2.63	0.47
1:C:704:HIS:CD2	1:C:716:SER:OG	2.66	0.47
1:D:81:ALA:O	1:D:82:GLU:HB3	2.13	0.47
1:D:175:LYS:HE3	1:D:180:LEU:O	2.15	0.47
1:A:435:GLN:OE1	1:A:437:ASN:OD1	2.32	0.47
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.49	0.47
1:A:75:ASN:HB3	1:A:92:ASN:H	1.77	0.47
1:A:150:ASN:O	1:A:151:ASN:HB2	2.15	0.47
1:A:177:GLU:HB2	1:A:180:LEU:HB2	1.97	0.47
1:B:643:GLY:HA2	6:B:1631:HOH:O	2.14	0.47
1:B:438:ASP:OD2	1:B:441:LYS:HE3	2.15	0.46
1:B:184:ARG:HD3	1:B:186:THR:O	2.16	0.46
1:C:73:GLU:CD	4:C:768(A):NAG:H61	2.40	0.46
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.15	0.46
1:C:516:VAL:HG12	1:C:517:ILE:N	2.29	0.46
1:C:533:HIS:O	1:C:534:PHE:C	2.57	0.46
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.80	0.46
1:B:482:LEU:O	1:B:490:GLU:O	2.32	0.46
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.51	0.46
1:B:435:GLN:OE1	1:B:441:LYS:HD2	2.16	0.46
1:D:75:ASN:HD22	1:D:91:GLU:HA	1.79	0.46
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.97	0.46
1:D:379:GLU:HG2	1:D:381:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:TYR:CA	1:A:436:LEU:HD13	2.45	0.46
1:A:477:LEU:HD12	1:A:501:ASP:HB2	1.98	0.46
1:A:517:ILE:HD11	1:A:578:PHE:CE1	2.50	0.46
1:C:503:MET:HE2	1:C:503:MET:HB2	1.74	0.46
1:D:177:GLU:CB	1:D:180:LEU:HD23	2.46	0.46
1:A:78:LEU:O	4:A:767(A):NAG:H81	2.15	0.46
1:A:81:ALA:O	1:A:492:ARG:NH1	2.48	0.46
1:C:57:PHE:HA	1:C:480:TYR:CE1	2.51	0.46
1:C:345:HIS:HE1	1:C:389:THR:O	1.99	0.46
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.80	0.46
1:D:543:LEU:HD22	1:D:759:LEU:HD11	1.98	0.46
1:B:516:VAL:CG1	1:B:517:ILE:N	2.79	0.46
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.51	0.46
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.98	0.46
1:D:425:MET:HG2	1:D:525:TRP:CH2	2.51	0.46
1:A:415:LEU:C	1:A:415:LEU:CD1	2.88	0.45
1:D:345:HIS:HD2	6:D:1728:HOH:O	1.98	0.45
1:A:686:SER:HA	2:F:1:NAG:H82	1.98	0.45
1:B:528:MET:HG2	1:B:576:ALA:HB2	1.98	0.45
1:B:136:ASP:O	1:B:140:ARG:HA	2.16	0.45
1:C:142:LEU:HD23	1:C:143:ILE:O	2.16	0.45
1:C:415:LEU:HD23	1:C:415:LEU:C	2.41	0.45
1:D:77:LEU:HB2	1:D:79:PHE:CE2	2.50	0.45
1:B:660:GLU:CG	6:B:1520:HOH:O	2.64	0.45
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.52	0.45
1:D:600:THR:O	1:D:603:VAL:HG13	2.16	0.45
1:C:175:LYS:CG	1:C:182:SER:HB3	2.46	0.45
1:C:432:TYR:CE2	1:C:444:CYS:HB2	2.52	0.45
1:D:219:ASN:HB2	1:D:308:GLU:CD	2.42	0.45
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.45
1:C:41:ARG:HH11	1:C:507:VAL:HG12	1.82	0.45
1:B:704:HIS:CD2	1:B:716:SER:OG	2.65	0.45
1:C:612:GLN:O	1:C:615:LYS:CG	2.64	0.45
1:B:73:GLU:HB3	3:G:1:NAG:H4	1.99	0.45
1:C:150:ASN:O	1:C:151:ASN:HB2	2.18	0.45
1:A:67:GLU:HB3	1:A:78:LEU:HD11	1.99	0.44
1:B:345:HIS:HE1	1:B:389:THR:O	2.00	0.44
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.99	0.44
1:C:414:TYR:CA	1:C:436:LEU:HD13	2.46	0.44
1:A:136:ASP:O	1:A:140:ARG:HA	2.17	0.44
1:B:437:ASN:C	1:B:437:ASN:OD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:LYS:HG2	6:C:1747:HOH:O	2.16	0.44
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.52	0.44
1:D:379:GLU:HG2	1:D:381:TYR:HD1	1.82	0.44
1:C:535:ASP:O	1:C:536:LYS:HB3	2.18	0.44
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.00	0.44
1:D:206:GLU:OE2	1:D:663:ASP:OD2	2.34	0.44
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.44
1:D:603:VAL:HG23	1:D:639:VAL:CG2	2.48	0.44
1:A:85:ASN:ND2	4:A:767(A):NAG:O7	2.51	0.44
1:C:125:ARG:HB3	6:C:1518:HOH:O	2.16	0.44
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.98	0.44
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.82	0.44
1:D:370:SER:HB2	1:D:387:PHE:O	2.18	0.44
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.18	0.44
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.52	0.44
1:B:691:ARG:HH11	1:B:691:ARG:CG	2.27	0.44
1:C:77:LEU:CD2	1:C:88:ILE:HG12	2.48	0.44
1:C:92:ASN:O	1:C:95:PHE:HD2	2.01	0.44
1:A:60:LEU:HD12	1:A:60:LEU:C	2.43	0.44
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.15	0.44
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.47	0.44
1:C:76:ILE:HD12	1:C:90:LEU:CD1	2.48	0.44
1:C:733:MET:HA	1:D:732:THR:HG21	2.00	0.44
1:D:590:ILE:HG12	6:D:1722:HOH:O	2.18	0.44
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.47	0.43
1:C:515:ASP:HB3	1:C:526:TYR:CZ	2.53	0.43
1:B:72:GLN:HG2	1:B:73:GLU:HG2	1.99	0.43
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.53	0.43
1:C:543:LEU:HD22	1:C:759:LEU:HD11	1.99	0.43
1:B:393:ASN:HD22	1:B:393:ASN:H	1.66	0.43
1:B:673:LEU:HD12	1:B:673:LEU:N	2.33	0.43
1:C:67:GLU:HB3	1:C:78:LEU:HD11	2.01	0.43
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.83	0.43
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.82	0.43
1:C:114:ILE:HG22	1:C:135:TYR:HB3	2.01	0.43
1:C:316:ILE:HG22	1:C:323:SER:HB2	2.00	0.43
3:J:1:NAG:H62	3:J:2:NAG:HN2	1.83	0.43
1:A:125:ARG:HB3	6:A:1550:HOH:O	2.19	0.43
1:A:377:ASN:ND2	6:A:1745:HOH:O	2.50	0.43
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.49	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:SER:O	1:C:760:LYS:HG3	2.19	0.43
1:D:516:VAL:CG1	1:D:517:ILE:N	2.82	0.43
1:A:397:ILE:HD12	1:A:434:ILE:HD13	2.01	0.43
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.54	0.43
1:A:612:GLN:HE21	1:A:612:GLN:HB3	1.66	0.43
1:C:463:ASN:N	1:C:463:ASN:ND2	2.67	0.43
1:A:516:VAL:HG12	1:A:517:ILE:N	2.32	0.43
1:B:175:LYS:CG	1:B:182:SER:HB3	2.48	0.43
1:C:183:GLN:HE22	1:C:278:PRO:N	2.17	0.43
1:D:67:GLU:CD	1:D:111:ARG:HH12	2.26	0.43
1:A:42:THR:HB	1:A:569:SER:OG	2.19	0.42
1:A:127:SER:HB3	1:A:211:TYR:CG	2.54	0.42
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.00	0.42
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.34	0.42
1:C:732:THR:HG22	1:D:732:THR:HG23	2.01	0.42
1:A:415:LEU:HD13	1:A:416:TYR:N	2.33	0.42
1:C:135:TYR:CD2	1:C:137:LEU:HD23	2.54	0.42
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.84	0.42
1:D:515:ASP:HB3	1:D:526:TYR:CE2	2.54	0.42
1:A:91:GLU:C	1:A:92:ASN:O	2.59	0.42
1:B:673:LEU:HD11	6:B:1720:HOH:O	2.18	0.42
1:C:53:PHE:CZ	1:C:507:VAL:HG11	2.55	0.42
1:C:75:ASN:ND2	1:C:92:ASN:HB2	2.29	0.42
1:B:73:GLU:O	1:B:74:ASN:HB2	2.19	0.42
1:B:143:ILE:HD12	1:B:143:ILE:N	2.34	0.42
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.54	0.42
1:C:612:GLN:HE21	1:C:612:GLN:HB3	1.65	0.42
1:C:615:LYS:CG	1:C:616:MET:N	2.82	0.42
1:D:377:ASN:HB2	1:D:381:TYR:H	1.84	0.42
1:D:500:LEU:HA	1:D:503:MET:HE3	2.01	0.42
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.80	0.42
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.00	0.42
1:C:114:ILE:CG2	1:C:135:TYR:HB3	2.50	0.42
1:A:490:GLU:O	1:A:492:ARG:N	2.53	0.42
1:B:524:PHE:CE2	1:B:590:ILE:HD12	2.54	0.42
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.84	0.42
1:B:289:PRO:HG2	1:B:294:LEU:HG	2.01	0.42
1:D:112:GLN:HG2	1:D:138:ASN:HD21	1.84	0.42
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.55	0.42
1:D:610:THR:HA	1:D:613:PHE:CD2	2.55	0.42
1:A:92:ASN:C	1:A:94:THR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HD11	1:B:320:GLN:HA	2.02	0.42
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.84	0.42
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.42
1:B:134:ILE:O	1:B:143:ILE:HD13	2.20	0.42
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.55	0.42
1:D:457:TYR:HA	1:D:471:ARG:O	2.20	0.42
1:A:704:HIS:HE1	1:A:711:VAL:O	2.02	0.42
1:B:654:ALA:N	1:B:655:PRO:CD	2.82	0.42
1:D:107:VAL:HG12	1:D:114:ILE:HG13	2.01	0.42
1:D:114:ILE:HG22	1:D:135:TYR:HB3	2.01	0.42
1:A:502:LYS:HD2	1:A:505:GLN:OE1	2.20	0.41
1:A:626:ILE:HG23	1:A:636:THR:HG23	2.02	0.41
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.50	0.41
1:D:39:SER:N	6:D:1670:HOH:O	2.52	0.41
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.55	0.41
1:B:677:GLU:H	1:B:677:GLU:CD	2.28	0.41
1:C:159:PRO:HG2	1:C:217:SER:O	2.19	0.41
1:D:288:VAL:HG12	1:D:289:PRO:CD	2.49	0.41
1:D:405:ILE:HG13	1:D:429:ARG:CD	2.50	0.41
1:D:482:LEU:HD23	1:D:483:HIS:H	1.85	0.41
1:D:603:VAL:HG23	1:D:639:VAL:HG22	2.01	0.41
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.41
1:D:134:ILE:CG2	1:D:143:ILE:HD12	2.51	0.41
1:D:150:ASN:O	1:D:151:ASN:HB2	2.21	0.41
1:D:237:GLU:HA	1:D:252:VAL:O	2.20	0.41
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.35	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:D:757:HIS:CE1	6:D:1744:HOH:O	2.73	0.41
1:B:107:VAL:HG22	1:B:114:ILE:HD12	2.03	0.41
1:D:82:GLU:HA	1:D:491:LEU:HD13	2.03	0.41
1:D:82:GLU:N	1:D:491:LEU:HD13	2.36	0.41
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.35	0.41
1:B:519:LEU:HB3	1:B:520:HIS:CE1	2.56	0.41
1:A:322:TYR:CD1	1:A:322:TYR:C	2.99	0.41
1:A:328:CYS:HA	1:A:338:ILE:O	2.21	0.41
1:D:515:ASP:HB3	1:D:526:TYR:CZ	2.55	0.41
1:C:491:LEU:N	1:C:491:LEU:HD22	2.36	0.41
1:D:184:ARG:HD2	1:D:187:TRP:CD2	2.55	0.41
1:A:157:TRP:CZ3	1:A:164:LEU:HG	2.56	0.41
1:A:527:GLN:HB3	1:A:555:VAL:HG13	2.02	0.41
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:LEU:HD12	1:B:436:LEU:HA	1.87	0.41
1:C:232:GLU:HB3	1:C:262:GLU:HG2	2.03	0.41
1:C:483:HIS:CA	1:C:491:LEU:HD23	2.50	0.41
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.90	0.41
1:D:105:TYR:HA	1:D:115:LEU:O	2.21	0.41
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.36	0.41
1:D:169:ASN:O	1:D:170:ASN:HB2	2.21	0.41
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.56	0.41
1:D:516:VAL:HG12	1:D:517:ILE:N	2.35	0.41
1:D:516:VAL:HG13	1:D:524:PHE:O	2.20	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.03	0.41
1:A:486:SER:OG	1:A:487:SER:N	2.54	0.41
1:A:616:MET:HB3	1:A:618:PHE:CE2	2.55	0.41
1:B:60:LEU:C	1:B:60:LEU:HD12	2.46	0.41
1:B:660:GLU:HG3	6:B:1520:HOH:O	2.21	0.41
1:C:134:ILE:HG21	1:C:178:PRO:HB3	2.03	0.41
1:B:507:VAL:HG22	1:B:508:GLN:N	2.36	0.40
1:B:610:THR:HA	1:B:613:PHE:CD2	2.56	0.40
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.55	0.40
1:B:418:ILE:HD11	6:B:1506:HOH:O	2.20	0.40
1:C:345:HIS:HD2	6:C:1610:HOH:O	2.05	0.40
1:B:504:LEU:HA	1:B:507:VAL:HG12	2.03	0.40
1:C:282:VAL:HG12	1:C:284:SER:OG	2.22	0.40
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.56	0.40
1:D:599:GLY:O	1:D:603:VAL:HG11	2.20	0.40
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.56	0.40
1:D:242:SER:HB3	1:D:246:LEU:HD12	2.02	0.40
1:B:405:ILE:HG13	1:B:429:ARG:HD3	2.04	0.40
1:C:41:ARG:NH1	1:C:507:VAL:HG12	2.36	0.40
1:C:76:ILE:HB	1:C:90:LEU:HD12	2.03	0.40
1:D:71:LYS:HA	1:D:75:ASN:O	2.21	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	726/728 (100%)	689 (95%)	34 (5%)	3 (0%)	30	19
1	B	726/728 (100%)	699 (96%)	25 (3%)	2 (0%)	36	25
1	C	726/728 (100%)	685 (94%)	35 (5%)	6 (1%)	16	6
1	D	726/728 (100%)	698 (96%)	28 (4%)	0	100	100
All	All	2904/2912 (100%)	2771 (95%)	122 (4%)	11 (0%)	30	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	B	491	LEU
1	C	103	ASN
1	C	104	ASP
1	C	535	ASP
1	C	536	LYS
1	A	491	LEU
1	B	40	ARG
1	A	97	GLU
1	C	74	ASN
1	C	99	GLY

