



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:36 AM UTC

PDB ID : 1R9M / pdb_00001r9m
Title : Crystal Structure of Human Dipeptidyl Peptidase IV at 2.1 Ang. Resolution.
Authors : Aertgeerts, K.; Ye, S.; Tennant, M.G.; Collins, B.; Rogers, J.; Sang, B.C.;
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Deposited on : 2003-10-30
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

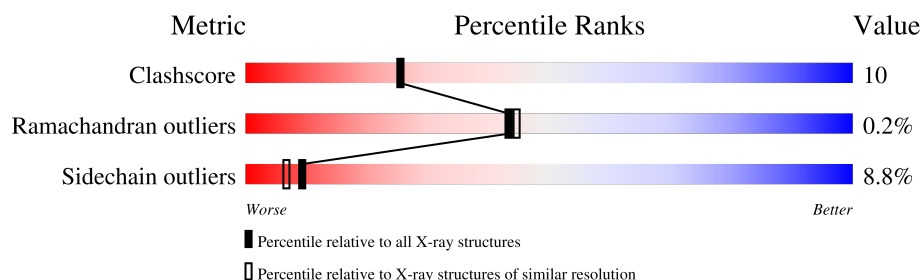
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	733	72% 23% . .
1	B	733	75% 22% .
1	C	733	74% 22% . .
1	D	733	77% 19% . .
2	E	2	100%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	 50% 50%
2	L	2	 50% 50%
3	F	3	 67% 33%
4	K	4	 75% 25%

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
2	NAG	I	2	X	-	-	-
4	MAN	K	4	X	-	-	-
5	NAG	A	6851	X	-	-	-
5	NAG	C	1501	X	-	-	-
5	NAG	D	2191	X	-	-	-
5	NAG	D	5201	X	-	-	-
5	NAG	D	6851	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26111 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	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 20 discrepancies between the modelled and reference sequences:

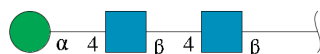
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- 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	G	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	J	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			

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



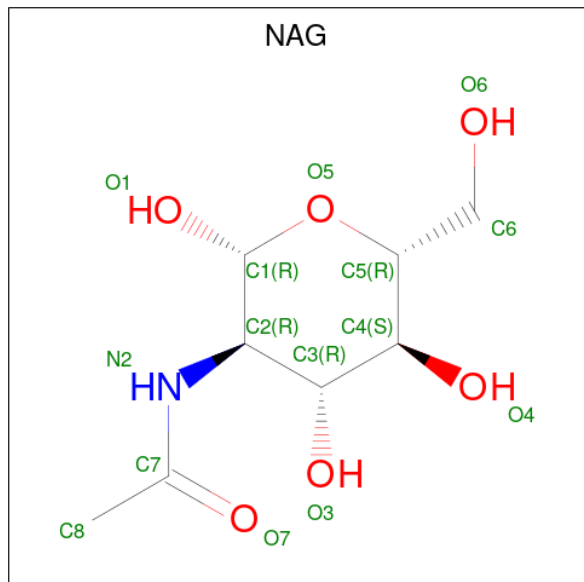
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-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
4	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



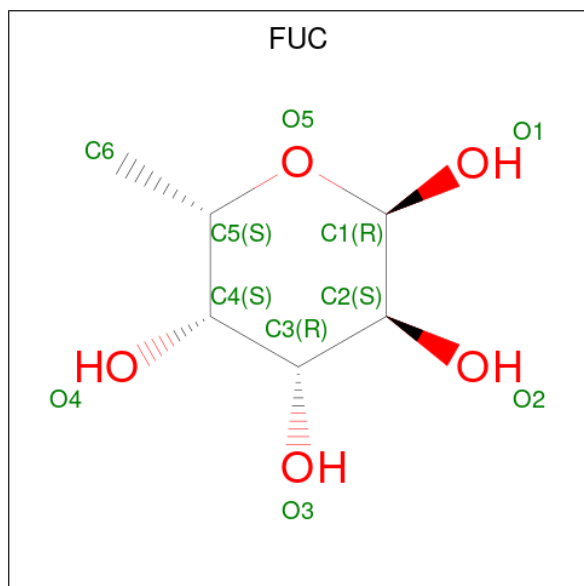
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

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

- Molecule 6 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

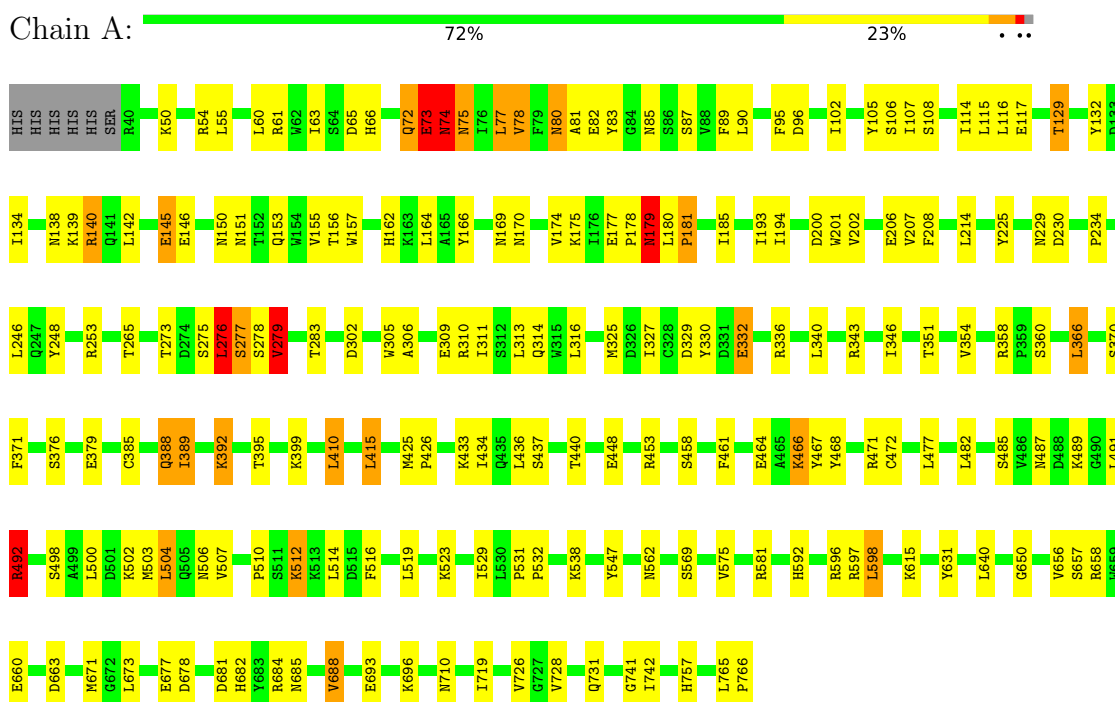
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	466	Total 466	O 466	0	0
7	B	467	Total 467	O 467	0	0
7	C	334	Total 334	O 334	0	0
7	D	411	Total 411	O 411	0	0

3 Residue-property plots [i](#)

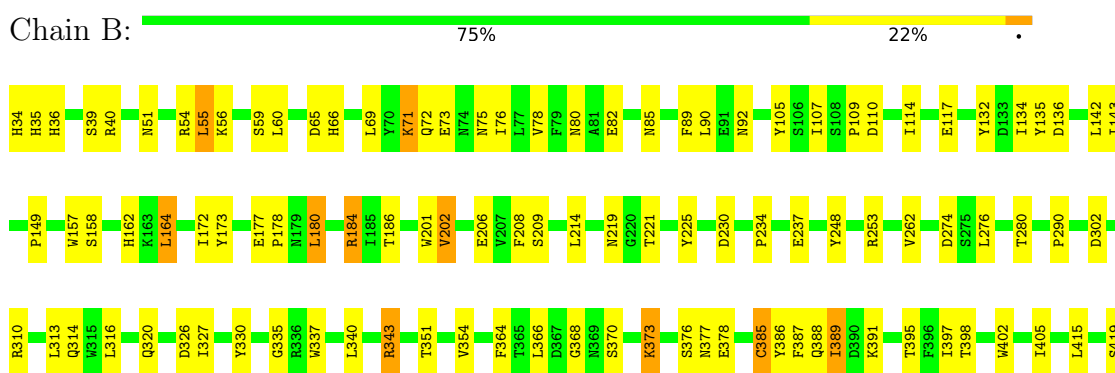
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

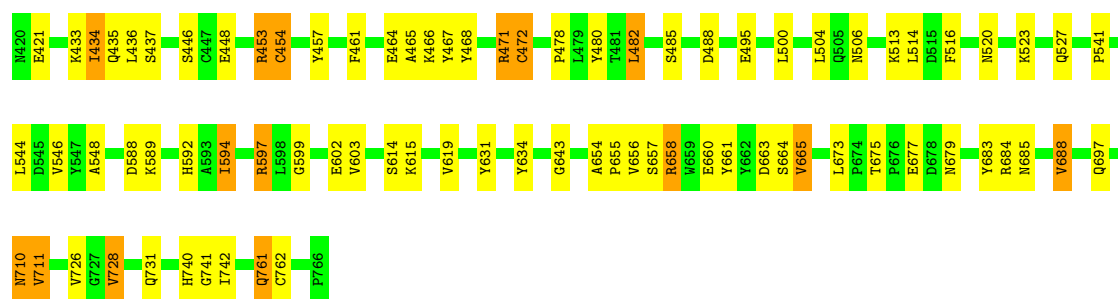
Note EDS was not executed.

• Molecule 1: Dipeptidyl peptidase IV



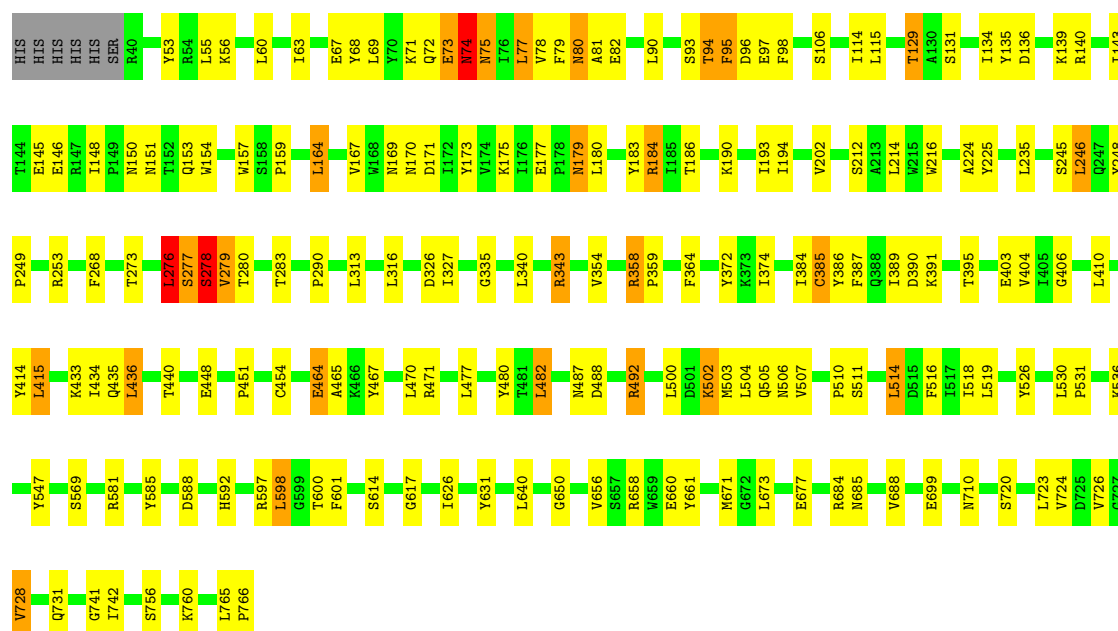
• Molecule 1: Dipeptidyl peptidase IV





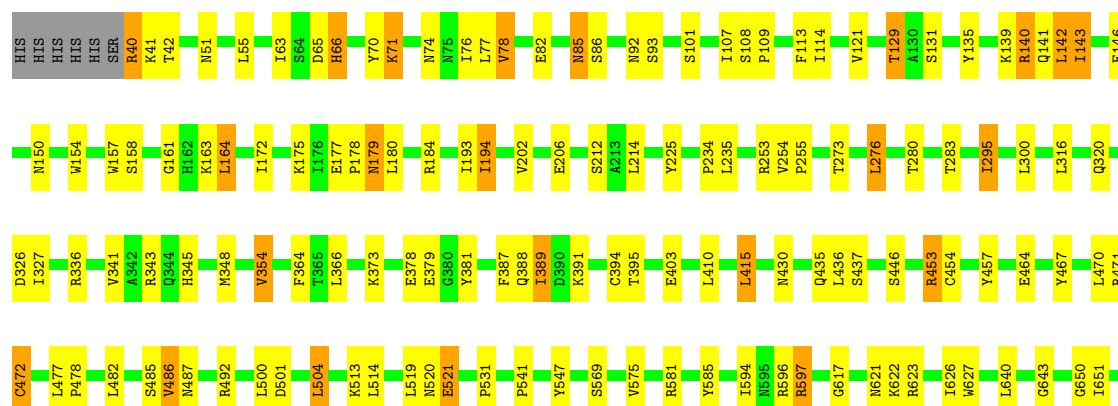
• Molecule 1: Dipeptidyl peptidase IV

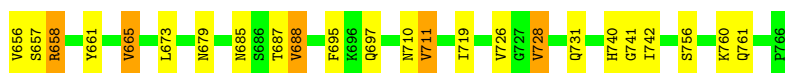
Chain C: 74% 22%



• Molecule 1: Dipeptidyl peptidase IV

Chain D: 77% 19%





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

Chain E:  100%



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

Chain G:  100%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain L:  50% 50%



