



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:36 PM UTC

PDB ID : 1FZD / pdb_00001fzd
Title : STRUCTURE OF RECOMBINANT ALPHAEC DOMAIN FROM HUMAN FIBRINOGEN-420
Authors : Spraggon, G.; Applegate, D.; Everse, S.J.; Zhang, J.-Z.; Veerapandian, L.; Redman, C.; Doolittle, R.F.; Griening, G.
Deposited on : 1998-06-22
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

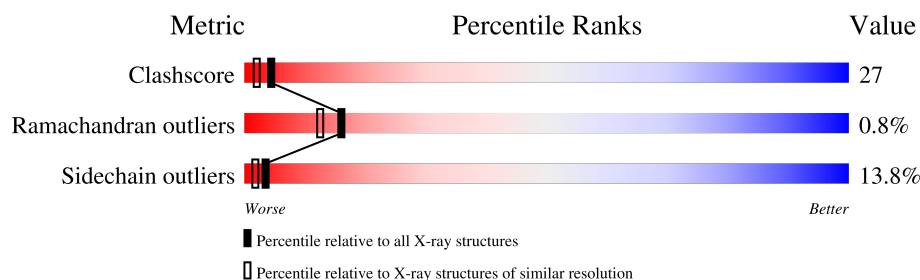
1 Overall quality at a glance

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)

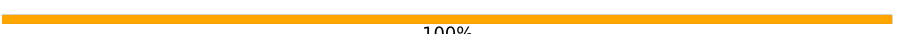
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	201	64% 24% 7% . .
1	B	201	67% 21% 7% . .
1	C	201	65% 25% 5% . .
1	D	201	68% 23% . . .
1	E	201	58% 28% 10% . .
1	F	201	61% 26% 9% . .
1	G	201	53% 33% 9% . .
1	H	201	47% 38% 11% . .

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Mol	Chain	Length	Quality of chain
2	I	6	 33% 67%
2	K	6	 17% 17% 67%
2	L	6	 50% 50%
3	J	6	 17% 83%
4	M	2	 100%
4	N	2	 50% 50%

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	MAN	I	3	X	-	X	-
2	MAN	I	4	-	-	X	-
2	MAN	I	6	-	-	X	-
2	MAN	K	3	X	-	X	-
2	MAN	K	4	-	-	X	-
2	NAG	K	5	-	-	X	-
2	MAN	K	6	X	-	-	-
2	NAG	L	1	-	X	-	-
2	MAN	L	4	-	-	X	-
2	NAG	L	5	-	-	X	-
2	MAN	L	6	X	-	-	-
3	NAG	J	1	-	X	-	-
3	MAN	J	3	X	-	X	-
3	MAN	J	4	-	-	X	-
3	NAG	J	5	-	-	X	-
4	NAG	M	1	-	X	X	-
6	NAG	G	10	-	-	X	-
6	NAG	G	11	-	-	X	-
6	NAG	H	10	-	-	X	-
6	NAG	H	11	-	-	X	-

2 Entry composition [i](#)

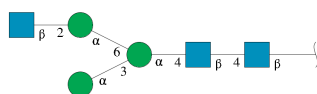
There are 7 unique types of molecules in this entry. The entry contains 13595 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FIBRINOGEN-420.

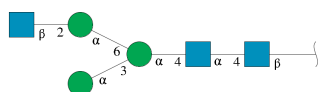
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	B	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	C	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	D	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	E	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	F	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	G	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	H	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
2	I	6	Total	C	N	O	0	0	0
			75	42	3	30			
2	K	6	Total	C	N	O	0	0	0
			75	42	3	30			
2	L	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	6	Total	C	N	O	0	0	0
			74	42	3	29			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	1	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

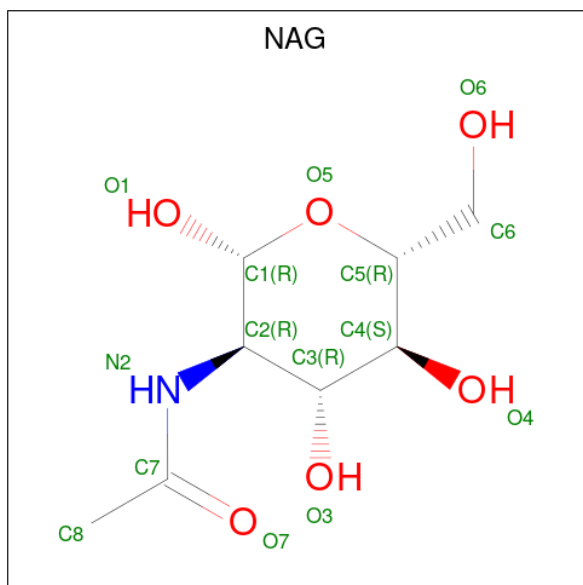
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	G	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	70	Total	O	0	0
			70	70		
7	B	76	Total	O	0	0
			76	76		
7	C	71	Total	O	0	0
			71	71		
7	D	74	Total	O	0	0
			74	74		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	52	Total 52	O 52	0	0
7	F	63	Total 63	O 63	0	0
7	G	56	Total 56	O 56	0	0
7	H	34	Total 34	O 34	0	0

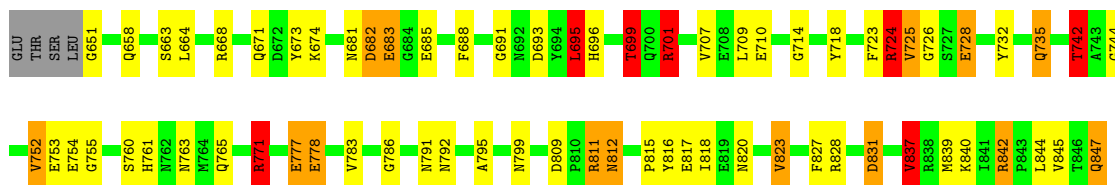
3 Residue-property plots

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

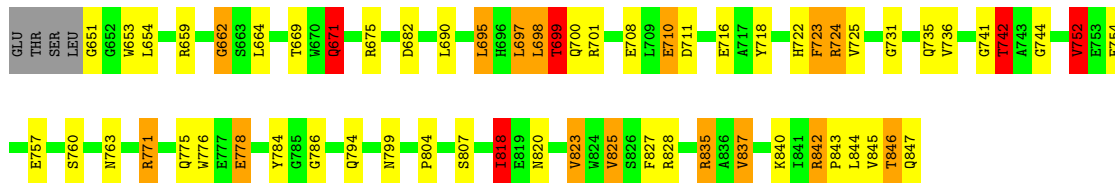
• Molecule 1: FIBRINOGEN-420

Chain A: 



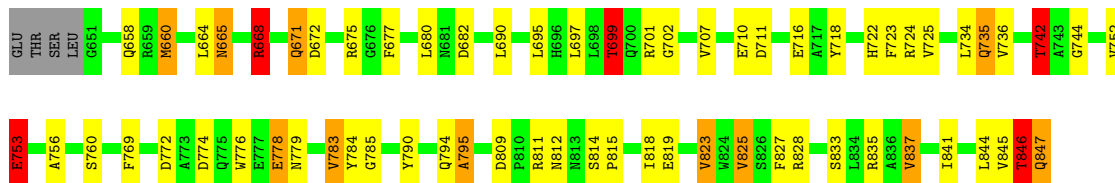
• Molecule 1: FIBRINOGEN-420

Chain B: 



• Molecule 1: FIBRINOGEN-420

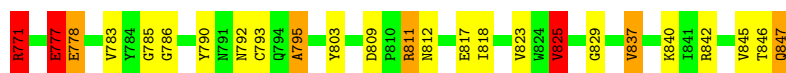
Chain C: 



• Molecule 1: FIBRINOGEN-420

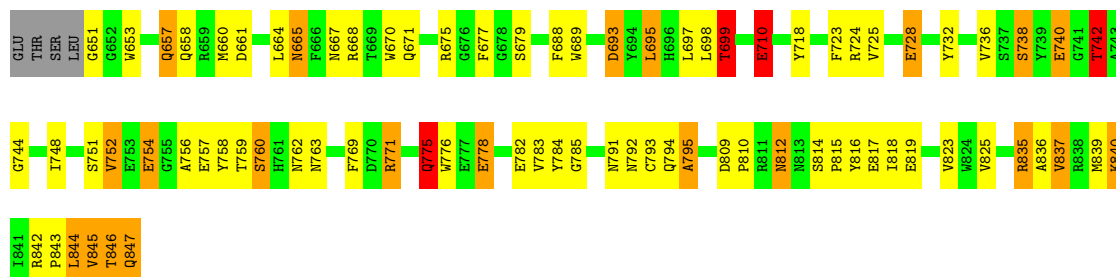
Chain D: 





• Molecule 1: FIBRINOGEN-420

Chain E: 58% 28% 10% ..



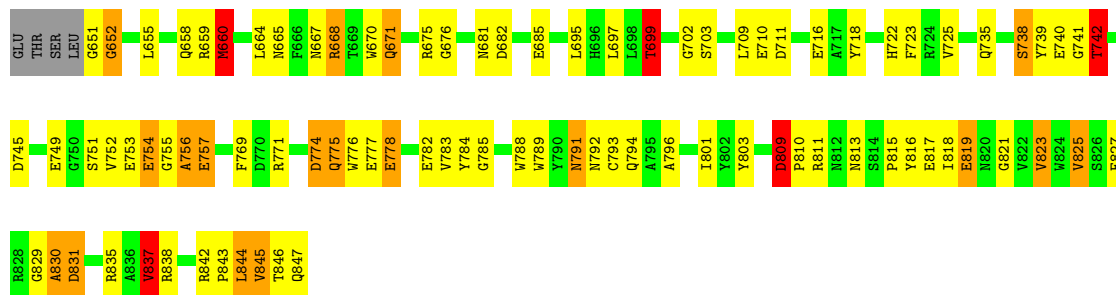
• Molecule 1: FIBRINOGEN-420

Chain F: 61% 26% 9% ..



• Molecule 1: FIBRINOGEN-420

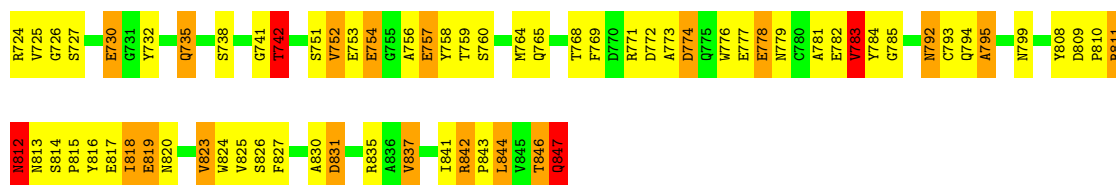
Chain G: 53% 33% 9% ..



• Molecule 1: FIBRINOGEN-420

Chain H: 47% 38% 11% ..





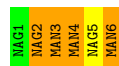
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 33% 67%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 17% 17% 67%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 17% 83%



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

Chain M: 100%



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

Chain N:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.25Å 105.18Å 71.14Å 104.60° 108.95° 71.47°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13595	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.03	0/1628	2.22	63/2208 (2.9%)
1	B	0.99	1/1628 (0.1%)	2.05	48/2208 (2.2%)
1	C	0.95	1/1628 (0.1%)	1.98	49/2208 (2.2%)
1	D	0.98	1/1628 (0.1%)	1.95	40/2208 (1.8%)
1	E	0.73	0/1628	1.75	36/2208 (1.6%)
1	F	0.71	0/1628	1.70	27/2208 (1.2%)
1	G	0.71	0/1628	1.71	27/2208 (1.2%)
1	H	0.64	0/1628	1.68	35/2208 (1.6%)
All	All	0.86	3/13024 (0.0%)	1.89	325/17664 (1.8%)

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	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	G	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	823	VAL	N-CA	5.29	1.52	1.46
1	D	744	GLY	CA-C	5.16	1.57	1.51
1	C	846	THR	N-CA	-5.09	1.39	1.46

