



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 AM UTC

PDB ID : 1L5G / pdb_0000115g
Title : CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN AVB3 IN COMPLEX WITH AN ARG-GLY-ASP LIGAND
Authors : Xiong, J.-P.; Stehle, T.; Zhang, R.; Joachimiak, A.; Frech, M.; Goodman, S.L.; Arnaout, M.A.
Deposited on : 2002-03-06
Resolution : 3.20 Å(reported)

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

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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

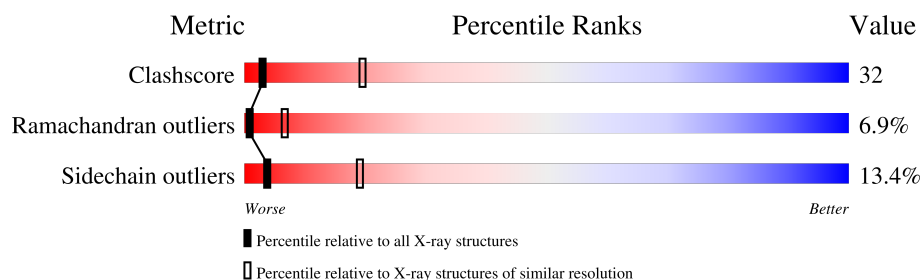
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	957	
2	B	692	
3	C	5	
4	D	2	
4	E	2	
4	F	2	
4	H	2	
5	G	2	

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Mol	Chain	Length	Quality of chain
5	I	2	 50%50%
5	J	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11700 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 INTEGRIN ALPHA V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	927	Total	C	N	O	S	0	0	0
			7216	4568	1224	1389	35			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	539	Total	C	N	O	S	0	0	0
			4182	2594	700	842	46			

- Molecule 3 is a protein called CYCLIC ARG-GLY-ASP PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			42	27	8	7			

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



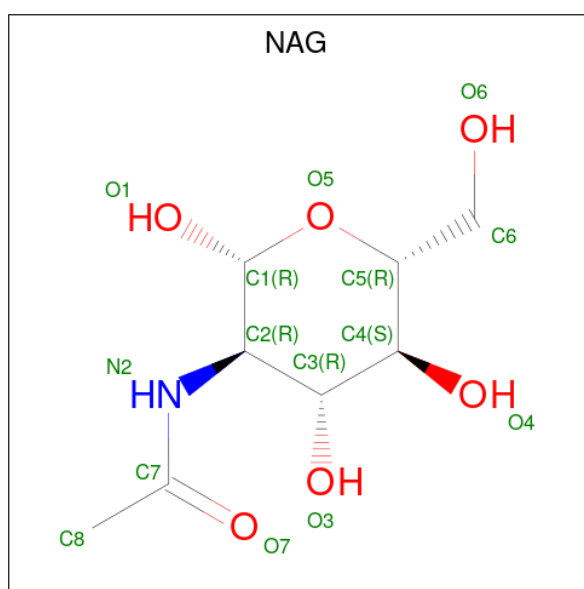
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

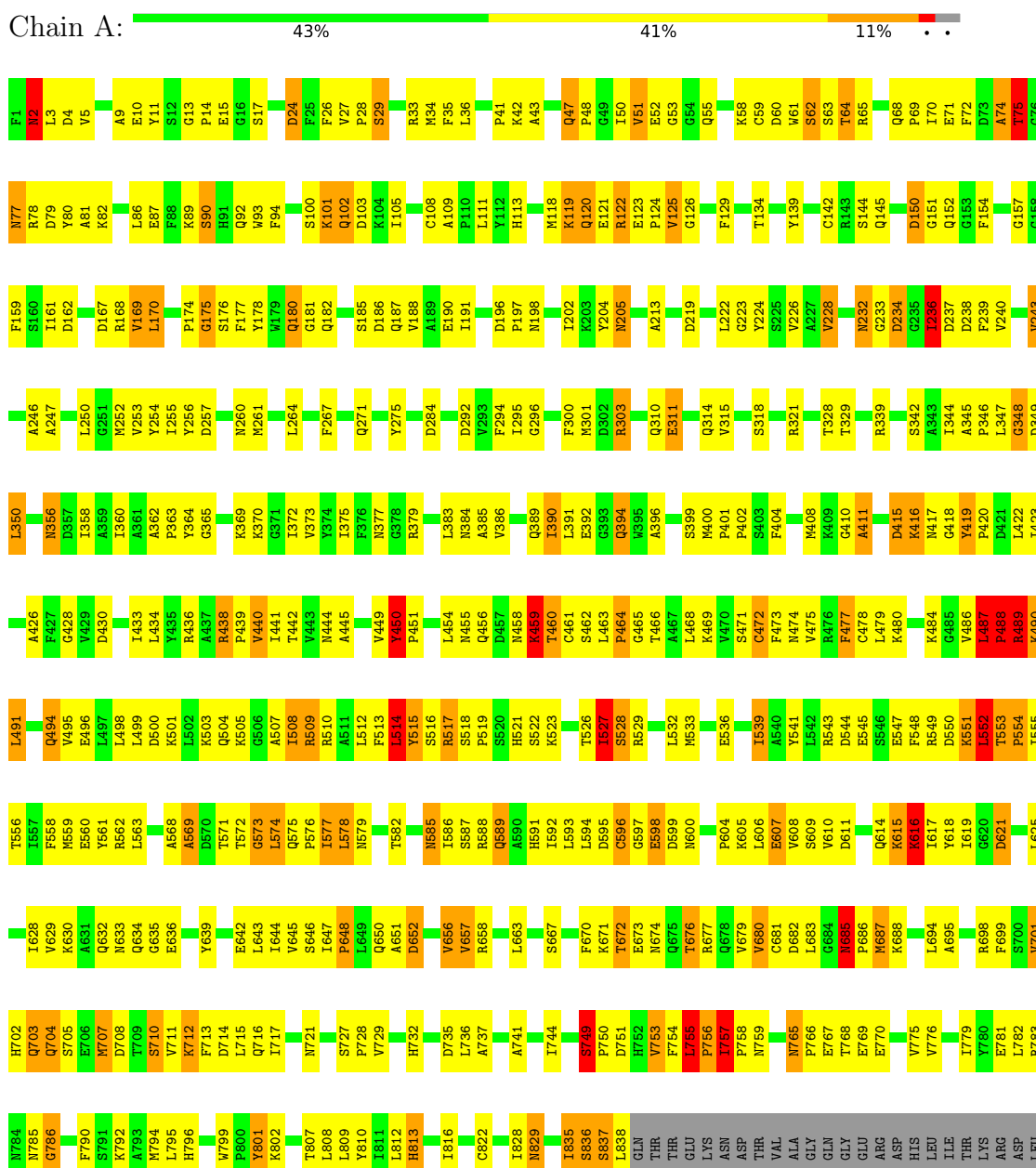
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	Mn 5	0	0
7	B	3	Total 3	Mn 3	0	0

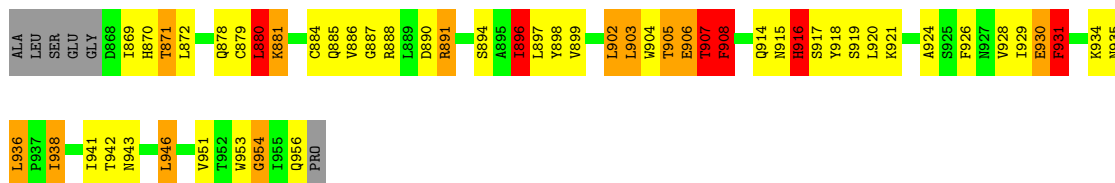
3 Residue-property plots

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.