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

Chain F:  67% 33%

MAG1
MAG2
MAN3

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

Chain K:  75% 25%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.82Å 124.06Å 144.49Å 90.00° 114.71° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.218 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26111	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	2/6123 (0.0%)	1.04	28/8329 (0.3%)
1	B	0.54	0/6190	0.95	10/8419 (0.1%)
1	C	0.52	1/6123 (0.0%)	1.03	25/8329 (0.3%)
1	D	0.53	0/6129	0.98	14/8336 (0.2%)
All	All	0.55	3/24565 (0.0%)	1.00	77/33413 (0.2%)

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	A	0	6
1	C	2	3
All	All	2	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	ARG	C-N	7.44	1.42	1.33
1	C	279	VAL	C-O	-5.49	1.18	1.24
1	A	73	GLU	C-N	5.01	1.40	1.33

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	VAL	CA-C-O	16.74	135.27	119.20
1	C	279	VAL	O-C-N	-15.87	106.68	122.23
1	A	279	VAL	O-C-N	-11.63	108.03	122.57
1	D	93	SER	N-CA-C	-9.14	99.45	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	THR	N-CA-C	-8.97	101.89	112.92
1	C	74	ASN	CA-CB-CG	8.87	121.47	112.60
1	C	75	ASN	CA-CB-CG	8.51	121.11	112.60
1	A	277	SER	CA-C-O	-8.36	111.88	121.58
1	A	276	LEU	O-C-N	-8.32	112.50	122.65
1	A	73	GLU	O-C-N	8.05	133.30	122.59
1	D	41	LYS	O-C-N	-7.94	113.21	122.89
1	A	140	ARG	CA-C-O	7.68	131.49	120.51
1	C	73	GLU	O-C-N	-7.61	112.47	122.59
1	C	74	ASN	O-C-N	-7.44	97.96	122.06
1	B	202	VAL	CB-CA-C	-7.32	102.12	112.22
1	B	335	GLY	N-CA-C	-7.01	104.95	115.32
1	A	74	ASN	CA-C-N	6.81	133.92	121.94
1	A	74	ASN	C-N-CA	6.81	133.92	121.94
1	A	275	SER	CA-C-N	-6.78	108.32	121.06
1	A	275	SER	C-N-CA	-6.78	108.32	121.06
1	A	277	SER	O-C-N	-6.72	113.74	122.94
1	C	390	ASP	N-CA-C	6.63	120.36	112.93
1	C	454	CYS	N-CA-C	6.61	119.78	108.02
1	C	335	GLY	N-CA-C	-6.60	106.13	115.30
1	C	74	ASN	CB-CA-C	6.57	123.25	110.57
1	D	139	LYS	CB-CA-C	-6.47	97.89	110.11
1	D	41	LYS	N-CA-C	6.28	119.58	110.28
1	A	276	LEU	N-CA-C	6.28	118.13	110.41
1	D	40	ARG	CA-C-N	6.22	129.70	120.87
1	D	40	ARG	C-N-CA	6.22	129.70	120.87
1	C	391	LYS	N-CA-C	6.20	118.49	109.07
1	A	74	ASN	CA-CB-CG	6.15	118.75	112.60
1	C	74	ASN	CA-C-O	6.03	139.45	118.58
1	B	454	CYS	N-CA-C	5.97	118.13	108.34
1	C	73	GLU	CB-CG-CD	5.94	122.70	112.60
1	B	541	PRO	N-CA-C	-5.94	101.94	111.38
1	A	74	ASN	N-CA-C	5.86	121.15	113.30
1	C	547	TYR	N-CA-C	-5.84	102.64	111.34
1	A	279	VAL	CA-CB-CG1	5.66	120.02	110.40
1	D	617	GLY	N-CA-C	5.64	120.39	113.79
1	A	150	ASN	N-CA-C	-5.63	102.95	110.55
1	B	391	LYS	N-CA-C	5.61	118.55	109.40
1	C	276	LEU	CA-C-N	-5.61	112.97	122.67
1	C	276	LEU	C-N-CA	-5.61	112.97	122.67
1	A	75	ASN	N-CA-CB	-5.60	100.99	111.13
1	C	656	VAL	N-CA-C	-5.59	101.61	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	LYS	N-CA-CB	5.58	118.17	109.97
1	C	617	GLY	N-CA-C	5.53	122.40	115.21
1	B	656	VAL	N-CA-C	-5.51	102.47	109.80
1	A	75	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	102	ILE	N-CA-C	5.47	116.11	108.89
1	C	63	ILE	N-CA-C	-5.45	107.48	113.43
1	D	140	ARG	CB-CA-C	5.45	121.26	110.42
1	D	656	VAL	N-CA-C	-5.44	101.81	109.21
1	C	277	SER	CA-C-O	-5.42	115.00	121.89
1	A	656	VAL	N-CA-C	-5.41	101.85	109.21
1	A	492	ARG	N-CA-C	5.33	116.55	108.07
1	A	547	TYR	N-CA-C	-5.33	103.40	111.34
1	C	507	VAL	N-CA-C	5.32	116.33	108.45
1	C	73	GLU	N-CA-CB	-5.31	101.52	110.49
1	A	75	ASN	O-C-N	-5.31	117.20	123.41
1	C	93	SER	N-CA-C	5.30	118.74	107.67
1	C	139	LYS	N-CA-C	-5.26	106.86	113.28
1	A	179	ASN	N-CA-C	5.24	119.77	113.17
1	B	548	ALA	N-CA-C	5.23	119.61	113.23
1	A	388	GLN	N-CA-C	-5.22	100.66	109.07
1	D	300	LEU	N-CA-C	-5.21	100.74	109.24
1	A	139	LYS	CA-C-N	5.17	131.42	121.54
1	A	139	LYS	C-N-CA	5.17	131.42	121.54
1	D	547	TYR	N-CA-C	-5.15	103.67	111.34
1	B	201	TRP	N-CA-C	5.12	117.26	111.11
1	D	41	LYS	CB-CA-C	5.08	118.34	109.65
1	A	202	VAL	N-CA-C	5.05	115.82	110.72
1	A	332	GLU	N-CA-C	5.04	117.15	111.11
1	B	664	SER	N-CA-C	5.03	117.15	111.11
1	D	531	PRO	O-C-N	5.03	123.62	121.31
1	B	320	GLN	N-CA-C	5.03	120.04	113.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	73	GLU	CA
1	C	74	ASN	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	277	SER	Mainchain
1	A	279	VAL	Mainchain
1	A	72	GLN	Peptide
1	A	74	ASN	Peptide,Mainchain
1	C	277	SER	Mainchain
1	C	278	SER	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5951	0	5660	119	0
1	B	6013	0	5710	114	1
1	C	5951	0	5660	124	0
1	D	5957	0	5673	103	1
2	E	28	0	25	0	0
2	G	28	0	24	0	0
2	H	28	0	25	1	0
2	I	28	0	25	3	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
3	F	39	0	34	2	0
4	K	50	0	41	1	0
5	A	56	0	52	10	0
5	B	84	0	77	9	0
5	C	70	0	65	3	0
5	D	84	0	78	4	0
6	B	10	0	10	3	0
7	A	466	0	0	3	0
7	B	467	0	0	3	0
7	C	334	0	0	0	0
7	D	411	0	0	0	0
All	All	26111	0	23209	458	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (458) 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:731:GLN:NE2	1:D:731:GLN:HE22	1.46	1.13
1:A:327:ILE:HD13	1:A:389:ILE:CD1	1.80	1.12
5:B:1501:NAG:O6	6:B:1502:FUC:C1	2.00	1.10
1:C:731:GLN:HE22	1:D:731:GLN:NE2	1.50	1.08
1:C:731:GLN:NE2	1:D:731:GLN:NE2	2.03	1.06
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.36	1.04
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.60	1.01
1:C:153:GLN:HE22	1:C:170:ASN:H	1.08	0.99
1:A:72:GLN:HG3	1:A:77:LEU:CD2	1.94	0.97
1:A:72:GLN:HG3	1:A:77:LEU:HD21	1.45	0.97
1:C:72:GLN:HB3	1:C:77:LEU:HD21	1.47	0.96
1:A:153:GLN:HE22	1:A:170:ASN:H	1.10	0.96
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.48	0.95
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.08	0.93
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.92	0.92
1:D:711:VAL:HG13	1:D:740:HIS:CE1	2.04	0.91
1:A:500:LEU:HA	1:A:503:MET:HE3	1.54	0.89
1:A:72:GLN:O	1:A:74:ASN:N	2.05	0.87
1:C:660:GLU:OE2	1:C:684:ARG:NH2	2.07	0.87
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.57	0.87
1:B:435:GLN:NE2	1:B:437:SER:OG	2.08	0.87
1:B:599:GLY:N	1:B:602:GLU:OE2	2.07	0.86
2:I:2:NAG:O7	2:I:2:NAG:O3	1.93	0.86
1:C:72:GLN:HB3	1:C:77:LEU:CD2	2.06	0.85
1:D:486:VAL:HG12	1:D:487:ASN:ND2	1.95	0.82
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.75	0.82
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.62	0.81
1:A:325:MET:HE3	1:A:327:ILE:CD1	2.10	0.81
1:B:78:VAL:HG13	5:B:851:NAG:H81	1.64	0.80
1:B:471:ARG:HG3	1:B:480:TYR:CE1	2.17	0.80
1:C:731:GLN:HE22	1:D:731:GLN:HE21	1.29	0.79
5:A:2191:NAG:H82	5:A:2191:NAG:O3	1.82	0.79
1:C:290:PRO:HG3	1:C:326:ASP:OD1	1.82	0.78
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.63	0.78
1:D:82:GLU:HG2	1:D:467:TYR:OH	1.84	0.78
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.65	0.78
1:A:660:GLU:OE2	1:A:684:ARG:NH2	2.15	0.77
1:A:153:GLN:NE2	1:A:170:ASN:H	1.82	0.77
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.77	0.76
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.21	0.76
1:C:153:GLN:NE2	1:C:170:ASN:H	1.83	0.76
1:A:325:MET:CE	1:A:327:ILE:HD11	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.22	0.75
1:C:190:LYS:HE2	1:C:193:ILE:HD12	1.68	0.74
1:C:157:TRP:CE3	1:C:164:LEU:HD13	2.24	0.73
1:C:184:ARG:HD3	1:C:186:THR:O	1.88	0.73
1:C:153:GLN:HE22	1:C:170:ASN:N	1.84	0.73
1:A:146:GLU:O	1:A:175:LYS:NZ	2.17	0.72
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.72	0.72
1:D:140:ARG:O	1:D:141:GLN:HG3	1.89	0.72
1:A:153:GLN:HE22	1:A:170:ASN:N	1.86	0.72
1:C:327:ILE:HD13	1:C:389:ILE:CD1	2.19	0.71
1:C:183:TYR:CD2	1:C:276:LEU:HD23	2.24	0.71
1:D:726:VAL:HG23	1:D:728:VAL:HG12	1.71	0.71
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.74	0.71
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.25	0.71
1:B:75:ASN:HD22	1:B:92:ASN:H	1.38	0.70
1:C:190:LYS:HE2	1:C:193:ILE:CD1	2.21	0.70
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.75	0.70
1:C:173:TYR:CE1	1:C:184:ARG:HG3	2.26	0.70
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.26	0.70
1:B:184:ARG:HD3	1:B:186:THR:O	1.92	0.70
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.74	0.69
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.27	0.69
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.73	0.69
1:A:325:MET:HE1	1:A:371:PHE:CE2	2.28	0.68
1:B:370:SER:OG	1:B:386:TYR:CE2	2.47	0.68
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.23	0.68
1:D:82:GLU:CG	1:D:467:TYR:OH	2.43	0.67
1:D:85:ASN:OD1	1:D:85:ASN:C	2.38	0.67
1:A:194:ILE:HD12	3:F:1:NAG:H82	1.75	0.67
1:C:385:CYS:HB3	1:C:387:PHE:CE2	2.30	0.67
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.29	0.67
1:C:81:ALA:O	1:C:492:ARG:NH1	2.28	0.66
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.78	0.66
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.76	0.66
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.78	0.66
1:A:327:ILE:CD1	1:A:389:ILE:CD1	2.68	0.65
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.60	0.65
1:C:60:LEU:C	1:C:60:LEU:HD12	2.22	0.65
1:A:82:GLU:HG2	1:A:467:TYR:OH	1.96	0.64
1:A:129:THR:HG23	1:A:151:ASN:HA	1.78	0.64