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	ARG	CD-NE-CZ	36.75	175.85	124.40
1	B	771	ARG	CD-NE-CZ	27.74	163.23	124.40
1	C	845	VAL	CA-C-N	16.16	152.40	121.54
1	C	845	VAL	C-N-CA	16.16	152.40	121.54
1	C	742	THR	N-CA-CB	-14.30	92.11	110.98
1	B	840	LYS	CA-CB-CG	14.08	142.26	114.10
1	B	742	THR	N-CA-CB	-12.70	94.01	110.90
1	A	752	VAL	CB-CA-C	-12.52	95.64	112.04
1	D	742	THR	N-CA-CB	-12.40	94.41	110.90
1	D	825	VAL	CB-CA-C	-12.16	96.32	111.88
1	A	742	THR	N-CA-CB	-12.04	94.26	110.88
1	F	723	PHE	CA-CB-CG	11.85	125.65	113.80
1	C	723	PHE	CA-CB-CG	11.70	125.50	113.80
1	B	723	PHE	CA-CB-CG	11.66	125.47	113.80
1	A	823	VAL	N-CA-CB	-11.58	90.52	111.93
1	B	671	GLN	CB-CG-CD	11.33	131.86	112.60
1	D	840	LYS	CA-CB-CG	11.18	136.46	114.10
1	A	723	PHE	CA-CB-CG	11.04	124.83	113.80
1	H	723	PHE	CA-CB-CG	10.99	124.79	113.80
1	H	774	ASP	CA-CB-CG	10.81	123.41	112.60
1	G	723	PHE	CA-CB-CG	10.42	124.22	113.80
1	E	742	THR	N-CA-CB	-10.23	97.47	110.98
1	F	693	ASP	CA-CB-CG	-9.79	102.81	112.60
1	G	676	GLY	CA-C-O	-9.77	115.49	122.23
1	D	771	ARG	CD-NE-CZ	9.76	138.06	124.40
1	B	699	THR	N-CA-CB	-9.47	96.04	110.73
1	D	699	THR	N-CA-CB	-9.39	96.43	110.61
1	E	723	PHE	CA-CB-CG	9.32	123.12	113.80
1	H	658	GLN	CB-CG-CD	9.24	128.31	112.60
1	H	769	PHE	CA-CB-CG	9.22	123.03	113.80
1	B	752	VAL	CB-CA-C	-9.20	99.99	112.04
1	A	847	GLN	CB-CG-CD	9.17	128.18	112.60
1	F	676	GLY	CA-C-O	-9.13	116.28	122.22
1	G	742	THR	N-CA-CB	-9.11	98.78	110.90
1	E	785	GLY	N-CA-C	9.11	127.47	115.36
1	G	699	THR	N-CA-CB	-9.07	96.91	110.61
1	H	724	ARG	CD-NE-CZ	9.05	137.06	124.40
1	A	755	GLY	CA-C-O	8.96	130.03	122.24
1	B	827	PHE	CA-CB-CG	8.84	122.64	113.80
1	D	723	PHE	CA-CB-CG	8.80	122.60	113.80
1	A	688	PHE	N-CA-CB	-8.79	98.20	111.56
1	F	823	VAL	N-CA-CB	-8.75	93.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	668	ARG	NE-CZ-NH2	-8.72	111.35	119.20
1	A	792	ASN	OD1-CG-ND2	-8.63	113.97	122.60
1	A	701	ARG	CD-NE-CZ	8.63	136.48	124.40
1	D	825	VAL	N-CA-CB	8.46	119.90	110.51
1	A	765	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	F	837	VAL	N-CA-CB	-8.28	96.44	111.92
1	C	699	THR	N-CA-CB	-8.27	97.91	110.73
1	C	760	SER	CA-C-O	-8.24	111.93	121.16
1	E	699	THR	N-CA-CB	-8.23	98.54	110.65
1	G	823	VAL	N-CA-CB	-8.18	97.15	111.39
1	E	840	LYS	CA-CB-CG	8.18	130.46	114.10
1	B	818	ILE	N-CA-CB	-8.10	99.09	112.06
1	A	752	VAL	N-CA-CB	8.06	120.55	110.47
1	A	693	ASP	CA-CB-CG	-7.99	104.61	112.60
1	D	825	VAL	CA-C-O	-7.99	112.96	121.27
1	G	823	VAL	N-CA-C	7.91	119.87	108.48
1	B	823	VAL	N-CA-CB	-7.90	97.32	111.93
1	G	785	GLY	N-CA-C	7.90	124.09	114.69
1	E	688	PHE	N-CA-CB	-7.89	99.34	111.56
1	C	837	VAL	N-CA-CB	-7.87	96.67	111.62
1	A	778	GLU	CB-CG-CD	-7.81	99.32	112.60
1	A	671	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	A	699	THR	N-CA-CB	-7.78	98.87	110.61
1	A	688	PHE	CA-CB-CG	7.69	121.49	113.80
1	E	837	VAL	N-CA-CB	-7.66	97.07	111.62
1	E	688	PHE	CA-CB-CG	7.60	121.40	113.80
1	C	823	VAL	N-CA-CB	-7.60	96.18	111.91
1	A	681	ASN	CA-C-N	7.60	130.46	120.28
1	A	681	ASN	C-N-CA	7.60	130.46	120.28
1	E	847	GLN	CB-CG-CD	7.59	125.50	112.60
1	C	677	PHE	CA-CB-CG	7.59	121.39	113.80
1	G	791	ASN	CA-CB-CG	7.48	120.08	112.60
1	A	671	GLN	CB-CG-CD	7.45	125.27	112.60
1	D	825	VAL	N-CA-C	7.44	118.17	110.36
1	H	827	PHE	CA-CB-CG	7.43	121.23	113.80
1	H	722	HIS	N-CA-C	-7.42	97.50	109.96
1	E	769	PHE	CA-CB-CG	7.32	121.12	113.80
1	D	837	VAL	N-CA-CB	-7.31	97.72	111.62
1	E	823	VAL	N-CA-C	7.19	119.81	108.89
1	C	841	ILE	O-C-N	7.15	130.62	122.97
1	A	840	LYS	CA-CB-CG	7.13	128.36	114.10
1	B	711	ASP	CA-CB-CG	7.13	119.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	659	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	G	830	ALA	N-CA-C	7.08	121.17	112.54
1	F	701	ARG	CD-NE-CZ	7.07	134.30	124.40
1	D	660	MET	CA-C-O	-7.07	110.40	120.51
1	A	827	PHE	CA-CB-CG	7.05	120.85	113.80
1	F	742	THR	N-CA-CB	-7.02	101.72	110.98
1	A	791	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	H	722	HIS	CA-C-O	-6.96	112.91	120.92
1	A	658	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	G	754	GLU	N-CA-C	-6.90	106.06	114.75
1	G	809	ASP	CA-CB-CG	6.85	119.45	112.60
1	F	699	THR	N-CA-CB	-6.83	100.61	110.80
1	E	752	VAL	CB-CA-C	-6.80	102.96	112.14
1	C	668	ARG	CD-NE-CZ	6.78	133.90	124.40
1	D	785	GLY	N-CA-C	6.74	124.33	115.36
1	E	679	SER	CA-C-O	-6.70	114.06	121.23
1	C	823	VAL	N-CA-C	6.69	119.15	108.85
1	G	660	MET	CA-C-O	-6.69	110.95	120.51
1	D	837	VAL	CA-C-O	-6.68	114.31	121.19
1	B	736	VAL	CA-C-O	-6.62	113.60	121.28
1	C	690	LEU	CA-C-O	-6.62	113.87	120.82
1	C	835	ARG	CD-NE-CZ	6.59	133.62	124.40
1	C	779	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	B	659	ARG	NE-CZ-NH2	6.53	125.08	119.20
1	B	842	ARG	NE-CZ-NH2	6.53	125.07	119.20
1	A	847	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	G	722	HIS	N-CA-C	-6.48	99.96	110.20
1	D	786	GLY	CA-C-N	-6.46	115.30	121.57
1	D	786	GLY	C-N-CA	-6.46	115.30	121.57
1	C	772	ASP	CA-CB-CG	6.46	119.06	112.60
1	D	842	ARG	CD-NE-CZ	6.46	133.44	124.40
1	D	690	LEU	CA-C-O	-6.45	113.72	120.55
1	F	794	GLN	N-CA-C	6.41	118.59	108.79
1	B	799	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	B	731	GLY	CA-C-N	6.39	131.47	122.46
1	B	731	GLY	C-N-CA	6.39	131.47	122.46
1	A	837	VAL	N-CA-CB	-6.38	99.50	111.62
1	A	707	VAL	O-C-N	-6.38	115.95	123.03
1	F	766	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	760	SER	CA-C-O	-6.33	114.66	121.56
1	C	828	ARG	CD-NE-CZ	-6.33	115.54	124.40
1	C	785	GLY	N-CA-C	6.31	124.02	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	779	ASN	CA-C-N	6.29	128.62	120.44
1	C	779	ASN	C-N-CA	6.29	128.62	120.44
1	H	672	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	744	GLY	N-CA-C	-6.27	104.89	112.48
1	C	769	PHE	CA-CB-CG	6.27	120.07	113.80
1	E	752	VAL	N-CA-CB	6.25	119.04	110.54
1	A	761	HIS	CA-CB-CG	-6.25	107.55	113.80
1	G	722	HIS	N-CA-CB	6.25	119.49	110.06
1	C	671	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	C	845	VAL	CA-C-O	6.21	128.54	120.78
1	H	742	THR	N-CA-CB	-6.21	101.52	110.65
1	F	795	ALA	N-CA-C	-6.20	106.31	114.31
1	H	692	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	D	659	ARG	NH1-CZ-NH2	-6.18	111.27	119.30
1	C	845	VAL	O-C-N	-6.17	114.86	122.57
1	F	834	LEU	CA-C-N	6.16	128.81	120.44
1	F	834	LEU	C-N-CA	6.16	128.81	120.44
1	E	661	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	837	VAL	N-CA-CB	-6.13	99.97	111.62
1	E	665	ASN	CA-CB-CG	-6.13	106.47	112.60
1	H	837	VAL	N-CA-CB	-6.12	99.99	111.62
1	H	779	ASN	CA-CB-CG	6.11	118.71	112.60
1	F	770	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	825	VAL	CA-C-O	-6.10	114.60	120.95
1	D	738	SER	CB-CA-C	-6.08	103.25	111.89
1	E	740	GLU	CA-CB-CG	6.08	126.26	114.10
1	B	794	GLN	CA-C-O	-6.08	114.19	120.99
1	D	756	ALA	N-CA-C	6.06	117.89	111.28
1	G	796	ALA	CA-C-O	-6.05	114.04	121.06
1	C	794	GLN	N-CA-C	6.04	118.03	108.79
1	E	723	PHE	N-CA-CB	-6.01	100.36	111.13
1	H	681	ASN	CA-CB-CG	6.01	118.61	112.60
1	B	752	VAL	N-CA-CB	5.98	117.95	110.47
1	A	728	GLU	CB-CG-CD	5.98	122.76	112.60
1	C	723	PHE	N-CA-C	5.98	119.22	109.06
1	A	755	GLY	O-C-N	-5.97	115.70	122.56
1	G	827	PHE	CA-CB-CG	5.96	119.76	113.80
1	G	794	GLN	N-CA-C	5.96	118.18	108.76
1	C	707	VAL	CA-C-O	-5.94	114.21	120.57
1	E	795	ALA	N-CA-C	-5.94	106.64	114.31
1	B	742	THR	CB-CA-C	5.92	118.97	109.02
1	A	786	GLY	O-C-N	-5.90	118.54	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	763	ASN	CA-CB-CG	-5.89	106.71	112.60
1	C	756	ALA	CA-C-N	5.89	128.45	120.38
1	C	756	ALA	C-N-CA	5.89	128.45	120.38
1	A	663	SER	CA-C-N	5.89	131.13	123.00
1	A	663	SER	C-N-CA	5.89	131.13	123.00
1	E	794	GLN	N-CA-C	5.86	117.76	108.79
1	F	736	VAL	CA-C-O	-5.86	115.51	121.67
1	D	702	GLY	CA-C-O	-5.82	117.57	122.29
1	A	714	GLY	CA-C-O	-5.82	112.56	119.02
1	C	660	MET	CA-CB-CG	5.81	125.72	114.10
1	H	811	ARG	CD-NE-CZ	5.79	132.50	124.40
1	D	701	ARG	CD-NE-CZ	5.77	132.48	124.40
1	D	823	VAL	N-CA-C	5.77	118.27	108.86
1	C	790	TYR	N-CA-C	5.77	119.31	110.20
1	C	744	GLY	CA-C-O	-5.75	117.39	121.88
1	A	695	LEU	O-C-N	-5.74	116.03	122.12
1	C	742	THR	CB-CA-C	5.74	118.69	109.27
1	D	790	TYR	N-CA-C	5.73	118.58	110.50
1	E	653	TRP	CA-C-O	-5.71	114.66	121.11
1	H	812	ASN	CA-CB-CG	5.70	118.30	112.60
1	C	665	ASN	CA-C-O	-5.70	114.20	120.69
1	F	660	MET	CA-C-O	-5.68	112.39	120.51
1	B	823	VAL	CA-CB-CG2	5.67	120.04	110.40
1	D	742	THR	OG1-CB-CG2	5.66	120.63	109.30
1	A	725	VAL	CA-C-O	-5.66	114.05	120.67
1	C	753	GLU	CA-C-O	-5.66	115.07	120.90
1	B	828	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	D	777	GLU	CB-CG-CD	5.64	122.19	112.60
1	E	835	ARG	CD-NE-CZ	5.64	132.30	124.40
1	B	804	PRO	CA-C-O	-5.64	114.54	121.31
1	B	690	LEU	CA-C-O	-5.63	113.74	120.10
1	H	785	GLY	N-CA-C	5.63	122.53	115.21
1	H	799	ASN	OD1-CG-ND2	5.63	128.23	122.60
1	E	825	VAL	N-CA-C	5.62	116.27	110.36
1	H	660	MET	CA-C-O	-5.61	112.49	120.51
1	C	701	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	H	783	VAL	CB-CA-C	-5.60	104.73	112.24
1	B	835	ARG	CB-CG-CD	5.59	124.17	111.30
1	D	715	ASN	CA-CB-CG	-5.58	107.02	112.60
1	E	846	THR	CA-C-O	-5.56	115.09	121.82
1	D	742	THR	CB-CA-C	5.55	118.35	109.02
1	E	665	ASN	OD1-CG-ND2	5.55	128.15	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	667	ASN	CA-CB-CG	5.55	118.15	112.60
1	B	698	LEU	N-CA-C	5.55	119.15	112.38
1	C	846	THR	N-CA-C	5.51	122.55	110.80
1	F	840	LYS	CA-CB-CG	5.50	125.11	114.10
1	E	710	GLU	CA-CB-CG	5.50	125.10	114.10
1	G	777	GLU	N-CA-C	-5.50	105.83	112.54
1	A	682	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	823	VAL	CB-CA-C	5.45	119.41	110.69
1	D	700	GLN	CA-C-O	-5.45	114.74	120.63
1	B	722	HIS	CA-CB-CG	-5.45	108.36	113.80
1	E	775	GLN	CA-CB-CG	5.44	124.98	114.10
1	C	795	ALA	CA-C-O	5.43	124.80	118.77
1	G	837	VAL	N-CA-CB	-5.43	103.07	111.05
1	B	763	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	E	677	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	724	ARG	CA-C-N	-5.41	115.59	123.06
1	A	724	ARG	C-N-CA	-5.41	115.59	123.06
1	C	702	GLY	CA-C-O	-5.41	117.59	122.57
1	H	777	GLU	N-CA-C	-5.40	106.86	113.50
1	G	774	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	699	THR	CA-CB-CG2	5.39	119.66	110.50
1	A	837	VAL	CA-CB-CG1	5.38	119.55	110.40
1	E	699	THR	CA-C-N	5.38	128.23	120.38
1	E	699	THR	C-N-CA	5.38	128.23	120.38
1	B	763	ASN	CA-CB-CG	-5.37	107.23	112.60
1	G	711	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	668	ARG	CD-NE-CZ	5.36	131.91	124.40
1	A	691	GLY	CA-C-O	-5.36	115.01	121.98
1	B	735	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	B	701	ARG	CD-NE-CZ	5.35	131.89	124.40
1	C	671	GLN	CB-CG-CD	5.35	121.70	112.60
1	H	795	ALA	CA-C-O	5.35	124.70	118.97
1	A	811	ARG	CD-NE-CZ	5.34	131.88	124.40
1	H	699	THR	CA-CB-CG2	5.33	119.56	110.50
1	G	745	ASP	N-CA-C	5.33	117.86	109.39
1	A	828	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	C	833	SER	O-C-N	-5.32	117.26	123.27
1	A	831	ASP	OD1-CG-OD2	5.32	135.66	122.90
1	C	711	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	755	GLY	CA-C-N	5.31	127.83	120.29
1	A	755	GLY	C-N-CA	5.31	127.83	120.29
1	E	658	GLN	OE1-CD-NE2	-5.31	117.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	B	662	GLY	O-C-N	-5.29	115.32	122.35
1	B	818	ILE	CB-CA-C	5.29	119.53	110.38
1	A	777	GLU	CA-C-O	-5.28	113.11	119.49
1	C	828	ARG	CA-C-O	-5.27	112.96	119.18
1	B	708	GLU	O-C-N	5.26	129.47	123.31
1	B	744	GLY	N-CA-C	-5.26	106.11	112.48
1	D	771	ARG	NH1-CZ-NH2	-5.26	112.46	119.30
1	E	724	ARG	CD-NE-CZ	5.26	131.76	124.40
1	C	774	ASP	CA-C-O	-5.25	114.93	121.50
1	A	673	TYR	CA-C-O	5.25	126.01	119.97
1	B	700	GLN	CA-CB-CG	-5.25	103.60	114.10
1	E	657	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	760	SER	CA-CB-OG	-5.24	100.62	111.10
1	H	741	GLY	N-CA-C	5.24	117.95	110.46
1	F	697	LEU	N-CA-CB	5.24	117.56	109.91
1	D	795	ALA	N-CA-C	-5.23	107.56	114.31
1	H	794	GLN	N-CA-C	5.22	117.33	109.23
1	F	774	ASP	CA-CB-CG	5.21	117.81	112.60
1	F	823	VAL	CA-C-N	5.21	131.25	122.76
1	F	823	VAL	C-N-CA	5.21	131.25	122.76
1	D	656	ILE	N-CA-C	-5.21	108.21	113.47
1	H	823	VAL	N-CA-C	5.21	117.11	108.99
1	F	658	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	763	ASN	CA-CB-CG	-5.18	107.42	112.60
1	B	820	ASN	N-CA-CB	-5.18	102.67	111.17
1	B	823	VAL	O-C-N	-5.18	117.46	123.00
1	C	734	LEU	CA-C-O	-5.17	114.97	120.92
1	E	693	ASP	CA-CB-CG	-5.17	107.43	112.60
1	H	667	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	799	ASN	CB-CG-ND2	5.16	124.15	116.40
1	H	706	ARG	NE-CZ-NH2	-5.16	114.55	119.20
1	G	699	THR	CB-CA-C	5.15	118.87	110.17
1	G	829	GLY	CA-C-O	-5.15	118.12	122.29
1	A	839	MET	CG-SD-CE	-5.14	89.60	100.90
1	G	825	VAL	CA-C-O	-5.13	115.71	121.05
1	D	829	GLY	N-CA-C	-5.13	106.54	112.29
1	E	757	GLU	CA-C-O	-5.13	115.11	120.55
1	B	786	GLY	CA-C-N	-5.13	116.02	121.45
1	B	786	GLY	C-N-CA	-5.13	116.02	121.45
1	G	803	TYR	CA-C-O	-5.12	113.58	119.32
1	H	847	GLN	CB-CG-CD	5.12	121.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	657	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	C	779	ASN	CB-CG-ND2	5.12	124.08	116.40
1	D	744	GLY	N-CA-C	-5.12	106.29	112.48
1	H	792	ASN	CA-CB-CG	5.10	117.70	112.60
1	F	751	SER	CA-C-N	5.09	127.71	120.53
1	F	751	SER	C-N-CA	5.09	127.71	120.53
1	A	760	SER	CA-C-O	-5.09	115.12	120.92
1	D	723	PHE	N-CA-C	5.09	117.71	109.06
1	E	744	GLY	N-CA-C	-5.09	106.33	112.48
1	F	825	VAL	N-CA-C	5.08	115.70	110.36
1	B	754	GLU	N-CA-C	-5.08	106.93	113.23
1	A	695	LEU	CA-C-O	5.08	125.93	120.55
1	A	696	HIS	CA-C-O	5.07	126.14	120.82
1	A	753	GLU	CA-C-O	-5.07	115.48	120.70
1	C	827	PHE	CA-CB-CG	5.06	118.86	113.80
1	C	825	VAL	N-CA-C	5.06	116.39	110.62
1	A	842	ARG	NE-CZ-NH1	5.05	126.56	121.50
1	H	735	GLN	N-CA-CB	5.05	118.78	110.90
1	A	792	ASN	CA-CB-CG	5.05	117.65	112.60
1	B	741	GLY	N-CA-C	5.04	116.83	110.38
1	A	691	GLY	O-C-N	5.03	129.09	122.55
1	H	841	ILE	N-CA-C	5.03	117.25	108.95
1	B	710	GLU	OE1-CD-OE2	5.03	134.97	122.90
1	D	840	LYS	CA-C-N	-5.02	114.29	122.57
1	D	840	LYS	C-N-CA	-5.02	114.29	122.57
1	C	835	ARG	CA-C-O	-5.02	113.88	120.00
1	A	812	ASN	CA-CB-CG	5.01	117.61	112.60
1	F	697	LEU	CA-C-O	-5.01	115.73	121.00
1	D	731	GLY	CA-C-O	-5.01	113.61	119.72
1	G	769	PHE	CA-CB-CG	5.01	118.81	113.80
1	H	722	HIS	N-CA-CB	5.00	118.34	110.23

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	795	ALA	Mainchain
1	B	723	PHE	Mainchain
1	C	846	THR	Mainchain
1	D	666	PHE	Mainchain
1	D	803	TYR	Mainchain
1	E	738	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	E	840	LYS	Mainchain
1	G	825	VAL	Mainchain

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	1585	0	1421	29	0
1	B	1585	0	1418	43	0
1	C	1585	0	1420	32	5
1	D	1585	0	1421	34	1
1	E	1585	0	1422	59	0
1	F	1585	0	1421	108	0
1	G	1585	0	1422	111	0
1	H	1585	0	1422	118	6
2	I	75	0	64	19	0
2	K	75	0	64	27	0
2	L	75	0	64	12	0
3	J	74	0	58	30	0
4	M	28	0	26	19	0
4	N	28	0	25	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	G	28	0	26	13	0
6	H	28	0	26	17	0
7	A	70	0	0	4	0
7	B	76	0	0	8	0
7	C	71	0	0	0	0
7	D	74	0	0	7	0
7	E	52	0	0	5	0
7	F	63	0	0	3	0
7	G	56	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	34	0	0	6	0
All	All	13595	0	11720	654	6

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 27.