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	652/652 (100%)	629 (96%)	23 (4%)	32	19
1	B	652/652 (100%)	627 (96%)	25 (4%)	29	17
1	C	652/652 (100%)	627 (96%)	25 (4%)	29	17
1	D	652/652 (100%)	622 (95%)	30 (5%)	24	12
All	All	2608/2608 (100%)	2505 (96%)	103 (4%)	28	16

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	74	ASN
1	A	90	LEU
1	A	119	ASN
1	A	142	LEU
1	A	180	LEU
1	A	219	ASN
1	A	246	LEU
1	A	294	LEU
1	A	367	ASP
1	A	399	LYS
1	A	415	LEU
1	A	471	ARG
1	A	491	LEU
1	A	492	ARG
1	A	520	HIS
1	A	536	LYS
1	A	542	LEU
1	A	543	LEU
1	A	561	LEU
1	A	701	LEU
1	A	718	GLN
1	A	761	GLN
1	B	86	SER
1	B	91	GLU
1	B	180	LEU
1	B	246	LEU
1	B	294	LEU
1	B	378	GLU
1	B	379	GLU
1	B	385	CYS
1	B	436	LEU
1	B	450	ASN
1	B	472	CYS
1	B	478	PRO
1	B	491	LEU
1	B	506	ASP
1	B	520	HIS
1	B	535	ASP
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU

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Mol	Chain	Res	Type
1	B	561	LEU
1	B	701	LEU
1	B	702	LEU
1	B	718	GLN
1	B	732	THR
1	B	761	GLN
1	C	41	ARG
1	C	75	ASN
1	C	90	LEU
1	C	147	ARG
1	C	246	LEU
1	C	277	SER
1	C	294	LEU
1	C	385	CYS
1	C	399	LYS
1	C	442	VAL
1	C	448	GLU
1	C	482	LEU
1	C	503	MET
1	C	507	VAL
1	C	520	HIS
1	C	535	ASP
1	C	536	LYS
1	C	542	LEU
1	C	561	LEU
1	C	679	ASN
1	C	701	LEU
1	C	732	THR
1	C	746	MET
1	C	759	LEU
1	C	761	GLN
1	D	71	LYS
1	D	91	GLU
1	D	103	ASN
1	D	107	VAL
1	D	111	ARG
1	D	142	LEU
1	D	145	GLU
1	D	246	LEU
1	D	253	ARG
1	D	276	LEU
1	D	294	LEU

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Mol	Chain	Res	Type
1	D	358	ARG
1	D	399	LYS
1	D	412	SER
1	D	436	LEU
1	D	448	GLU
1	D	482	LEU
1	D	507	VAL
1	D	535	ASP
1	D	536	LYS
1	D	561	LEU
1	D	581	ARG
1	D	603	VAL
1	D	608	GLU
1	D	673	LEU
1	D	701	LEU
1	D	702	LEU
1	D	718	GLN
1	D	759	LEU
1	D	760	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	75	ASN
1	A	141	GLN
1	A	150	ASN
1	A	170	ASN
1	A	176	ASN
1	A	179	ASN
1	A	183	GLN
1	A	192	ASN
1	A	247	GLN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	430	ASN
1	A	435	GLN
1	A	463	ASN
1	A	483	HIS
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	595	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	B	61	GLN
1	B	72	GLN
1	B	75	ASN
1	B	103	ASN
1	B	138	ASN
1	B	169	ASN
1	B	170	ASN
1	B	176	ASN
1	B	183	GLN
1	B	192	ASN
1	B	345	HIS
1	B	369	ASN
1	B	393	ASN
1	B	422	HIS
1	B	435	GLN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	533	HIS
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	757	HIS
1	B	761	GLN
1	C	72	GLN
1	C	123	GLN
1	C	141	GLN
1	C	169	ASN
1	C	170	ASN
1	C	176	ASN
1	C	183	GLN
1	C	192	ASN

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Mol	Chain	Res	Type
1	C	247	GLN
1	C	345	HIS
1	C	369	ASN
1	C	393	ASN
1	C	422	HIS
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN
1	C	586	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN
1	C	757	HIS
1	C	761	GLN
1	D	72	GLN
1	D	75	ASN
1	D	103	ASN
1	D	112	GLN
1	D	123	GLN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	247	GLN
1	D	345	HIS
1	D	369	ASN
1	D	383	HIS
1	D	393	ASN
1	D	422	HIS
1	D	463	ASN
1	D	483	HIS
1	D	505	GLN
1	D	586	GLN
1	D	612	GLN
1	D	679	ASN

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Mol	Chain	Res	Type
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	745	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.76	0	17,19,21	0.61	0
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.71	0	17,19,21	0.69	0
2	NAG	F	2	2	14,14,15	0.53	0	17,19,21	0.72	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.52	0	17,19,21	0.72	0
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	0.67	0
3	BMA	G	3	3	11,11,12	0.46	0	15,15,17	0.63	0
2	NAG	H	1	1,2	14,14,15	0.48	0	17,19,21	0.71	0
2	NAG	H	2	2	14,14,15	0.52	0	17,19,21	0.81	0
2	NAG	I	1	1,2	14,14,15	0.73	0	17,19,21	0.76	0
2	NAG	I	2	2	14,14,15	0.62	0	17,19,21	0.79	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.62	0	17,19,21	0.82	1 (5%)
3	NAG	J	2	3	14,14,15	0.44	0	17,19,21	0.71	0
3	BMA	J	3	3	11,11,12	0.63	0	15,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	1	1,2	14,14,15	0.66	0	17,19,21	0.55	0
2	NAG	K	2	2	14,14,15	0.49	0	17,19,21	0.66	0
2	NAG	L	1	1,2	14,14,15	0.73	0	17,19,21	0.81	0
2	NAG	L	2	2	14,14,15	0.63	0	17,19,21	0.72	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.72	0	17,19,21	0.62	0
2	NAG	M	2	2	14,14,15	0.57	0	17,19,21	1.08	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	NAG	C1-C2-N2	2.68	114.66	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C2-N2-C7	-2.47	119.59	122.90
2	F	2	NAG	C2-N2-C7	-2.21	119.94	122.90
3	J	1	NAG	C2-N2-C7	-2.20	119.95	122.90
2	E	2	NAG	C2-N2-C7	-2.18	119.98	122.90
2	M	2	NAG	O5-C1-C2	-2.15	107.97	111.29
2	L	2	NAG	C2-N2-C7	-2.13	120.04	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