5:B:1501:NAG:O6	6:B:1502:FUC:O5	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:GLN:HG3	1:B:762:CYS:N	2.13	0.64
1:C:502:LYS:HA	1:C:505:GLN:HE21	1.63	0.63
1:A:162:HIS:NE2	1:A:177:GLU:OE1	2.31	0.63
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.80	0.63
1:D:146:GLU:O	1:D:175:LYS:HE2	1.99	0.63
1:B:35:HIS:CD2	1:B:35:HIS:H	2.17	0.63
1:A:500:LEU:HG	1:A:504:LEU:HD22	1.79	0.62
1:C:72:GLN:CB	1:C:77:LEU:HD21	2.26	0.62
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.16	0.62
1:C:756:SER:O	1:C:760:LYS:HG3	2.00	0.62
1:C:60:LEU:HD12	1:C:60:LEU:O	2.00	0.61
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.80	0.61
5:A:6851:NAG:O7	5:A:6851:NAG:O3	2.17	0.61
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.82	0.61
1:A:346:ILE:H	1:A:392:LYS:NZ	1.99	0.61
1:D:193:ILE:HG22	1:D:194:ILE:CD1	2.29	0.61
1:C:598:LEU:HG	1:C:631:TYR:OH	2.01	0.61
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.83	0.61
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.83	0.61
1:C:246:LEU:HD13	1:C:248:TYR:O	2.01	0.61
1:D:710:ASN:C	1:D:710:ASN:HD22	2.09	0.60
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.36	0.60
1:B:76:ILE:HD12	1:B:90:LEU:HD23	1.82	0.60
1:B:710:ASN:C	1:B:710:ASN:HD22	2.09	0.60
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.01	0.60
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.83	0.60
1:B:711:VAL:CG1	1:B:740:HIS:CE1	2.85	0.59
1:C:710:ASN:C	1:C:710:ASN:HD22	2.10	0.59
1:A:87:SER:OG	5:A:851:NAG:H83	2.02	0.59
1:C:136:ASP:O	1:C:140:ARG:HA	2.03	0.59
1:C:414:TYR:CE2	1:C:433:LYS:HE2	2.38	0.59
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.89	0.59
1:D:135:TYR:CZ	1:D:140:ARG:HA	2.37	0.59
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.68	0.58
1:C:129:THR:HG23	1:C:151:ASN:HA	1.84	0.58
1:B:597:ARG:NH1	1:B:679:ASN:OD1	2.36	0.58
1:C:114:ILE:HG22	1:C:135:TYR:HB2	1.86	0.58
1:A:155:VAL:HG12	1:A:166:TYR:HB3	1.85	0.58
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.84	0.58
1:C:340:LEU:HB2	1:C:343:ARG:HG3	1.84	0.58
1:C:157:TRP:CZ3	1:C:164:LEU:HD13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:HB2	1:A:132:TYR:CE2	2.39	0.58
1:C:581:ARG:CZ	5:C:5201:NAG:H5	2.34	0.58
1:D:206:GLU:HB3	1:D:665:VAL:HG22	1.87	0.57
1:D:214:LEU:HD23	1:D:225:TYR:CB	2.34	0.57
1:A:81:ALA:O	1:A:492:ARG:NH1	2.35	0.57
1:A:581:ARG:NH2	5:A:5201:NAG:H3	2.19	0.57
1:B:597:ARG:HG2	7:B:7141:HOH:O	2.04	0.57
1:C:179:ASN:HD22	1:C:179:ASN:H	1.52	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:B:82:GLU:CG	1:B:467:TYR:OH	2.46	0.57
1:C:731:GLN:HE21	1:D:731:GLN:HE22	1.44	0.57
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.34	0.56
1:A:83:TYR:HB2	1:A:85:ASN:OD1	2.04	0.56
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.40	0.56
1:A:60:LEU:HD12	1:A:60:LEU:C	2.30	0.56
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.87	0.56
1:D:214:LEU:CD2	1:D:225:TYR:HB3	2.35	0.56
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.41	0.56
1:A:72:GLN:C	1:A:74:ASN:N	2.53	0.56
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.40	0.56
1:C:80:ASN:HD22	1:C:81:ALA:N	2.02	0.56
1:A:87:SER:OG	5:A:851:NAG:C8	2.53	0.56
1:B:453:ARG:HG3	1:B:454:CYS:SG	2.45	0.56
1:B:65:ASP:OD2	1:B:464:GLU:N	2.34	0.56
1:D:520:ASN:O	1:D:521:GLU:HB2	2.05	0.56
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.87	0.56
1:B:56:LYS:HE3	1:B:495:GLU:OE2	2.05	0.56
1:B:136:ASP:HB2	1:B:143:ILE:HD11	1.88	0.56
1:D:55:LEU:HD12	1:D:500:LEU:HD22	1.88	0.56
1:A:657:SER:HA	1:A:688:VAL:HG13	1.88	0.55
1:C:95:PHE:O	1:C:98:PHE:HB2	2.06	0.55
1:B:378:GLU:CD	1:B:378:GLU:H	2.13	0.55
1:C:69:LEU:HD23	1:C:78:VAL:HA	1.87	0.55
1:D:726:VAL:HG23	1:D:728:VAL:CG1	2.36	0.55
1:C:723:LEU:HB3	1:C:728:VAL:HG13	1.88	0.55
1:D:581:ARG:HD3	5:D:5201:NAG:H5	1.87	0.55
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.87	0.55
1:A:273:THR:O	1:A:276:LEU:HD22	2.07	0.55
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.89	0.55
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.88	0.55
1:D:131:SER:OG	1:D:150:ASN:OD1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:O	1:C:94:THR:HG22	2.06	0.55
1:D:135:TYR:OH	1:D:140:ARG:HA	2.05	0.54
1:A:72:GLN:HG3	1:A:77:LEU:HD23	1.87	0.54
1:C:169:ASN:O	1:C:170:ASN:HB2	2.07	0.54
1:D:42:THR:HB	1:D:569:SER:OG	2.06	0.54
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.87	0.54
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.07	0.54
1:D:364:PHE:HE2	1:D:389:ILE:HD11	1.72	0.54
1:A:145:GLU:HG3	1:A:179:ASN:HB2	1.90	0.54
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.37	0.54
1:A:200:ASP:OD1	1:A:230:ASP:OD2	2.26	0.54
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.91	0.54
1:B:415:LEU:C	1:B:415:LEU:HD23	2.32	0.54
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.89	0.54
7:A:7174:HOH:O	3:F:2:NAG:H81	2.08	0.54
1:C:95:PHE:O	1:C:98:PHE:CB	2.56	0.53
1:C:114:ILE:CG2	1:C:135:TYR:HB2	2.37	0.53
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.89	0.53
1:A:155:VAL:HG12	1:A:166:TYR:CB	2.38	0.53
1:C:385:CYS:HB3	1:C:387:PHE:HE2	1.71	0.53
1:C:760:LYS:NZ	1:C:766:PRO:O	2.42	0.53
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.90	0.53
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.43	0.53
1:B:39:SER:OG	1:B:506:ASN:HA	2.08	0.53
1:B:208:PHE:O	1:B:209:SER:HB2	2.08	0.53
1:B:75:ASN:ND2	1:B:92:ASN:H	2.06	0.53
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.44	0.53
1:C:414:TYR:CE2	1:C:435:GLN:HG3	2.44	0.53
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.39	0.53
1:B:92:ASN:OD1	1:B:92:ASN:C	2.51	0.53
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.91	0.53
1:D:109:PRO:HD2	1:D:161:GLY:O	2.08	0.53
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.43	0.52
1:A:72:GLN:CG	1:A:77:LEU:CD2	2.79	0.52
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.91	0.52
1:A:177:GLU:HB2	1:A:180:LEU:HD12	1.91	0.52
1:B:340:LEU:HB2	1:B:343:ARG:HG3	1.91	0.52
1:D:430:ASN:ND2	1:D:446:SER:OG	2.29	0.52
5:C:2191:NAG:O7	5:C:2191:NAG:H3	2.09	0.52
1:D:756:SER:O	1:D:760:LYS:HG3	2.10	0.52
1:D:477:LEU:HD12	1:D:501:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:HD11	1:C:95:PHE:CZ	2.46	0.51
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.92	0.51
1:A:681:ASP:HB3	5:A:6851:NAG:H2	1.91	0.51
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.45	0.51
1:B:433:LYS:NZ	1:B:488:ASP:OD1	2.37	0.51
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.91	0.51
1:B:465:ALA:O	1:B:485:SER:OG	2.26	0.51
1:B:657:SER:HA	1:B:688:VAL:CG1	2.40	0.51
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.46	0.51
1:D:435:GLN:NE2	1:D:437:SER:OG	2.36	0.51
1:A:169:ASN:O	1:A:170:ASN:HB2	2.11	0.51
1:C:741:GLY:O	1:C:742:ILE:C	2.53	0.51
1:A:207:VAL:HG12	1:A:208:PHE:CD1	2.46	0.51
1:B:71:LYS:H	1:B:71:LYS:HD2	1.76	0.51
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.46	0.51
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.41	0.51
1:D:113:PHE:CZ	1:D:178:PRO:HG2	2.46	0.51
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.93	0.51
1:B:602:GLU:HG3	1:B:603:VAL:H	1.75	0.51
1:D:594:ILE:C	1:D:594:ILE:HD12	2.36	0.51
1:B:78:VAL:HG13	5:B:851:NAG:C8	2.39	0.50
1:D:500:LEU:HG	1:D:504:LEU:HD22	1.92	0.50
1:A:741:GLY:O	1:A:742:ILE:C	2.53	0.50
1:B:684:ARG:HB3	5:B:6851:NAG:C8	2.42	0.50
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.42	0.50
1:A:410:LEU:HD23	1:A:410:LEU:O	2.12	0.50
1:A:87:SER:CB	5:A:851:NAG:H83	2.41	0.50
1:D:741:GLY:O	1:D:742:ILE:C	2.53	0.50
1:A:72:GLN:O	1:A:75:ASN:HB2	2.12	0.50
1:C:372:TYR:OH	1:C:436:LEU:HG	2.12	0.50
1:A:106:SER:HG	1:A:157:TRP:CD1	2.30	0.50
1:A:366:LEU:HD12	1:A:366:LEU:O	2.11	0.50
1:B:658:ARG:O	1:B:658:ARG:HG3	2.11	0.50
1:B:684:ARG:HB3	5:B:6851:NAG:H81	1.93	0.50
5:D:5201:NAG:O7	5:D:5201:NAG:H3	2.12	0.50
1:C:410:LEU:HD11	1:C:436:LEU:HD21	1.94	0.50
1:D:596:ARG:O	1:D:597:ARG:NE	2.35	0.50
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.46	0.49
1:B:173:TYR:CZ	1:B:184:ARG:HG3	2.47	0.49
1:D:485:SER:O	1:D:486:VAL:C	2.53	0.49
1:D:142:LEU:HD12	1:D:143:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ASN:HD22	1:A:710:ASN:C	2.20	0.49
1:C:660:GLU:CD	1:C:684:ARG:HH21	2.09	0.49
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.94	0.49
1:A:180:LEU:O	1:A:181:PRO:C	2.54	0.49
1:B:675:THR:HB	1:B:677:GLU:OE1	2.12	0.49
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.78	0.49
1:B:55:LEU:HD12	1:B:500:LEU:CD2	2.43	0.49
1:A:757:HIS:HD2	7:A:7143:HOH:O	1.96	0.48
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.95	0.48
1:C:177:GLU:HB2	1:C:180:LEU:HG	1.96	0.48
1:C:179:ASN:HD22	1:C:179:ASN:N	2.10	0.48
1:C:516:PHE:CE1	1:C:518:ILE:HD11	2.48	0.48
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.47	0.48
2:I:2:NAG:HO3	2:I:2:NAG:C7	2.16	0.48
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.48	0.48
1:A:491:LEU:O	1:A:492:ARG:HB3	2.13	0.48
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.95	0.48
1:C:372:TYR:CE1	1:C:386:TYR:CD2	3.02	0.48