All (654) 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:F:758:TYR:CD1	1:F:792:ASN:HB3	1.25	1.63
3:J:1:NAG:C3	3:J:1:NAG:C2	1.76	1.61
1:E:667:ASN:HD21	4:M:1:NAG:C1	0.99	1.61
1:F:842:ARG:CZ	1:F:847:GLN:HB2	1.25	1.61
1:F:842:ARG:CZ	1:F:847:GLN:CB	1.83	1.56
1:F:843:PRO:HG2	1:F:846:THR:CG2	1.34	1.55
1:G:667:ASN:HD21	6:G:10:NAG:C1	0.97	1.55
1:H:667:ASN:HD21	6:H:10:NAG:C1	1.25	1.50
4:M:1:NAG:C4	4:M:1:NAG:O4	1.64	1.45
1:F:843:PRO:CG	1:F:846:THR:HG21	1.48	1.44
1:F:842:ARG:NE	1:F:847:GLN:HB2	1.15	1.43
4:M:1:NAG:C1	4:M:1:NAG:O5	1.68	1.42
1:F:843:PRO:CD	1:F:846:THR:HG21	1.51	1.39
1:G:671:GLN:NE2	1:G:675:ARG:HE	1.18	1.39
1:F:758:TYR:CD1	1:F:792:ASN:CB	2.07	1.36
2:K:3:MAN:H62	2:K:4:MAN:C5	1.53	1.33
1:H:846:THR:HB	1:H:847:GLN:OE1	1.21	1.33
1:F:842:ARG:CG	1:F:846:THR:HG23	1.58	1.32
4:M:1:NAG:O5	4:M:1:NAG:C5	1.77	1.31
1:F:842:ARG:HG2	1:F:846:THR:CG2	1.64	1.27
1:F:843:PRO:CG	1:F:846:THR:CG2	2.07	1.27
1:F:819:GLU:OE2	1:F:831:ASP:HB3	1.17	1.26
1:F:758:TYR:CE1	1:F:792:ASN:CB	2.20	1.25
1:H:818:ILE:HD13	1:H:819:GLU:N	1.51	1.24
1:E:846:THR:O	1:E:847:GLN:CG	1.85	1.24
1:F:842:ARG:NH1	1:F:847:GLN:CB	1.99	1.23
1:F:843:PRO:HG2	1:F:846:THR:CB	1.69	1.22
1:G:702:GLY:C	1:G:844:LEU:CD1	2.13	1.22
1:F:842:ARG:CZ	1:F:847:GLN:HB3	1.71	1.20
2:K:4:MAN:H4	2:K:5:NAG:C1	1.70	1.20
1:G:702:GLY:C	1:G:844:LEU:HD12	1.68	1.18
1:G:784:TYR:OH	1:G:818:ILE:HD11	1.44	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3:MAN:H61	3:J:4:MAN:C5	1.75	1.17
2:K:3:MAN:H61	2:K:4:MAN:H3	1.18	1.13
2:L:3:MAN:H61	2:L:4:MAN:C5	1.78	1.12
1:G:671:GLN:NE2	1:G:675:ARG:NE	1.96	1.12
3:J:3:MAN:H3	3:J:6:MAN:C3	1.72	1.12
1:E:846:THR:O	1:E:847:GLN:HG2	0.94	1.11
3:J:3:MAN:C6	3:J:4:MAN:H5	1.80	1.11
4:M:1:NAG:O4	4:M:2:NAG:H2	1.49	1.10
1:G:652:GLY:HA3	1:G:847:GLN:OE1	1.49	1.10
2:K:3:MAN:C6	2:K:4:MAN:H5	1.80	1.10
1:F:843:PRO:HD2	1:F:846:THR:HG21	1.28	1.09
2:L:3:MAN:H61	2:L:4:MAN:H5	1.21	1.09
1:F:843:PRO:O	1:F:846:THR:HG22	1.52	1.09
3:J:3:MAN:H3	3:J:6:MAN:H3	1.08	1.07
1:F:842:ARG:HG2	1:F:846:THR:HG23	1.10	1.06
1:F:758:TYR:CE1	1:F:792:ASN:HB2	1.84	1.06
1:F:819:GLU:OE2	1:F:831:ASP:CB	2.04	1.06
3:J:4:MAN:H4	3:J:5:NAG:C1	1.87	1.05
4:M:1:NAG:O4	4:M:2:NAG:C2	2.04	1.04
1:F:842:ARG:NH1	1:F:847:GLN:HB3	1.68	1.04
1:E:783:VAL:HG12	1:E:818:ILE:HD13	1.39	1.04
1:B:825:VAL:HB	7:B:492:HOH:O	1.54	1.03
1:F:842:ARG:CD	1:F:847:GLN:HB2	1.87	1.03
1:F:842:ARG:NH1	1:F:847:GLN:CG	2.20	1.03
1:G:782:GLU:OE2	1:G:816:TYR:OH	1.78	1.02
1:G:703:SER:N	1:G:844:LEU:HD11	1.74	1.02
1:E:710:GLU:HG3	1:E:836:ALA:HB3	1.41	1.02
1:B:843:PRO:HB2	1:B:846:THR:HG22	1.38	1.01
1:G:842:ARG:HD2	1:G:847:GLN:OXT	1.60	1.01
1:G:843:PRO:HD2	1:G:847:GLN:HB3	1.40	1.01
1:H:754:GLU:HG3	1:H:759:THR:HG21	1.41	1.01
1:F:758:TYR:CZ	1:F:792:ASN:ND2	2.28	1.00
1:F:842:ARG:HH11	1:F:847:GLN:HG3	1.26	1.00
1:D:846:THR:O	1:D:847:GLN:HG3	1.60	1.00
1:G:847:GLN:HA	7:G:438:HOH:O	1.61	1.00
1:H:818:ILE:HD13	1:H:819:GLU:H	0.84	1.00
1:F:842:ARG:NH1	1:F:847:GLN:HG3	1.76	0.99
1:F:842:ARG:HD2	1:F:846:THR:O	1.61	0.99
1:F:843:PRO:CD	1:F:846:THR:CG2	2.38	0.99
1:H:751:SER:CB	1:H:754:GLU:HB2	1.93	0.99
1:F:842:ARG:NH2	1:F:844:LEU:O	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:818:ILE:CD1	1:H:819:GLU:H	1.76	0.98
2:K:3:MAN:C6	2:K:4:MAN:H3	1.94	0.98
1:H:751:SER:HB3	1:H:754:GLU:HB2	1.42	0.98
1:F:845:VAL:O	1:F:847:GLN:N	1.98	0.97
1:G:703:SER:N	1:G:844:LEU:CD1	2.27	0.97
3:J:3:MAN:H61	3:J:4:MAN:H5	0.97	0.97
2:K:4:MAN:C4	2:K:5:NAG:C1	2.42	0.97
1:D:846:THR:O	1:D:847:GLN:CG	2.13	0.96
1:E:844:LEU:HD12	7:E:478:HOH:O	1.63	0.96
1:E:695:LEU:O	1:E:699:THR:HB	1.65	0.96
2:K:3:MAN:C6	2:K:4:MAN:C5	2.41	0.96
1:F:842:ARG:NE	1:F:847:GLN:CB	2.12	0.95
2:K:2:NAG:O3	2:K:3:MAN:H2	1.66	0.95
1:E:846:THR:C	1:E:847:GLN:HG2	1.91	0.95
1:F:681:ASN:HD21	1:F:685:GLU:CD	1.74	0.95
1:G:819:GLU:OE2	1:G:831:ASP:HB3	1.67	0.95
1:G:681:ASN:HD21	1:G:685:GLU:CG	1.79	0.94
1:H:782:GLU:HG3	6:H:10:NAG:O4	1.69	0.93
1:H:710:GLU:OE2	1:H:835:ARG:NH2	2.01	0.93
1:H:757:GLU:OE1	1:H:758:TYR:CE1	2.20	0.93
2:I:3:MAN:H62	2:I:3:MAN:O2	1.69	0.93
4:M:1:NAG:O5	4:M:1:NAG:C6	2.15	0.92
1:F:758:TYR:HD1	1:F:792:ASN:HB3	1.27	0.92
1:E:783:VAL:CG1	1:E:818:ILE:HD13	2.00	0.92
1:F:842:ARG:HH11	1:F:847:GLN:CG	1.80	0.92
1:D:783:VAL:HG13	1:D:818:ILE:HD13	1.51	0.92
1:F:843:PRO:HG2	1:F:846:THR:HB	1.47	0.92
1:D:699:THR:HG21	1:D:725:VAL:H	1.35	0.92
1:A:845:VAL:HG23	7:A:905:HOH:O	1.69	0.91
1:G:681:ASN:HD21	1:G:685:GLU:HG2	1.36	0.90
1:H:667:ASN:HD21	6:H:10:NAG:C2	1.82	0.90
1:G:681:ASN:ND2	1:G:685:GLU:HG2	1.86	0.90
1:G:784:TYR:OH	1:G:818:ILE:CD1	2.20	0.90
1:C:699:THR:HG21	1:C:725:VAL:H	1.36	0.90
1:E:844:LEU:CD1	7:E:478:HOH:O	2.17	0.90
1:H:846:THR:CB	1:H:847:GLN:OE1	2.16	0.90
1:G:842:ARG:CD	1:G:847:GLN:OXT	2.18	0.90
1:H:653:TRP:CE3	1:H:842:ARG:HG3	2.07	0.89
1:H:776:TRP:CE2	1:H:778:GLU:HB2	2.07	0.89
1:B:843:PRO:HB2	1:B:846:THR:CG2	2.01	0.89
1:G:776:TRP:HA	1:G:792:ASN:HD21	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3:MAN:H61	2:K:4:MAN:C3	2.01	0.88
1:C:783:VAL:HG13	1:C:818:ILE:HD13	1.56	0.88
1:H:818:ILE:CD1	1:H:819:GLU:N	2.35	0.88
1:F:842:ARG:HD3	1:F:847:GLN:HG2	1.56	0.88
1:F:842:ARG:CD	1:F:847:GLN:HG2	2.04	0.87
2:L:3:MAN:C6	2:L:4:MAN:H5	2.02	0.87
1:G:702:GLY:O	1:G:844:LEU:HD12	1.74	0.87
1:G:776:TRP:HA	1:G:792:ASN:ND2	1.88	0.87
1:A:818:ILE:HD11	1:A:820:ASN:HB3	1.54	0.86
1:G:671:GLN:HE22	1:G:675:ARG:NE	1.60	0.86
2:K:3:MAN:C6	2:K:4:MAN:C3	2.52	0.86
1:E:758:TYR:HB3	1:E:792:ASN:HB3	1.59	0.85
3:J:1:NAG:C2	3:J:1:NAG:O3	2.22	0.85
1:G:842:ARG:CB	1:G:847:GLN:OXT	2.24	0.84
3:J:1:NAG:C3	3:J:1:NAG:N2	2.40	0.84
1:A:815:PRO:HG2	1:A:816:TYR:CE1	2.11	0.84
2:I:6:MAN:O2	2:I:6:MAN:H61	1.78	0.84
1:H:718:TYR:H	1:H:742:THR:HG22	1.42	0.84
3:J:1:NAG:C3	3:J:1:NAG:C1	2.56	0.84
2:L:4:MAN:O5	2:L:5:NAG:C1	2.26	0.84
1:H:816:TYR:HB2	7:H:389:HOH:O	1.76	0.84
1:F:843:PRO:HG2	1:F:846:THR:HG22	1.58	0.83
1:G:681:ASN:ND2	1:G:685:GLU:CG	2.42	0.83
1:B:842:ARG:HE	1:B:847:GLN:HA	1.44	0.83
1:H:765:GLN:HE22	1:H:771:ARG:HH22	1.26	0.83
1:F:758:TYR:CE1	1:F:792:ASN:ND2	2.46	0.83
1:G:843:PRO:HD2	1:G:847:GLN:CB	2.09	0.83
4:M:1:NAG:HO4	4:M:2:NAG:H2	1.43	0.82
1:E:842:ARG:NH2	1:E:847:GLN:O	2.12	0.82
1:F:718:TYR:H	1:F:742:THR:HG22	1.44	0.82
1:C:724:ARG:HB2	1:C:735:GLN:HG3	1.62	0.82
3:J:4:MAN:C4	3:J:5:NAG:C1	2.54	0.82
1:E:699:THR:CG2	1:E:725:VAL:H	1.91	0.82
1:H:671:GLN:CD	1:H:675:ARG:HH21	1.88	0.82
1:H:754:GLU:HG3	1:H:759:THR:CG2	2.09	0.82
1:G:702:GLY:C	1:G:844:LEU:HD11	2.02	0.81
6:H:10:NAG:C4	6:H:11:NAG:C1	2.58	0.81
2:K:3:MAN:H62	2:K:4:MAN:H5	0.84	0.81
1:H:795:ALA:O	1:H:825:VAL:HG13	1.81	0.81
1:G:809:ASP:OD1	1:G:811:ARG:HG3	1.80	0.80
1:G:819:GLU:HG2	1:G:830:ALA:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:776:TRP:CD2	1:H:778:GLU:HB2	2.16	0.80
1:F:758:TYR:CG	1:F:792:ASN:HB3	2.14	0.80
1:H:752:VAL:HG23	1:H:753:GLU:H	1.46	0.80
1:C:795:ALA:O	1:C:825:VAL:HG23	1.81	0.80
1:H:751:SER:HB3	1:H:754:GLU:CB	2.11	0.80
2:L:3:MAN:C6	2:L:4:MAN:C5	2.57	0.80
2:K:4:MAN:O6	2:K:5:NAG:H61	1.80	0.80
1:G:671:GLN:HE21	1:G:675:ARG:HE	1.30	0.80
1:H:754:GLU:CG	1:H:759:THR:HG21	2.11	0.80
3:J:3:MAN:C3	3:J:6:MAN:H3	2.02	0.79
1:G:671:GLN:HE22	1:G:675:ARG:HE	0.80	0.79
1:E:776:TRP:CZ3	1:E:778:GLU:HB3	2.18	0.79
1:E:810:PRO:O	1:E:817:GLU:HA	1.83	0.79
2:I:3:MAN:H2	2:I:6:MAN:H3	1.66	0.78
1:G:842:ARG:HB2	1:G:847:GLN:OXT	1.83	0.78
1:G:846:THR:OG1	1:G:847:GLN:N	2.12	0.78
1:F:758:TYR:HE1	1:F:792:ASN:HB2	1.47	0.78
1:G:784:TYR:HH	1:G:818:ILE:HD11	1.45	0.77
1:C:671:GLN:HG2	1:C:675:ARG:HE	1.48	0.77
1:E:718:TYR:H	1:E:742:THR:HG22	1.48	0.77
1:F:681:ASN:ND2	1:F:685:GLU:OE2	2.17	0.77
1:D:783:VAL:CG1	1:D:818:ILE:HD13	2.13	0.77
1:G:749:GLU:O	1:G:756:ALA:HB2	1.86	0.76
1:F:842:ARG:CD	1:F:847:GLN:CB	2.61	0.76
1:A:724:ARG:HB3	1:A:735:GLN:HG3	1.66	0.76
1:F:842:ARG:HG3	1:F:846:THR:HG23	1.68	0.76
1:G:665:ASN:O	1:G:668:ARG:HD3	1.84	0.76
1:A:701:ARG:HG2	1:A:701:ARG:HH11	1.51	0.76
1:H:815:PRO:HG2	1:H:816:TYR:CE1	2.21	0.75
1:F:842:ARG:CD	1:F:846:THR:HG23	2.16	0.75
2:K:6:MAN:H62	2:K:6:MAN:O2	1.87	0.75
1:G:845:VAL:HG13	1:G:846:THR:H	1.51	0.74
1:G:842:ARG:HD2	1:G:847:GLN:C	2.11	0.74
1:D:722:HIS:CD2	7:D:494:HOH:O	2.39	0.74
1:G:718:TYR:H	1:G:742:THR:HG22	1.53	0.74
1:H:699:THR:CG2	1:H:725:VAL:H	2.00	0.74
1:F:758:TYR:CE1	1:F:792:ASN:HB3	1.91	0.74
1:A:699:THR:CG2	1:A:725:VAL:H	2.00	0.74
1:F:681:ASN:CG	1:F:685:GLU:HG2	2.13	0.73
1:G:671:GLN:HE21	1:G:675:ARG:NE	1.86	0.73
1:H:751:SER:OG	1:H:754:GLU:HB2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3:MAN:H3	2:I:6:MAN:O4	1.89	0.73
1:B:776:TRP:CE3	1:B:778:GLU:HB3	2.23	0.73
1:E:699:THR:HG21	1:E:725:VAL:H	1.52	0.73
1:F:845:VAL:O	1:F:847:GLN:OXT	2.06	0.73
1:B:842:ARG:NE	1:B:847:GLN:HA	2.03	0.72
2:K:4:MAN:C6	2:K:5:NAG:H5	2.19	0.72
6:G:10:NAG:O4	6:G:11:NAG:C1	2.38	0.72
6:H:10:NAG:H4	6:H:11:NAG:C1	2.20	0.72
4:M:1:NAG:O5	4:M:1:NAG:C2	2.33	0.72
2:I:3:MAN:O2	2:I:3:MAN:C6	2.38	0.72
1:H:667:ASN:ND2	6:H:10:NAG:C2	2.47	0.72
2:I:2:NAG:O3	2:I:6:MAN:H3	1.88	0.72
2:I:4:MAN:H4	2:I:5:NAG:C1	2.20	0.72
3:J:3:MAN:C6	3:J:4:MAN:C5	2.51	0.72
2:I:3:MAN:C2	2:I:6:MAN:H3	2.20	0.71
4:M:1:NAG:O5	4:M:1:NAG:H62	1.89	0.71
1:E:776:TRP:CE3	1:E:778:GLU:HB3	2.25	0.71
1:F:845:VAL:CG1	1:F:846:THR:N	2.53	0.71
2:K:4:MAN:H61	2:K:5:NAG:H5	1.73	0.71
1:F:699:THR:CG2	1:F:725:VAL:H	2.03	0.71
3:J:3:MAN:H61	3:J:4:MAN:C3	2.21	0.71
1:A:718:TYR:H	1:A:742:THR:HG22	1.54	0.71
1:D:699:THR:CG2	1:D:725:VAL:H	2.03	0.71
1:F:843:PRO:CG	1:F:846:THR:HG22	2.13	0.71
1:H:815:PRO:HG2	1:H:816:TYR:CD1	2.26	0.71
1:C:846:THR:OG1	1:C:847:GLN:N	2.20	0.71
1:B:653:TRP:CH2	1:B:842:ARG:NH1	2.58	0.70
1:F:699:THR:HG21	1:F:725:VAL:H	1.56	0.70
1:A:817:GLU:C	1:A:818:ILE:HG23	2.17	0.70
1:G:695:LEU:O	1:G:699:THR:HB	1.92	0.70
1:F:810:PRO:HG3	1:F:819:GLU:HG3	1.74	0.70
1:F:842:ARG:CD	1:F:847:GLN:CG	2.69	0.70
1:G:818:ILE:CG1	1:G:819:GLU:H	2.05	0.70
1:A:817:GLU:C	1:A:818:ILE:CG2	2.65	0.69
1:H:776:TRP:CZ3	1:H:778:GLU:HB3	2.27	0.69
1:G:681:ASN:CG	1:G:685:GLU:HG2	2.16	0.69
3:J:3:MAN:H61	3:J:4:MAN:H3	1.73	0.69
2:K:4:MAN:O6	2:K:5:NAG:C5	2.40	0.69
1:F:783:VAL:HG12	1:F:784:TYR:CD1	2.28	0.69
1:C:718:TYR:H	1:C:742:THR:HG22	1.57	0.69
1:B:784:TYR:OH	1:B:818:ILE:HD11	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:771:ARG:CD	7:D:427:HOH:O	2.40	0.69
1:F:842:ARG:CD	1:F:846:THR:O	2.38	0.69
1:H:823:VAL:HG23	7:H:379:HOH:O	1.92	0.69
1:D:777:GLU:HG2	1:D:778:GLU:OE1	1.93	0.69
1:G:843:PRO:CD	1:G:847:GLN:HB3	2.20	0.69
1:G:699:THR:CG2	1:G:725:VAL:H	2.06	0.68
1:C:809:ASP:OD2	1:C:812:ASN:OD1	2.11	0.68
1:F:843:PRO:C	1:F:846:THR:HG22	2.18	0.68
1:H:765:GLN:NE2	1:H:771:ARG:HH22	1.90	0.68
2:K:4:MAN:O6	2:K:5:NAG:C6	2.41	0.68
1:F:745:ASP:OD2	1:F:748:ILE:HB	1.94	0.67
1:G:755:GLY:O	1:G:757:GLU:N	2.27	0.67
2:K:6:MAN:O2	2:K:6:MAN:C6	2.43	0.67
1:A:771:ARG:NH2	7:A:917:HOH:O	2.20	0.67
1:C:671:GLN:HE21	1:C:675:ARG:NE	1.92	0.67
1:F:843:PRO:HG2	1:F:846:THR:HG21	1.13	0.67
1:F:842:ARG:CG	1:F:846:THR:CG2	2.39	0.67
6:G:10:NAG:C4	6:G:11:NAG:C1	2.73	0.66
1:G:658:GLN:HE21	1:G:838:ARG:HE	1.43	0.66
1:F:774:ASP:OD2	1:F:780:CYS:SG	2.53	0.66
1:G:776:TRP:CA	1:G:792:ASN:ND2	2.58	0.66
2:I:3:MAN:C1	2:I:6:MAN:O4	2.43	0.66
2:K:3:MAN:H62	2:K:4:MAN:C4	2.24	0.66
1:H:665:ASN:O	1:H:668:ARG:HD3	1.94	0.66
1:G:819:GLU:OE2	1:G:831:ASP:CB	2.43	0.66
1:B:651:GLY:N	1:B:847:GLN:OXT	2.29	0.65
1:E:844:LEU:HD12	1:E:845:VAL:H	1.61	0.65
1:C:710:GLU:HG2	1:C:716:GLU:HG2	1.78	0.65
1:F:775:GLN:HG3	1:F:791:ASN:OD1	1.96	0.65
1:F:845:VAL:C	1:F:847:GLN:H	1.96	0.65
1:F:843:PRO:HD2	1:F:846:THR:CG2	2.14	0.65
1:D:724:ARG:HB2	1:D:735:GLN:HG3	1.79	0.65
1:G:703:SER:N	1:G:844:LEU:HD12	2.03	0.65
1:G:842:ARG:HB2	1:G:847:GLN:HB3	1.79	0.65
1:F:681:ASN:ND2	1:F:685:GLU:CG	2.60	0.64
4:M:1:NAG:O4	4:M:1:NAG:C5	2.43	0.64
1:H:846:THR:O	1:H:847:GLN:HG2	1.98	0.64
1:F:681:ASN:HD21	1:F:685:GLU:CG	2.09	0.64
1:F:782:GLU:HG3	4:N:1:NAG:O4	1.97	0.64
1:H:782:GLU:CD	6:H:11:NAG:H2	2.23	0.64
1:E:775:GLN:CG	1:E:791:ASN:OD1	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:10:NAG:H4	6:G:11:NAG:O5	1.96	0.64
1:B:776:TRP:CE2	1:B:778:GLU:HB2	2.33	0.64
1:G:818:ILE:HG13	1:G:819:GLU:H	1.62	0.64
1:D:771:ARG:HD3	7:D:427:HOH:O	1.98	0.64
1:A:699:THR:HG21	1:A:725:VAL:H	1.63	0.63
1:F:758:TYR:CE1	1:F:792:ASN:CG	2.76	0.63
1:G:702:GLY:CA	1:G:844:LEU:CD1	2.76	0.63
1:G:775:GLN:O	1:G:792:ASN:ND2	2.31	0.63
1:E:748:ILE:O	1:E:760:SER:OG	2.15	0.63
1:C:671:GLN:NE2	1:C:675:ARG:CZ	2.61	0.63
1:F:681:ASN:OD1	1:F:685:GLU:HG2	1.99	0.63
1:G:740:GLU:HG2	1:G:741:GLY:N	2.12	0.63
1:C:699:THR:CG2	1:C:725:VAL:H	2.11	0.63
1:H:846:THR:HB	1:H:847:GLN:CD	2.17	0.63
1:H:699:THR:HG23	1:H:725:VAL:H	1.62	0.63
1:B:776:TRP:CZ3	1:B:778:GLU:HB3	2.34	0.63
1:E:756:ALA:O	1:E:760:SER:HB2	1.99	0.63
1:F:842:ARG:HD3	1:F:847:GLN:CG	2.27	0.63
1:A:818:ILE:CD1	1:A:820:ASN:HB3	2.28	0.62
3:J:1:NAG:C2	3:J:1:NAG:C4	2.75	0.62
1:C:671:GLN:NE2	1:C:675:ARG:NH2	2.47	0.62
1:F:681:ASN:ND2	1:F:685:GLU:HG2	2.14	0.62
3:J:5:NAG:C3	3:J:5:NAG:O7	2.47	0.62
1:G:652:GLY:CA	1:G:847:GLN:OE1	2.38	0.62
1:C:814:SER:HA	1:C:815:PRO:C	2.24	0.62
1:H:776:TRP:CZ2	1:H:778:GLU:HB2	2.34	0.62
1:B:699:THR:CG2	1:B:725:VAL:H	2.12	0.62
1:B:784:TYR:CZ	1:B:818:ILE:CD1	2.82	0.62
1:B:662:GLY:HA2	7:B:98:HOH:O	2.00	0.62
1:E:697:LEU:HD23	1:E:698:LEU:HD23	1.81	0.62
1:F:843:PRO:O	1:F:846:THR:CG2	2.40	0.62
1:D:783:VAL:O	1:D:818:ILE:HD11	1.98	0.62
1:A:695:LEU:O	1:A:699:THR:HB	2.01	0.61
1:D:783:VAL:CG1	1:D:818:ILE:CD1	2.78	0.61
1:H:809:ASP:OD1	1:H:811:ARG:HB2	2.00	0.61
6:G:10:NAG:H62	6:G:11:NAG:C1	2.31	0.61
1:B:784:TYR:OH	1:B:818:ILE:CD1	2.49	0.61
1:C:783:VAL:HG13	1:C:818:ILE:CD1	2.30	0.61
1:G:810:PRO:O	1:G:817:GLU:HG2	2.01	0.61
1:D:783:VAL:HG13	1:D:818:ILE:CD1	2.29	0.61
1:E:665:ASN:O	1:E:668:ARG:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:681:ASN:OD1	1:D:684:GLY:N	2.33	0.60
1:A:817:GLU:O	1:A:818:ILE:HG22	2.01	0.60
1:H:782:GLU:CG	6:H:10:NAG:O4	2.47	0.60
1:G:818:ILE:CG1	1:G:819:GLU:N	2.64	0.60
1:H:667:ASN:ND2	6:H:10:NAG:H2	2.16	0.60
1:H:842:ARG:NE	1:H:847:GLN:OE1	2.35	0.60
1:G:775:GLN:C	1:G:792:ASN:HD22	2.09	0.60