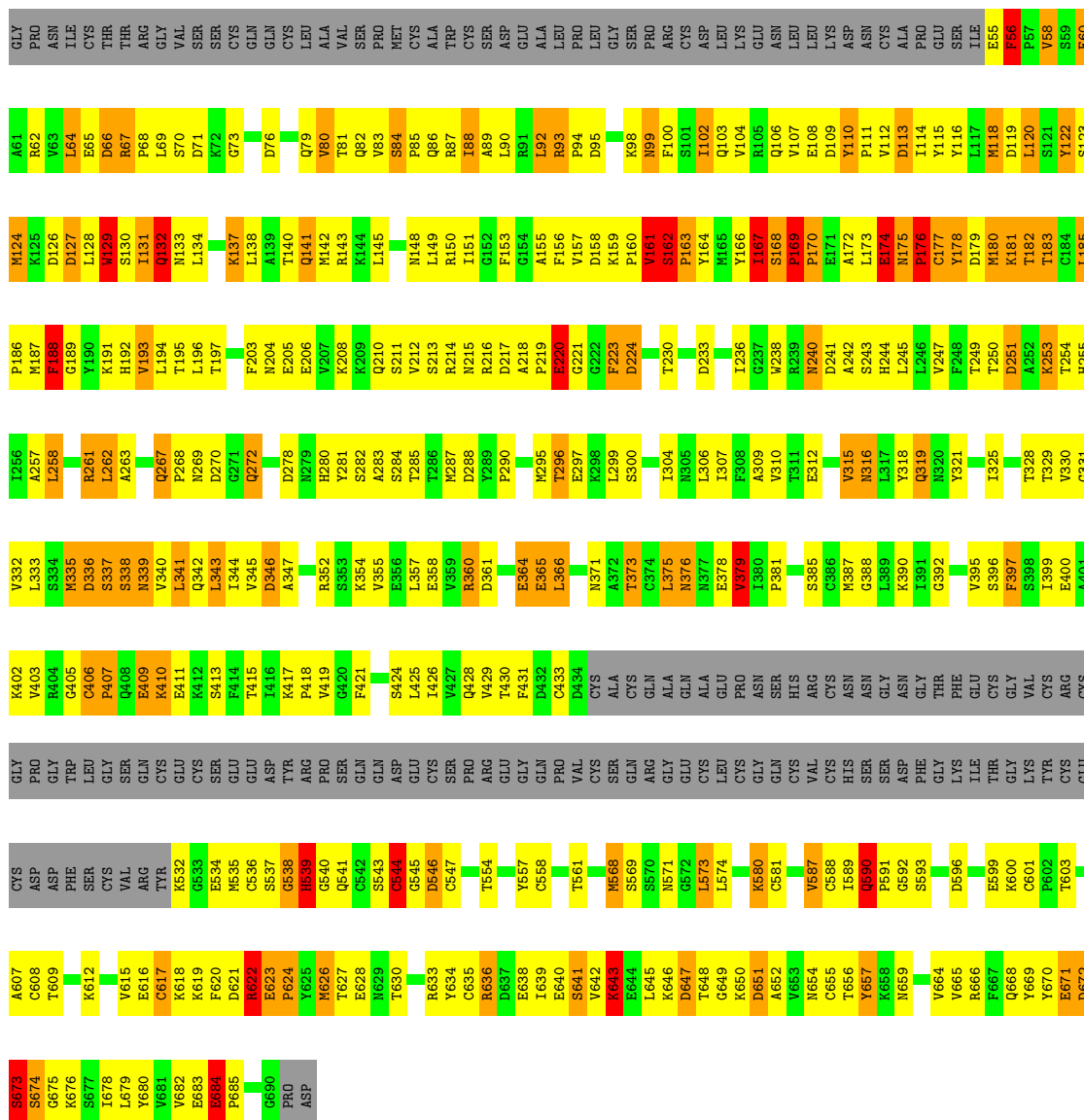
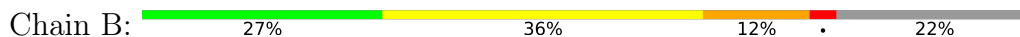
Note EDS was not executed.

• Molecule 1: INTEGRIN ALPHA V

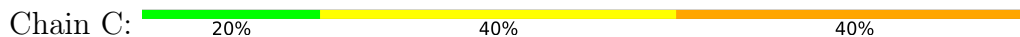




- Molecule 2: INTEGRIN BETA-3



- Molecule 3: CYCLIC ARG-GLY-ASP PEPTIDE

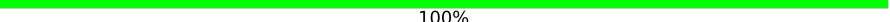


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%



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

Chain E:  100%



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

Chain F:  50% 50%



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

Chain H:  50% 50%

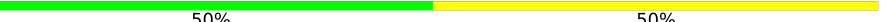


- Molecule 5: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

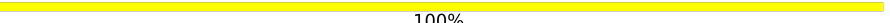


- Molecule 5: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



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

Chain J:  100%

MAG1
MDG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.79Å 129.79Å 308.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.248 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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: NDG, MVA, NAG, MN

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	0.62	2/7372 (0.0%)	1.25	109/9994 (1.1%)
2	B	0.60	0/4256	1.32	66/5754 (1.1%)
3	C	0.41	0/34	0.90	0/43
All	All	0.61	2/11662 (0.0%)	1.27	175/15791 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	THR	CA-CB	10.03	1.70	1.53
1	A	907	THR	CA-CB	7.68	1.62	1.52