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.78	0.48
1:C:414:TYR:CZ	1:C:433:LYS:HE2	2.48	0.48
1:D:415:LEU:CD1	1:D:415:LEU:C	2.87	0.48
1:D:688:VAL:HG22	1:D:719:ILE:HG12	1.96	0.48
1:A:433:LYS:O	1:A:433:LYS:HG2	2.13	0.48
1:D:71:LYS:H	1:D:71:LYS:HD2	1.79	0.48
1:B:677:GLU:CD	1:B:677:GLU:H	2.22	0.48
1:C:131:SER:OG	1:C:150:ASN:OD1	2.30	0.48
1:B:206:GLU:HB3	1:B:665:VAL:HG22	1.95	0.48
1:C:80:ASN:HD22	1:C:80:ASN:C	2.22	0.47
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.29	0.47
1:A:54:ARG:HE	1:D:40:ARG:NH1	2.13	0.47
1:C:67:GLU:HA	1:C:79:PHE:O	2.14	0.47
1:C:94:THR:C	1:C:95:PHE:CD1	2.92	0.47
1:C:448:GLU:HA	1:C:451:PRO:HG3	1.96	0.47
1:D:295:ILE:HD13	1:D:295:ILE:O	2.14	0.47
1:C:514:LEU:HD23	1:C:526:TYR:O	2.14	0.47
1:C:60:LEU:C	1:C:60:LEU:CD1	2.88	0.47
1:C:246:LEU:CD1	1:C:248:TYR:O	2.63	0.47
1:C:278:SER:HB3	1:C:279:VAL:HG23	1.97	0.47
1:A:129:THR:CG2	1:A:151:ASN:HA	2.44	0.47
1:C:343:ARG:HD2	1:C:389:ILE:HG22	1.97	0.47
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:HD22	1:A:81:ALA:N	2.13	0.46
1:D:453:ARG:O	1:D:453:ARG:HG3	2.07	0.46
1:D:457:TYR:HA	1:D:471:ARG:O	2.15	0.46
1:B:643:GLY:HA2	1:B:697:GLN:HE22	1.80	0.46
1:B:366:LEU:C	1:B:366:LEU:HD13	2.41	0.46
1:D:74:ASN:O	1:D:92:ASN:HB2	2.16	0.46
1:D:107:ILE:HG22	1:D:108:SER:O	2.15	0.46
1:C:374:ILE:CD1	1:C:406:GLY:HA2	2.46	0.46
1:C:487:ASN:O	1:C:488:ASP:HB2	2.15	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.56	0.46
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.97	0.46
1:D:472:CYS:O	1:D:478:PRO:HA	2.14	0.46
1:B:741:GLY:O	1:B:742:ILE:C	2.58	0.46
1:D:157:TRP:CZ3	1:D:164:LEU:CD2	2.99	0.46
1:C:98:PHE:CD2	1:C:135:TYR:OH	2.69	0.46
1:D:658:ARG:HG2	1:D:661:TYR:CE2	2.50	0.46
1:C:358:ARG:HB2	1:C:359:PRO:HD2	1.96	0.45
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.34	0.45
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.97	0.45
1:C:94:THR:O	1:C:95:PHE:CD1	2.70	0.45
1:D:486:VAL:CG1	1:D:487:ASN:ND2	2.72	0.45
1:A:306:ALA:HB3	1:A:310:ARG:HG2	1.98	0.45
1:B:65:ASP:OD1	1:B:466:LYS:HB2	2.16	0.45
1:C:470:LEU:HA	1:C:470:LEU:HD23	1.79	0.45
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.47	0.45
1:D:453:ARG:HG3	1:D:454:CYS:SG	2.57	0.45
1:D:657:SER:HA	1:D:688:VAL:HG13	1.99	0.45
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.69	0.45
1:A:500:LEU:HA	1:A:503:MET:CE	2.39	0.45
1:B:59:SER:HB3	1:B:71:LYS:HE3	1.99	0.45
1:B:614:SER:HA	1:B:619:VAL:HB	1.98	0.45
1:A:562:ASN:HB2	7:A:6872:HOH:O	2.17	0.45
1:B:516:PHE:CD1	1:B:523:LYS:HG2	2.52	0.45
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.81	0.45
1:D:202:VAL:CG2	1:D:665:VAL:HG13	2.47	0.45
1:A:65:ASP:CG	1:A:466:LYS:HB2	2.42	0.44
1:D:78:VAL:O	1:D:86:SER:HB2	2.17	0.44
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.98	0.44
1:A:512:LYS:HG2	1:A:529:ILE:HD13	1.99	0.44
1:C:214:LEU:HD23	1:C:225:TYR:CB	2.45	0.44
1:A:107:ILE:HG22	1:A:108:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ARG:NH2	1:B:368:GLY:O	2.48	0.44
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.53	0.44
1:C:464:GLU:O	1:C:465:ALA:HB3	2.18	0.44
1:A:60:LEU:HD12	1:A:60:LEU:O	2.17	0.44
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.53	0.44
1:C:55:LEU:HD23	1:C:500:LEU:HD22	2.00	0.44
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.98	0.44
1:A:115:LEU:HD21	1:A:155:VAL:CG2	2.45	0.44
1:A:458:SER:OG	1:A:471:ARG:HB3	2.18	0.44
1:A:693:GLU:OE1	1:A:696:LYS:NZ	2.29	0.44
1:C:510:PRO:HD3	1:C:569:SER:HB2	2.00	0.44
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.99	0.44
1:B:373:LYS:HE2	7:B:7148:HOH:O	2.18	0.44
1:B:594:ILE:CD1	1:B:594:ILE:H	2.30	0.44
1:C:53:TYR:CD1	1:C:503:MET:HE2	2.53	0.44
1:D:65:ASP:HB3	1:D:66:HIS:CE1	2.53	0.44
1:D:121:VAL:HB	1:D:129:THR:HG22	2.00	0.44
1:C:516:PHE:HE1	1:C:518:ILE:HD11	1.82	0.43
1:C:626:ILE:O	1:C:650:GLY:HA2	2.18	0.43
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.43
1:C:157:TRP:CE3	1:C:164:LEU:CD1	3.00	0.43
1:C:193:ILE:HG22	1:C:194:ILE:CD1	2.45	0.43
1:D:594:ILE:C	1:D:594:ILE:CD1	2.91	0.43
1:A:87:SER:HB3	5:A:851:NAG:H83	1.99	0.43
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.99	0.43
1:C:471:ARG:HG3	1:C:480:TYR:CE1	2.54	0.43
1:A:596:ARG:NH2	1:A:678:ASP:OD2	2.41	0.43
1:C:106:SER:HB3	1:C:115:LEU:HB3	2.01	0.43
1:D:626:ILE:O	1:D:650:GLY:HA2	2.19	0.43
1:C:415:LEU:HB3	1:C:434:ILE:HG23	2.00	0.43
5:C:2191:NAG:O7	5:C:2191:NAG:C3	2.67	0.43
1:C:55:LEU:HD23	1:C:500:LEU:HD21	2.00	0.43
1:C:74:ASN:HD22	1:C:74:ASN:HA	1.76	0.43
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.52	0.43
2:H:2:NAG:O7	2:H:2:NAG:C1	2.66	0.43
1:A:174:VAL:HG23	1:A:185:ILE:CD1	2.49	0.43
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.19	0.43
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.53	0.43
1:B:214:LEU:HD23	1:B:225:TYR:HB3	2.00	0.43
1:B:544:LEU:HG	1:B:546:VAL:CG1	2.49	0.43
1:A:329:ASP:OD2	1:A:343:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:PRO:HG3	1:D:623:ARG:CZ	2.48	0.43
1:D:627:TRP:HB2	1:D:651:ILE:HB	2.01	0.43
1:C:72:GLN:CB	1:C:77:LEU:CD2	2.87	0.42
1:D:378:GLU:CD	1:D:378:GLU:H	2.27	0.42
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.54	0.42
1:C:96:ASP:OD2	1:C:97:GLU:N	2.53	0.42
1:B:397:ILE:HD12	1:B:434:ILE:HD13	2.00	0.42
1:C:273:THR:HA	1:C:276:LEU:HD13	2.01	0.42
1:A:598:LEU:HG	1:A:631:TYR:OH	2.20	0.42
1:B:60:LEU:C	1:B:60:LEU:HD12	2.45	0.42
1:B:290:PRO:HG3	1:B:326:ASP:OD1	2.20	0.42
1:C:482:LEU:HD23	1:C:482:LEU:HA	1.89	0.42
1:C:600:THR:OG1	1:C:601:PHE:N	2.46	0.42
1:D:273:THR:HA	1:D:276:LEU:HD22	1.99	0.42
1:B:631:TYR:O	1:B:634:TYR:HB3	2.19	0.42
1:A:201:TRP:CZ2	1:A:710:ASN:HA	2.54	0.42
1:A:389:ILE:HA	1:A:389:ILE:HD13	1.81	0.42
5:A:5201:NAG:H3	5:A:5201:NAG:O7	2.19	0.42
1:B:117:GLU:HG3	1:B:132:TYR:CE2	2.55	0.42
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.19	0.42
1:D:179:ASN:OD1	1:D:179:ASN:N	2.52	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.20	0.42
1:B:206:GLU:CB	1:B:665:VAL:HG22	2.49	0.42
1:A:54:ARG:NE	1:D:40:ARG:NH1	2.67	0.42
1:C:146:GLU:O	1:C:175:LYS:NZ	2.46	0.42
1:D:320:GLN:O	1:D:354:VAL:HG12	2.20	0.42
1:D:486:VAL:HG12	1:D:487:ASN:HD21	1.80	0.42
1:D:711:VAL:HG13	1:D:740:HIS:ND1	2.33	0.42
1:B:405:ILE:HG12	1:B:419:SER:HA	2.02	0.41
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.55	0.41
1:D:202:VAL:HG22	1:D:665:VAL:HG13	2.02	0.41
1:D:387:PHE:CE1	1:D:394:CYS:HB3	2.55	0.41
1:A:415:LEU:C	1:A:415:LEU:HD13	2.44	0.41
1:B:482:LEU:HD23	1:B:482:LEU:HA	1.83	0.41
1:C:248:TYR:HA	1:C:249:PRO:HD3	1.95	0.41
1:A:415:LEU:C	1:A:415:LEU:CD1	2.93	0.41
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.36	0.41
1:D:70:TYR:CG	1:D:71:LYS:N	2.87	0.41
1:D:157:TRP:CZ3	1:D:164:LEU:HD21	2.55	0.41
1:B:588:ASP:O	1:B:592:HIS:HB2	2.20	0.41
1:D:172:ILE:CD1	1:D:214:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:VAL:HA	1:D:255:PRO:HD3	1.95	0.41
1:D:379:GLU:HB3	1:D:381:TYR:HD1	1.85	0.41
1:B:69:LEU:HD13	1:B:107:ILE:HD12	2.02	0.41
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.75	0.41
1:B:520:ASN:OD1	5:B:5201:NAG:H2	2.08	0.41
1:C:167:VAL:HA	1:C:171:ASP:O	2.21	0.41
1:C:588:ASP:O	1:C:592:HIS:HB2	2.21	0.41
1:D:658:ARG:HB2	1:D:687:THR:HG22	2.01	0.41
2:I:2:NAG:O3	2:I:2:NAG:C7	2.65	0.41
1:B:237:GLU:HG2	1:B:253:ARG:HG2	2.01	0.41
1:B:602:GLU:CD	1:B:631:TYR:HH	2.29	0.41
1:A:487:ASN:OD1	1:A:487:ASN:N	2.54	0.41
1:B:366:LEU:HD22	1:B:366:LEU:HA	1.87	0.41
1:C:720:SER:O	1:C:724:VAL:HG23	2.21	0.41
1:D:520:ASN:HB2	5:D:5201:NAG:H61	2.02	0.41
1:D:622:LYS:HB2	1:D:622:LYS:HE2	1.60	0.41
1:B:435:GLN:HE21	1:B:437:SER:HG	1.54	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.80	0.41
4:K:2:NAG:H82	4:K:2:NAG:H2	1.92	0.41
1:A:731:GLN:NE2	1:B:731:GLN:HE22	2.19	0.41
1:B:149:PRO:HA	5:B:1501:NAG:H83	2.02	0.41
1:A:531:PRO:HA	1:A:532:PRO:HD3	1.94	0.40
1:B:92:ASN:ND2	7:B:7058:HOH:O	2.52	0.40
1:B:513:LYS:O	1:B:527:GLN:HA	2.22	0.40
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.40
5:B:1501:NAG:HO6	6:B:1502:FUC:C1	2.04	0.40
1:C:68:TYR:CD1	1:C:68:TYR:C	2.99	0.40
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.96	0.40
1:A:87:SER:CB	5:A:851:NAG:C8	2.99	0.40
1:B:172:ILE:HD13	1:B:214:LEU:HD21	2.03	0.40
1:B:472:CYS:O	1:B:478:PRO:HA	2.21	0.40
1:A:95:PHE:CZ	1:A:116:LEU:HD11	2.57	0.40
1:A:309:GLU:HB3	1:A:330:TYR:HB3	2.03	0.40
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.83	0.40
1:C:598:LEU:HB2	1:C:671:MET:SD	2.60	0.40
1:D:157:TRP:CZ3	1:D:164:LEU:HD22	2.57	0.40
1:D:581:ARG:NH2	5:D:5201:NAG:O7	2.54	0.40
1:A:174:VAL:HG23	1:A:185:ILE:HD11	2.03	0.40
1:B:214:LEU:CD2	1:B:225:TYR:HB3	2.52	0.40
1:B:377:ASN:OD1	1:B:377:ASN:C	2.65	0.40
1:B:654:ALA:N	1:B:655:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLU:HG3	1:B:683:TYR:CD1	2.56	0.40
1:D:695:PHE:HB3	1:D:728:VAL:HG21	2.02	0.40
1:A:425:MET:HA	1:A:426:PRO:HD3	1.94	0.40
1:B:219:ASN:OD1	1:B:219:ASN:C	2.64	0.40
1:B:221:THR:HG23	1:B:274:ASP:OD2	2.22	0.40
1:D:345:HIS:HE1	1:D:391:LYS:O	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:HIS:ND1	1:D:388:GLN:OE1[2_645]	1.96	0.24