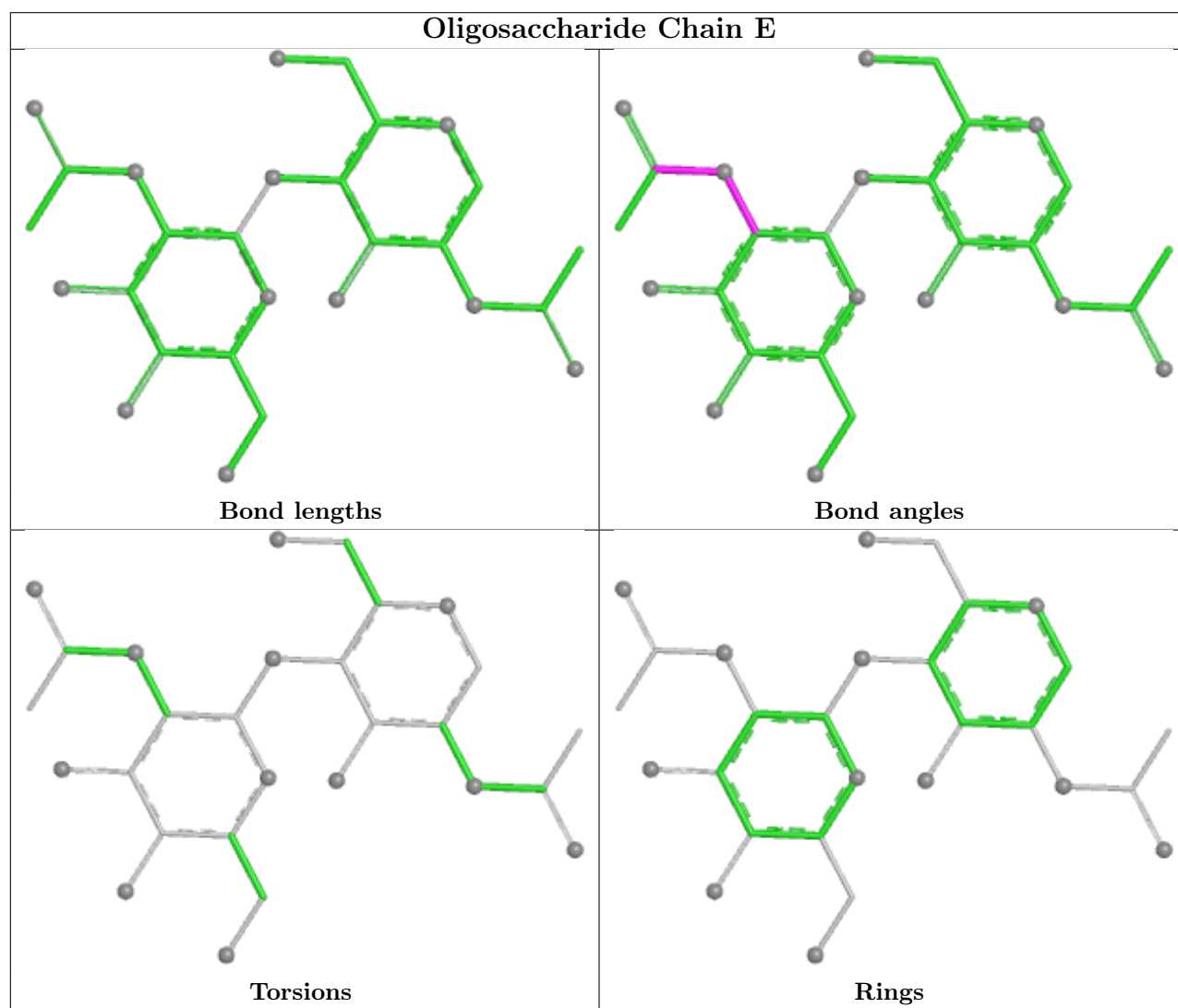
Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
2	K	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C8-C7-N2-C2
3	G	3	BMA	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
2	L	2	NAG	C8-C7-N2-C2
2	L	1	NAG	C4-C5-C6-O6
2	L	2	NAG	O7-C7-N2-C2

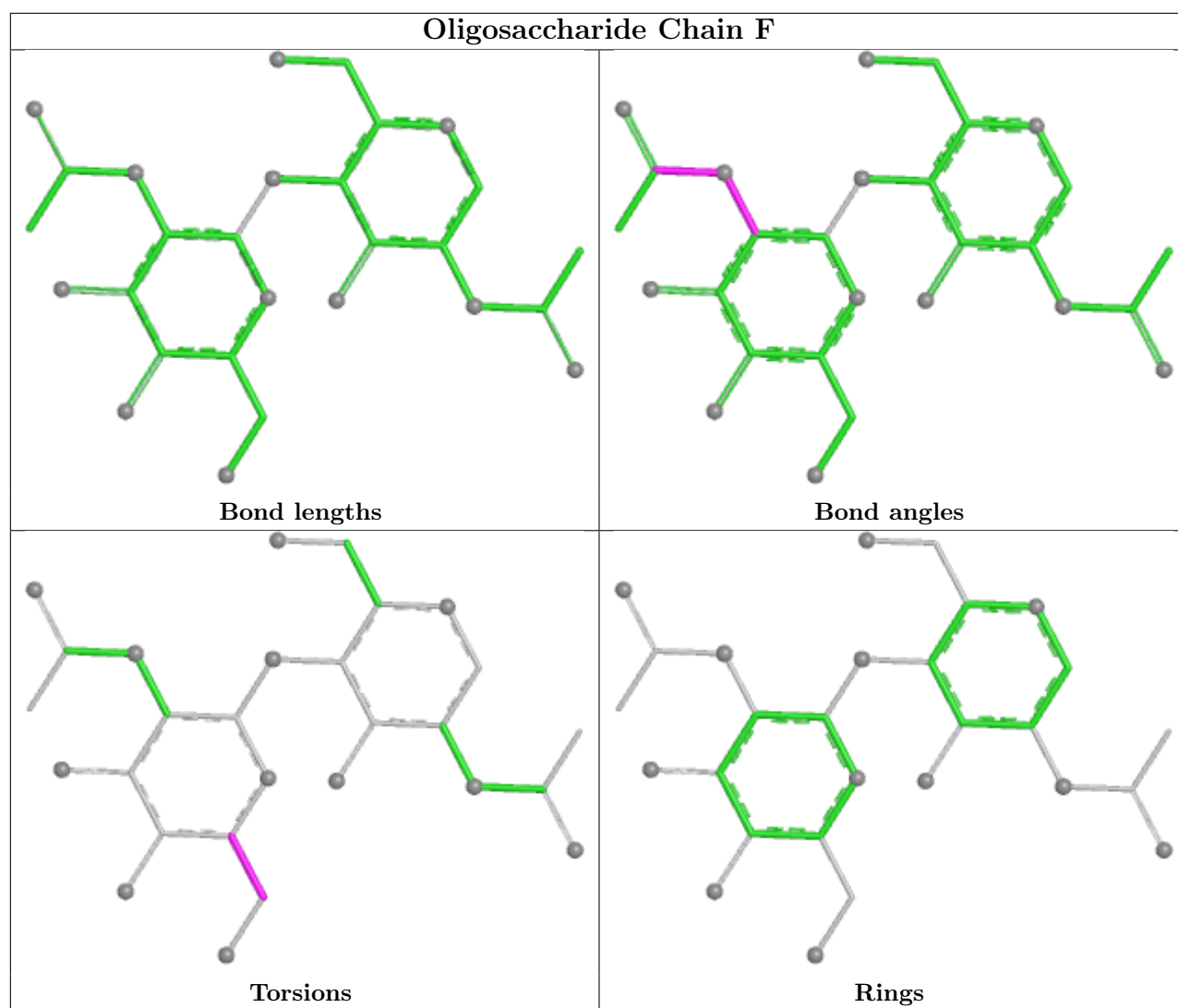
There are no ring outliers.

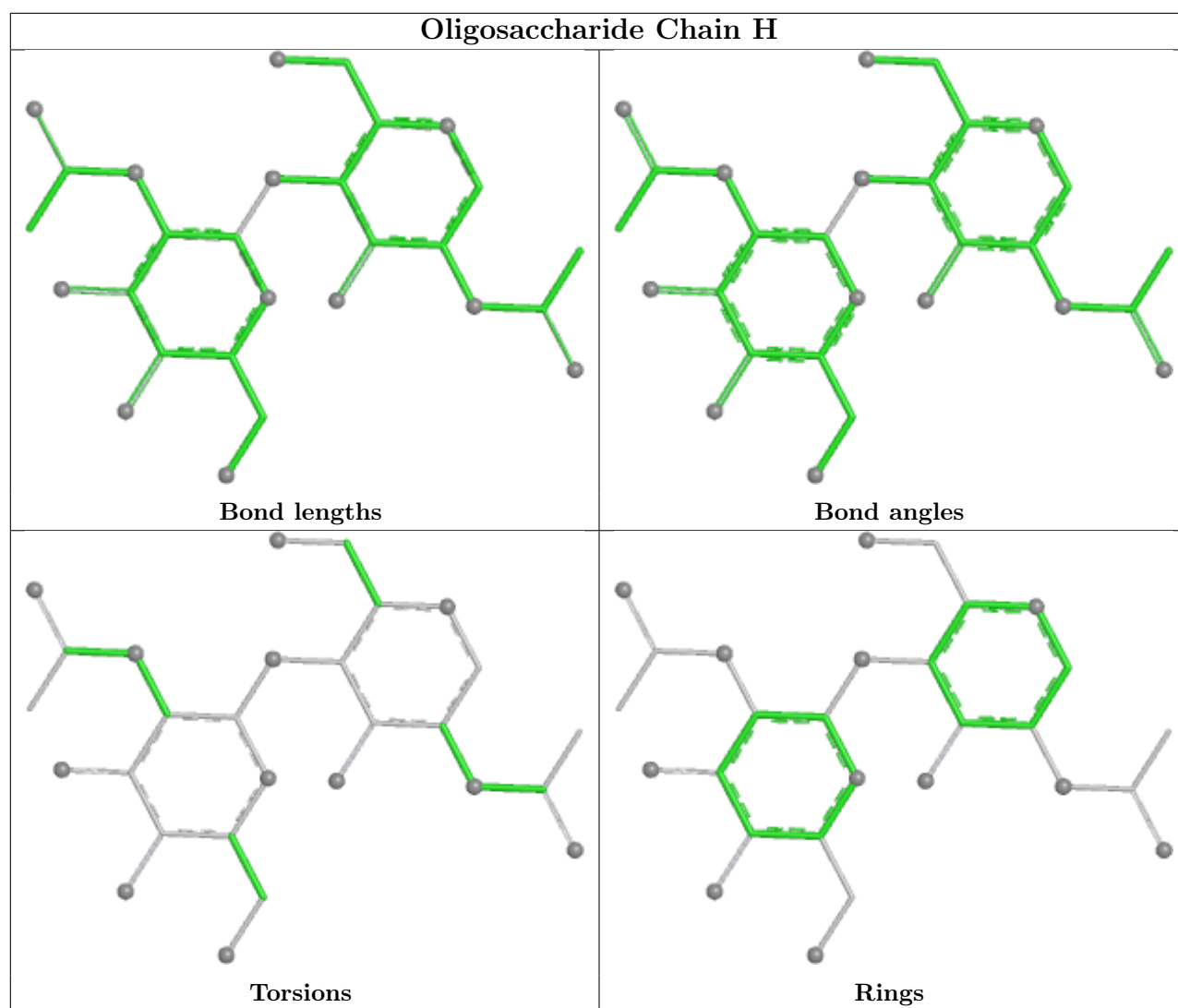
4 monomers are involved in 3 short contacts:

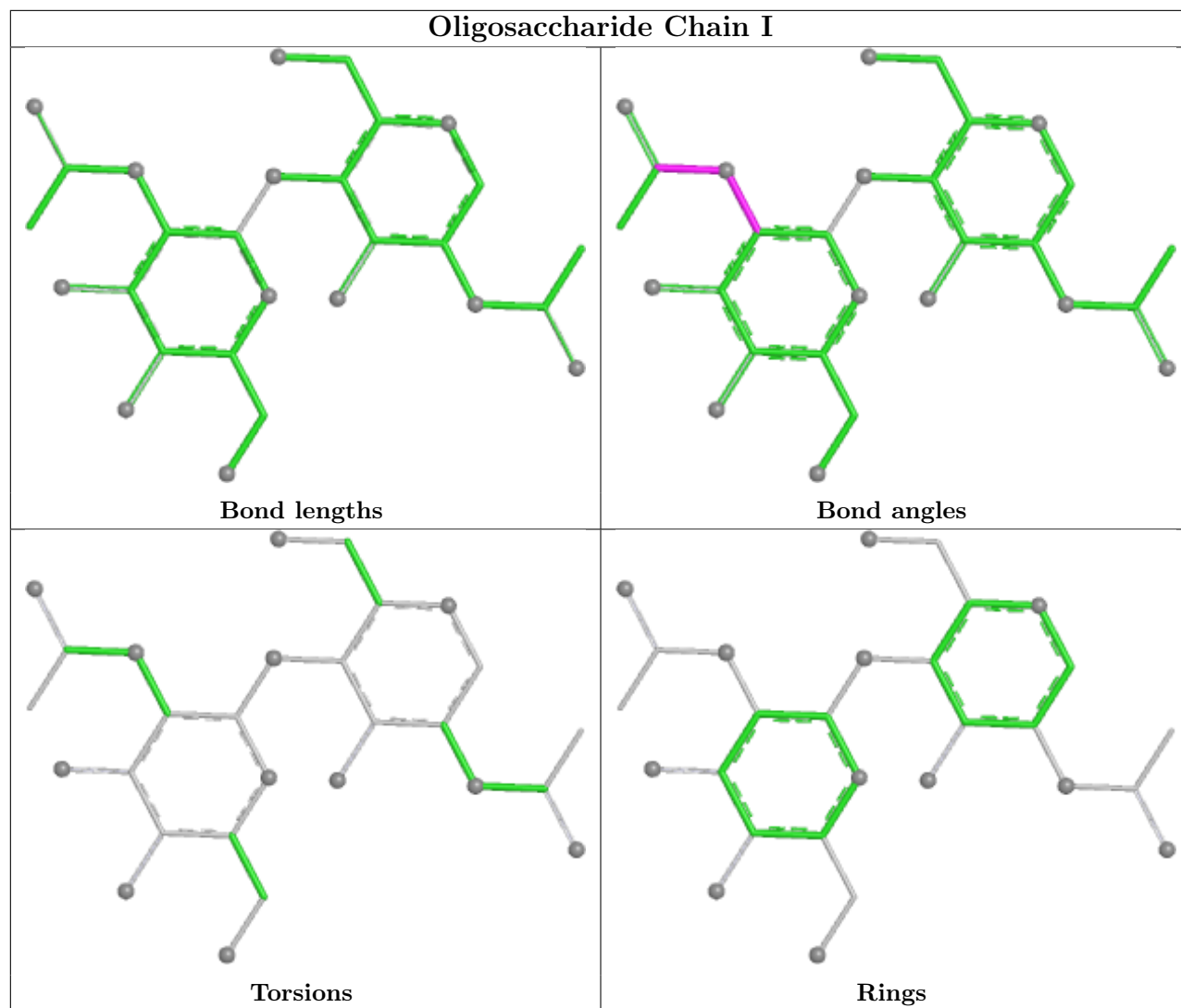
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
3	J	1	NAG	1	0
3	J	2	NAG	1	0
3	G	1	NAG	1	0

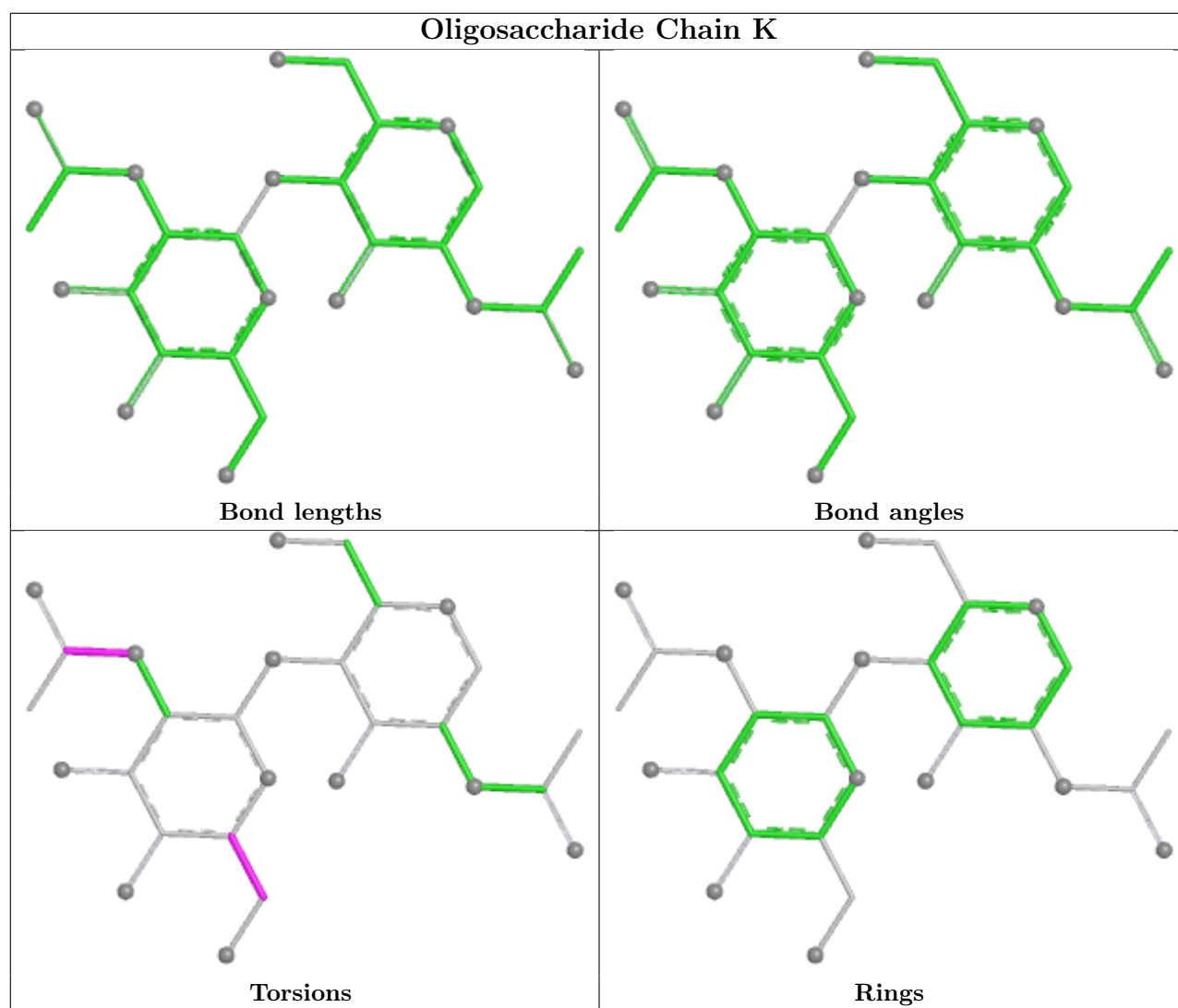
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