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	THR	N-CA-C	14.21	129.94	111.75
1	A	907	THR	N-CA-C	-13.67	91.68	110.68
2	B	175	ASN	CA-C-N	13.03	136.12	119.84
2	B	175	ASN	C-N-CA	13.03	136.12	119.84
2	B	169	PRO	N-CA-C	-11.97	96.10	110.70
1	A	150	ASP	N-CA-C	-11.49	101.52	114.62
2	B	132	GLN	N-CA-C	-11.44	98.89	111.36
1	A	908	PHE	N-CA-C	11.30	124.00	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	ARG	N-CA-C	10.57	126.78	111.87
1	A	569	ALA	N-CA-C	9.74	123.98	110.24
2	B	674	SER	N-CA-C	-9.56	102.84	112.97
1	A	188	VAL	N-CA-C	9.51	119.53	110.30
1	A	64	THR	N-CA-C	-9.49	100.06	112.68
1	A	599	ASP	N-CA-C	-9.43	100.88	112.38
2	B	92	LEU	N-CA-C	9.42	124.25	108.90
2	B	684	GLU	CA-C-N	9.15	128.91	119.76
2	B	684	GLU	C-N-CA	9.15	128.91	119.76
2	B	336	ASP	N-CA-C	-9.12	91.38	110.80
2	B	223	PHE	N-CA-C	-8.92	101.46	111.71
1	A	75	THR	N-CA-CB	8.78	125.33	110.49
1	A	488	PRO	N-CA-C	8.66	130.32	112.47
2	B	673	SER	N-CA-C	8.53	124.18	113.43
1	A	896	ILE	N-CA-C	8.50	120.36	108.12
1	A	672	THR	N-CA-C	-8.43	95.56	108.96
2	B	544	CYS	N-CA-C	8.37	123.18	109.96
1	A	749	SER	CA-C-N	-8.32	109.44	119.84
1	A	749	SER	C-N-CA	-8.32	109.44	119.84
2	B	590	GLN	N-CA-C	8.14	127.81	109.81
1	A	596	CYS	N-CA-C	-8.06	101.24	112.45
2	B	168	SER	CA-C-N	-8.01	112.13	120.38
2	B	168	SER	C-N-CA	-8.01	112.13	120.38
2	B	365	GLU	N-CA-C	7.98	120.98	111.33
2	B	169	PRO	CA-C-N	-7.94	111.41	119.99
2	B	169	PRO	C-N-CA	-7.94	111.41	119.99
1	A	553	THR	N-CA-C	-7.79	91.65	108.64
2	B	137	LYS	N-CA-C	7.76	120.63	111.71
1	A	362	ALA	CA-C-N	7.56	127.60	119.28
1	A	362	ALA	C-N-CA	7.56	127.60	119.28
2	B	138	LEU	N-CA-C	-7.43	102.78	111.03
2	B	315	VAL	N-CA-C	7.43	117.51	110.30
1	A	801	TYR	N-CA-C	7.40	120.78	111.24
1	A	673	GLU	N-CA-C	-7.37	102.24	112.12
1	A	415	ASP	N-CA-C	7.31	117.61	108.19
1	A	385	ALA	N-CA-C	7.24	121.56	112.87
1	A	461	CYS	N-CA-C	7.23	120.92	109.50
1	A	224	TYR	N-CA-C	-7.21	103.51	111.36
1	A	349	ASP	N-CA-C	-7.17	93.69	108.53
2	B	66	ASP	N-CA-C	-7.08	101.16	110.43
2	B	568	MET	N-CA-C	7.08	121.21	109.46
2	B	409	GLU	N-CA-C	7.04	119.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	916	HIS	N-CA-C	7.03	125.77	110.80
2	B	335	MET	N-CA-C	-7.00	95.89	110.80
1	A	490	LYS	N-CA-C	6.94	120.80	108.24
2	B	161	VAL	N-CA-C	6.90	118.09	108.23
1	A	450	TYR	CA-C-N	-6.84	112.40	120.13
1	A	450	TYR	C-N-CA	-6.84	112.40	120.13
1	A	228	VAL	N-CA-C	6.83	117.37	108.35
1	A	712	LYS	N-CA-C	6.71	119.62	109.23
1	A	80	TYR	N-CA-C	-6.68	105.41	113.97
2	B	545	GLY	N-CA-C	-6.67	97.37	113.18
2	B	174	GLU	N-CA-C	-6.57	105.14	113.02
1	A	829	ASN	CA-C-N	6.55	126.68	119.87
1	A	829	ASN	C-N-CA	6.55	126.68	119.87
1	A	568	ALA	N-CA-C	6.53	119.83	109.65
1	A	710	SER	N-CA-C	6.51	119.05	108.76
1	A	438	ARG	CA-C-N	6.47	126.70	119.90
1	A	438	ARG	C-N-CA	6.47	126.70	119.90
1	A	386	VAL	N-CA-C	6.45	114.99	107.77
2	B	193	VAL	N-CA-C	6.45	118.41	111.58
1	A	879	CYS	N-CA-C	6.38	118.92	108.52
1	A	144	SER	N-CA-C	6.32	117.77	108.86
1	A	616	LYS	N-CA-C	6.28	118.62	109.07
1	A	880	LEU	N-CA-C	-6.28	97.47	108.20
1	A	243	VAL	CA-C-N	6.26	126.74	119.47
1	A	243	VAL	C-N-CA	6.26	126.74	119.47
1	A	589	GLN	N-CA-C	6.25	119.68	109.24
1	A	24	ASP	N-CA-C	6.23	117.61	108.14
1	A	931	PHE	CA-C-N	6.22	125.85	119.56
1	A	931	PHE	C-N-CA	6.22	125.85	119.56
1	A	744	ILE	N-CA-C	6.18	116.54	106.72
1	A	77	ASN	N-CA-C	6.17	119.57	109.76
2	B	162	SER	N-CA-C	6.13	123.36	109.81
1	A	27	VAL	CA-C-N	6.08	126.02	119.76
1	A	27	VAL	C-N-CA	6.08	126.02	119.76
1	A	917	SER	N-CA-C	6.05	119.40	108.69
2	B	170	PRO	N-CA-C	-6.04	101.00	111.32
1	A	755	LEU	N-CA-C	6.00	123.07	109.81
1	A	489	ARG	N-CA-C	5.99	123.56	110.80
2	B	319	GLN	N-CA-C	-5.97	104.11	111.40
2	B	84	SER	CA-C-N	-5.97	112.38	119.84
2	B	84	SER	C-N-CA	-5.97	112.38	119.84
2	B	124	MET	N-CA-C	-5.96	106.01	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	GLY	N-CA-C	-5.95	104.15	112.13
2	B	588	CYS	N-CA-C	5.94	118.82	109.96
1	A	491	LEU	N-CA-C	5.94	119.15	107.98
1	A	232	ASN	N-CA-C	-5.86	103.20	110.41
1	A	651	ALA	N-CA-C	5.80	118.02	110.53
1	A	440	VAL	N-CA-C	5.79	116.13	107.51
1	A	757	ILE	N-CA-C	5.79	121.38	108.88
1	A	704	GLN	N-CA-C	-5.78	103.58	111.56
1	A	202	ILE	N-CA-C	5.77	116.51	108.89
2	B	282	SER	N-CA-C	5.76	117.23	111.07
1	A	47	GLN	CA-C-N	5.75	127.02	119.84
1	A	47	GLN	C-N-CA	5.75	127.02	119.84
2	B	267	GLN	CA-C-N	5.73	125.64	119.85
2	B	267	GLN	C-N-CA	5.73	125.64	119.85
2	B	179	ASP	N-CA-C	-5.73	104.93	112.72
1	A	757	ILE	CA-C-N	5.72	126.05	119.93
1	A	757	ILE	C-N-CA	5.72	126.05	119.93
2	B	93	ARG	N-CA-C	-5.68	101.95	110.24
1	A	765	ASN	CA-C-N	5.65	125.97	119.92
1	A	765	ASN	C-N-CA	5.65	125.97	119.92
1	A	180	GLN	N-CA-C	-5.63	105.06	111.14
1	A	2	ASN	N-CA-C	5.59	118.55	108.48
1	A	597	GLY	N-CA-C	5.59	126.43	113.18
1	A	671	LYS	N-CA-C	5.59	116.70	107.20
2	B	118	MET	N-CA-C	5.57	118.04	109.07
1	A	74	ALA	O-C-N	-5.55	115.21	122.59
1	A	345	ALA	CA-C-N	5.54	125.47	119.76
1	A	345	ALA	C-N-CA	5.54	125.47	119.76
2	B	569	SER	N-CA-C	5.50	117.01	110.19
1	A	619	ILE	N-CA-C	5.46	116.31	108.93
1	A	871	THR	N-CA-C	5.42	118.17	110.10
1	A	433	ILE	N-CA-C	5.39	115.72	108.17
2	B	601	CYS	CA-C-N	5.39	124.90	119.19
2	B	601	CYS	C-N-CA	5.39	124.90	119.19
1	A	342	SER	N-CA-C	5.38	117.57	111.11
1	A	487	LEU	CA-C-N	5.38	126.56	119.84
1	A	487	LEU	C-N-CA	5.38	126.56	119.84
1	A	588	ARG	N-CA-C	-5.38	100.90	109.23
2	B	181	LYS	N-CA-C	5.36	122.21	110.80
2	B	587	VAL	N-CA-C	-5.35	97.08	106.61
2	B	70	SER	N-CA-C	5.33	117.87	109.39
1	A	419	TYR	CA-C-N	5.32	125.24	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	TYR	C-N-CA	5.32	125.24	119.76
1	A	75	THR	CB-CA-C	-5.32	99.83	110.42
1	A	615	LYS	N-CA-C	5.32	122.13	110.80
2	B	655	CYS	N-CA-C	5.32	118.30	110.59
1	A	507	ALA	N-CA-C	5.31	118.91	111.90
2	B	406	CYS	N-CA-C	5.28	118.83	109.58
1	A	168	ARG	N-CA-C	-5.27	100.72	108.99
1	A	472	CYS	N-CA-C	5.24	118.77	109.96
2	B	110	TYR	CA-C-N	5.22	125.14	119.76
2	B	110	TYR	C-N-CA	5.22	125.14	119.76
2	B	176	PRO	N-CA-C	5.21	123.21	112.47
1	A	489	ARG	CB-CA-C	5.21	120.79	110.42
1	A	698	ARG	N-CA-C	5.21	117.24	108.96
2	B	188	PHE	N-CA-C	5.20	121.88	110.80
1	A	786	GLY	CA-C-N	5.20	124.65	119.24
1	A	786	GLY	C-N-CA	5.20	124.65	119.24
2	B	538	GLY	N-CA-C	-5.19	100.88	113.18
1	A	899	VAL	CB-CA-C	-5.18	104.69	110.96
1	A	459	LYS	N-CA-C	5.16	119.29	113.15
2	B	325	ILE	N-CA-C	-5.15	97.75	108.88
1	A	475	VAL	N-CA-C	5.15	115.39	107.77
2	B	113	ASP	N-CA-C	-5.14	101.32	109.59
1	A	356	ASN	N-CA-C	5.13	117.48	110.55
1	A	234	ASP	N-CA-C	5.13	115.01	108.24
1	A	611	ASP	N-CA-C	5.12	117.95	109.85
1	A	157	GLY	N-CA-C	-5.12	106.04	111.93
2	B	657	TYR	N-CA-C	5.12	115.29	108.38
2	B	593	SER	N-CA-C	5.09	117.60	109.81
1	A	123	GLU	CA-C-N	5.09	126.20	119.84
1	A	123	GLU	C-N-CA	5.09	126.20	119.84
2	B	535	MET	N-CA-C	5.08	119.20	113.15
1	A	175	GLY	N-CA-C	5.08	125.22	113.18
1	A	13	GLY	CA-C-N	5.06	125.06	119.90
1	A	13	GLY	C-N-CA	5.06	125.06	119.90
1	A	489	ARG	CB-CG-CD	5.05	122.92	111.30
2	B	390	LYS	N-CA-C	-5.05	101.92	109.95
2	B	220	GLU	N-CA-C	5.05	120.06	112.94
2	B	80	VAL	N-CA-C	5.04	115.91	109.30
2	B	56	PHE	N-CA-C	5.03	120.93	109.81
2	B	194	LEU	N-CA-C	5.02	116.49	107.80
1	A	629	VAL	N-CA-C	5.02	116.43	109.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	5004	PHE	CA