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	725/733 (99%)	693 (96%)	29 (4%)	3 (0%)	30	28
1	B	731/733 (100%)	703 (96%)	28 (4%)	0	100	100
1	C	725/733 (99%)	691 (95%)	33 (5%)	1 (0%)	48	50
1	D	725/733 (99%)	693 (96%)	30 (4%)	2 (0%)	36	36
All	All	2906/2932 (99%)	2780 (96%)	120 (4%)	6 (0%)	43	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	D	486	VAL
1	C	73	GLU
1	A	140	ARG

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Mol	Chain	Res	Type
1	D	621	ASN
1	A	181	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/658 (99%)	580 (89%)	71 (11%)	6	4
1	B	658/658 (100%)	608 (92%)	50 (8%)	12	9
1	C	651/658 (99%)	600 (92%)	51 (8%)	11	9
1	D	652/658 (99%)	594 (91%)	58 (9%)	9	6
All	All	2612/2632 (99%)	2382 (91%)	230 (9%)	9	7

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	61	ARG
1	A	63	ILE
1	A	66	HIS
1	A	73	GLU
1	A	74	ASN
1	A	77	LEU
1	A	78	VAL
1	A	80	ASN
1	A	96	ASP
1	A	129	THR
1	A	138	ASN
1	A	142	LEU
1	A	145	GLU
1	A	156	THR
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	278	SER

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Mol	Chain	Res	Type
1	A	279	VAL
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	332	GLU
1	A	336	ARG
1	A	340	LEU
1	A	354	VAL
1	A	358	ARG
1	A	360	SER
1	A	366	LEU
1	A	370	SER
1	A	376	SER
1	A	379	GLU
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	392	LYS
1	A	395	THR
1	A	399	LYS
1	A	410	LEU
1	A	415	LEU
1	A	436	LEU
1	A	437	SER
1	A	440	THR
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	466	LYS
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	485	SER
1	A	489	LYS
1	A	492	ARG
1	A	498	SER
1	A	502	LYS
1	A	504	LEU
1	A	506	ASN
1	A	507	VAL
1	A	512	LYS
1	A	514	LEU

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Mol	Chain	Res	Type
1	A	519	LEU
1	A	538	LYS
1	A	575	VAL
1	A	598	LEU
1	A	615	LYS
1	A	658	ARG
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	688	VAL
1	B	34	HIS
1	B	40	ARG
1	B	51	ASN
1	B	54	ARG
1	B	55	LEU
1	B	66	HIS
1	B	71	LYS
1	B	72	GLN
1	B	73	GLU
1	B	142	LEU
1	B	164	LEU
1	B	180	LEU
1	B	184	ARG
1	B	202	VAL
1	B	230	ASP
1	B	262	VAL
1	B	276	LEU
1	B	280	THR
1	B	313	LEU
1	B	316	LEU
1	B	343	ARG
1	B	354	VAL
1	B	373	LYS
1	B	376	SER
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	395	THR
1	B	434	ILE
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG

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Mol	Chain	Res	Type
1	B	471	ARG
1	B	472	CYS
1	B	482	LEU
1	B	504	LEU
1	B	514	LEU
1	B	589	LYS
1	B	594	ILE
1	B	597	ARG
1	B	615	LYS
1	B	658	ARG
1	B	665	VAL
1	B	673	LEU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	B	711	VAL
1	B	728	VAL
1	B	761	GLN
1	C	56	LYS
1	C	71	LYS
1	C	74	ASN
1	C	75	ASN
1	C	77	LEU
1	C	80	ASN
1	C	95	PHE
1	C	129	THR
1	C	143	ILE
1	C	145	GLU
1	C	164	LEU
1	C	179	ASN
1	C	184	ARG
1	C	202	VAL
1	C	235	LEU
1	C	245	SER
1	C	246	LEU
1	C	276	LEU
1	C	278	SER
1	C	280	THR
1	C	283	THR
1	C	313	LEU
1	C	316	LEU
1	C	343	ARG

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Mol	Chain	Res	Type
1	C	354	VAL
1	C	358	ARG
1	C	385	CYS
1	C	395	THR
1	C	415	LEU
1	C	436	LEU
1	C	440	THR
1	C	464	GLU
1	C	477	LEU
1	C	482	LEU
1	C	492	ARG
1	C	502	LYS
1	C	504	LEU
1	C	506	ASN
1	C	511	SER
1	C	514	LEU
1	C	519	LEU
1	C	536	LYS
1	C	597	ARG
1	C	598	LEU
1	C	614	SER
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	699	GLU
1	C	728	VAL
1	D	51	ASN
1	D	63	ILE
1	D	66	HIS
1	D	71	LYS
1	D	76	ILE
1	D	77	LEU
1	D	78	VAL
1	D	85	ASN
1	D	101	SER
1	D	129	THR
1	D	142	LEU
1	D	143	ILE
1	D	164	LEU
1	D	177	GLU
1	D	179	ASN

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Mol	Chain	Res	Type
1	D	180	LEU
1	D	184	ARG
1	D	194	ILE
1	D	235	LEU
1	D	276	LEU
1	D	280	THR
1	D	283	THR
1	D	295	ILE
1	D	316	LEU
1	D	326	ASP
1	D	327	ILE
1	D	336	ARG
1	D	341	VAL
1	D	348	MET
1	D	354	VAL
1	D	366	LEU
1	D	373	LYS
1	D	389	ILE
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	453	ARG
1	D	464	GLU
1	D	470	LEU
1	D	472	CYS
1	D	482	LEU
1	D	492	ARG
1	D	504	LEU
1	D	513	LYS
1	D	514	LEU
1	D	519	LEU
1	D	521	GLU
1	D	575	VAL
1	D	597	ARG
1	D	658	ARG
1	D	665	VAL
1	D	673	LEU
1	D	685	ASN
1	D	688	VAL
1	D	711	VAL
1	D	728	VAL

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Mol	Chain	Res	Type
1	D	761	GLN

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

Mol	Chain	Res	Type
1	A	51	ASN
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	338	ASN
1	A	344	GLN
1	A	345	HIS
1	A	388	GLN
1	A	455	GLN
1	A	506	ASN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	B	35	HIS
1	B	72	GLN
1	B	75	ASN
1	B	169	ASN
1	B	196	ASN
1	B	344	GLN
1	B	435	GLN
1	B	505	GLN
1	B	572	ASN
1	B	592	HIS
1	B	595	ASN
1	B	697	GLN
1	B	710	ASN
1	B	731	GLN
1	C	74	ASN
1	C	80	ASN
1	C	138	ASN
1	C	141	GLN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	179	ASN

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Mol	Chain	Res	Type
1	C	314	GLN
1	C	344	GLN
1	C	455	GLN
1	C	505	GLN
1	C	572	ASN
1	C	592	HIS
1	C	606	GLN
1	C	697	GLN
1	C	710	ASN
1	C	731	GLN
1	D	75	ASN
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	345	HIS
1	D	487	ASN
1	D	505	GLN
1	D	595	ASN
1	D	606	GLN
1	D	697	GLN
1	D	710	ASN
1	D	731	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 ⓘ

19 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	0.65	0	17,19,21	2.06	4 (23%)
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	1.61	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.62	0
3	MAN	F	3	3	11,11,12	0.33	0	15,15,17	0.87	1 (6%)
2	NAG	G	1	1,2	14,14,15	0.63	0	17,19,21	4.62	9 (52%)
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	1.21	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.44	0	17,19,21	0.95	0
2	NAG	H	2	2	14,14,15	0.52	0	17,19,21	1.08	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.82	1 (7%)	17,19,21	1.25	1 (5%)
2	NAG	I	2	2	14,14,15	1.09	1 (7%)	17,19,21	2.57	6 (35%)
2	NAG	J	1	1,2	14,14,15	0.34	0	17,19,21	1.11	1 (5%)
2	NAG	J	2	2	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	K	1	1,4	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	1.07	3 (17%)
4	MAN	K	3	4	11,11,12	0.42	0	15,15,17	1.98	5 (33%)
4	MAN	K	4	4	11,11,12	0.32	0	15,15,17	1.52	2 (13%)
2	NAG	L	1	1,2	14,14,15	0.30	0	17,19,21	0.92	0
2	NAG	L	2	2	14,14,15	0.35	0	17,19,21	1.23	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	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	MAN	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	1/1/4/5	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C1-C2	3.70	1.57	1.52
2	I	1	NAG	O4-C4	2.23	1.48	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-C2-N2	10.79	127.43	110.43
2	G	1	NAG	C4-C3-C2	-9.64	96.89	111.02
2	G	1	NAG	C2-N2-C7	7.64	133.14	122.90
2	G	1	NAG	O5-C1-C2	-7.52	99.65	111.29
2	I	2	NAG	O5-C1-C2	-6.12	101.82	111.29
2	I	2	NAG	C1-C2-N2	5.27	118.74	110.43
2	E	1	NAG	C4-C3-C2	-5.21	103.39	111.02
4	K	3	MAN	C6-C5-C4	-4.66	101.58	113.02
2	E	2	NAG	C1-O5-C5	4.33	117.99	112.19
2	I	2	NAG	C2-N2-C7	4.08	128.37	122.90
3	F	1	NAG	C2-N2-C7	-3.84	117.75	122.90
2	E	2	NAG	C2-N2-C7	-3.40	118.34	122.90
2	E	1	NAG	O4-C4-C3	3.39	118.37	110.38
2	G	1	NAG	C1-O5-C5	3.32	116.64	112.19
2	E	1	NAG	C2-N2-C7	3.24	127.25	122.90
4	K	3	MAN	C1-C2-C3	3.10	114.16	109.64
2	I	1	NAG	O4-C4-C3	3.10	117.67	110.38
2	E	1	NAG	C3-C4-C5	-3.07	104.66	110.23
2	L	2	NAG	C1-O5-C5	-2.97	108.20	112.19
2	I	2	NAG	C4-C3-C2	-2.96	106.69	111.02
4	K	4	MAN	O5-C1-C2	-2.94	103.78	110.79
4	K	4	MAN	C1-O5-C5	2.89	116.06	112.19
4	K	3	MAN	C1-O5-C5	-2.79	108.45	112.19
4	K	3	MAN	O6-C6-C5	-2.78	101.86	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	NAG	C1-C2-N2	2.53	114.42	110.43
2	G	2	NAG	C2-N2-C7	2.50	126.24	122.90
2	G	1	NAG	C8-C7-N2	-2.49	111.99	116.12
2	J	1	NAG	C2-N2-C7	-2.32	119.79	122.90
4	K	1	NAG	O5-C5-C6	2.31	112.17	107.66
4	K	2	NAG	C1-C2-N2	2.29	114.03	110.43
2	G	2	NAG	C1-O5-C5	2.28	115.24	112.19
2	I	2	NAG	C1-O5-C5	2.28	115.24	112.19
2	G	1	NAG	O4-C4-C5	2.25	114.86	109.32
2	H	2	NAG	O5-C1-C2	-2.23	107.84	111.29
2	L	2	NAG	O5-C1-C2	-2.22	107.85	111.29
4	K	2	NAG	O5-C5-C6	2.13	111.81	107.66
2	G	1	NAG	O5-C5-C6	2.11	111.77	107.66
2	I	2	NAG	O7-C7-N2	2.11	125.71	121.98
4	K	2	NAG	C4-C3-C2	-2.10	107.94	111.02
4	K	3	MAN	C3-C4-C5	2.08	114.01	110.23
3	F	1	NAG	O5-C1-C2	-2.08	108.07	111.29
2	G	1	NAG	O7-C7-N2	2.08	125.66	121.98
3	F	3	MAN	C3-C4-C5	2.06	113.96	110.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	2	NAG	C1
4	K	4	MAN	C1