1:D:771:ARG:NE	7:D:427:HOH:O	2.32	0.60
1:D:795:ALA:O	1:D:825:VAL:HG22	2.01	0.60
1:B:843:PRO:CB	1:B:846:THR:CG2	2.77	0.60
1:G:819:GLU:OE2	1:G:831:ASP:OD2	2.18	0.60
1:G:671:GLN:NE2	1:G:675:ARG:CZ	2.63	0.60
1:H:842:ARG:CZ	1:H:847:GLN:OE1	2.50	0.60
1:H:754:GLU:CB	1:H:759:THR:HG21	2.32	0.59
1:A:815:PRO:HG2	1:A:816:TYR:CD1	2.37	0.59
1:B:842:ARG:HE	1:B:847:GLN:CA	2.13	0.59
2:L:4:MAN:O5	2:L:5:NAG:O5	2.18	0.59
1:H:653:TRP:CZ3	1:H:842:ARG:HG3	2.36	0.59
1:G:778:GLU:HG2	7:G:339:HOH:O	2.02	0.59
1:B:695:LEU:O	1:B:699:THR:HB	2.03	0.59
1:E:699:THR:HG23	1:E:725:VAL:H	1.67	0.59
1:A:710:GLU:OE1	7:A:916:HOH:O	2.17	0.59
1:A:844:LEU:HB2	7:A:905:HOH:O	2.02	0.59
1:H:792:ASN:N	1:H:793:CYS:HA	2.17	0.58
3:J:3:MAN:H4	3:J:4:MAN:H3	1.83	0.58
1:E:809:ASP:O	1:E:812:ASN:HB2	2.03	0.58
2:K:4:MAN:O6	2:K:5:NAG:H5	2.03	0.58
1:E:844:LEU:HG	7:E:271:HOH:O	2.03	0.58
1:G:783:VAL:HG12	1:G:818:ILE:HG21	1.84	0.58
2:I:2:NAG:O4	2:I:3:MAN:H62	2.03	0.58
1:B:718:TYR:H	1:B:742:THR:HG22	1.68	0.58
1:D:680:LEU:HD13	1:D:684:GLY:C	2.28	0.58
1:E:783:VAL:CG1	1:E:818:ILE:CD1	2.80	0.58
1:F:845:VAL:HG12	1:F:846:THR:H	1.69	0.58
2:K:3:MAN:O3	2:K:6:MAN:H62	2.03	0.58
2:K:4:MAN:O5	2:K:5:NAG:O5	2.21	0.58
1:G:681:ASN:OD1	1:G:685:GLU:HG2	2.03	0.57
1:H:784:TYR:CE1	1:H:818:ILE:HD12	2.38	0.57
1:E:845:VAL:HB	7:E:478:HOH:O	2.03	0.57
1:F:815:PRO:HG2	1:F:816:TYR:CE2	2.39	0.57
1:B:675:ARG:NH1	7:B:437:HOH:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:775:GLN:HB2	1:G:791:ASN:O	2.05	0.57
1:H:653:TRP:CZ2	1:H:842:ARG:HD3	2.39	0.57
1:E:775:GLN:HG3	1:E:791:ASN:OD1	2.04	0.57
1:H:810:PRO:HA	1:H:813:ASN:OD1	2.04	0.57
1:D:699:THR:HG21	1:D:725:VAL:N	2.13	0.57
1:D:846:THR:O	1:D:847:GLN:CB	2.52	0.57
1:G:681:ASN:HD21	1:G:685:GLU:CD	2.12	0.57
1:C:671:GLN:HE21	1:C:675:ARG:CZ	2.18	0.57
1:C:671:GLN:CD	1:C:675:ARG:HH21	2.13	0.56
1:E:784:TYR:CZ	1:E:818:ILE:HD11	2.40	0.56
1:G:755:GLY:C	1:G:757:GLU:H	2.12	0.56
1:G:652:GLY:O	1:G:847:GLN:HG3	2.06	0.56
1:G:784:TYR:CZ	1:G:818:ILE:CD1	2.89	0.56
6:G:10:NAG:C4	6:G:11:NAG:O5	2.54	0.56
1:G:782:GLU:HG3	6:G:10:NAG:O4	2.06	0.56
1:B:710:GLU:OE1	1:B:835:ARG:NH1	2.39	0.56
1:H:756:ALA:O	1:H:760:SER:HB3	2.06	0.56
1:H:846:THR:HG22	1:H:847:GLN:H	1.70	0.56
1:E:759:THR:HB	1:E:795:ALA:HB2	1.88	0.55
1:H:703:SER:HB2	1:H:842:ARG:O	2.06	0.55
1:D:722:HIS:CG	7:D:494:HOH:O	2.58	0.55
1:F:842:ARG:HH21	1:F:844:LEU:C	2.12	0.55
1:B:699:THR:HG23	1:B:724:ARG:HA	1.87	0.55
1:F:665:ASN:O	1:F:668:ARG:HD3	2.06	0.55
1:C:783:VAL:HG12	1:C:784:TYR:CD2	2.42	0.55
1:E:775:GLN:HG2	1:E:791:ASN:OD1	2.06	0.55
1:F:842:ARG:NH2	1:F:847:GLN:HB3	2.20	0.55
3:J:4:MAN:C5	3:J:5:NAG:H5	2.36	0.55
2:L:4:MAN:C1	2:L:5:NAG:O5	2.53	0.55
1:B:697:LEU:HD23	1:B:698:LEU:N	2.22	0.55
1:H:662:GLY:HA2	7:H:391:HOH:O	2.07	0.55
1:H:783:VAL:HG13	1:H:816:TYR:CD2	2.41	0.55
1:D:811:ARG:HA	1:D:817:GLU:HG2	1.87	0.54
1:H:823:VAL:HG22	1:H:824:TRP:N	2.21	0.54
1:H:656:ILE:HG22	1:H:690:LEU:HD22	1.89	0.54
6:H:10:NAG:C3	6:H:11:NAG:C1	2.85	0.54
1:H:810:PRO:HB2	1:H:817:GLU:O	2.07	0.54
1:H:846:THR:C	1:H:847:GLN:CG	2.81	0.54
6:H:10:NAG:H4	6:H:11:NAG:N2	2.22	0.54
2:L:4:MAN:H4	2:L:5:NAG:C1	2.38	0.54
1:A:683:GLU:HG3	1:A:685:GLU:CD	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:776:TRP:CZ3	1:H:778:GLU:CB	2.90	0.54
4:M:1:NAG:C4	4:M:1:NAG:HO4	2.07	0.54
3:J:4:MAN:O5	3:J:5:NAG:C5	2.56	0.54
1:A:817:GLU:O	1:A:818:ILE:CG2	2.55	0.54
6:H:10:NAG:O4	6:H:11:NAG:C1	2.55	0.54
2:L:4:MAN:C4	2:L:5:NAG:C1	2.86	0.54
1:G:671:GLN:NE2	1:G:675:ARG:HH21	2.07	0.53
1:H:717:ALA:HB1	1:H:742:THR:CG2	2.39	0.53
1:F:842:ARG:HD2	1:F:847:GLN:HG2	1.85	0.53
1:F:845:VAL:HG12	1:F:846:THR:N	2.24	0.53
1:F:845:VAL:N	7:F:314:HOH:O	2.38	0.53
1:H:776:TRP:CH2	1:H:778:GLU:CB	2.91	0.53
1:H:809:ASP:HB3	1:H:812:ASN:ND2	2.22	0.53
3:J:3:MAN:C4	3:J:4:MAN:H3	2.38	0.53
2:L:4:MAN:C5	2:L:5:NAG:C1	2.87	0.53
1:G:670:TRP:CZ3	1:G:771:ARG:HD2	2.44	0.52
2:I:2:NAG:O3	2:I:3:MAN:H2	2.09	0.52
1:B:710:GLU:HG2	1:B:716:GLU:HG2	1.90	0.52
1:A:699:THR:HG23	1:A:725:VAL:H	1.74	0.52
1:G:792:ASN:N	1:G:793:CYS:HA	2.22	0.52
1:E:651:GLY:C	1:E:842:ARG:HH12	2.17	0.52
1:H:670:TRP:CZ3	1:H:771:ARG:HD3	2.44	0.52
1:B:784:TYR:CZ	1:B:818:ILE:HD12	2.44	0.52
1:G:709:LEU:HD23	1:G:837:VAL:HG22	1.92	0.52
1:H:846:THR:C	1:H:847:GLN:HG2	2.34	0.52
1:H:818:ILE:HD13	1:H:819:GLU:CA	2.37	0.52
1:C:695:LEU:O	1:C:699:THR:HB	2.10	0.52
1:E:667:ASN:ND2	4:M:1:NAG:O5	2.42	0.52
6:G:10:NAG:H4	6:G:11:NAG:C1	2.39	0.52
1:H:816:TYR:CB	7:H:389:HOH:O	2.48	0.52
1:F:695:LEU:O	1:F:699:THR:HB	2.09	0.52
1:H:670:TRP:CE3	1:H:771:ARG:HD2	2.45	0.52
1:G:835:ARG:HD2	7:G:419:HOH:O	2.09	0.51
1:H:696:HIS:HD2	7:H:370:HOH:O	1.93	0.51
2:I:4:MAN:O3	2:I:5:NAG:N2	2.43	0.51
1:E:815:PRO:HG2	1:E:816:TYR:CE2	2.45	0.51
1:F:845:VAL:HG13	1:F:846:THR:N	2.25	0.51
1:D:751:SER:C	7:D:214:HOH:O	2.53	0.51
1:B:697:LEU:HD23	1:B:697:LEU:C	2.35	0.51
1:B:845:VAL:HG13	1:B:846:THR:N	2.25	0.51
1:E:810:PRO:O	1:E:817:GLU:CA	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:776:TRP:CE3	1:F:778:GLU:HB3	2.46	0.51
1:H:670:TRP:CD2	1:H:771:ARG:HD2	2.45	0.51
1:B:699:THR:HG21	1:B:725:VAL:H	1.76	0.51
1:B:825:VAL:CB	7:B:492:HOH:O	2.30	0.51
1:H:772:ASP:OD1	1:H:773:ALA:N	2.44	0.51
2:I:4:MAN:C4	2:I:5:NAG:C1	2.83	0.51
2:K:2:NAG:O3	2:K:3:MAN:C2	2.49	0.51
1:G:703:SER:CA	1:G:844:LEU:HD12	2.41	0.51
1:G:842:ARG:CG	1:G:847:GLN:OXT	2.58	0.51
1:B:842:ARG:NH1	7:B:113:HOH:O	2.43	0.51
2:K:3:MAN:C6	2:K:4:MAN:C4	2.87	0.50
1:C:671:GLN:CG	1:C:675:ARG:HE	2.21	0.50
1:F:842:ARG:NE	1:F:846:THR:C	2.70	0.50
1:G:671:GLN:NE2	1:G:675:ARG:NH2	2.60	0.50
6:G:10:NAG:O4	6:G:11:NAG:C2	2.60	0.50
1:A:709:LEU:HD23	1:A:837:VAL:HG22	1.94	0.50
1:E:728:GLU:HB2	1:E:732:TYR:CZ	2.46	0.50
1:F:819:GLU:CD	1:F:831:ASP:HB3	2.23	0.50
1:G:778:GLU:HB3	7:G:339:HOH:O	2.11	0.50
1:H:695:LEU:O	1:H:699:THR:HB	2.12	0.50
1:H:752:VAL:HG23	1:H:753:GLU:N	2.22	0.50
1:H:842:ARG:HD2	1:H:847:GLN:HE22	1.76	0.50
1:C:809:ASP:OD2	1:C:811:ARG:HB2	2.12	0.50
1:F:753:GLU:O	1:F:755:GLY:N	2.44	0.50
1:G:703:SER:CA	1:G:844:LEU:CD1	2.88	0.50
1:G:835:ARG:CD	7:G:419:HOH:O	2.59	0.50
3:J:4:MAN:O5	3:J:5:NAG:H5	2.12	0.50
1:F:845:VAL:C	1:F:847:GLN:N	2.60	0.50
1:G:699:THR:HG21	1:G:725:VAL:H	1.77	0.50
1:G:702:GLY:HA3	1:G:844:LEU:HD13	1.94	0.50
1:H:754:GLU:HB3	1:H:759:THR:HG21	1.92	0.50
1:H:652:GLY:O	1:H:842:ARG:HG2	2.12	0.50
1:H:671:GLN:CG	1:H:675:ARG:HH21	2.25	0.50
1:C:844:LEU:O	1:C:846:THR:HG22	2.12	0.49
1:D:792:ASN:N	1:D:793:CYS:HA	2.27	0.49
3:J:5:NAG:O7	3:J:5:NAG:O3	2.25	0.49
1:G:658:GLN:NE2	1:G:838:ARG:HE	2.08	0.49
1:G:751:SER:O	1:G:755:GLY:N	2.36	0.49
1:G:813:ASN:O	1:G:817:GLU:HG3	2.12	0.49
1:H:776:TRP:CE3	1:H:778:GLU:HB2	2.46	0.49
1:H:776:TRP:CE3	1:H:778:GLU:CB	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:GLY:HA2	1:A:842:ARG:HH12	1.77	0.49
1:G:699:THR:HG23	1:G:725:VAL:H	1.77	0.49
4:M:1:NAG:O4	4:M:1:NAG:H5	2.12	0.49
1:E:710:GLU:CG	1:E:836:ALA:HB3	2.29	0.49
6:G:10:NAG:O4	6:G:11:NAG:H2	2.13	0.49
1:B:843:PRO:CB	1:B:846:THR:HG22	2.28	0.49
1:D:846:THR:C	1:D:847:GLN:CG	2.80	0.49
1:H:823:VAL:CG2	1:H:824:TRP:N	2.76	0.49
1:F:843:PRO:CA	1:F:846:THR:HG22	2.43	0.48
1:D:717:ALA:HB1	1:D:742:THR:HG22	1.95	0.48
1:G:651:GLY:O	1:G:847:GLN:O	2.31	0.48
1:H:653:TRP:CH2	1:H:842:ARG:HD3	2.48	0.48
1:H:825:VAL:HG23	1:H:826:SER:N	2.28	0.48
1:D:811:ARG:HE	1:D:811:ARG:HB2	1.44	0.48
1:H:671:GLN:HG2	1:H:675:ARG:NH2	2.28	0.48
1:A:674:LYS:NZ	1:A:728:GLU:OE1	2.42	0.48
1:F:683:GLU:HB2	1:F:685:GLU:OE2	2.13	0.48
1:H:783:VAL:CG1	1:H:816:TYR:CD2	2.96	0.48
3:J:3:MAN:C6	3:J:4:MAN:H3	2.43	0.48
2:K:4:MAN:O5	2:K:5:NAG:C1	2.62	0.48
1:B:843:PRO:HD2	1:B:846:THR:HG23	1.95	0.48
1:E:776:TRP:CE2	1:E:778:GLU:HB2	2.48	0.48
1:G:819:GLU:HG2	1:G:830:ALA:C	2.38	0.48
1:H:670:TRP:CZ3	1:H:771:ARG:CD	2.97	0.48
1:C:665:ASN:O	1:C:668:ARG:HD3	2.14	0.48
1:D:783:VAL:HG12	1:D:818:ILE:CD1	2.44	0.48
1:E:651:GLY:N	1:E:847:GLN:O	2.47	0.48
1:H:783:VAL:HG12	1:H:816:TYR:CG	2.48	0.48
1:H:808:TYR:CE1	1:H:831:ASP:HA	2.49	0.48
1:C:752:VAL:HG13	1:C:753:GLU:N	2.28	0.48
1:H:813:ASN:HB3	1:H:816:TYR:O	2.13	0.48
1:B:776:TRP:CD2	1:B:778:GLU:CB	2.98	0.47
1:C:783:VAL:O	1:C:818:ILE:HD11	2.14	0.47
1:F:843:PRO:CG	1:F:846:THR:HB	2.31	0.47
1:H:705:LEU:O	1:H:720:GLU:HA	2.14	0.47
1:H:727:SER:OG	1:H:730:GLU:OE1	2.31	0.47
1:E:782:GLU:O	4:M:1:NAG:N2	2.31	0.47
1:E:792:ASN:N	1:E:793:CYS:HA	2.29	0.47
1:F:758:TYR:HD1	1:F:792:ASN:CB	1.98	0.47
1:G:755:GLY:C	1:G:757:GLU:N	2.73	0.47
2:K:4:MAN:C6	2:K:5:NAG:C5	2.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:759:THR:HB	1:H:795:ALA:HB2	1.96	0.47
1:C:671:GLN:CD	1:C:675:ARG:NH2	2.72	0.47
1:D:752:VAL:HA	7:D:214:HOH:O	2.14	0.47
1:G:702:GLY:HA3	1:G:844:LEU:CD1	2.43	0.47
1:G:771:ARG:O	1:G:771:ARG:HD3	2.15	0.47
1:H:764:MET:HE2	1:H:764:MET:HA	1.97	0.47
2:I:3:MAN:O4	2:I:4:MAN:H5	2.14	0.47
2:K:4:MAN:C5	2:K:5:NAG:C1	2.93	0.47
1:H:699:THR:HG21	1:H:725:VAL:H	1.78	0.47
1:G:815:PRO:HG2	1:G:816:TYR:CE1	2.50	0.47
6:H:10:NAG:H3	6:H:11:NAG:C1	2.45	0.47
1:C:699:THR:HG21	1:C:725:VAL:N	2.18	0.47
1:E:776:TRP:CH2	1:E:778:GLU:HB3	2.48	0.47
1:H:809:ASP:OD1	1:H:811:ARG:HD3	2.14	0.47
1:F:792:ASN:N	1:F:793:CYS:HA	2.26	0.46
6:H:10:NAG:C4	6:H:11:NAG:N2	2.78	0.46
6:H:10:NAG:H5	6:H:11:NAG:H82	1.95	0.46
1:E:667:ASN:CG	4:M:1:NAG:C1	2.77	0.46
1:E:699:THR:HG21	1:E:725:VAL:N	2.26	0.46
1:H:813:ASN:O	1:H:816:TYR:C	2.57	0.46
1:H:842:ARG:HB3	1:H:843:PRO:HD2	1.96	0.46
2:I:3:MAN:H3	2:I:6:MAN:C4	2.45	0.46
3:J:6:MAN:O2	3:J:6:MAN:C6	2.64	0.46
1:H:667:ASN:ND2	6:H:10:NAG:O5	2.43	0.46
1:B:752:VAL:HA	7:B:102:HOH:O	2.15	0.46
1:D:809:ASP:O	1:D:812:ASN:HB2	2.16	0.46
1:G:775:GLN:HB2	1:G:791:ASN:C	2.41	0.46
1:E:651:GLY:N	1:E:842:ARG:HH22	2.14	0.46
1:A:699:THR:HG21	1:A:725:VAL:N	2.31	0.46
1:G:658:GLN:HE21	1:G:838:ARG:NE	2.11	0.46
1:H:776:TRP:CZ2	1:H:778:GLU:CB	2.98	0.46
2:L:4:MAN:O5	2:L:5:NAG:C5	2.64	0.46
1:H:809:ASP:HB3	1:H:812:ASN:HD21	1.81	0.46
1:B:843:PRO:CG	1:B:846:THR:CG2	2.93	0.46
1:F:843:PRO:CB	1:F:846:THR:HG22	2.45	0.46
1:F:842:ARG:NH2	1:F:847:GLN:CB	2.65	0.46
1:B:669:THR:OG1	1:B:671:GLN:HG3	2.15	0.45
1:C:776:TRP:CZ3	1:C:778:GLU:HB3	2.52	0.45
1:F:668:ARG:NE	1:F:672:ASP:OD2	2.46	0.45
1:H:776:TRP:CH2	1:H:778:GLU:HB3	2.51	0.45
3:J:4:MAN:O5	3:J:5:NAG:O5	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:752:VAL:HG23	7:F:475:HOH:O	2.15	0.45
1:F:846:THR:OG1	7:F:487:HOH:O	2.20	0.45
2:I:3:MAN:C4	2:I:4:MAN:H5	2.47	0.45
1:E:657:GLN:HG3	1:E:689:TRP:CZ3	2.51	0.45
1:C:672:ASP:OD1	1:C:675:ARG:NH2	2.50	0.45
1:D:683:GLU:OE1	1:D:685:GLU:OE2	2.34	0.45
1:G:775:GLN:C	1:G:792:ASN:ND2	2.74	0.45
1:G:811:ARG:HA	1:G:817:GLU:HG2	1.99	0.45
2:L:4:MAN:O6	2:L:5:NAG:H5	2.16	0.45
1:G:703:SER:HA	1:G:844:LEU:HD12	1.97	0.45
1:H:717:ALA:HB1	1:H:742:THR:HG23	1.99	0.45
3:J:2:NDG:O3	3:J:3:MAN:C1	2.64	0.45
1:F:768:THR:O	1:F:769:PHE:C	2.59	0.45
1:E:783:VAL:HG11	1:E:818:ILE:CD1	2.46	0.45
1:C:658:GLN:CD	1:C:660:MET:HE3	2.42	0.45
1:H:816:TYR:CA	7:H:389:HOH:O	2.65	0.45
1:E:670:TRP:CZ3	1:E:771:ARG:HD3	2.53	0.44
1:E:843:PRO:HA	7:E:271:HOH:O	2.17	0.44
2:I:2:NAG:O3	2:I:6:MAN:C3	2.63	0.44
1:C:671:GLN:NE2	1:C:675:ARG:NE	2.63	0.44
1:H:670:TRP:CE3	1:H:771:ARG:CD	3.01	0.44
1:F:847:GLN:OE1	1:F:847:GLN:HA	2.18	0.44
1:B:776:TRP:CD2	1:B:778:GLU:HB3	2.52	0.44
1:F:776:TRP:CZ3	1:F:778:GLU:HB3	2.53	0.44
1:H:813:ASN:CB	1:H:816:TYR:O	2.65	0.44
1:G:843:PRO:CD	1:G:847:GLN:CB	2.89	0.44
1:C:722:HIS:O	1:C:736:VAL:HA	2.17	0.43
1:D:817:GLU:C	1:D:818:ILE:HG23	2.42	0.43
1:G:739:TYR:CG	1:G:740:GLU:N	2.86	0.43
1:E:844:LEU:HD12	1:E:845:VAL:N	2.30	0.43
1:F:758:TYR:CE2	1:F:792:ASN:ND2	2.77	0.43
1:G:845:VAL:HG22	1:G:846:THR:N	2.34	0.43
1:B:825:VAL:CG1	7:B:492:HOH:O	2.66	0.43
1:H:768:THR:C	1:H:781:ALA:CB	2.92	0.43
1:F:843:PRO:N	1:F:846:THR:CG2	2.80	0.43
1:G:816:TYR:HE1	6:G:10:NAG:O3	2.01	0.43
6:G:10:NAG:C6	6:G:11:NAG:C1	2.97	0.43
1:G:667:ASN:CG	6:G:10:NAG:C1	2.77	0.43
1:E:754:GLU:H	1:E:754:GLU:HG2	1.65	0.43
1:G:774:ASP:C	1:G:775:GLN:HE21	2.27	0.43
1:H:784:TYR:HE1	1:H:818:ILE:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:GLY:CA	1:A:842:ARG:HH12	2.32	0.42
1:H:810:PRO:O	1:H:817:GLU:HA	2.18	0.42
3:J:3:MAN:H5	3:J:6:MAN:H3	2.00	0.42
1:H:671:GLN:HG2	1:H:675:ARG:HH21	1.82	0.42
1:B:845:VAL:CG1	1:B:846:THR:N	2.83	0.42
1:G:788:TRP:CG	1:G:789:TRP:H	2.36	0.42
1:H:717:ALA:HA	1:H:742:THR:CG2	2.49	0.42
1:H:718:TYR:N	1:H:742:THR:HG22	2.21	0.42
1:A:809:ASP:O	1:A:812:ASN:HB2	2.19	0.42
1:H:809:ASP:OD1	1:H:811:ARG:CB	2.66	0.42
1:G:660:MET:HB2	7:G:321:HOH:O	2.19	0.42
4:M:1:NAG:C1	4:M:1:NAG:C5	2.94	0.42
1:F:795:ALA:O	1:F:825:VAL:HB	2.19	0.42
1:H:842:ARG:CZ	1:H:847:GLN:CD	2.93	0.42
1:A:701:ARG:HG2	1:A:701:ARG:NH1	2.22	0.42
3:J:4:MAN:C1	3:J:5:NAG:O5	2.67	0.42
1:F:717:ALA:HB1	1:F:742:THR:HG23	2.01	0.42
2:I:3:MAN:C1	2:I:6:MAN:H3	2.49	0.42
1:E:667:ASN:ND2	4:M:1:NAG:C2	2.67	0.42
1:E:651:GLY:CA	1:E:842:ARG:HH12	2.33	0.41
1:G:842:ARG:HB3	1:G:847:GLN:OXT	2.15	0.41
1:H:726:GLY:O	1:H:732:TYR:HA	2.20	0.41
1:B:842:ARG:HE	1:B:847:GLN:CB	2.32	0.41
1:H:752:VAL:O	1:H:753:GLU:C	2.64	0.41
1:E:657:GLN:HB3	1:E:839:MET:HB2	2.02	0.41
1:F:671:GLN:O	1:F:675:ARG:HG3	2.19	0.41
1:D:809:ASP:OD2	1:D:811:ARG:CZ	2.68	0.41
1:G:738:SER:O	1:G:739:TYR:C	2.64	0.41
4:M:1:NAG:C4	4:M:1:NAG:O5	2.58	0.41
1:A:724:ARG:O	1:A:735:GLN:HG2	2.21	0.41
1:H:819:GLU:HB3	1:H:830:ALA:O	2.20	0.41
6:H:11:NAG:H61	6:H:11:NAG:O3	2.20	0.41
1:E:842:ARG:CZ	1:E:847:GLN:HA	2.51	0.41
1:E:846:THR:O	1:E:847:GLN:CB	2.60	0.41
1:G:778:GLU:CB	7:G:339:HOH:O	2.69	0.41
1:F:739:TYR:CG	1:F:740:GLU:N	2.88	0.40
1:G:801:ILE:O	1:G:821:GLY:HA2	2.21	0.40
2:I:3:MAN:O4	2:I:4:MAN:C5	2.68	0.40
1:B:843:PRO:O	1:B:844:LEU:C	2.63	0.40
1:E:762:ASN:O	1:E:763:ASN:HB2	2.22	0.40
1:B:775:GLN:NE2	7:B:106:HOH:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:751:SER:HB2	1:D:825:VAL:HG21	2.02	0.40
1:G:818:ILE:HG12	1:G:819:GLU:H	1.84	0.40
3:J:3:MAN:C6	3:J:4:MAN:C3	2.96	0.40
1:A:726:GLY:O	1:A:732:TYR:HA	2.21	0.40
1:B:776:TRP:CE2	1:B:778:GLU:CB	3.02	0.40
1:H:818:ILE:HG23	1:H:820:ASN:HB3	2.04	0.40
1:H:842:ARG:HD2	1:H:847:GLN:NE2	2.36	0.40