There are no planarity outliers.

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	7216	0	7035	413	0
2	B	4182	0	4029	311	0
3	C	42	0	39	8	0
4	D	28	0	25	5	0
4	E	28	0	25	0	0
4	F	28	0	25	3	0
4	H	28	0	25	3	0
5	G	28	0	24	7	0
5	I	28	0	24	0	0
5	J	28	0	24	8	0
6	A	28	0	26	8	0
6	B	28	0	26	5	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
All	All	11700	0	11327	736	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (736) 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)
5:G:1:NAG:H2	5:G:1:NAG:H61	1.34	1.06
1:A:487:LEU:HD23	1:A:488:PRO:HD3	1.37	1.05
1:A:236:ILE:HD13	1:A:236:ILE:H	1.21	1.02
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.46	0.95
2:B:371:ASN:ND2	6:B:3371:NAG:H62	1.81	0.95
1:A:741:ALA:H	1:A:786:GLY:HA3	1.28	0.93
2:B:185:LEU:H	2:B:185:LEU:HD23	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PRO:HB2	2:B:170:PRO:HD3	1.48	0.93
2:B:157:VAL:HG11	2:B:188:PHE:H	1.31	0.92
2:B:316:ASN:HD22	2:B:316:ASN:H	1.12	0.92
1:A:416:LYS:H	1:A:416:LYS:HD2	1.38	0.89
2:B:157:VAL:HG12	2:B:189:GLY:H	1.36	0.89
2:B:129:TRP:HB2	2:B:208:LYS:HE3	1.55	0.88
1:A:585:ASN:ND2	4:F:1:NAG:H61	1.90	0.87
1:A:751:ASP:HB2	4:H:1:NAG:H81	1.57	0.86
1:A:685:ASN:HB3	1:A:686:PRO:HD3	1.55	0.85
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.58	0.84
1:A:379:ARG:HE	1:A:384:ASN:HB2	1.44	0.83
1:A:608:VAL:HG22	1:A:717:ILE:HG13	1.62	0.82
2:B:99:ASN:HD22	2:B:99:ASN:H	1.25	0.81
1:A:51:VAL:H	1:A:90:SER:HB3	1.45	0.81
1:A:77:ASN:HD21	1:A:89:LYS:H	1.26	0.81
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.62	0.81
1:A:228:VAL:HG22	1:A:237:ASP:HB3	1.60	0.81
1:A:444:ASN:HB2	1:A:480:LYS:HG2	1.63	0.80
2:B:178:TYR:HA	2:B:181:LYS:HD2	1.62	0.80
1:A:633:ASN:HB2	1:A:687:MET:HE2	1.64	0.80
2:B:650:LYS:HB2	5:J:2:NDG:H6C2	1.63	0.79
2:B:316:ASN:H	2:B:316:ASN:ND2	1.79	0.79
2:B:373:THR:HB	2:B:379:VAL:HG12	1.62	0.79
2:B:343:LEU:HD22	2:B:343:LEU:H	1.48	0.78
1:A:236:ILE:H	1:A:236:ILE:CD1	1.96	0.78
5:G:1:NAG:H61	5:G:1:NAG:C2	2.13	0.78
2:B:88:ILE:HG22	2:B:425:LEU:HD11	1.65	0.77
2:B:119:ASP:O	2:B:124:MET:HG3	1.84	0.77
2:B:371:ASN:HD22	6:B:3371:NAG:H62	1.47	0.77
1:A:441:ILE:HD11	1:A:563:LEU:HD22	1.67	0.76
2:B:157:VAL:HG13	2:B:158:ASP:H	1.49	0.76
1:A:672:THR:HG22	1:A:677:ARG:HA	1.68	0.76
2:B:141:GLN:HB3	2:B:345:VAL:HG21	1.66	0.76
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.69	0.75
2:B:157:VAL:CG1	2:B:188:PHE:H	1.98	0.75
2:B:64:LEU:HB2	2:B:87:ARG:HB3	1.68	0.74
2:B:650:LYS:HD2	5:J:2:NDG:H6C1	1.69	0.74
2:B:141:GLN:HE21	2:B:345:VAL:HG21	1.51	0.74
1:A:608:VAL:HG21	1:A:716:GLN:HA	1.69	0.74
1:A:450:TYR:HB2	1:A:451:PRO:HD3	1.70	0.73
1:A:301:MET:HA	1:A:310:GLN:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LEU:HD23	1:A:694:LEU:HD23	1.70	0.73
2:B:84:SER:HB3	2:B:85:PRO:HD3	1.68	0.73
2:B:112:VAL:HG22	2:B:243:SER:HB3	1.71	0.73
5:G:2:NDG:H2	5:G:2:NDG:H6C1	1.70	0.73
1:A:650:GLN:HE21	1:A:711:VAL:HG12	1.55	0.72
1:A:650:GLN:HB3	1:A:701:VAL:HG23	1.69	0.72
1:A:236:ILE:HD13	1:A:236:ILE:N	2.02	0.72
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.25	0.72
3:C:5005:MVA:HG22	3:C:5005:MVA:HN2	1.72	0.71
1:A:178:TYR:HD2	3:C:5001:ARG:CZ	2.03	0.71
2:B:654:ASN:HD22	5:J:1:NAG:H62	1.56	0.71
1:A:500:ASP:HB2	1:A:555:ILE:HG23	1.73	0.71
1:A:539:ILE:H	1:A:539:ILE:HD12	1.56	0.71
1:A:459:LYS:O	1:A:469:LYS:HB3	1.90	0.70
2:B:157:VAL:CG1	2:B:189:GLY:H	2.03	0.70
1:A:74:ALA:O	1:A:75:THR:HG23	1.92	0.70
2:B:623:GLU:HG2	2:B:624:PRO:HD2	1.71	0.70
2:B:127:ASP:O	2:B:128:LEU:HD12	1.91	0.70
1:A:228:VAL:CG2	1:A:237:ASP:HB3	2.21	0.70
2:B:650:LYS:HD2	5:J:2:NDG:C6	2.21	0.69
1:A:741:ALA:H	1:A:786:GLY:CA	2.02	0.69
2:B:642:VAL:HB	2:B:680:TYR:HB3	1.73	0.69
2:B:249:THR:HA	2:B:309:ALA:O	1.93	0.69
1:A:657:VAL:HG23	1:A:658:ARG:H	1.55	0.69
1:A:790:PHE:O	1:A:888:ARG:HA	1.92	0.69
1:A:756:PRO:HD3	1:A:954:GLY:H	1.58	0.68
2:B:617:CYS:SG	2:B:618:LYS:N	2.66	0.68
2:B:618:LYS:HB2	2:B:639:ILE:HD12	1.72	0.68
1:A:710:SER:HA	1:A:736:LEU:HD13	1.75	0.68
1:A:228:VAL:HG23	1:A:238:ASP:O	1.93	0.68
1:A:551:LYS:HB2	1:A:551:LYS:HZ3	1.59	0.68
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.29	0.67