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
4	K	3	MAN	C4-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	3	MAN	O5-C5-C6-O6
4	K	4	MAN	C4-C5-C6-O6
3	F	3	MAN	C4-C5-C6-O6

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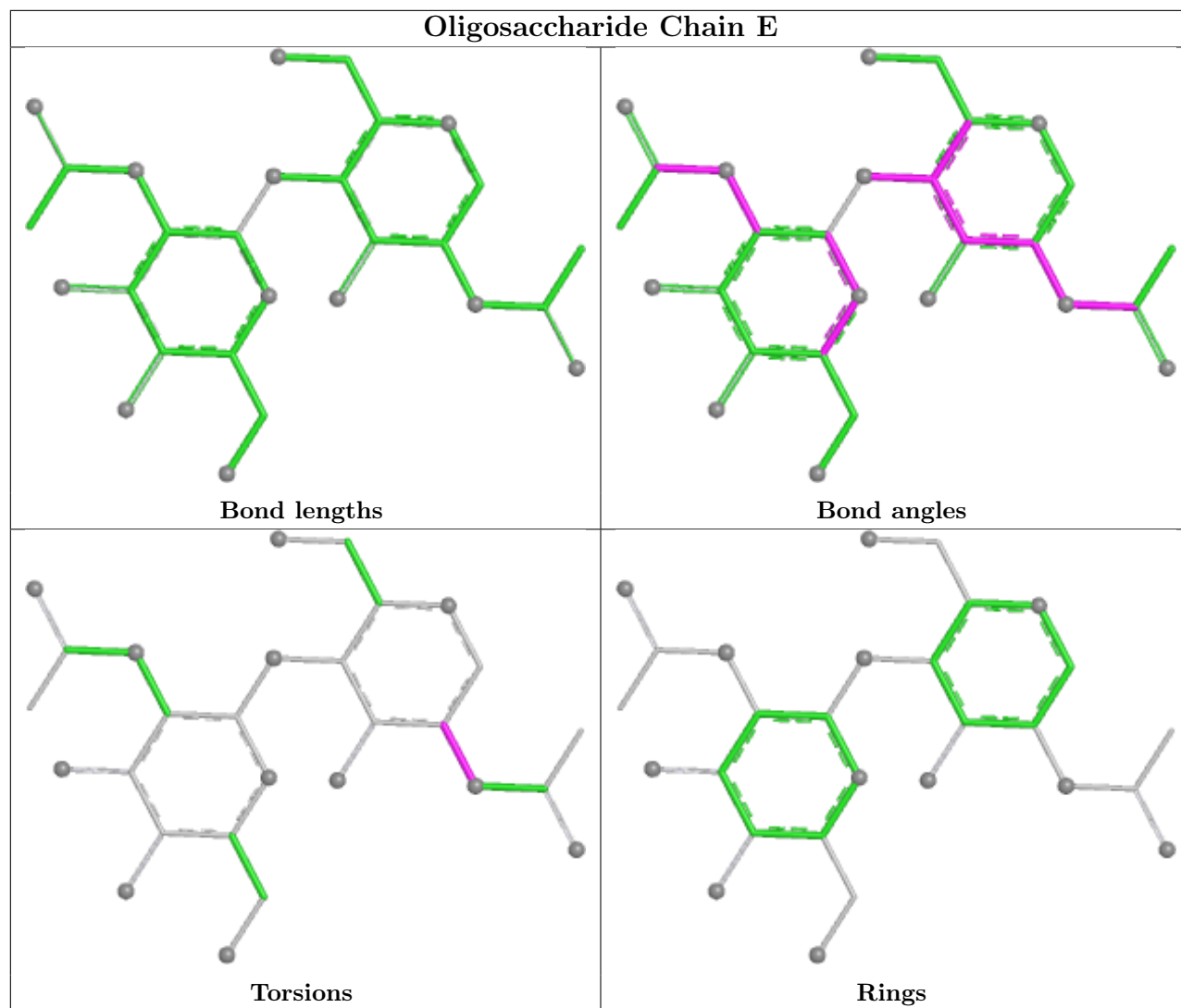
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	F	3	MAN	O5-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6

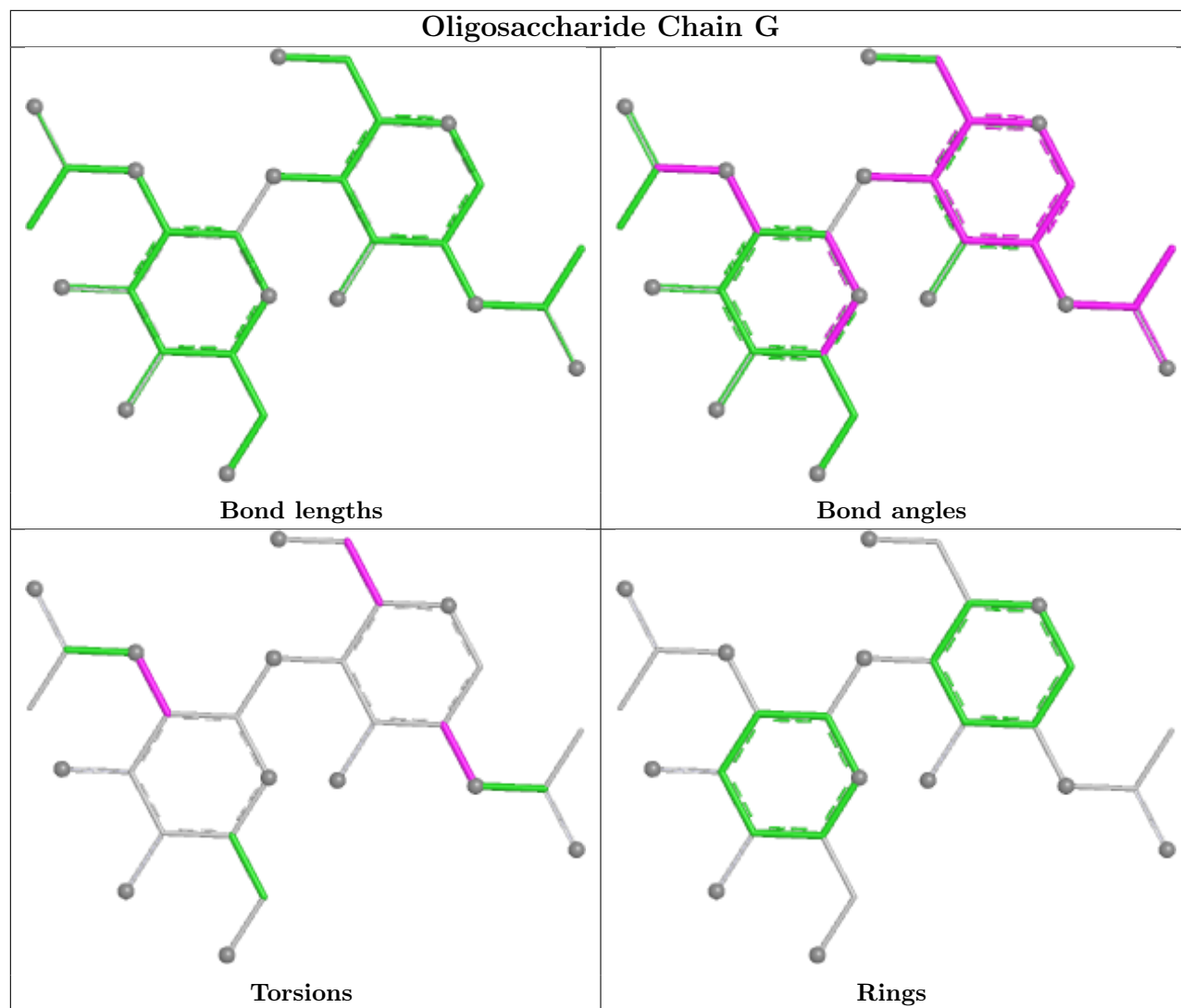
There are no ring outliers.

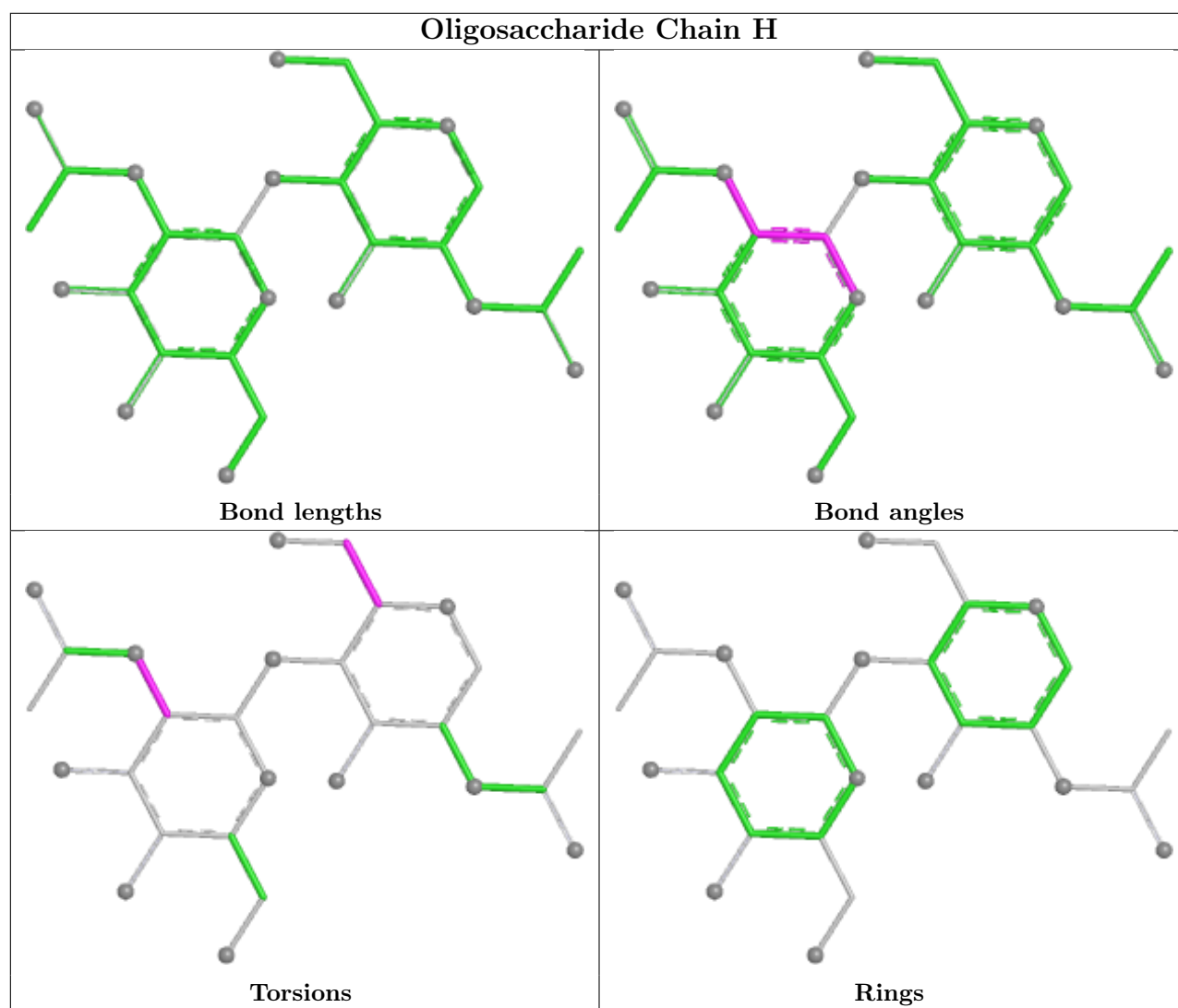
5 monomers are involved in 7 short contacts:

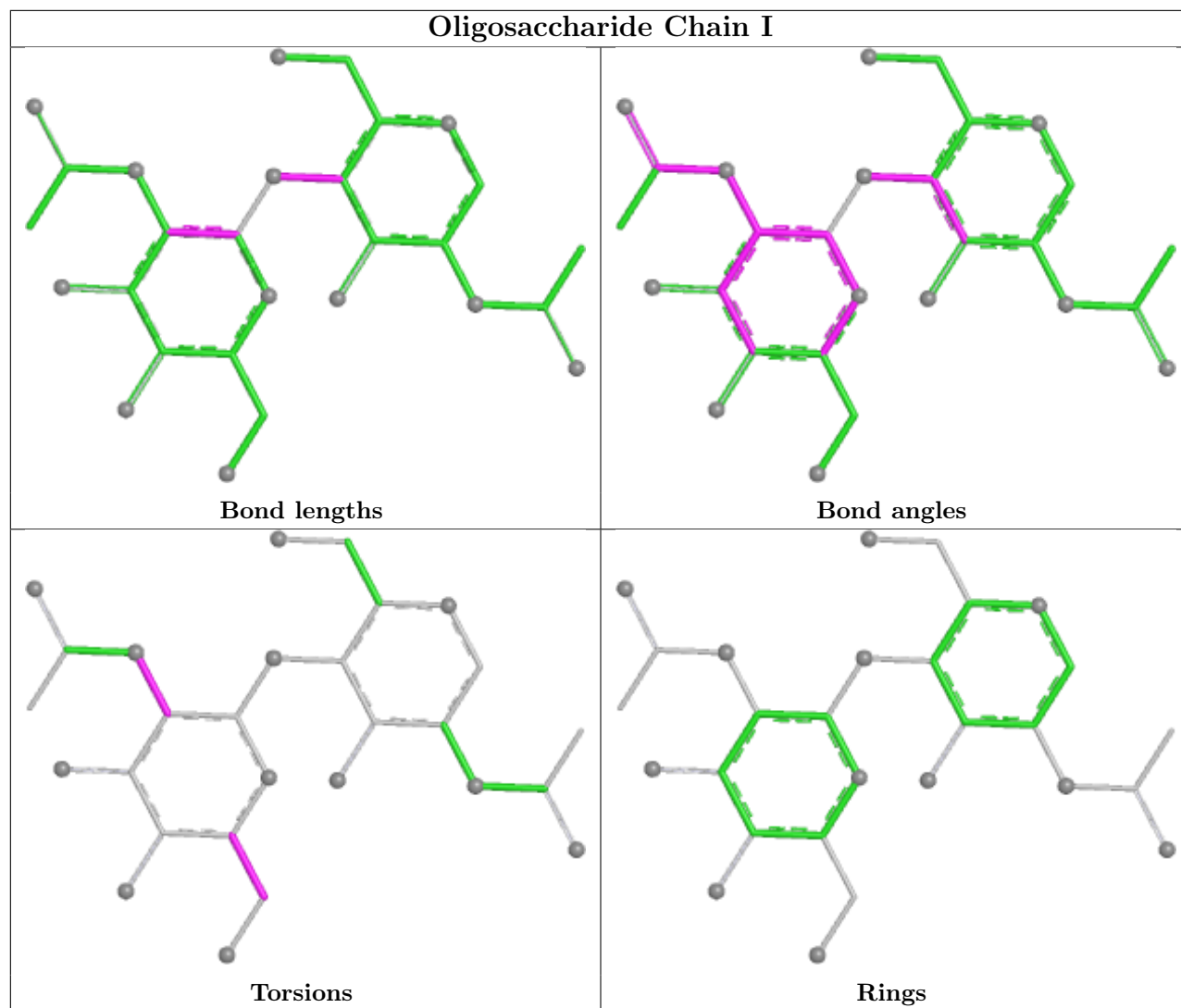
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
4	K	2	NAG	1	0
3	F	2	NAG	1	0
2	I	2	NAG	3	0
2	H	2	NAG	1	0

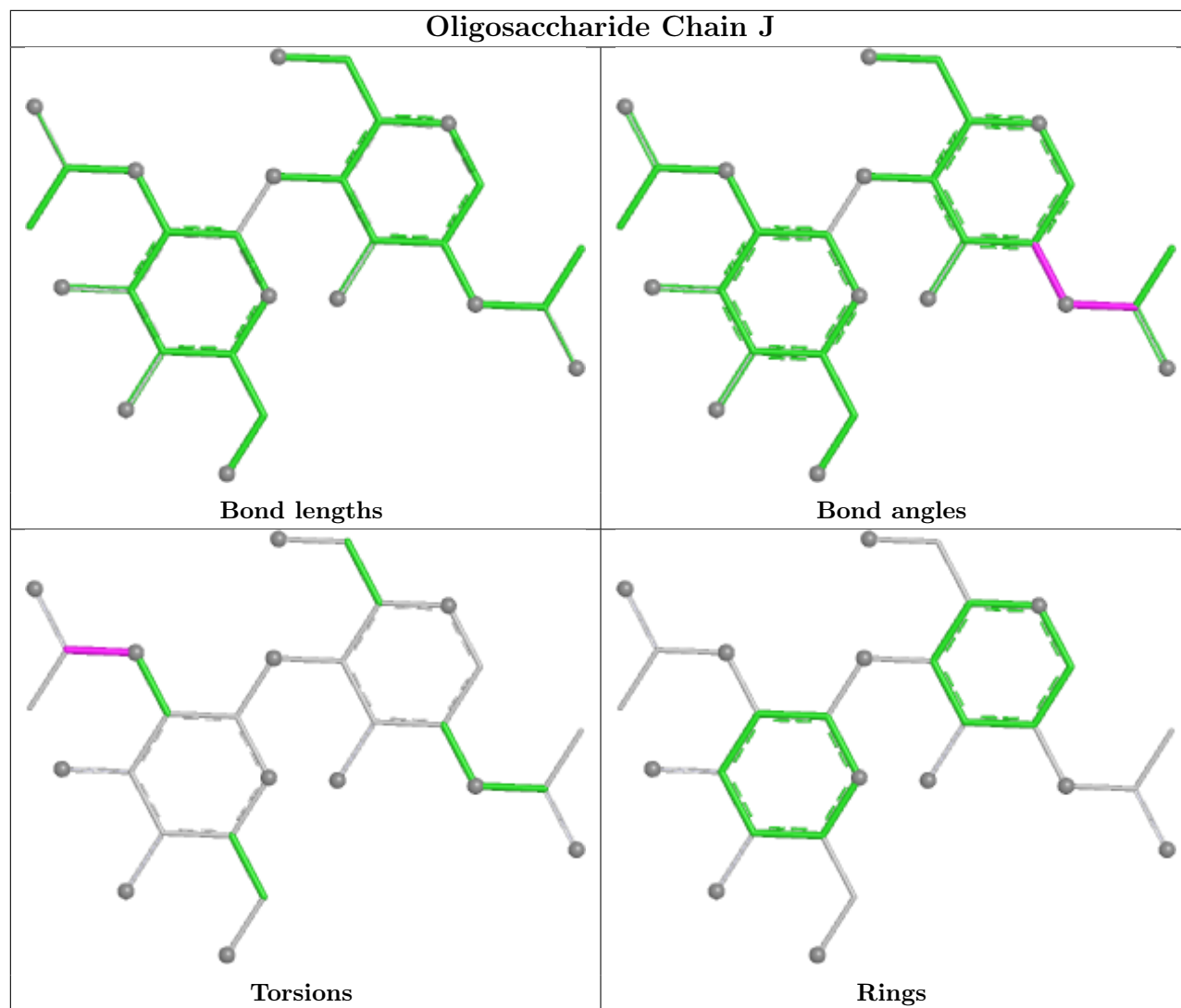
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