All (6) 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:C:847:GLN:OXT	1:H:678:GLY:O[1_445]	0.94	1.26
1:D:847:GLN:O	1:H:722:HIS:ND1[1_545]	1.73	0.47
1:C:847:GLN:C	1:H:678:GLY:O[1_445]	1.88	0.32
1:C:847:GLN:NE2	1:H:680:LEU:O[1_445]	2.03	0.17
1:C:847:GLN:OXT	1:H:678:GLY:C[1_445]	2.13	0.07
1:C:680:LEU:O	1:H:847:GLN:O[1_445]	2.18	0.02

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	195/201 (97%)	184 (94%)	11 (6%)	0	100	100
1	B	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
1	C	195/201 (97%)	184 (94%)	10 (5%)	1 (0%)	24	22
1	D	195/201 (97%)	183 (94%)	11 (6%)	1 (0%)	24	22
1	E	195/201 (97%)	187 (96%)	7 (4%)	1 (0%)	24	22
1	F	195/201 (97%)	181 (93%)	10 (5%)	4 (2%)	5	2
1	G	195/201 (97%)	176 (90%)	16 (8%)	3 (2%)	8	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	195/201 (97%)	175 (90%)	17 (9%)	3 (2%)	8	4
All	All	1560/1608 (97%)	1458 (94%)	89 (6%)	13 (1%)	16	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	846	THR
1	G	756	ALA
1	C	846	THR
1	F	754	GLU
1	H	652	GLY
1	F	753	GLU
1	G	652	GLY
1	H	752	VAL
1	F	661	ASP
1	H	844	LEU
1	E	660	MET
1	G	845	VAL
1	D	755	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	159/163 (98%)	139 (87%)	20 (13%)	4	2
1	B	159/163 (98%)	141 (89%)	18 (11%)	5	3
1	C	159/163 (98%)	144 (91%)	15 (9%)	8	6
1	D	159/163 (98%)	140 (88%)	19 (12%)	5	3
1	E	159/163 (98%)	133 (84%)	26 (16%)	2	1
1	F	159/163 (98%)	132 (83%)	27 (17%)	2	1
1	G	159/163 (98%)	133 (84%)	26 (16%)	2	1
1	H	159/163 (98%)	135 (85%)	24 (15%)	3	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1272/1304 (98%)	1097 (86%)	175 (14%)	3 2