4:D:1:NAG:C6	4:D:2:NAG:C1	2.72	0.67
1:A:55:GLN:NE2	1:A:69:PRO:HB3	2.09	0.67
2:B:157:VAL:HG11	2:B:188:PHE:N	2.08	0.67
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.77	0.67
2:B:571:ASN:ND2	2:B:573:LEU:HB2	2.10	0.67
2:B:185:LEU:HB2	2:B:186:PRO:HD2	1.76	0.67
2:B:580:LYS:NZ	2:B:580:LYS:HB2	2.10	0.67
1:A:344:ILE:HG22	1:A:358:ILE:HD11	1.77	0.66
1:A:656:VAL:HG23	1:A:657:VAL:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:THR:HG22	1:A:589:GLN:HB3	1.78	0.66
2:B:130:SER:HB3	2:B:338:SER:CB	2.24	0.66
2:B:133:ASN:O	2:B:137:LYS:N	2.28	0.65
2:B:122:TYR:HB2	2:B:213:SER:O	1.95	0.65
1:A:670:PHE:CE1	1:A:672:THR:HG23	2.32	0.65
1:A:169:VAL:O	1:A:185:SER:HA	1.96	0.65
1:A:501:LYS:HD2	1:A:509:ARG:HH12	1.61	0.65
1:A:869:ILE:HG13	1:A:870:HIS:HD2	1.61	0.65
1:A:159:PHE:CZ	2:B:261:ARG:HD2	2.32	0.65
1:A:544:ASP:O	1:A:547:GLU:HG2	1.97	0.65
2:B:157:VAL:HG13	2:B:158:ASP:N	2.12	0.64
2:B:616:GLU:HG2	2:B:657:TYR:OH	1.97	0.64
1:A:776:VAL:HB	1:A:809:LEU:HD21	1.79	0.64
2:B:140:THR:HG22	2:B:143:ARG:HH21	1.62	0.64
2:B:366:LEU:HA	2:B:402:LYS:O	1.98	0.64
2:B:657:TYR:CE2	2:B:665:VAL:HB	2.32	0.64
5:G:2:NDG:H2	5:G:2:NDG:C6	2.27	0.64
1:A:871:THR:HA	1:A:919:SER:HB3	1.80	0.64
2:B:129:TRP:C	2:B:131:ILE:H	2.03	0.64
1:A:608:VAL:HG11	1:A:715:LEU:HB3	1.78	0.64
2:B:129:TRP:CD1	2:B:130:SER:H	2.16	0.64
2:B:142:MET:SD	2:B:345:VAL:HG22	2.38	0.64
1:A:808:LEU:HD13	1:A:920:LEU:HD22	1.80	0.64
2:B:185:LEU:H	2:B:185:LEU:CD2	2.05	0.63
1:A:609:SER:HB3	1:A:630:LYS:HB3	1.80	0.63
1:A:487:LEU:CD2	1:A:488:PRO:HD3	2.21	0.63
1:A:769:GLU:HG2	1:A:902:LEU:HD21	1.80	0.63
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.32	0.63
1:A:812:LEU:HD21	1:A:902:LEU:HD22	1.80	0.63
1:A:578:LEU:H	1:A:578:LEU:HD22	1.64	0.63
1:A:61:TRP:C	1:A:63:SER:H	2.08	0.62
1:A:111:LEU:HD21	2:B:262:LEU:O	1.99	0.62
2:B:388:GLY:HA2	2:B:636:ARG:NH1	2.15	0.62
1:A:835:ILE:HG12	1:A:836:SER:N	2.15	0.62
1:A:348:GLY:HA3	1:A:420:PRO:HG2	1.81	0.62
2:B:638:GLU:O	2:B:678:ILE:HD12	2.00	0.62
2:B:120:LEU:HD21	2:B:210:GLN:HB3	1.79	0.62
2:B:534:GLU:HB3	2:B:544:CYS:SG	2.39	0.62
1:A:711:VAL:HG13	1:A:736:LEU:HD11	1.82	0.62
2:B:88:ILE:CG2	2:B:425:LEU:HD11	2.30	0.61
1:A:751:ASP:HB2	4:H:1:NAG:C8	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:LYS:HD2	2:B:668:GLN:HE21	1.65	0.61
1:A:177:PHE:HB2	1:A:180:GLN:HG3	1.83	0.61
2:B:114:ILE:HD13	2:B:344:ILE:HG21	1.82	0.61
2:B:159:LYS:HE3	2:B:284:SER:O	2.01	0.61
1:A:379:ARG:NE	1:A:384:ASN:HB2	2.13	0.61
1:A:375:ILE:O	1:A:375:ILE:HG13	2.01	0.61
2:B:100:PHE:CE1	2:B:399:ILE:HD13	2.36	0.61
1:A:347:LEU:HD13	1:A:350:LEU:HD22	1.82	0.60
2:B:221:GLY:H	2:B:255:HIS:H	1.48	0.60
1:A:464:PRO:HD3	1:A:514:LEU:HD13	1.81	0.60
1:A:41:PRO:O	1:A:42:LYS:HB2	2.01	0.60
1:A:458:ASN:O	1:A:471:SER:HA	2.01	0.60
1:A:442:THR:HG22	1:A:579:ASN:HB2	1.82	0.60
2:B:130:SER:C	2:B:132:GLN:H	2.07	0.60
1:A:390:ILE:O	1:A:390:ILE:HG13	1.99	0.60
1:A:539:ILE:HD12	1:A:539:ILE:N	2.15	0.60
1:A:808:LEU:HD12	1:A:808:LEU:O	2.02	0.60
1:A:375:ILE:HG12	1:A:389:GLN:HB3	1.82	0.60
1:A:650:GLN:NE2	1:A:711:VAL:HG12	2.15	0.59
2:B:169:PRO:CB	2:B:170:PRO:HD3	2.28	0.59
2:B:671:GLU:HA	2:B:676:LYS:O	2.01	0.59
2:B:104:VAL:HG13	2:B:395:VAL:HG23	1.84	0.59
2:B:62:ARG:HD2	2:B:85:PRO:HB3	1.83	0.59
2:B:161:VAL:HG22	2:B:162:SER:H	1.67	0.59
1:A:474:ASN:OD1	1:A:539:ILE:HG23	2.02	0.59
1:A:58:LYS:HB2	1:A:70:ILE:HD11	1.85	0.59
1:A:415:ASP:HB2	1:A:416:LYS:HD2	1.83	0.59
1:A:727:SER:HB2	1:A:728:PRO:HD2	1.83	0.59
2:B:64:LEU:HB3	2:B:86:GLN:HB2	1.85	0.59
2:B:157:VAL:O	2:B:220:GLU:HG3	2.03	0.59
1:A:510:ARG:HH12	1:A:553:THR:HB	1.67	0.59
1:A:741:ALA:N	1:A:786:GLY:HA3	2.09	0.59
2:B:156:PHE:HB2	2:B:189:GLY:O	2.03	0.59
1:A:370:LYS:O	1:A:404:PHE:HB3	2.02	0.59
1:A:552:LEU:HD11	1:A:591:HIS:HD2	1.68	0.58
2:B:371:ASN:OD1	2:B:381:PRO:HA	2.03	0.58
1:A:903:LEU:HD13	1:A:905:THR:H	1.69	0.58
1:A:410:GLY:O	1:A:411:ALA:HB2	2.03	0.58
1:A:559:MET:HE2	1:A:586:ILE:HG22	1.85	0.58
2:B:185:LEU:HD23	2:B:185:LEU:N	2.13	0.58
1:A:159:PHE:HZ	2:B:261:ARG:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:CYS:SG	2:B:635:CYS:O	2.61	0.58