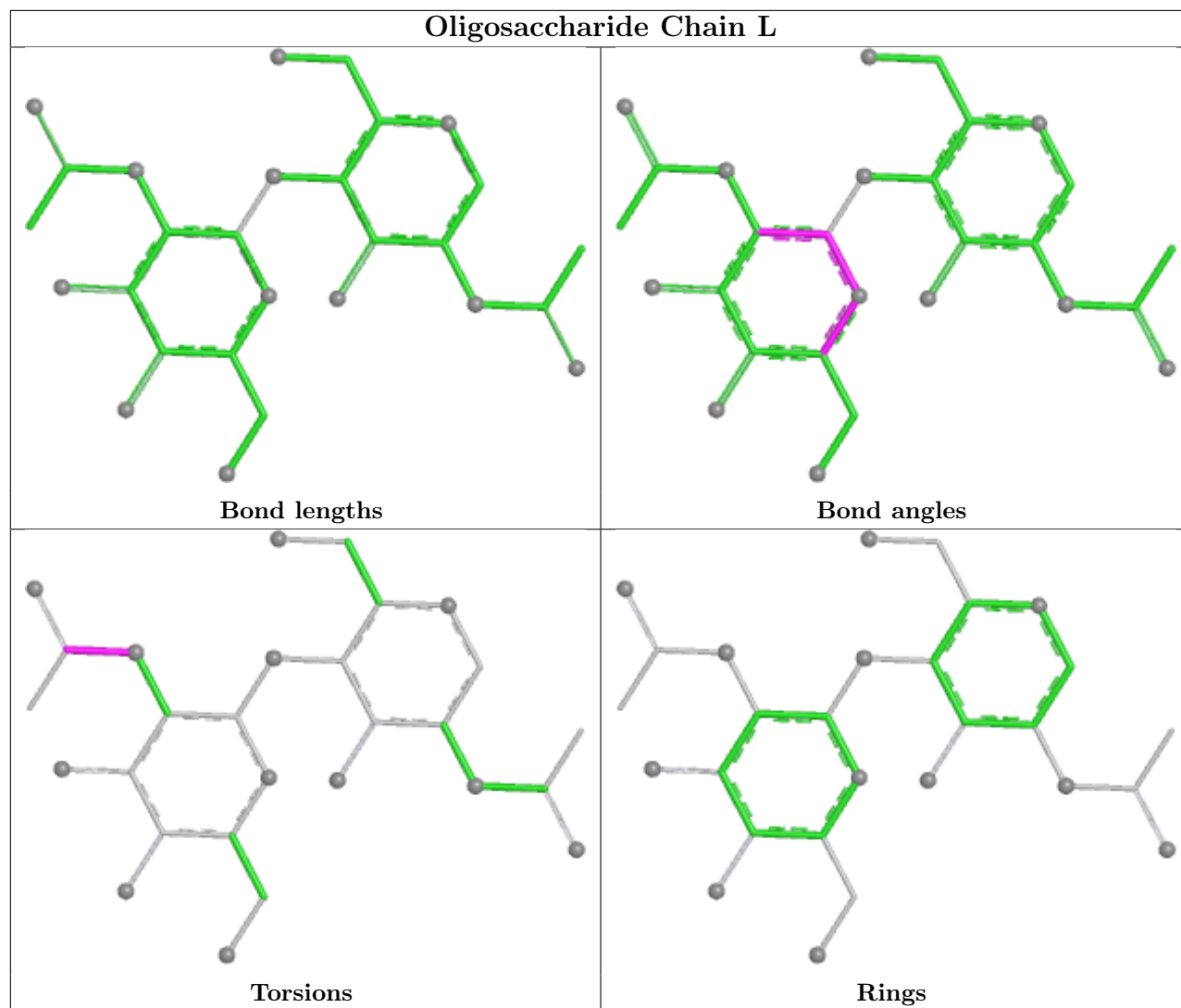


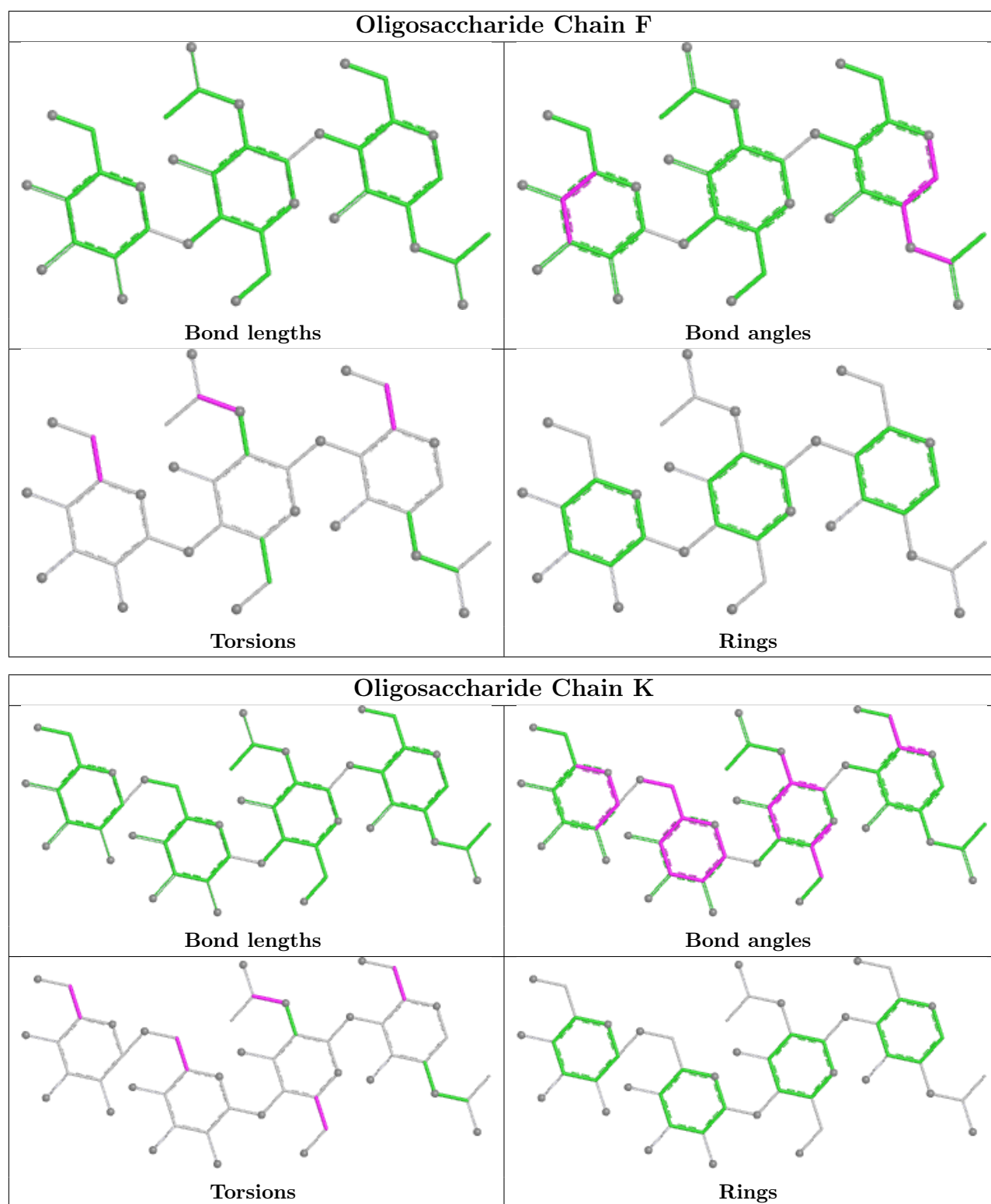












5.6 Ligand geometry [i](#)

22 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	D	2811	1	14,14,15	0.35	0	17,19,21	0.77	0
5	NAG	D	2191	1	14,14,15	0.34	0	17,19,21	0.58	0
5	NAG	B	851	1	14,14,15	0.32	0	17,19,21	1.23	2 (11%)
5	NAG	B	1501	1	14,14,15	0.40	0	17,19,21	1.27	2 (11%)
5	NAG	C	2191	1	14,14,15	0.29	0	17,19,21	0.82	0
5	NAG	A	2191	1	14,14,15	0.28	0	17,19,21	1.92	2 (11%)
5	NAG	C	1501	1	14,14,15	0.38	0	17,19,21	0.88	1 (5%)
5	NAG	C	3211	1	14,14,15	0.40	0	17,19,21	1.10	1 (5%)
5	NAG	A	851	1	14,14,15	0.30	0	17,19,21	2.51	5 (29%)
5	NAG	D	6851	1	14,14,15	0.43	0	17,19,21	1.62	3 (17%)
5	NAG	A	6851	1	14,14,15	0.38	0	17,19,21	1.82	3 (17%)
5	NAG	B	2811	1	14,14,15	0.34	0	17,19,21	0.83	0
5	NAG	D	1501	1	14,14,15	0.35	0	17,19,21	1.24	2 (11%)
5	NAG	D	5201	1	14,14,15	0.33	0	17,19,21	1.38	1 (5%)
5	NAG	B	3211	1	14,14,15	0.32	0	17,19,21	1.10	2 (11%)
5	NAG	C	5201	1	14,14,15	0.53	0	17,19,21	1.57	3 (17%)
5	NAG	A	5201	1	14,14,15	0.38	0	17,19,21	1.93	5 (29%)
5	NAG	C	2811	1	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
5	NAG	B	5201	1	14,14,15	0.50	0	17,19,21	3.87	6 (35%)
5	NAG	B	6851	1	14,14,15	0.30	0	17,19,21	1.05	2 (11%)
6	FUC	B	1502	-	10,10,11	0.41	0	14,14,16	1.14	1 (7%)
5	NAG	D	3211	1	14,14,15	0.27	0	17,19,21	1.30	3 (17%)

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	D	2811	1	-	0/6/23/26	0/1/1/1
5	NAG	B	851	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	2191	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	B	1501	1	-	4/6/23/26	0/1/1/1
5	NAG	C	2191	1	-	3/6/23/26	0/1/1/1
5	NAG	A	2191	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1501	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	C	3211	1	-	2/6/23/26	0/1/1/1
5	NAG	A	851	1	-	3/6/23/26	0/1/1/1
5	NAG	D	6851	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	6851	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	D	5201	1	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	B	2811	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1501	1	-	4/6/23/26	0/1/1/1
5	NAG	B	3211	1	-	0/6/23/26	0/1/1/1
5	NAG	C	5201	1	-	1/6/23/26	0/1/1/1
5	NAG	A	5201	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
5	NAG	B	5201	1	-	1/6/23/26	0/1/1/1
5	NAG	B	6851	1	-	0/6/23/26	0/1/1/1
6	FUC	B	1502	-	-	-	0/1/1/1
5	NAG	D	3211	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5201	NAG	C2-N2-C7	12.29	139.37	122.90
5	B	5201	NAG	C1-C2-N2	5.91	119.74	110.43
5	A	2191	NAG	C4-C3-C2	-5.72	102.63	111.02
5	A	851	NAG	C4-C3-C2	-5.72	102.64	111.02
5	A	851	NAG	C1-C2-N2	5.54	119.17	110.43
5	B	5201	NAG	C8-C7-N2	-5.09	107.68	116.12
5	D	5201	NAG	C2-N2-C7	4.60	129.07	122.90
5	A	6851	NAG	O5-C1-C2	-4.55	104.25	111.29
5	A	5201	NAG	C2-N2-C7	4.54	128.98	122.90
5	A	2191	NAG	O5-C1-C2	-4.22	104.77	111.29
5	B	5201	NAG	O7-C7-N2	3.94	128.94	121.98
5	C	3211	NAG	O5-C1-C2	-3.78	105.44	111.29
5	A	5201	NAG	C1-O5-C5	3.55	116.95	112.19
5	B	1501	NAG	C4-C3-C2	-3.55	105.82	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5201	NAG	C1-O5-C5	3.48	116.84	112.19
5	A	851	NAG	O5-C1-C2	-3.43	105.98	111.29
5	D	6851	NAG	C1-O5-C5	3.41	116.76	112.19
5	C	5201	NAG	C1-C2-N2	3.41	115.80	110.43
5	A	851	NAG	C1-O5-C5	3.35	116.68	112.19
5	A	851	NAG	C2-N2-C7	3.32	127.34	122.90
5	D	3211	NAG	C2-N2-C7	-3.27	118.52	122.90
5	A	5201	NAG	O5-C5-C6	3.20	113.89	107.66
5	B	5201	NAG	C4-C3-C2	3.18	115.67	111.02
5	A	6851	NAG	C4-C3-C2	-3.17	106.37	111.02
5	D	6851	NAG	C1-C2-N2	3.11	115.33	110.43
5	B	3211	NAG	C2-N2-C7	-3.07	118.78	122.90
5	D	3211	NAG	O5-C1-C2	-2.91	106.79	111.29
5	C	1501	NAG	C4-C3-C2	-2.90	106.76	111.02
5	A	5201	NAG	C4-C3-C2	-2.89	106.78	111.02
5	A	6851	NAG	C2-N2-C7	2.86	126.73	122.90
6	B	1502	FUC	C1-C2-C3	2.85	113.79	109.64
5	D	6851	NAG	O5-C1-C2	-2.73	107.06	111.29
5	B	3211	NAG	O5-C1-C2	-2.73	107.06	111.29
5	C	5201	NAG	C2-N2-C7	2.71	126.53	122.90
5	B	5201	NAG	C1-O5-C5	2.69	115.80	112.19
5	C	2811	NAG	C2-N2-C7	-2.63	119.37	122.90
5	B	6851	NAG	C4-C3-C2	-2.59	107.22	111.02
5	B	1501	NAG	O3-C3-C2	2.47	114.53	109.40
5	A	5201	NAG	O5-C1-C2	2.36	114.94	111.29
5	D	1501	NAG	O5-C1-C2	-2.30	107.74	111.29
5	B	851	NAG	C1-C2-N2	-2.28	106.84	110.43
5	B	851	NAG	C2-N2-C7	2.28	125.95	122.90
5	D	1501	NAG	C3-C4-C5	2.23	114.27	110.23
5	B	6851	NAG	O5-C1-C2	-2.14	107.98	111.29
5	D	3211	NAG	C4-C3-C2	-2.12	107.91	111.02

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	6851	NAG	C1
5	C	1501	NAG	C1
5	D	2191	NAG	C1
5	D	5201	NAG	C1
5	D	6851	NAG	C1

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	851	NAG	C1-C2-N2-C7
5	A	5201	NAG	C3-C2-N2-C7
5	A	6851	NAG	C3-C2-N2-C7
5	B	1501	NAG	C1-C2-N2-C7
5	B	5201	NAG	C1-C2-N2-C7
5	C	2191	NAG	C3-C2-N2-C7
5	C	5201	NAG	C1-C2-N2-C7
5	D	5201	NAG	C3-C2-N2-C7
5	B	851	NAG	C4-C5-C6-O6
5	A	851	NAG	O5-C5-C6-O6
5	B	851	NAG	O5-C5-C6-O6
5	B	1501	NAG	O5-C5-C6-O6
5	C	1501	NAG	O5-C5-C6-O6
5	A	2191	NAG	O5-C5-C6-O6
5	C	2811	NAG	O5-C5-C6-O6
5	B	2811	NAG	O5-C5-C6-O6
5	A	851	NAG	C4-C5-C6-O6
5	B	2811	NAG	C4-C5-C6-O6
5	C	3211	NAG	O5-C5-C6-O6
5	B	1501	NAG	C4-C5-C6-O6
5	C	2811	NAG	C4-C5-C6-O6
5	C	1501	NAG	C4-C5-C6-O6
5	D	3211	NAG	O5-C5-C6-O6
5	C	3211	NAG	C4-C5-C6-O6
5	D	1501	NAG	C4-C5-C6-O6
5	A	2191	NAG	C8-C7-N2-C2
5	A	2191	NAG	O7-C7-N2-C2
5	D	6851	NAG	C8-C7-N2-C2
5	D	6851	NAG	O7-C7-N2-C2
5	D	1501	NAG	O5-C5-C6-O6
5	C	2191	NAG	O5-C5-C6-O6
5	A	2191	NAG	C4-C5-C6-O6
5	D	2191	NAG	O5-C5-C6-O6
5	D	2191	NAG	C4-C5-C6-O6
5	A	5201	NAG	O5-C5-C6-O6
5	D	3211	NAG	C4-C5-C6-O6
5	C	2191	NAG	C4-C5-C6-O6
5	C	1501	NAG	C1-C2-N2-C7
5	D	1501	NAG	C1-C2-N2-C7
5	A	6851	NAG	O5-C5-C6-O6
5	C	1501	NAG	C3-C2-N2-C7
5	D	1501	NAG	C3-C2-N2-C7
5	B	1501	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	851	NAG	2	0
5	B	1501	NAG	4	0
5	C	2191	NAG	2	0
5	A	2191	NAG	1	0
5	A	851	NAG	5	0
5	A	6851	NAG	2	0
5	D	5201	NAG	4	0
5	C	5201	NAG	1	0
5	A	5201	NAG	2	0
5	B	5201	NAG	1	0
5	B	6851	NAG	2	0
6	B	1502	FUC	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.