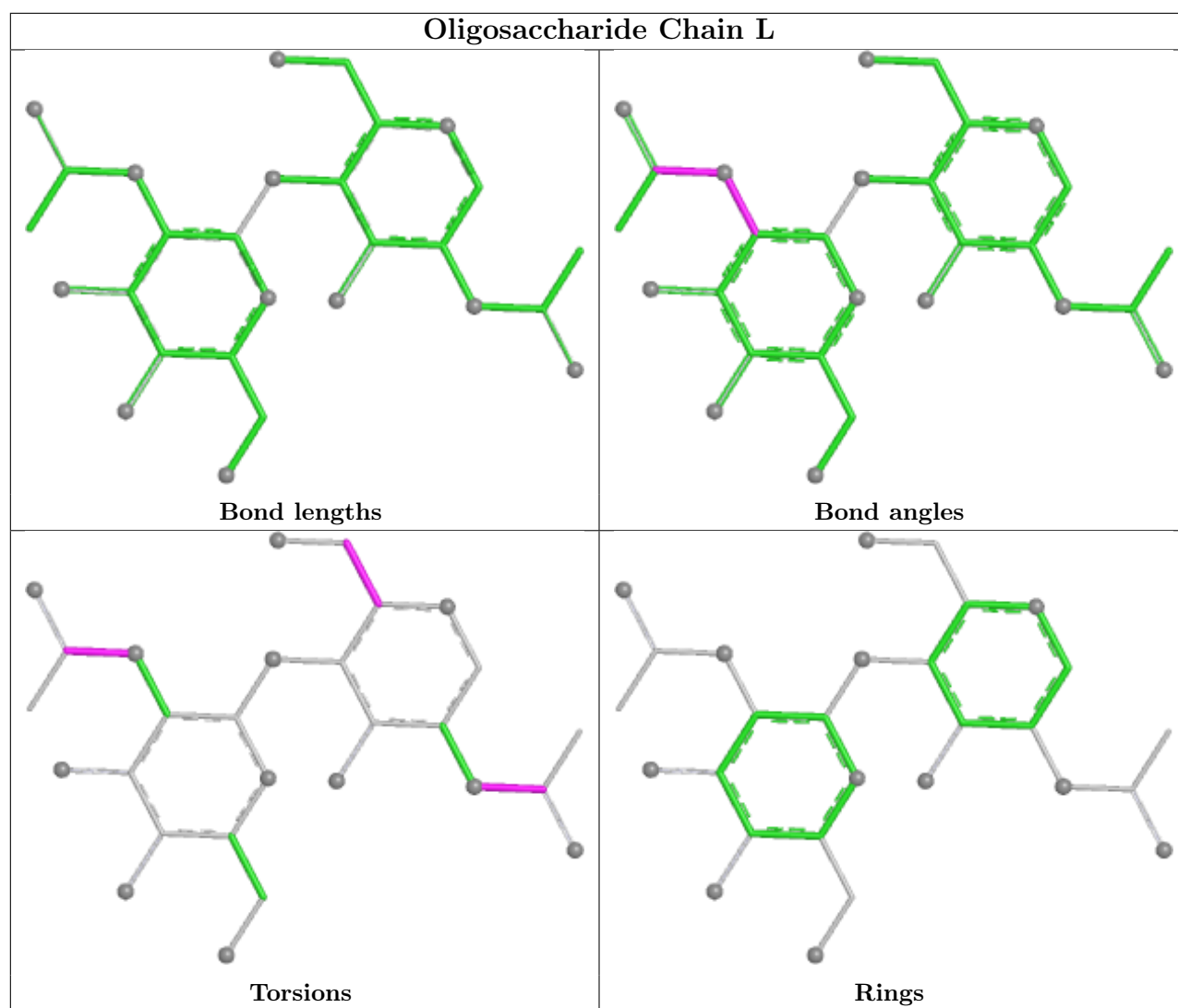


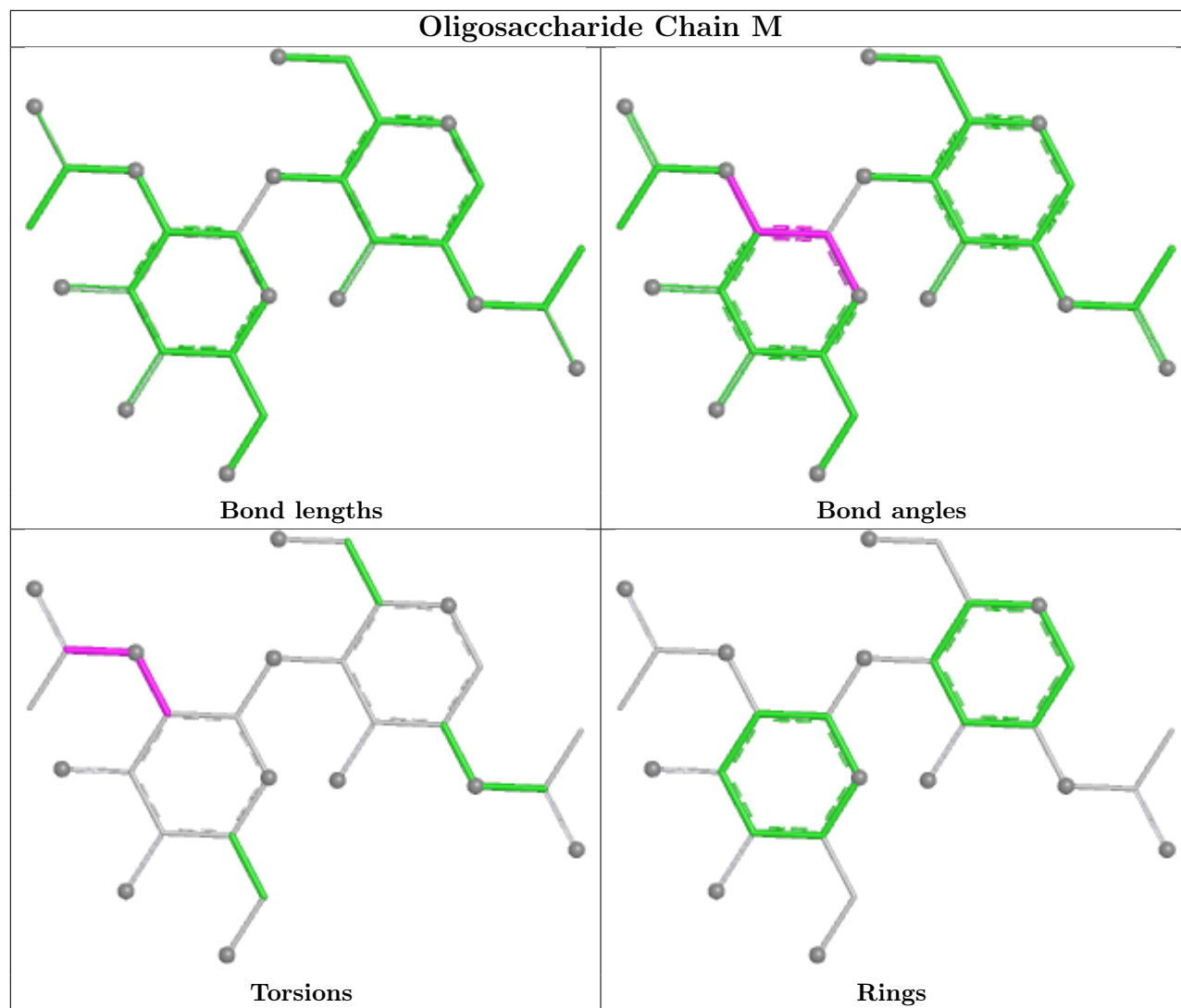


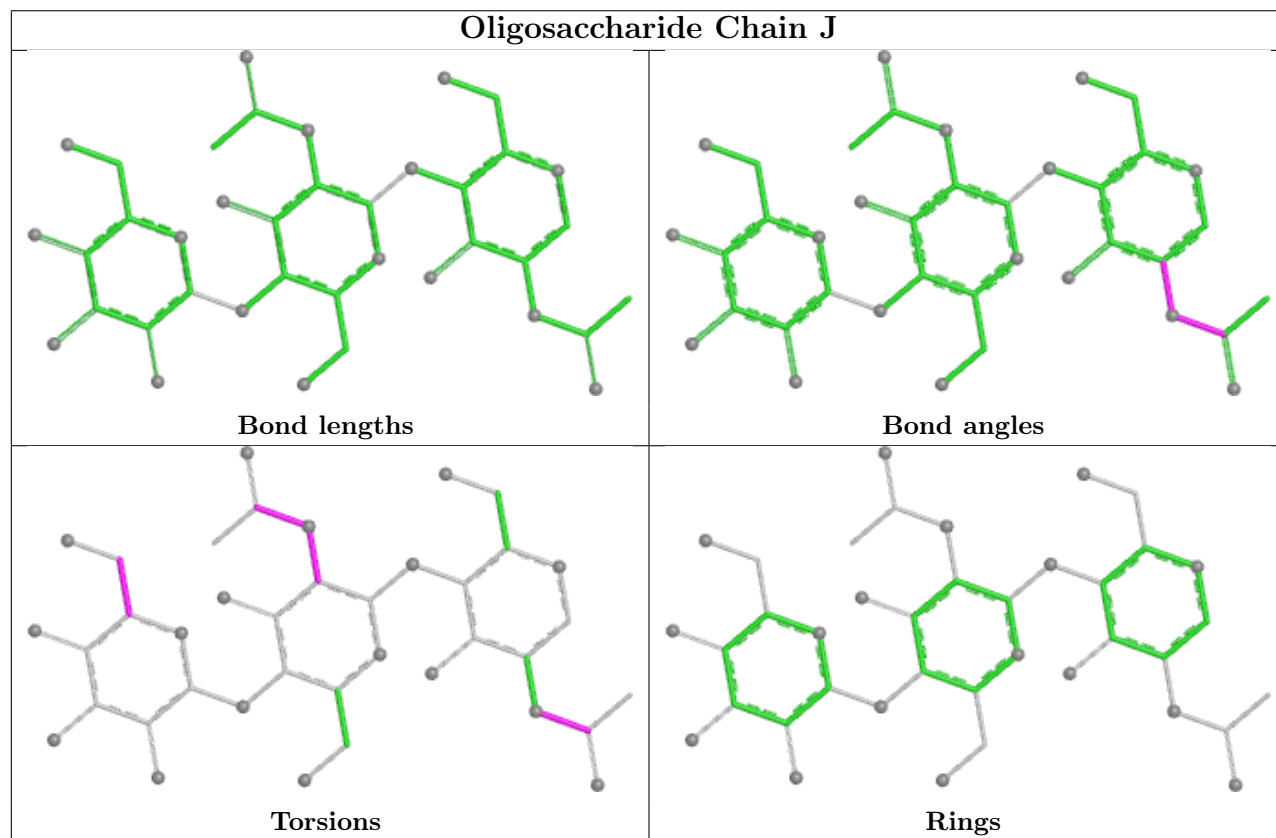
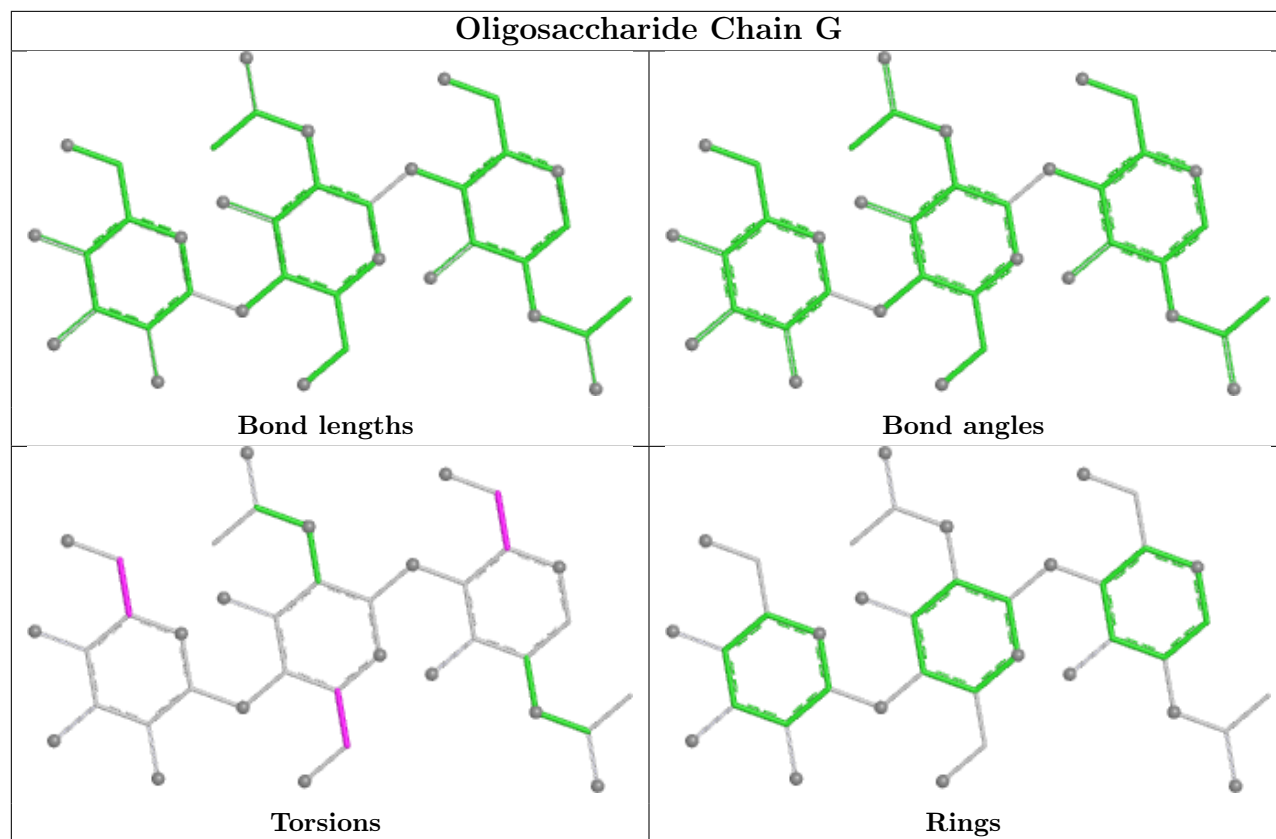