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	664	LEU
1	A	682	ASP
1	A	683	GLU
1	A	695	LEU
1	A	699	THR
1	A	701	ARG
1	A	724	ARG
1	A	735	GLN
1	A	742	THR
1	A	752	VAL
1	A	754	GLU
1	A	771	ARG
1	A	777	GLU
1	A	778	GLU
1	A	783	VAL
1	A	811	ARG
1	A	823	VAL
1	A	831	ASP
1	A	837	VAL
1	A	847	GLN
1	B	654	LEU
1	B	664	LEU
1	B	671	GLN
1	B	682	ASP
1	B	695	LEU
1	B	697	LEU
1	B	699	THR
1	B	724	ARG
1	B	742	THR
1	B	752	VAL
1	B	757	GLU
1	B	771	ARG
1	B	778	GLU
1	B	807	SER
1	B	818	ILE
1	B	823	VAL
1	B	837	VAL

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Mol	Chain	Res	Type
1	B	846	THR
1	C	664	LEU
1	C	668	ARG
1	C	682	ASP
1	C	697	LEU
1	C	699	THR
1	C	735	GLN
1	C	742	THR
1	C	753	GLU
1	C	778	GLU
1	C	783	VAL
1	C	819	GLU
1	C	823	VAL
1	C	837	VAL
1	C	846	THR
1	C	847	GLN
1	D	664	LEU
1	D	680	LEU
1	D	682	ASP
1	D	683	GLU
1	D	697	LEU
1	D	699	THR
1	D	735	GLN
1	D	742	THR
1	D	751	SER
1	D	753	GLU
1	D	757	GLU
1	D	771	ARG
1	D	777	GLU
1	D	778	GLU
1	D	811	ARG
1	D	825	VAL
1	D	837	VAL
1	D	845	VAL
1	D	847	GLN
1	E	664	LEU
1	E	671	GLN
1	E	675	ARG
1	E	693	ASP
1	E	695	LEU
1	E	699	THR
1	E	710	GLU

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Mol	Chain	Res	Type
1	E	728	GLU
1	E	736	VAL
1	E	738	SER
1	E	740	GLU
1	E	742	THR
1	E	751	SER
1	E	752	VAL
1	E	754	GLU
1	E	760	SER
1	E	771	ARG
1	E	775	GLN
1	E	778	GLU
1	E	812	ASN
1	E	814	SER
1	E	819	GLU
1	E	835	ARG
1	E	837	VAL
1	E	844	LEU
1	E	845	VAL
1	F	655	LEU
1	F	664	LEU
1	F	682	ASP
1	F	693	ASP
1	F	695	LEU
1	F	697	LEU
1	F	699	THR
1	F	735	GLN
1	F	736	VAL
1	F	738	SER
1	F	742	THR
1	F	752	VAL
1	F	753	GLU
1	F	757	GLU
1	F	758	TYR
1	F	771	ARG
1	F	775	GLN
1	F	778	GLU
1	F	783	VAL
1	F	812	ASN
1	F	819	GLU
1	F	823	VAL
1	F	825	VAL

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Mol	Chain	Res	Type
1	F	837	VAL
1	F	840	LYS
1	F	845	VAL
1	F	847	GLN
1	G	655	LEU
1	G	659	ARG
1	G	660	MET
1	G	664	LEU
1	G	668	ARG
1	G	671	GLN
1	G	682	ASP
1	G	697	LEU
1	G	699	THR
1	G	710	GLU
1	G	716	GLU
1	G	735	GLN
1	G	738	SER
1	G	742	THR
1	G	752	VAL
1	G	753	GLU
1	G	754	GLU
1	G	757	GLU
1	G	775	GLN
1	G	778	GLU
1	G	809	ASP
1	G	819	GLU
1	G	823	VAL
1	G	831	ASP
1	G	837	VAL
1	G	844	LEU
1	H	664	LEU
1	H	668	ARG
1	H	685	GLU
1	H	699	THR
1	H	701	ARG
1	H	730	GLU
1	H	735	GLN
1	H	738	SER
1	H	742	THR
1	H	754	GLU
1	H	757	GLU
1	H	774	ASP

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Mol	Chain	Res	Type
1	H	778	GLU
1	H	783	VAL
1	H	812	ASN
1	H	814	SER
1	H	818	ILE
1	H	819	GLU
1	H	831	ASP
1	H	837	VAL
1	H	842	ARG
1	H	844	LEU
1	H	846	THR
1	H	847	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	792	ASN
1	A	813	ASN
1	B	722	HIS
1	B	792	ASN
1	B	813	ASN
1	C	671	GLN
1	C	813	ASN
1	E	667	ASN
1	E	813	ASN
1	E	847	GLN
1	F	700	GLN
1	F	763	ASN
1	F	813	ASN
1	G	657	GLN
1	G	658	GLN
1	G	665	ASN
1	G	667	ASN
1	G	671	GLN
1	G	763	ASN
1	G	775	GLN
1	G	792	ASN
1	G	812	ASN
1	G	813	ASN
1	H	667	ASN
1	H	765	GLN
1	H	812	ASN

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Mol	Chain	Res	Type
1	H	813	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 ⓘ

28 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	I	1	2,1	14,14,15	0.90	1 (7%)	17,19,21	0.74	0
2	NAG	I	2	2	14,14,15	0.54	0	17,19,21	1.19	2 (11%)
2	MAN	I	3	2	11,11,12	0.90	1 (9%)	15,15,17	1.60	3 (20%)
2	MAN	I	4	2	11,11,12	0.80	0	15,15,17	0.70	0
2	NAG	I	5	2	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
2	MAN	I	6	2	11,11,12	0.97	0	15,15,17	1.61	2 (13%)
3	NAG	J	1	3,1	14,14,15	6.91	12 (85%)	17,19,21	4.34	11 (64%)
3	NDG	J	2	3	14,14,15	0.87	0	17,19,21	0.76	1 (5%)
3	MAN	J	3	3	11,11,12	0.85	0	15,15,17	1.97	2 (13%)
3	MAN	J	4	3	11,11,12	1.38	2 (18%)	15,15,17	1.57	3 (20%)
3	NAG	J	5	3	14,14,15	0.87	0	17,19,21	1.41	2 (11%)
3	MAN	J	6	3	10,10,12	0.79	0	14,14,17	0.93	0
2	NAG	K	1	2,1	14,14,15	0.47	0	17,19,21	0.71	0
2	NAG	K	2	2	14,14,15	0.69	1 (7%)	17,19,21	1.28	2 (11%)
2	MAN	K	3	2	11,11,12	0.59	0	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	K	4	2	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
2	NAG	K	5	2	14,14,15	0.93	0	17,19,21	0.75	0
2	MAN	K	6	2	11,11,12	1.00	1 (9%)	15,15,17	0.98	2 (13%)
2	NAG	L	1	2,1	14,14,15	6.34	11 (78%)	17,19,21	6.62	14 (82%)
2	NAG	L	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.83	1 (5%)
2	MAN	L	3	2	11,11,12	0.96	1 (9%)	15,15,17	1.58	2 (13%)
2	MAN	L	4	2	11,11,12	0.83	0	15,15,17	1.15	1 (6%)
2	NAG	L	5	2	14,14,15	0.91	0	17,19,21	2.02	5 (29%)
2	MAN	L	6	2	11,11,12	0.71	0	15,15,17	1.14	1 (6%)
4	NAG	M	1	4,1	14,14,15	8.57	11 (78%)	17,19,21	6.23	14 (82%)
4	NAG	M	2	4	14,14,15	0.62	0	17,19,21	0.73	1 (5%)
4	NAG	N	1	4,1	14,14,15	0.66	0	17,19,21	1.03	1 (5%)
4	NAG	N	2	4	14,14,15	0.80	0	17,19,21	1.47	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
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	MAN	I	3	2	1/1/4/5	1/2/19/22	1/1/1/1
2	MAN	I	4	2	-	2/2/19/22	0/1/1/1
2	NAG	I	5	2	-	0/6/23/26	0/1/1/1
2	MAN	I	6	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	1/6/23/26	0/1/1/1
3	NDG	J	2	3	-	2/6/23/26	0/1/1/1
3	MAN	J	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	NAG	J	5	3	-	2/6/23/26	0/1/1/1
3	MAN	J	6	3	-	-	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	MAN	K	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	2/2/19/22	0/1/1/1
2	NAG	K	5	2	-	2/6/23/26	0/1/1/1
2	MAN	K	6	2	1/1/4/5	2/2/19/22	1/1/1/1