1:A:445:ALA:HB1	1:A:559:MET:HE1	1.85	0.58
2:B:173:LEU:CD1	2:B:178:TYR:HB3	2.34	0.58
1:A:441:ILE:HG23	1:A:487:LEU:HD11	1.86	0.58
1:A:646:SER:HB2	1:A:714:ASP:HB2	1.84	0.58
2:B:620:PHE:O	2:B:622:ARG:HD3	2.04	0.58
1:A:2:ASN:HA	1:A:389:GLN:OE1	2.04	0.58
1:A:929:ILE:O	1:A:930:GLU:HB2	2.04	0.58
2:B:151:ILE:O	2:B:196:LEU:HA	2.04	0.57
2:B:219:PRO:HB2	2:B:255:HIS:CE1	2.39	0.57
1:A:621:ASP:HB3	1:A:891:ARG:NH2	2.20	0.57
2:B:623:GLU:CG	2:B:624:PRO:HD2	2.34	0.57
2:B:127:ASP:HB3	2:B:337:SER:HB3	1.85	0.57
2:B:102:ILE:HG22	2:B:399:ILE:HD11	1.87	0.57
1:A:489:ARG:HA	1:A:528:SER:OG	2.05	0.57
2:B:607:ALA:C	2:B:609:THR:H	2.11	0.57
1:A:61:TRP:CH2	1:A:415:ASP:HB3	2.39	0.57
1:A:472:CYS:N	6:A:2458:NAG:H61	2.19	0.57
2:B:103:GLN:HG3	2:B:396:SER:HB3	1.87	0.57
2:B:316:ASN:ND2	2:B:316:ASN:N	2.53	0.57
1:A:688:LYS:HE2	1:A:688:LYS:HA	1.86	0.57
1:A:813:HIS:HA	1:A:828:ILE:HD12	1.86	0.57
2:B:536:CYS:SG	2:B:543:SER:O	2.62	0.57
5:G:2:NDG:C6	5:G:2:NDG:C2	2.80	0.57
2:B:554:THR:O	2:B:558:CYS:HA	2.04	0.56
2:B:672:ASP:HB3	2:B:676:LYS:HE2	1.87	0.56
1:A:438:ARG:NH2	1:A:577:ILE:HG23	2.21	0.56
2:B:99:ASN:HD22	2:B:99:ASN:N	1.98	0.56
2:B:180:MET:HE3	2:B:214:ARG:NH2	2.20	0.56
2:B:219:PRO:HG3	2:B:253:LYS:HD2	1.85	0.56
2:B:73:GLY:HA3	2:B:109:ASP:HB3	1.88	0.56
2:B:173:LEU:HD13	2:B:178:TYR:HB3	1.86	0.56
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.88	0.56
1:A:252:MET:HE2	1:A:254:TYR:HE1	1.71	0.56
1:A:543:ARG:O	1:A:548:PHE:HE2	1.88	0.56
1:A:3:LEU:HD11	1:A:350:LEU:HD21	1.87	0.56
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.88	0.56
1:A:571:THR:C	1:A:573:GLY:H	2.14	0.56
2:B:333:LEU:HA	2:B:340:VAL:HG12	1.87	0.56
2:B:124:MET:SD	2:B:251:ASP:HB2	2.46	0.55
2:B:352:ARG:HH11	2:B:421:PHE:HZ	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:NAG:H5	4:D:2:NAG:HN2	1.71	0.55
2:B:111:PRO:HG2	2:B:242:ALA:HA	1.89	0.55
2:B:358:GLU:CD	2:B:419:VAL:HG12	2.32	0.55
1:A:271:GLN:HE22	1:A:301:MET:HB2	1.71	0.55
1:A:373:VAL:HG23	1:A:404:PHE:CE2	2.42	0.55
1:A:593:LEU:HD21	1:A:596:CYS:HB2	1.87	0.55
1:A:756:PRO:HD3	1:A:954:GLY:N	2.22	0.55
1:A:180:GLN:HE22	1:A:213:ALA:HB3	1.70	0.55
1:A:462:SER:HA	1:A:468:LEU:O	2.06	0.55
2:B:589:ILE:O	2:B:591:PRO:HD3	2.06	0.55
2:B:684:GLU:H	2:B:685:PRO:HD3	1.71	0.55
1:A:529:ARG:HB2	1:A:532:LEU:HB2	1.89	0.55
1:A:881:LYS:HB2	1:A:881:LYS:NZ	2.22	0.55
1:A:253:VAL:HG21	1:A:295:ILE:HG12	1.88	0.55
1:A:702:HIS:O	1:A:703:GLN:HB3	2.07	0.55
1:A:749:SER:CB	1:A:750:PRO:HD3	2.37	0.55
2:B:58:VAL:CG1	2:B:93:ARG:H	2.20	0.55
2:B:630:THR:O	2:B:634:TYR:HB3	2.06	0.55
2:B:94:PRO:O	2:B:95:ASP:HB2	2.07	0.55
2:B:250:THR:HG22	2:B:310:VAL:HG12	1.89	0.55
2:B:654:ASN:HD22	5:J:1:NAG:C6	2.19	0.55
2:B:169:PRO:HB2	2:B:170:PRO:CD	2.25	0.55
1:A:513:PHE:CE1	1:A:521:HIS:HB3	2.42	0.54
1:A:751:ASP:CB	4:H:1:NAG:H81	2.34	0.54
2:B:131:ILE:HG12	2:B:338:SER:O	2.07	0.54
2:B:657:TYR:O	2:B:664:VAL:HA	2.06	0.54
1:A:645:VAL:HB	1:A:679:VAL:HB	1.88	0.54
1:A:783:ARG:HB2	1:A:894:SER:OG	2.07	0.54
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.89	0.54
2:B:590:GLN:C	2:B:592:GLY:H	2.15	0.54
1:A:928:VAL:HB	1:A:941:ILE:HB	1.88	0.54
2:B:360:ARG:O	2:B:361:ASP:HB2	2.07	0.54
1:A:78:ARG:HG3	1:A:87:GLU:OE2	2.07	0.54
1:A:663:LEU:HD22	1:A:695:ALA:C	2.33	0.54
2:B:410:LYS:HG2	2:B:411:GLU:H	1.73	0.54
1:A:451:PRO:HD2	1:A:473:PHE:HB2	1.88	0.54
1:A:802:LYS:HG2	1:A:807:THR:HA	1.90	0.54
2:B:683:GLU:O	2:B:684:GLU:HB3	2.07	0.54
1:A:496:GLU:OE2	1:A:522:SER:HB3	2.07	0.54
1:A:543:ARG:HD3	1:A:547:GLU:HG3	1.90	0.54
2:B:99:ASN:H	2:B:99:ASN:ND2	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:C	1:A:62:SER:H	2.15	0.54
1:A:639:TYR:CD2	1:A:721:ASN:ND2	2.76	0.54
2:B:110:TYR:CD1	2:B:111:PRO:HD2	2.43	0.54
2:B:173:LEU:C	2:B:175:ASN:H	2.14	0.54
1:A:749:SER:HB3	1:A:750:PRO:HD3	1.89	0.54
2:B:622:ARG:NH2	2:B:659:ASN:HB2	2.22	0.54
1:A:458:ASN:HB3	6:A:2458:NAG:H62	1.91	0.53
1:A:529:ARG:HH11	1:A:529:ARG:HG2	1.74	0.53
2:B:71:ASP:HA	2:B:108:GLU:H	1.73	0.53
1:A:170:LEU:HG	1:A:239:PHE:CD2	2.44	0.53
1:A:758:PRO:HG2	2:B:666:ARG:NH1	2.23	0.53
2:B:652:ALA:HB1	2:B:669:TYR:O	2.08	0.53