5.6 Ligand geometry

19 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
4	NAG	C	770(A)	1	14,14,15	0.62	0	17,19,21	0.64	0
5	SO4	A	1500	-	4,4,4	0.58	0	6,6,6	0.65	0
5	SO4	D	1503	-	4,4,4	0.39	0	6,6,6	0.68	0
4	NAG	A	767(A)	1	14,14,15	0.66	0	17,19,21	0.65	0
4	NAG	C	769(A)	1	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
4	NAG	B	771(A)	1	14,14,15	0.70	0	17,19,21	0.60	0
4	NAG	B	773(A)	1	14,14,15	0.56	0	17,19,21	0.79	1 (5%)
4	NAG	B	772(A)	1	14,14,15	0.63	0	17,19,21	0.86	0
4	NAG	D	767(A)	1	14,14,15	0.63	0	17,19,21	0.83	1 (5%)
4	NAG	A	772(A)	1	14,14,15	0.58	0	17,19,21	0.79	0
4	NAG	A	771(A)	1	14,14,15	0.49	0	17,19,21	0.75	1 (5%)
5	SO4	C	1502	-	4,4,4	0.49	0	6,6,6	0.53	0
4	NAG	C	767(A)	1	14,14,15	0.46	0	17,19,21	0.72	1 (5%)
4	NAG	D	773(A)	1	14,14,15	0.64	0	17,19,21	0.69	0
5	SO4	B	1501	-	4,4,4	0.36	0	6,6,6	0.58	0
4	NAG	A	768(A)	1	14,14,15	0.58	0	17,19,21	0.73	0
4	NAG	B	767(A)	1	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
4	NAG	C	768(A)	1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
4	NAG	C	771(A)	1	14,14,15	0.51	0	17,19,21	0.91	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	A	768(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	767(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	D	767(A)	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	B	773(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	768(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	772(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	771(A)	1	-	3/6/23/26	0/1/1/1
4	NAG	C	770(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	767(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	D	773(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	C	771(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	B	772(A)	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	773(A)	NAG	C2-N2-C7	-2.59	119.43	122.90
4	D	767(A)	NAG	C2-N2-C7	-2.41	119.67	122.90
4	C	769(A)	NAG	C2-N2-C7	-2.27	119.86	122.90
4	A	771(A)	NAG	C2-N2-C7	-2.22	119.93	122.90
4	B	767(A)	NAG	C2-N2-C7	-2.22	119.93	122.90
4	C	768(A)	NAG	C2-N2-C7	-2.14	120.04	122.90
4	C	767(A)	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	768(A)	NAG	C8-C7-N2-C2
4	A	768(A)	NAG	O7-C7-N2-C2
4	A	771(A)	NAG	C8-C7-N2-C2
4	A	771(A)	NAG	O7-C7-N2-C2
4	C	768(A)	NAG	C8-C7-N2-C2
4	C	768(A)	NAG	O7-C7-N2-C2
4	C	771(A)	NAG	C8-C7-N2-C2
4	C	771(A)	NAG	O7-C7-N2-C2
4	D	773(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O7-C7-N2-C2
4	D	773(A)	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	772(A)	NAG	C8-C7-N2-C2
4	B	772(A)	NAG	O7-C7-N2-C2
4	C	770(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	C4-C5-C6-O6
4	C	770(A)	NAG	O7-C7-N2-C2
4	A	772(A)	NAG	C4-C5-C6-O6
4	B	773(A)	NAG	C4-C5-C6-O6
4	B	773(A)	NAG	O5-C5-C6-O6
4	A	772(A)	NAG	O5-C5-C6-O6
4	A	771(A)	NAG	O5-C5-C6-O6
4	D	767(A)	NAG	C8-C7-N2-C2
4	D	767(A)	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	767(A)	NAG	2	0
4	B	773(A)	NAG	1	0
4	D	767(A)	NAG	1	0
4	B	767(A)	NAG	1	0
4	C	768(A)	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	724/728 (99%)	0.45	62 (8%)	16	14	19, 33, 61, 90	13 (1%)
1	B	728/728 (100%)	0.21	27 (3%)	45	45	16, 30, 50, 71	12 (1%)
1	C	723/728 (99%)	0.31	43 (5%)	28	27	13, 31, 56, 97	12 (1%)
1	D	728/728 (100%)	0.55	54 (7%)	20	19	20, 36, 63, 87	10 (1%)
All	All	2903/2912 (99%)	0.38	186 (6%)	25	24	13, 32, 59, 97	47 (1%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	5.6
1	C	98	LEU	5.5
1	A	83	TYR	5.2
1	C	95	PHE	5.2
1	A	94	THR	5.1
1	C	104	ASP	5.0
1	C	535	ASP	4.9
1	B	83	TYR	4.7
1	A	101	SER	4.7
1	A	103	ASN	4.6
1	C	537	SER	4.6
1	D	98	LEU	4.4
1	C	90	LEU	4.3
1	D	83	TYR	4.3
1	A	491	LEU	4.2
1	D	143	ILE	4.1
1	A	93	SER	4.1
1	C	536	LYS	4.0
1	D	100	TYR	3.9
1	A	79	PHE	3.9
1	C	40	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	187	TRP	3.8
1	B	143	ILE	3.8
1	D	81	ALA	3.8
1	C	39	SER	3.7
1	B	506	ASP	3.7
1	D	377	ASN	3.7
1	D	99	GLY	3.6
1	A	89	PHE	3.6
1	C	295	ILE	3.6
1	B	39	SER	3.6
1	A	90	LEU	3.6
1	C	74	ASN	3.6
1	D	521	GLY	3.5
1	D	516	VAL	3.5
1	A	505	GLN	3.5
1	D	295	ILE	3.5
1	B	491	LEU	3.5
1	A	71	LYS	3.5
1	D	82	GLU	3.4
1	A	138	ASN	3.4
1	C	138	ASN	3.4
1	A	95	PHE	3.4
1	A	377	ASN	3.4
1	A	39	SER	3.4
1	A	102	THR	3.4
1	B	537	SER	3.3
1	A	69	LEU	3.3
1	A	88	ILE	3.3
1	D	79	PHE	3.3
1	A	86	SER	3.3
1	A	506	ASP	3.2
1	C	97	GLU	3.2
1	C	120	TYR	3.2
1	D	93	SER	3.2
1	D	537	SER	3.2
1	A	766	PRO	3.1
1	D	142	LEU	3.1
1	D	538	LYS	3.1
1	C	538	LYS	3.1
1	A	521	GLY	3.1
1	D	95	PHE	3.0
1	B	84	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	85	ASN	3.0
1	A	96	ASP	2.9
1	B	99	GLY	2.9
1	C	73	GLU	2.9
1	B	54	ARG	2.9
1	C	93	SER	2.9
1	C	96	ASP	2.9
1	D	486	SER	2.9
1	D	439	TYR	2.9
1	C	142	LEU	2.9
1	D	90	LEU	2.9
1	C	608	GLU	2.8
1	C	179	ASN	2.8
1	A	507	VAL	2.8
1	A	72	GLN	2.8
1	B	82	GLU	2.8
1	A	761	GLN	2.8
1	B	41	ARG	2.8
1	A	74	ASN	2.7
1	C	141	GLN	2.7
1	A	84	GLY	2.7
1	D	101	SER	2.7
1	D	447	CYS	2.7
1	D	389	THR	2.7
1	D	766	PRO	2.7
1	B	766	PRO	2.7
1	C	745	ASN	2.7
1	B	533	HIS	2.6
1	A	70	TYR	2.6
1	C	135	TYR	2.6
1	C	151	ASN	2.6
1	A	57	PHE	2.6
1	B	57	PHE	2.6
1	D	57	PHE	2.6
1	D	436	LEU	2.6
1	C	94	THR	2.6
1	B	40	ARG	2.5
1	A	179	ASN	2.5
1	C	440	THR	2.5
1	A	180	LEU	2.5
1	C	180	LEU	2.5
1	A	40	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	140	ARG	2.5
1	D	517	ILE	2.5
1	B	516	VAL	2.5
1	A	75	ASN	2.4
1	C	143	ILE	2.4
1	D	535	ASP	2.4
1	A	151	ASN	2.4
1	B	142	LEU	2.4
1	A	150	ASN	2.3
1	A	489	LYS	2.3
1	A	493	VAL	2.3
1	B	507	VAL	2.3
1	A	104	ASP	2.3
1	C	91	GLU	2.3
1	D	379	GLU	2.3
1	A	486	SER	2.3
1	A	243	ASP	2.3
1	C	762	CYS	2.3
1	A	142	LEU	2.3
1	A	504	LEU	2.3
1	B	520	HIS	2.3
1	A	467	TYR	2.3
1	D	682	TYR	2.3
1	D	181	SER	2.3
1	D	442	VAL	2.3
1	D	518	ASN	2.3
1	A	63	ILE	2.2
1	A	745	ASN	2.2
1	D	54	ARG	2.2
1	D	440	THR	2.2
1	B	98	LEU	2.2
1	B	388	GLN	2.2
1	C	506	ASP	2.2
1	C	766	PRO	2.2
1	D	72	GLN	2.2
1	D	96	ASP	2.2
1	A	80	ASN	2.2
1	D	506	ASP	2.2
1	D	414	TYR	2.2
1	A	76	ILE	2.2
1	A	187	TRP	2.2
1	A	464	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	40	ARG	2.2
1	D	505	GLN	2.2
1	C	367	ASP	2.2
1	A	447	CYS	2.2
1	D	401	ALA	2.2
1	D	492	ARG	2.2
1	C	83	TYR	2.1
1	A	87	SER	2.1
1	A	490	GLU	2.1
1	C	518	ASN	2.1
1	A	141	GLN	2.1
1	B	439	TYR	2.1
1	A	488	ASP	2.1
1	D	39	SER	2.1
1	C	54	ARG	2.1
1	B	378	GLU	2.1
1	C	533	HIS	2.1
1	A	463	ASN	2.1
1	B	141	GLN	2.1
1	D	88	ILE	2.1
1	A	440	THR	2.1
1	C	520	HIS	2.1
1	B	103	ASN	2.1
1	D	437	ASN	2.1
1	B	697	GLN	2.1
1	D	482	LEU	2.1
1	C	88	ILE	2.0
1	C	89	PHE	2.0
1	D	89	PHE	2.0
1	D	348	ILE	2.0
1	C	617	GLY	2.0
1	D	84	GLY	2.0
1	A	121	VAL	2.0
1	B	294	LEU	2.0
1	D	519	LEU	2.0
1	A	140	ARG	2.0
1	A	339	SER	2.0
1	D	485	SER	2.0
1	D	144	THR	2.0