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

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C5	17.67	1.77	1.43
4	M	1	NAG	C1-C2	-16.09	1.30	1.52
4	M	1	NAG	O5-C1	14.52	1.68	1.43
3	J	1	NAG	O3-C3	-13.33	1.10	1.43
3	J	1	NAG	C3-C2	11.34	1.76	1.52
2	L	1	NAG	C2-N2	11.30	1.65	1.46
2	L	1	NAG	C1-C2	10.23	1.66	1.52
3	J	1	NAG	O5-C1	10.18	1.60	1.43
2	L	1	NAG	O7-C7	-10.03	1.00	1.23
4	M	1	NAG	O4-C4	8.51	1.64	1.43
3	J	1	NAG	C7-N2	7.86	1.59	1.34
2	L	1	NAG	C8-C7	-7.64	1.34	1.50
2	L	1	NAG	O5-C1	7.36	1.56	1.43
4	M	1	NAG	C8-C7	6.76	1.64	1.50
4	M	1	NAG	C3-C2	6.69	1.66	1.52
2	L	1	NAG	C7-N2	6.49	1.55	1.34
3	J	1	NAG	C1-C2	-6.40	1.43	1.52
3	J	1	NAG	C4-C5	6.23	1.66	1.53
4	M	1	NAG	C2-N2	-5.06	1.37	1.46
3	J	1	NAG	C6-C5	-4.94	1.35	1.51
2	L	1	NAG	C6-C5	4.74	1.67	1.51
3	J	1	NAG	O6-C6	4.64	1.61	1.42
4	M	1	NAG	C7-N2	4.59	1.49	1.34
3	J	1	NAG	O4-C4	-4.56	1.31	1.43
3	J	1	NAG	O5-C5	4.54	1.52	1.43
4	M	1	NAG	O6-C6	4.35	1.60	1.42
2	L	1	NAG	O5-C5	4.14	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C4-C3	4.06	1.62	1.52
2	L	1	NAG	C3-C2	3.63	1.60	1.52
3	J	4	MAN	C2-C3	3.34	1.57	1.52
2	L	1	NAG	C4-C5	-2.96	1.46	1.53
4	M	1	NAG	C4-C3	2.93	1.59	1.52
3	J	1	NAG	C2-N2	-2.86	1.41	1.46
2	I	1	NAG	C1-C2	2.59	1.55	1.52
4	M	1	NAG	O7-C7	2.55	1.28	1.23
2	L	2	NAG	C1-C2	2.47	1.55	1.52
2	L	1	NAG	O4-C4	2.38	1.48	1.43
3	J	4	MAN	C1-C2	2.31	1.57	1.52
2	K	6	MAN	O5-C5	2.28	1.47	1.43
2	L	3	MAN	C2-C3	-2.13	1.49	1.52
2	K	2	NAG	C1-C2	2.08	1.55	1.52
2	I	3	MAN	O5-C1	2.06	1.47	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	O5-C1-C2	-15.01	88.07	111.29
4	M	1	NAG	O5-C5-C6	-13.20	81.97	107.66
2	L	1	NAG	O7-C7-C8	12.72	144.71	122.05
4	M	1	NAG	C2-N2-C7	-11.31	107.74	122.90
2	L	1	NAG	O7-C7-N2	-10.94	102.65	121.98
3	J	1	NAG	O7-C7-N2	-10.45	103.52	121.98
4	M	1	NAG	C6-C5-C4	8.97	135.04	113.02
4	M	1	NAG	C1-C2-N2	-7.96	97.89	110.43
3	J	1	NAG	C1-C2-N2	-7.83	98.10	110.43
2	L	1	NAG	O4-C4-C3	-7.80	91.99	110.38
4	M	1	NAG	O6-C6-C5	-7.12	87.10	111.33
2	L	1	NAG	O6-C6-C5	-6.57	88.96	111.33
2	L	1	NAG	C3-C4-C5	-6.19	99.01	110.23
2	L	5	NAG	C2-N2-C7	-5.82	115.09	122.90
4	M	1	NAG	O5-C1-C2	-5.63	102.58	111.29
4	M	1	NAG	C3-C4-C5	5.25	119.75	110.23
3	J	3	MAN	C3-C4-C5	-5.19	100.82	110.23
3	J	1	NAG	C8-C7-N2	5.12	124.61	116.12
4	M	1	NAG	O7-C7-C8	-4.73	113.63	122.05
3	J	1	NAG	O3-C3-C2	-4.73	99.58	109.40
4	M	1	NAG	C8-C7-N2	4.68	123.89	116.12
4	N	2	NAG	C4-C3-C2	4.54	117.67	111.02
3	J	1	NAG	O5-C5-C4	-4.46	99.96	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	MAN	C1-O5-C5	4.34	118.00	112.19
3	J	4	MAN	C3-C4-C5	-4.26	102.52	110.23
3	J	1	NAG	C6-C5-C4	4.22	123.37	113.02
2	L	3	MAN	C3-C4-C5	-4.19	102.64	110.23
3	J	1	NAG	C2-N2-C7	-4.12	117.38	122.90
4	M	1	NAG	O4-C4-C3	4.01	119.83	110.38
2	I	3	MAN	C2-C3-C4	-3.93	103.95	110.86
2	L	1	NAG	O3-C3-C2	-3.91	101.27	109.40
2	K	2	NAG	C4-C3-C2	-3.87	105.34	111.02
2	L	1	NAG	O4-C4-C5	-3.83	99.90	109.32
3	J	5	NAG	C1-O5-C5	-3.81	107.08	112.19
2	L	1	NAG	C4-C3-C2	3.74	116.50	111.02
3	J	1	NAG	O5-C1-C2	-3.72	105.54	111.29
3	J	3	MAN	C1-C2-C3	-3.66	104.32	109.64
2	I	6	MAN	C1-C2-C3	3.55	114.81	109.64
2	L	1	NAG	C6-C5-C4	3.52	121.67	113.02
4	M	1	NAG	C1-O5-C5	3.49	116.87	112.19
4	M	1	NAG	O4-C4-C5	-3.47	100.77	109.32
4	M	1	NAG	O5-C5-C4	-3.34	102.70	110.83
2	I	3	MAN	C1-C2-C3	-3.25	104.91	109.64
2	I	5	NAG	C2-N2-C7	-3.22	118.59	122.90
2	L	1	NAG	C2-N2-C7	-3.15	118.67	122.90
2	L	1	NAG	C1-O5-C5	3.13	116.38	112.19
3	J	1	NAG	O4-C4-C5	-3.00	101.93	109.32
2	L	1	NAG	C8-C7-N2	-3.00	111.14	116.12
2	L	5	NAG	C4-C3-C2	-2.82	106.88	111.02
2	L	5	NAG	C1-O5-C5	-2.75	108.50	112.19
2	L	1	NAG	O5-C5-C4	-2.73	104.18	110.83
4	N	1	NAG	C4-C3-C2	2.55	114.75	111.02
2	K	4	MAN	C1-O5-C5	2.52	115.57	112.19
2	K	6	MAN	C1-C2-C3	-2.48	106.03	109.64
2	I	5	NAG	O5-C1-C2	-2.44	107.51	111.29
3	J	1	NAG	C1-O5-C5	2.42	115.44	112.19
2	L	2	NAG	C2-N2-C7	-2.34	119.77	122.90
2	I	2	NAG	C3-C4-C5	2.34	114.47	110.23
2	L	5	NAG	O5-C1-C2	-2.33	107.69	111.29
3	J	4	MAN	C1-C2-C3	2.33	113.03	109.64
2	I	2	NAG	C4-C3-C2	2.32	114.42	111.02
2	L	3	MAN	C1-O5-C5	2.25	115.20	112.19
2	I	3	MAN	C3-C4-C5	-2.25	106.15	110.23
3	J	4	MAN	C6-C5-C4	2.25	118.54	113.02
2	L	4	MAN	C1-C2-C3	-2.22	106.41	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	NAG	O3-C3-C4	2.14	115.42	110.38
2	L	5	NAG	C6-C5-C4	2.14	118.27	113.02
4	N	2	NAG	C3-C4-C5	2.13	114.10	110.23
2	K	3	MAN	C2-C3-C4	-2.11	107.14	110.86
2	K	6	MAN	C2-C3-C4	-2.11	107.15	110.86
2	K	2	NAG	C2-N2-C7	-2.10	120.08	122.90
2	L	6	MAN	C1-C2-C3	-2.07	106.63	109.64
3	J	5	NAG	C3-C4-C5	2.06	113.97	110.23
4	N	2	NAG	C1-O5-C5	-2.04	109.45	112.19
3	J	1	NAG	C3-C4-C5	2.03	113.92	110.23
3	J	2	NDG	C2-N2-C7	-2.02	120.19	122.90
4	M	2	NAG	C2-N2-C7	-2.02	120.20	122.90

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	3	MAN	C1
2	K	3	MAN	C1
2	K	6	MAN	C1
2	L	6	MAN	C1
3	J	3	MAN	C1

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	5	NAG	C3-C2-N2-C7
3	J	2	NDG	C4-C5-C6-O6
2	I	4	MAN	O5-C5-C6-O6
2	K	4	MAN	O5-C5-C6-O6
2	L	3	MAN	O5-C5-C6-O6
3	J	3	MAN	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	K	4	MAN	C4-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
2	I	4	MAN	C4-C5-C6-O6
2	K	5	NAG	O5-C5-C6-O6
3	J	2	NDG	O5-C5-C6-O6
3	J	3	MAN	C4-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
2	K	5	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	M	2	NAG	O5-C5-C6-O6
2	L	3	MAN	C4-C5-C6-O6
2	K	6	MAN	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	K	3	MAN	C4-C5-C6-O6
2	L	5	NAG	C4-C5-C6-O6
2	K	3	MAN	O5-C5-C6-O6
3	J	5	NAG	O5-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
2	L	6	MAN	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
2	L	5	NAG	O5-C5-C6-O6
2	K	6	MAN	C4-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
2	L	4	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	MAN	C1-C2-C3-C4-C5-O5
2	K	6	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 108 short contacts:

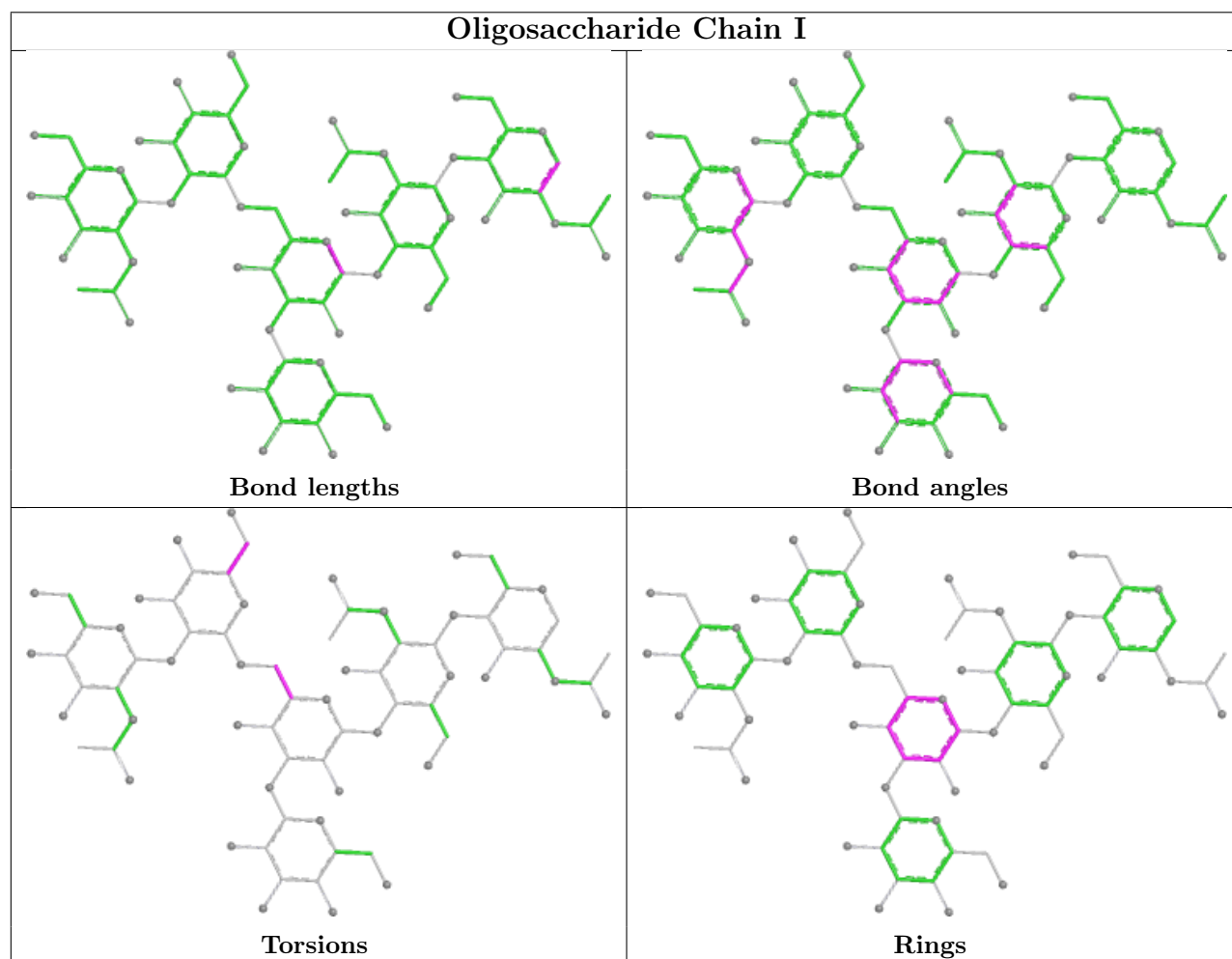
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	MAN	4	0
2	I	2	NAG	4	0
2	I	5	NAG	3	0
2	I	6	MAN	9	0
2	K	5	NAG	12	0
2	K	2	NAG	2	0
3	J	4	MAN	17	0
2	I	4	MAN	6	0
3	J	3	MAN	15	0
4	M	2	NAG	3	0
2	K	3	MAN	13	0
2	K	4	MAN	22	0
2	I	3	MAN	13	0
3	J	1	NAG	5	0
3	J	2	NDG	1	0
4	M	1	NAG	19	0
2	L	5	NAG	8	0