1:A:812:LEU:O	1:A:829:ASN:HB2	2.08	0.53
2:B:571:ASN:HD21	2:B:573:LEU:HB2	1.72	0.53
2:B:615:VAL:HG23	2:B:657:TYR:OH	2.09	0.53
2:B:683:GLU:O	2:B:684:GLU:CB	2.56	0.53
5:G:2:NDG:H6C1	5:G:2:NDG:C2	2.32	0.53
1:A:11:TYR:HE2	1:A:65:ARG:HA	1.73	0.53
1:A:477:PHE:N	1:A:477:PHE:CD2	2.76	0.53
2:B:158:ASP:HB3	2:B:187:MET:HE1	1.89	0.53
2:B:178:TYR:HB2	2:B:181:LYS:HZ3	1.74	0.53
2:B:673:SER:C	2:B:675:GLY:H	2.14	0.53
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.89	0.53
1:A:643:LEU:O	1:A:680:VAL:HA	2.08	0.53
2:B:309:ALA:HA	2:B:331:GLY:O	2.08	0.53
2:B:403:VAL:HG11	2:B:431:PHE:CE2	2.44	0.53
4:D:1:NAG:H62	4:D:2:NAG:C1	2.38	0.53
1:A:363:PRO:HA	1:A:404:PHE:O	2.09	0.53
1:A:456:GLN:NE2	1:A:545:GLU:HB3	2.24	0.53
2:B:82:GLN:O	2:B:104:VAL:HA	2.09	0.53
1:A:238:ASP:HB3	1:A:256:TYR:O	2.09	0.53
1:A:621:ASP:HB3	1:A:891:ARG:HH22	1.74	0.53
2:B:162:SER:OG	2:B:163:PRO:HD3	2.09	0.53
1:A:118:MET:SD	1:A:118:MET:N	2.82	0.53
1:A:450:TYR:CB	1:A:451:PRO:HD3	2.39	0.53
1:A:559:MET:HE3	1:A:561:TYR:CD2	2.44	0.53
2:B:375:LEU:HA	2:B:633:ARG:HH21	1.74	0.53
1:A:347:LEU:HD22	1:A:422:LEU:HD12	1.91	0.52
2:B:60:GLU:HB3	2:B:90:LEU:HD23	1.91	0.52
2:B:127:ASP:CB	2:B:337:SER:HB3	2.39	0.52
2:B:426:ILE:HD12	2:B:426:ILE:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:O	1:A:479:LEU:HD12	2.10	0.52
2:B:129:TRP:C	2:B:131:ILE:N	2.66	0.52
2:B:532:LYS:HD2	2:B:532:LYS:O	2.09	0.52
1:A:422:LEU:HD23	1:A:423:ILE:N	2.24	0.52
2:B:185:LEU:HD21	2:B:211:SER:OG	2.10	0.52
1:A:926:PHE:HE2	1:A:943:ASN:HB3	1.75	0.52
2:B:134:LEU:HB3	2:B:203:PHE:HE2	1.75	0.52
2:B:536:CYS:HB2	2:B:546:ASP:HA	1.92	0.52
2:B:158:ASP:OD1	2:B:159:LYS:N	2.39	0.52
1:A:139:TYR:OH	1:A:186:ASP:HB2	2.09	0.52
1:A:328:THR:HG22	1:A:329:THR:N	2.24	0.52
2:B:340:VAL:HG22	2:B:341:LEU:HG	1.92	0.52
1:A:178:TYR:HB2	3:C:5001:ARG:NH2	2.25	0.52
1:A:346:PRO:O	1:A:410:GLY:O	2.27	0.52
2:B:64:LEU:HD22	2:B:86:GLN:HB2	1.92	0.52
2:B:88:ILE:HG13	2:B:89:ALA:N	2.25	0.52
2:B:192:HIS:NE2	2:B:195:THR:HG22	2.24	0.52
2:B:540:GLY:O	2:B:558:CYS:HB2	2.08	0.52
2:B:544:CYS:C	2:B:546:ASP:H	2.17	0.52
2:B:134:LEU:CB	2:B:203:PHE:HE2	2.23	0.52
2:B:131:ILE:HG22	2:B:131:ILE:O	2.11	0.51
2:B:332:VAL:O	2:B:343:LEU:HD11	2.09	0.51
1:A:494:GLN:HE21	1:A:494:GLN:HA	1.74	0.51
1:A:628:ILE:HD12	1:A:663:LEU:HD21	1.92	0.51
2:B:417:LYS:HE2	2:B:424:SER:HB3	1.92	0.51
1:A:775:VAL:HG22	1:A:902:LEU:CD1	2.41	0.51
2:B:670:TYR:HB3	2:B:678:ILE:HG23	1.92	0.51
1:A:642:GLU:HA	1:A:681:CYS:O	2.10	0.51
2:B:167:ILE:O	2:B:169:PRO:CD	2.59	0.51
5:G:1:NAG:H2	5:G:1:NAG:C6	2.16	0.51
1:A:459:LYS:CB	1:A:469:LYS:HB3	2.41	0.51
1:A:586:ILE:HD12	1:A:587:SER:H	1.75	0.51
1:A:598:GLU:C	1:A:600:ASN:N	2.67	0.51
2:B:88:ILE:CG1	2:B:89:ALA:N	2.74	0.51
2:B:240:ASN:HD22	2:B:240:ASN:N	2.08	0.51
1:A:794:MET:O	1:A:926:PHE:HA	2.10	0.51
1:A:799:TRP:HB3	1:A:880:LEU:HB3	1.93	0.51
1:A:906:GLU:C	1:A:908:PHE:N	2.68	0.51
2:B:178:TYR:C	2:B:180:MET:H	2.18	0.51
1:A:257:ASP:HB3	1:A:261:MET:H	1.76	0.51
2:B:119:ASP:HB3	2:B:124:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:GLN:CD	2:B:342:GLN:HE21	2.19	0.51
2:B:167:ILE:O	2:B:169:PRO:HD3	2.10	0.51
1:A:113:HIS:HD2	1:A:122:ARG:O	1.94	0.50
2:B:88:ILE:HG13	2:B:89:ALA:H	1.76	0.50
2:B:233:ASP:HA	2:B:238:TRP:HD1	1.75	0.50
1:A:150:ASP:O	1:A:177:PHE:HA	2.11	0.50
1:A:560:GLU:OE2	4:F:1:NAG:H83	2.12	0.50
1:A:578:LEU:HD22	1:A:578:LEU:N	2.25	0.50
2:B:557:TYR:O	2:B:558:CYS:HB2	2.12	0.50
1:A:460:THR:OG1	6:A:2458:NAG:O5	2.29	0.50
1:A:125:VAL:HG22	1:A:142:CYS:HB3	1.94	0.50
2:B:164:TYR:CE1	2:B:263:ALA:HB2	2.46	0.50
2:B:684:GLU:N	2:B:685:PRO:HD3	2.26	0.50
1:A:478:CYS:HB3	1:A:533:MET:HE2	1.93	0.50
1:A:554:PRO:HG3	1:A:591:HIS:CD2	2.47	0.50
2:B:257:ALA:O	2:B:258:LEU:HB2	2.12	0.50
2:B:620:PHE:HB3	2:B:622:ARG:HE	1.77	0.50
4:D:2:NAG:H5	4:D:2:NAG:N2	2.26	0.50
1:A:869:ILE:HG13	1:A:870:HIS:CD2	2.45	0.50
2:B:185:LEU:CB	2:B:186:PRO:HD2	2.42	0.50
2:B:224:ASP:CG	2:B:281:TYR:HE2	2.20	0.50
2:B:373:THR:HA	2:B:379:VAL:HA	1.94	0.50
2:B:129:TRP:CD1	2:B:130:SER:N	2.80	0.50
2:B:399:ILE:HD12	2:B:399:ILE:H	1.75	0.50
2:B:188:PHE:N	2:B:188:PHE:CD1	2.80	0.49