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

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

6.3 Carbohydrates ⓘ

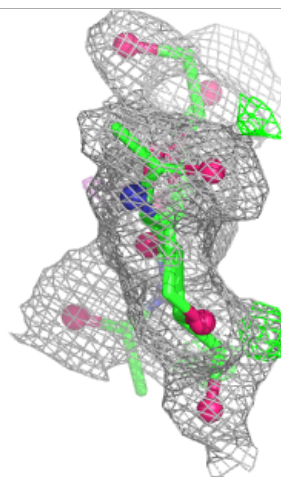
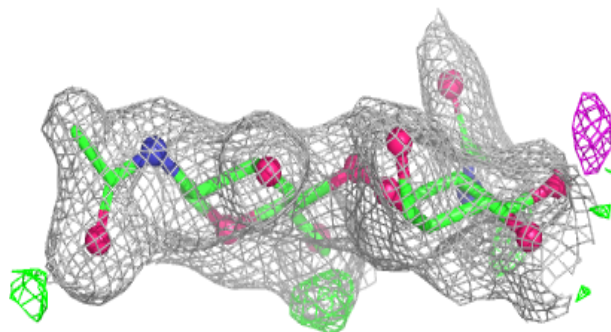
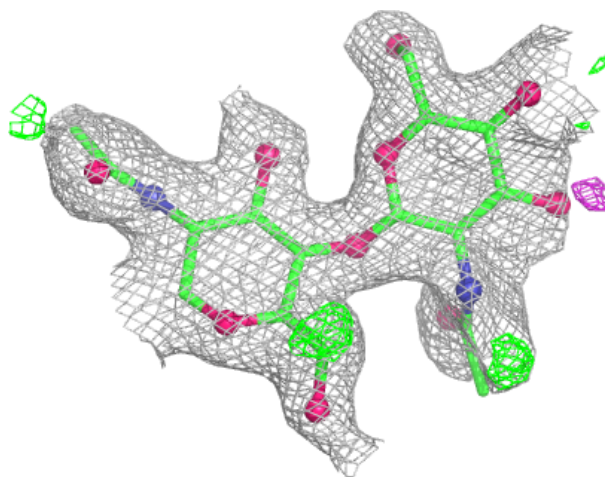
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	K	2	14/15	0.65	0.15	58,62,64,67	0
2	NAG	M	2	14/15	0.65	0.15	53,56,58,58	0
2	NAG	E	2	14/15	0.69	0.14	52,57,58,60	0
2	NAG	H	2	14/15	0.69	0.16	52,54,59,62	0
2	NAG	L	1	14/15	0.72	0.15	51,55,57,58	0
3	BMA	J	3	11/12	0.72	0.13	58,59,59,60	0
3	BMA	G	3	11/12	0.73	0.14	60,61,62,64	0
2	NAG	F	2	14/15	0.74	0.13	51,54,57,59	0
3	NAG	J	2	14/15	0.78	0.14	60,62,70,70	0
2	NAG	L	2	14/15	0.78	0.12	58,59,61,61	0
3	NAG	J	1	14/15	0.80	0.12	56,59,60,61	0
2	NAG	I	2	14/15	0.81	0.11	45,50,54,55	0
3	NAG	G	2	14/15	0.82	0.14	51,54,55,58	0
2	NAG	M	1	14/15	0.84	0.11	34,41,45,50	0
3	NAG	G	1	14/15	0.87	0.12	44,47,49,52	0
2	NAG	H	1	14/15	0.88	0.09	27,36,41,44	0
2	NAG	F	1	14/15	0.89	0.09	31,38,44,46	0
2	NAG	E	1	14/15	0.90	0.08	31,36,43,44	0
2	NAG	K	1	14/15	0.91	0.09	35,40,44,50	0
2	NAG	I	1	14/15	0.92	0.07	30,35,41,42	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.

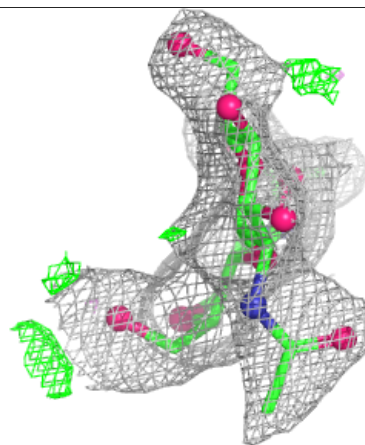
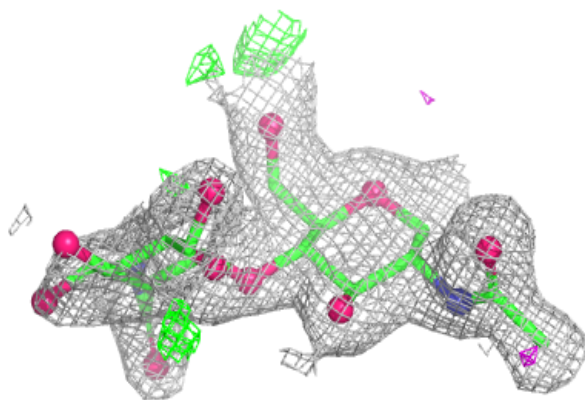
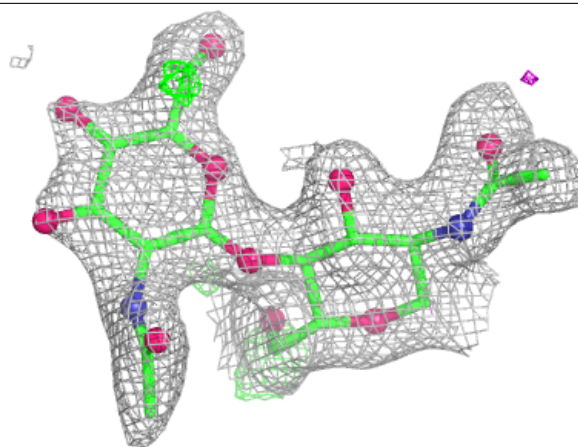
Electron density around Chain E:

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



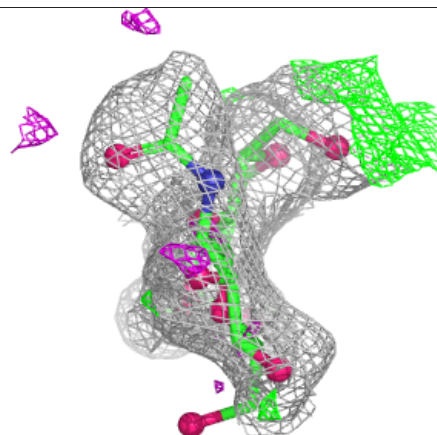
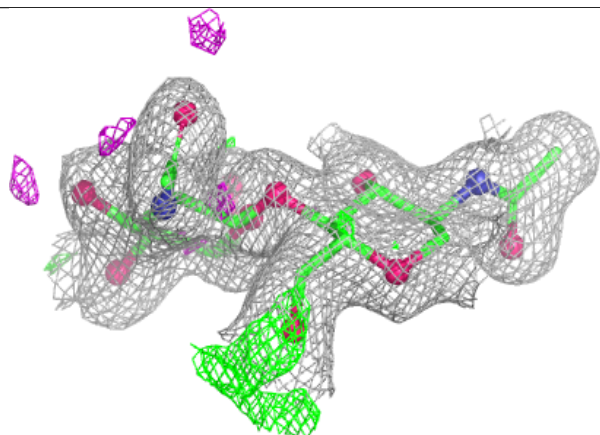
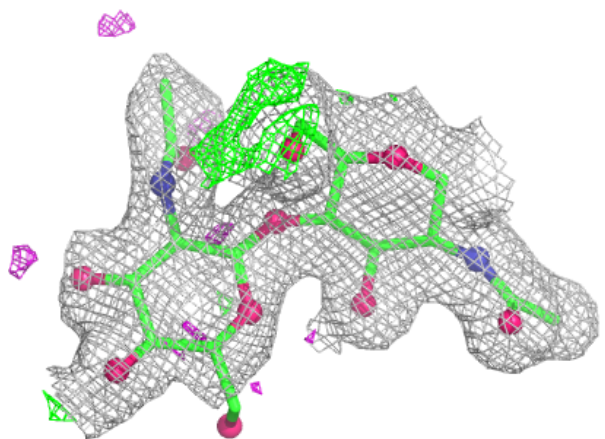
Electron density around Chain F:

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



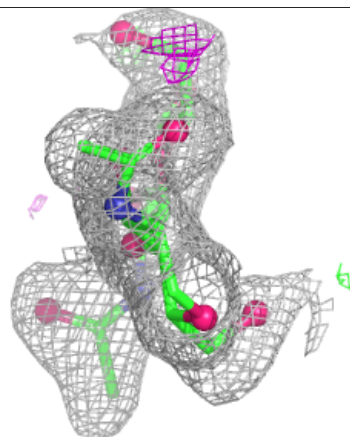
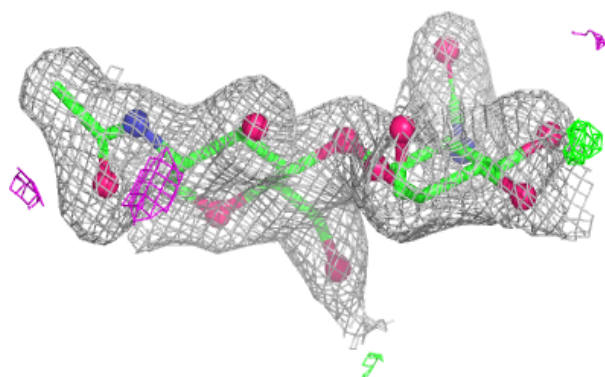
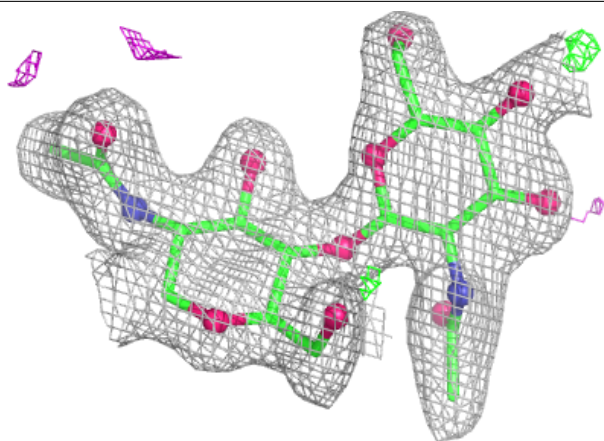
Electron density around Chain H:

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



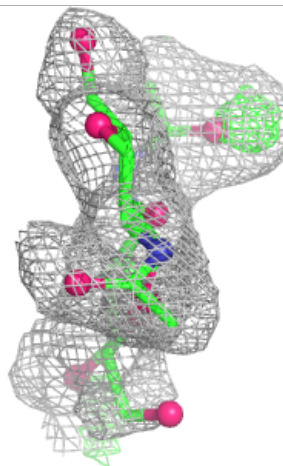
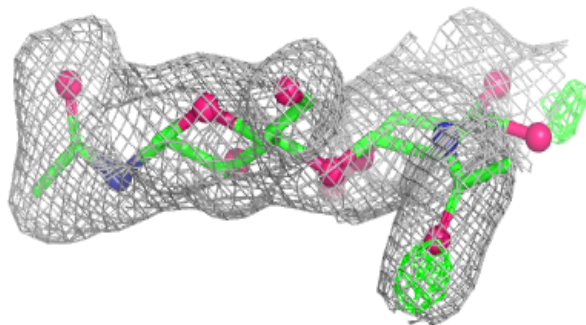
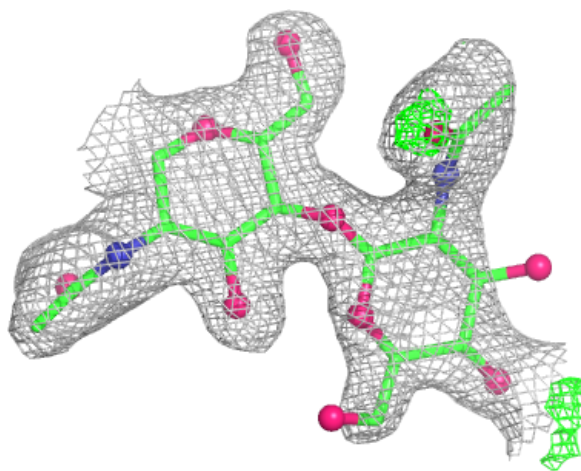
Electron density around Chain I:

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



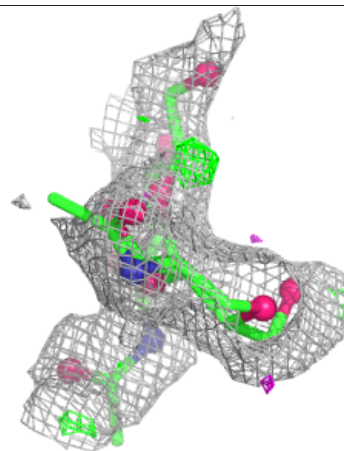
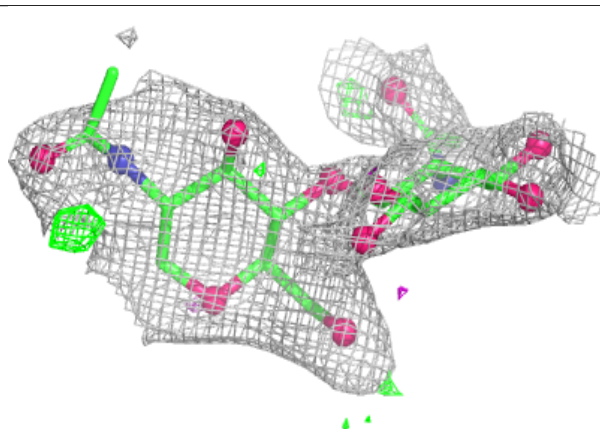
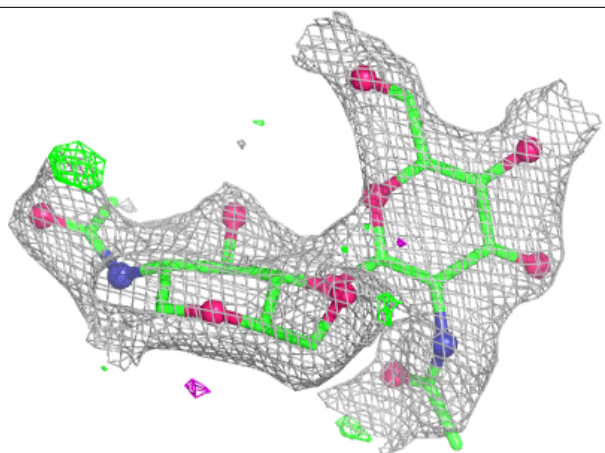
Electron density around Chain K:

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



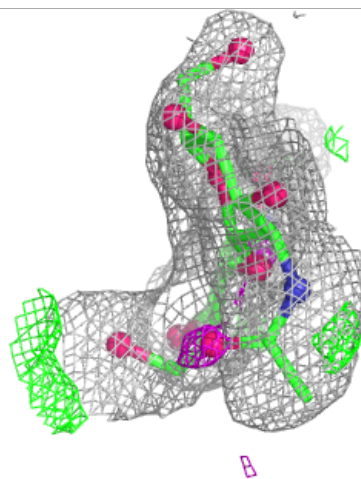
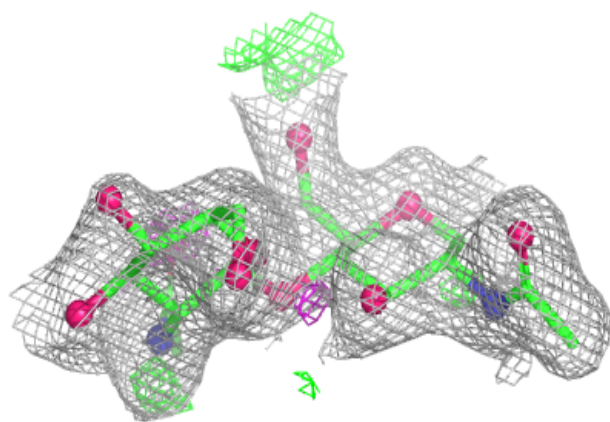
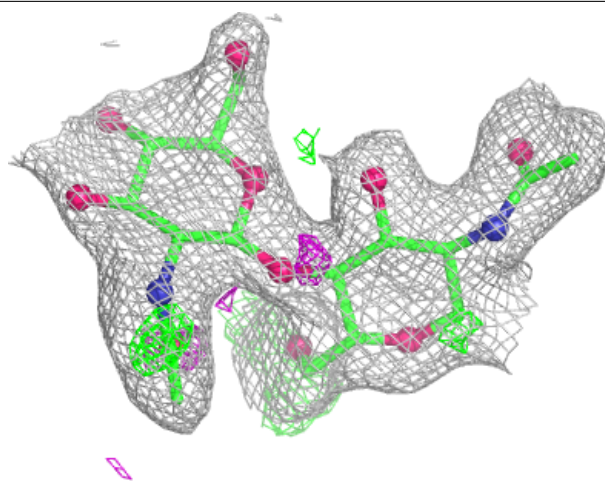
Electron density around Chain L:

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



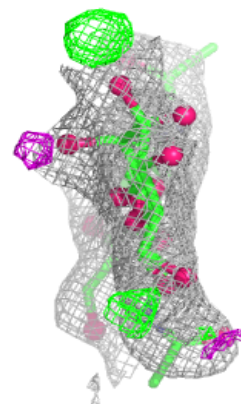
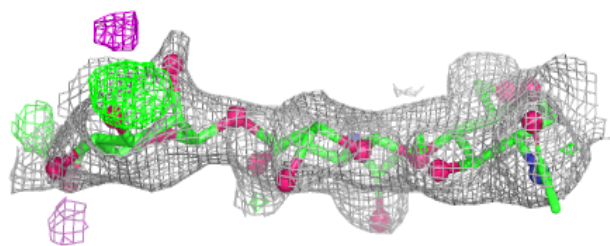
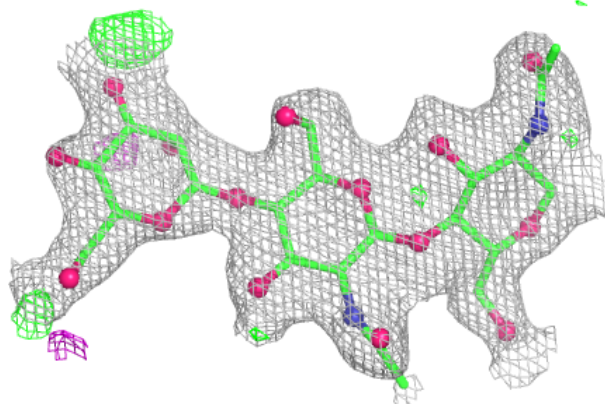
Electron density around Chain M:

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

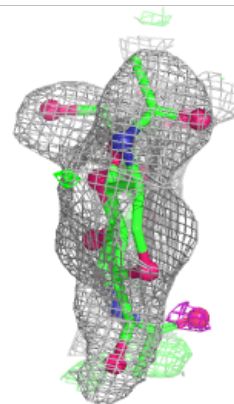
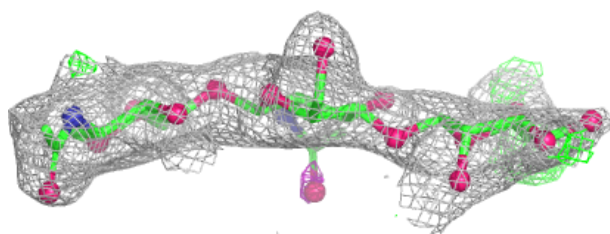
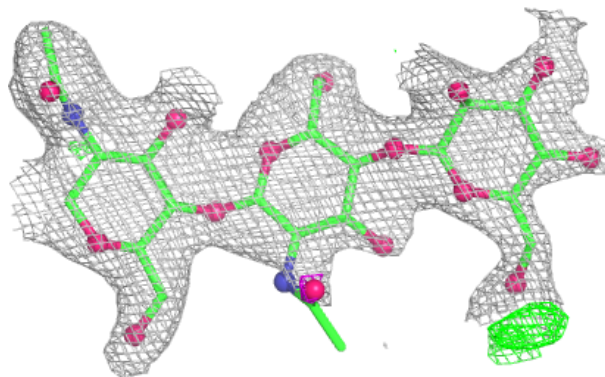


Electron density around Chain G:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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
4	NAG	D	767(A)	14/15	0.24	0.19	62,64,65,65	0
4	NAG	A	767(A)	14/15	0.43	0.16	70,73,73,74	0
4	NAG	D	773(A)	14/15	0.59	0.18	59,63,66,66	0
4	NAG	A	771(A)	14/15	0.63	0.17	50,53,55,56	3
4	NAG	C	771(A)	14/15	0.64	0.15	47,52,56,56	0
4	NAG	C	768(A)	14/15	0.66	0.18	82,84,87,87	0
4	NAG	C	767(A)	14/15	0.70	0.14	60,62,64,66	0
4	NAG	B	772(A)	14/15	0.75	0.13	45,47,50,51	0
4	NAG	A	768(A)	14/15	0.75	0.16	78,78,79,79	0
4	NAG	B	767(A)	14/15	0.76	0.15	65,66,69,70	0
4	NAG	C	770(A)	14/15	0.80	0.12	39,41,47,49	0
4	NAG	A	772(A)	14/15	0.81	0.12	44,48,54,54	0
4	NAG	B	773(A)	14/15	0.87	0.10	41,45,50,52	0
4	NAG	C	769(A)	14/15	0.88	0.10	31,36,40,43	0
4	NAG	B	771(A)	14/15	0.90	0.09	30,34,39,43	0
5	SO4	D	1503	5/5	0.93	0.10	38,40,41,42	0
5	SO4	B	1501	5/5	0.97	0.08	28,29,30,33	0
5	SO4	A	1500	5/5	0.97	0.08	33,34,35,37	0
5	SO4	C	1502	5/5	0.98	0.06	31,32,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.