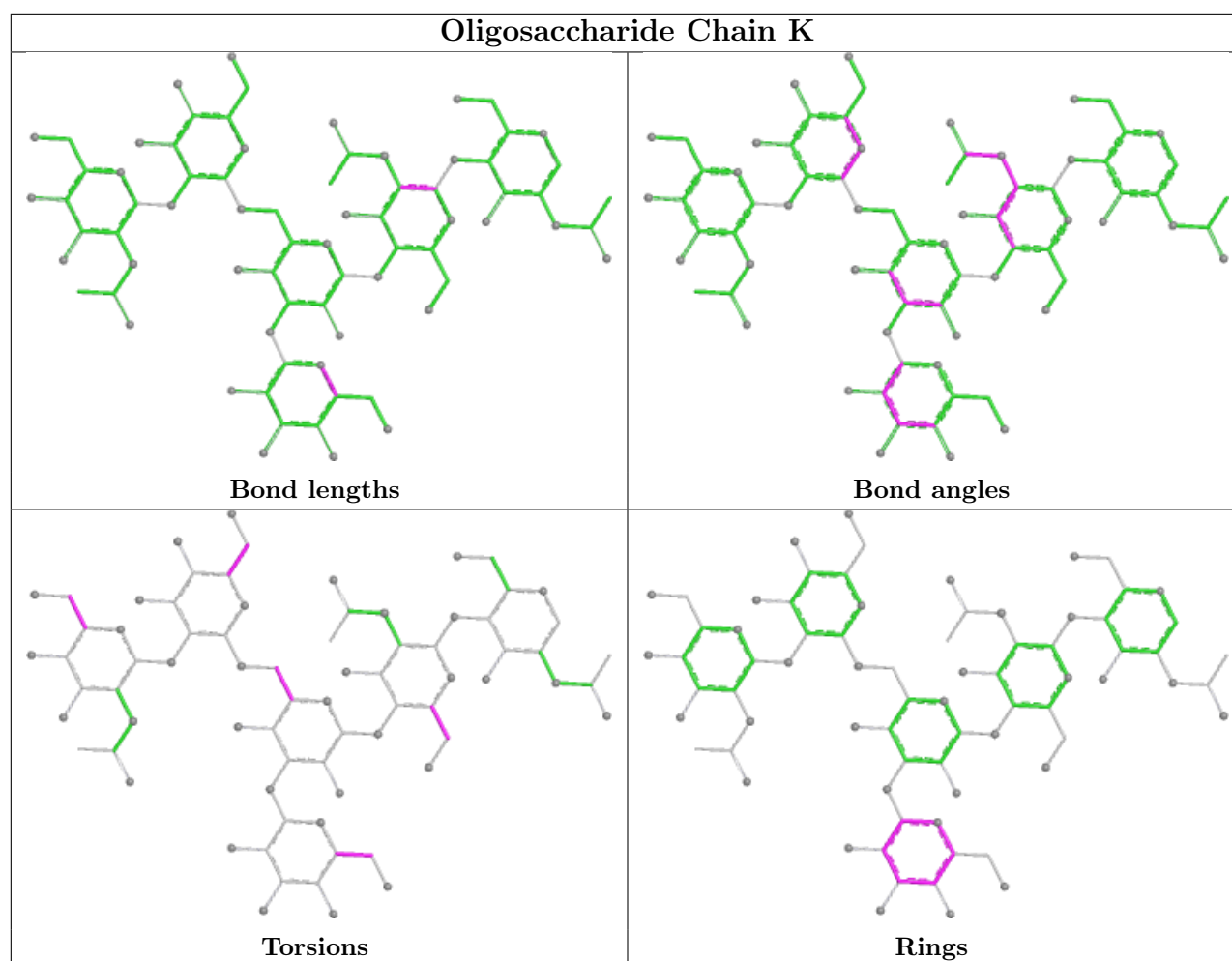
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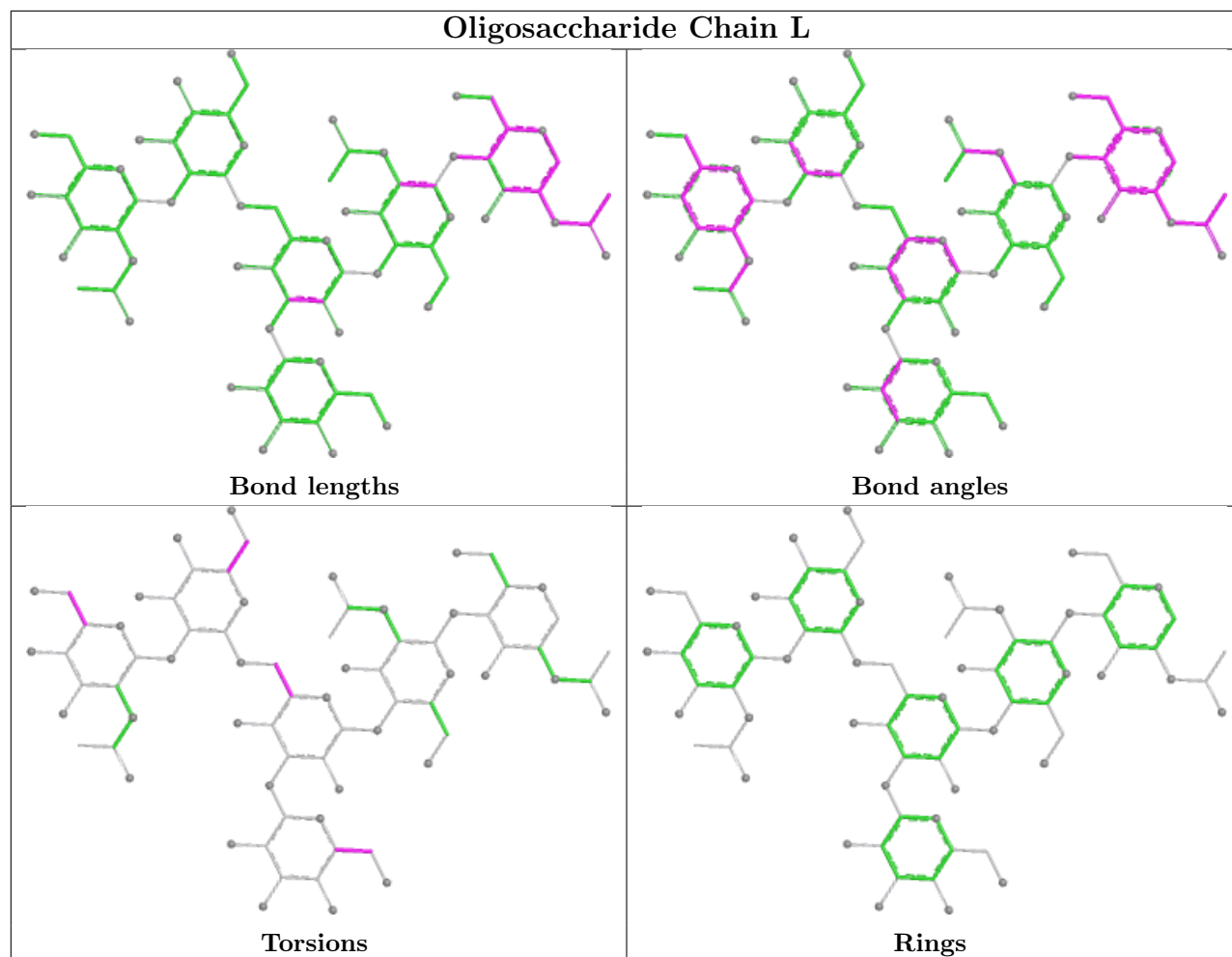
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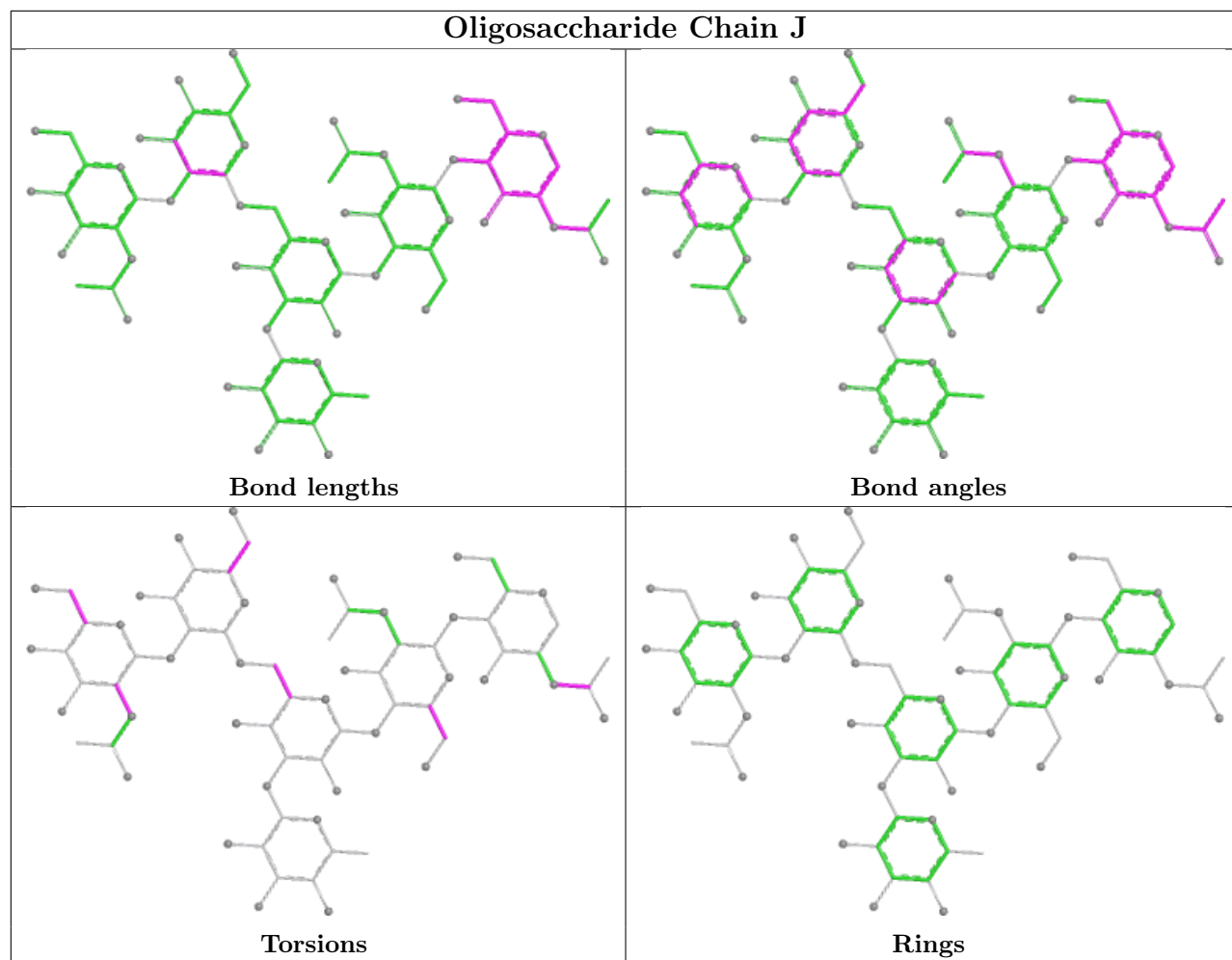
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	4	MAN	12	0
3	J	6	MAN	5	0
4	N	1	NAG	1	0
3	J	5	NAG	9	0
2	K	6	MAN	3	0

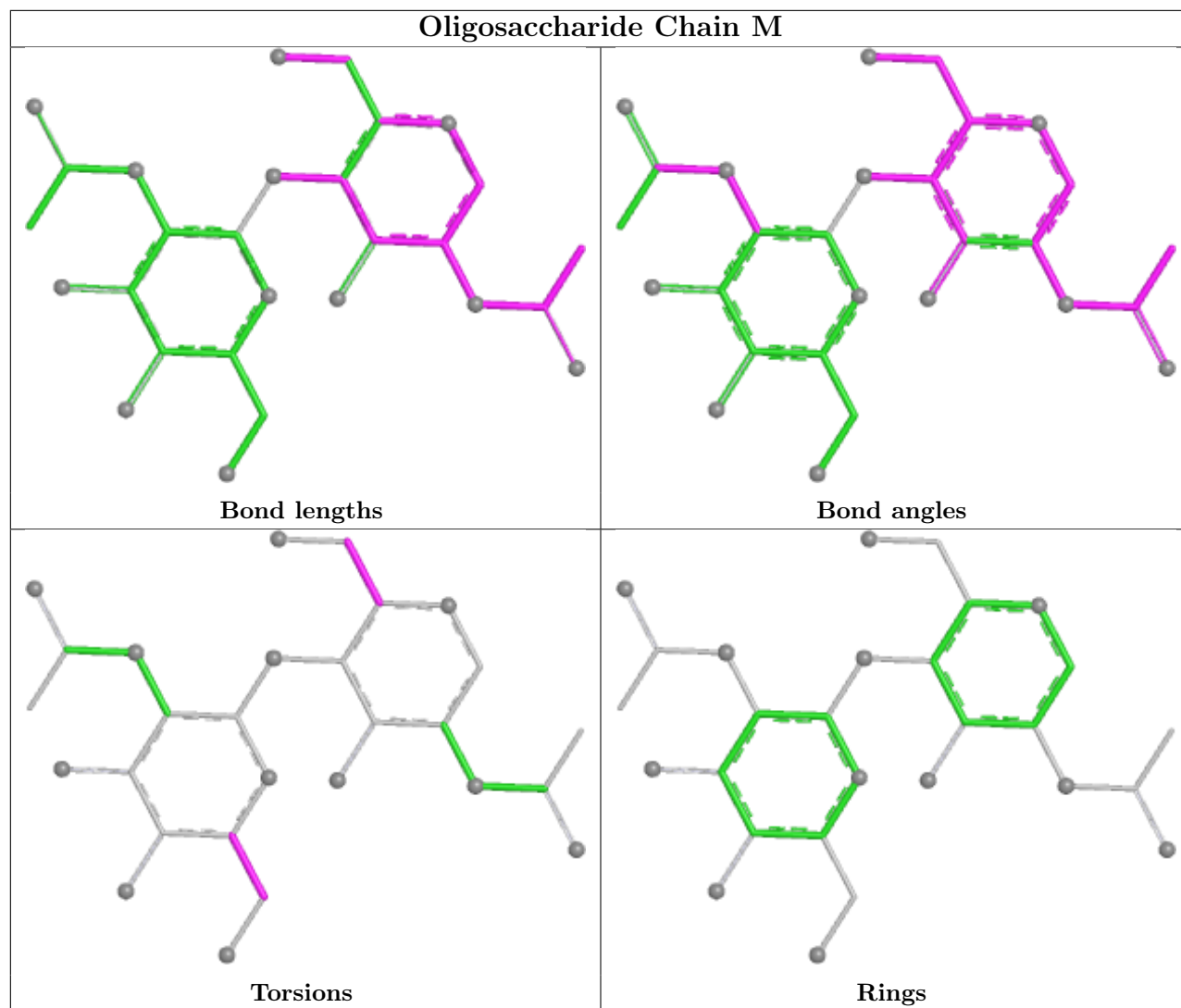
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

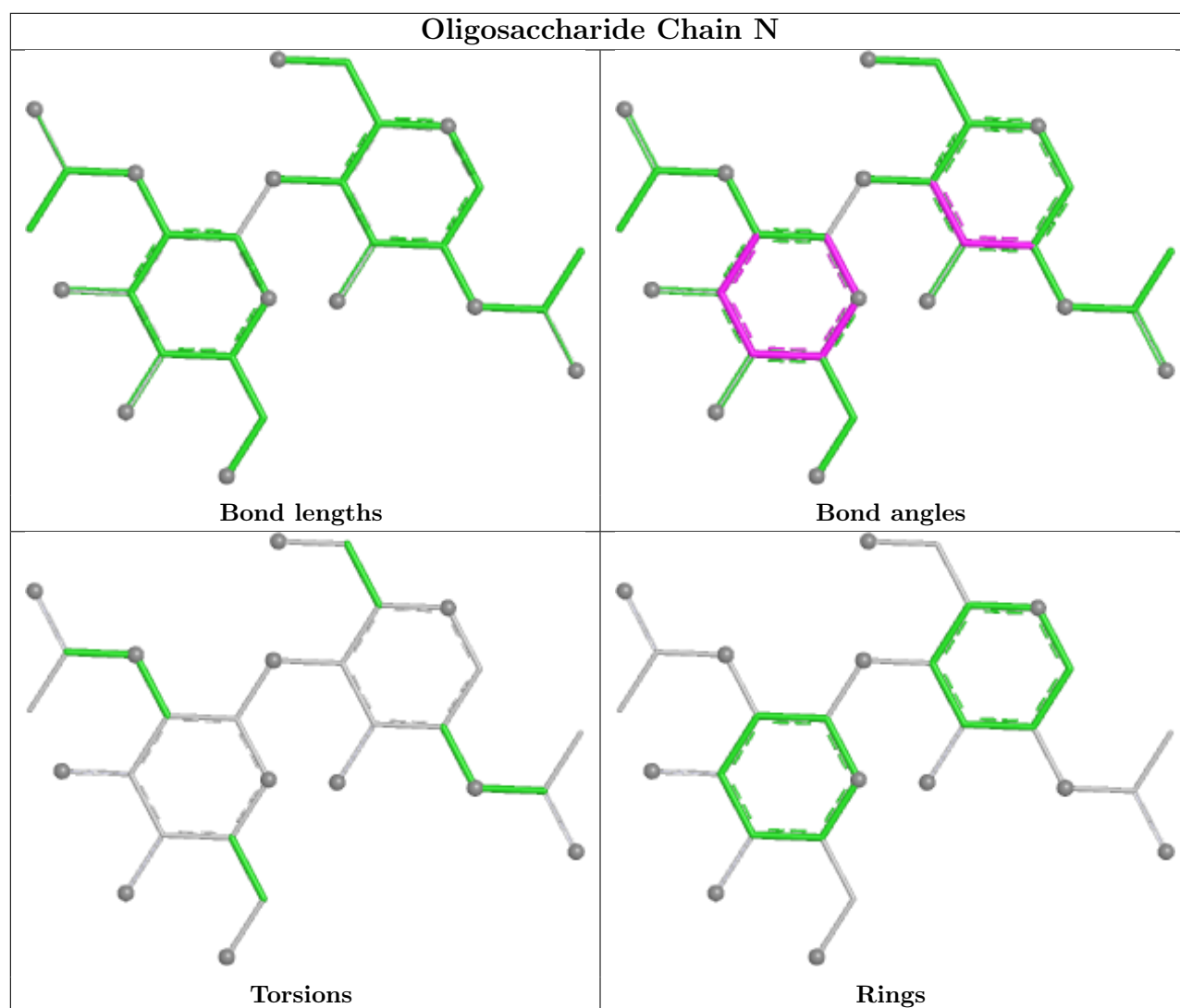












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	G	11	-	14,14,15	0.53	0	17,19,21	1.19	2 (11%)
6	NAG	G	10	1	14,14,15	0.55	0	17,19,21	1.35	2 (11%)
6	NAG	H	11	-	14,14,15	0.74	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	H	10	1	14,14,15	0.50	0	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	11	-	-	2/6/23/26	0/1/1/1
6	NAG	G	10	1	-	2/6/23/26	0/1/1/1
6	NAG	H	11	-	-	0/6/23/26	0/1/1/1
6	NAG	H	10	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	10	NAG	C3-C4-C5	3.69	116.93	110.23
6	G	11	NAG	C4-C3-C2	-3.19	106.34	111.02
6	H	10	NAG	C3-C4-C5	2.74	115.19	110.23
6	H	11	NAG	C2-N2-C7	-2.68	119.30	122.90
6	G	11	NAG	C2-N2-C7	-2.45	119.62	122.90
6	G	10	NAG	C2-N2-C7	-2.28	119.84	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	10	NAG	C4-C5-C6-O6
6	G	10	NAG	O5-C5-C6-O6
6	G	10	NAG	C4-C5-C6-O6
6	H	10	NAG	O5-C5-C6-O6
6	G	11	NAG	C4-C5-C6-O6
6	G	11	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	11	NAG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	10	NAG	13	0
6	H	11	NAG	10	0
6	H	10	NAG	15	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.