2:B:373:THR:CB	2:B:379:VAL:HG12	2.38	0.49
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.34	0.49
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.94	0.49
2:B:162:SER:CB	2:B:163:PRO:HD3	2.42	0.49
2:B:373:THR:HB	2:B:379:VAL:CG1	2.40	0.49
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.94	0.49
1:A:650:GLN:CG	1:A:704:GLN:HB2	2.43	0.49
2:B:187:MET:HE1	2:B:215:ASN:HD22	1.76	0.49
1:A:441:ILE:O	1:A:578:LEU:HA	2.12	0.49
1:A:604:PRO:HB3	1:A:636:GLU:O	2.12	0.49
1:A:3:LEU:HD21	1:A:350:LEU:HD11	1.93	0.49
1:A:931:PHE:N	1:A:931:PHE:CD2	2.80	0.49
2:B:355:VAL:O	2:B:385:SER:HA	2.11	0.49
2:B:623:GLU:HG2	2:B:624:PRO:CD	2.41	0.49
1:A:450:TYR:HD1	1:A:474:ASN:HB2	1.77	0.49
1:A:526:THR:HG22	1:A:527:ILE:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:GLU:O	2:B:410:LYS:HB2	2.13	0.49
2:B:346:ASP:OD1	2:B:346:ASP:N	2.46	0.49
1:A:683:LEU:HB3	1:A:687:MET:SD	2.53	0.49
1:A:178:TYR:HB2	3:C:5001:ARG:HH21	1.78	0.49
1:A:499:LEU:HD12	1:A:519:PRO:HA	1.94	0.49
1:A:663:LEU:CD2	1:A:694:LEU:HD23	2.42	0.49
1:A:35:PHE:HB3	1:A:59:CYS:O	2.13	0.48
1:A:191:ILE:HA	1:A:204:TYR:HE2	1.75	0.48
1:A:491:LEU:O	1:A:526:THR:HA	2.13	0.48
1:A:792:LYS:HB3	1:A:930:GLU:HB3	1.95	0.48
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.95	0.48
1:A:578:LEU:H	1:A:578:LEU:CD2	2.26	0.48
1:A:750:PRO:HD2	1:A:776:VAL:HA	1.96	0.48
1:A:914:GLN:HE21	1:A:916:HIS:HB3	1.78	0.48
2:B:587:VAL:HG23	2:B:587:VAL:O	2.13	0.48
1:A:372:ILE:HD12	1:A:392:GLU:HG2	1.94	0.48
2:B:67:ARG:O	2:B:69:LEU:HD12	2.13	0.48
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.42	0.48
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.78	0.48
1:A:487:LEU:H	1:A:488:PRO:HD2	1.77	0.48
1:A:579:ASN:HB3	1:A:582:THR:HG23	1.95	0.48
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.94	0.48
1:A:454:LEU:HD22	1:A:473:PHE:HB3	1.96	0.48
6:B:3371:NAG:O7	6:B:3371:NAG:H3	2.13	0.48
1:A:463:LEU:HG	1:A:464:PRO:HD2	1.95	0.48
2:B:148:ASN:C	2:B:148:ASN:HD22	2.22	0.48
2:B:371:ASN:ND2	6:B:3371:NAG:C6	2.63	0.48
1:A:72:PHE:HD2	1:A:129:PHE:HB3	1.78	0.48
1:A:938:ILE:N	1:A:938:ILE:HD13	2.29	0.48
2:B:174:GLU:O	2:B:186:PRO:HB3	2.14	0.48
2:B:267:GLN:HA	2:B:268:PRO:HD3	1.78	0.48
2:B:316:ASN:HB2	6:B:3320:NAG:H82	1.96	0.48
1:A:295:ILE:HD12	1:A:295:ILE:N	2.28	0.48
1:A:300:PHE:CE2	1:A:314:GLN:NE2	2.81	0.48
2:B:115:TYR:OH	2:B:192:HIS:ND1	2.45	0.48
1:A:377:ASN:O	1:A:383:LEU:HD12	2.14	0.47
1:A:439:PRO:HB2	1:A:487:LEU:HD13	1.96	0.47
1:A:449:VAL:HG23	1:A:474:ASN:O	2.14	0.47
1:A:648:PRO:O	1:A:677:ARG:HD3	2.14	0.47
2:B:180:MET:HG3	2:B:181:LYS:N	2.29	0.47
2:B:181:LYS:HA	2:B:181:LYS:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:LEU:O	2:B:328:THR:HG23	2.15	0.47
1:A:594:LEU:HD23	1:A:595:ASP:N	2.29	0.47
1:A:816:ILE:HD11	1:A:822:CYS:SG	2.54	0.47
1:A:886:VAL:HG12	1:A:887:GLY:N	2.30	0.47
2:B:343:LEU:O	2:B:347:ALA:N	2.43	0.47
2:B:574:LEU:HD11	2:B:581:CYS:HB2	1.96	0.47
1:A:102:GLN:HB2	1:A:103:ASP:H	1.55	0.47
1:A:271:GLN:NE2	1:A:301:MET:H	2.11	0.47
1:A:512:LEU:HD11	1:A:543:ARG:NH2	2.28	0.47
2:B:620:PHE:HB3	2:B:622:ARG:HD3	1.97	0.47
1:A:672:THR:HG22	1:A:677:ARG:CA	2.42	0.47
2:B:221:GLY:HA2	2:B:255:HIS:HB2	1.97	0.47
2:B:338:SER:O	2:B:339:ASN:HB2	2.13	0.47
2:B:410:LYS:HG2	2:B:411:GLU:N	2.29	0.47
2:B:411:GLU:OE1	2:B:428:GLN:HB3	2.13	0.47
1:A:271:GLN:HE22	1:A:301:MET:N	2.12	0.47
1:A:650:GLN:HE21	1:A:711:VAL:CG1	2.25	0.47
1:A:779:ILE:HD12	1:A:898:TYR:CD2	2.50	0.47
2:B:118:MET:SD	2:B:153:PHE:CD1	3.08	0.47
2:B:118:MET:SD	2:B:153:PHE:HD1	2.38	0.47
2:B:181:LYS:HZ1	2:B:183:THR:HA	1.80	0.47
1:A:674:ASN:HB3	1:A:676:THR:HG22	1.96	0.47
2:B:129:TRP:HD1	2:B:130:SER:H	1.63	0.47
2:B:130:SER:C	2:B:132:GLN:N	2.71	0.47
2:B:342:GLN:N	2:B:342:GLN:CD	2.73	0.47
2:B:187:MET:CE	2:B:215:ASN:HB3	2.45	0.47
2:B:646:LYS:HD2	2:B:668:GLN:NE2	2.30	0.47
1:A:441:ILE:HG23	1:A:487:LEU:CD1	2.44	0.46
1:A:527:ILE:O	1:A:528:SER:HB2	2.15	0.46
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.98	0.46
1:A:170:LEU:HD11	1:A:239:PHE:HB3	1.97	0.46
1:A:178:TYR:CD2	3:C:5001:ARG:CZ	2.93	0.46
1:A:754:PHE:CD1	2:B:656:THR:HG22	2.50	0.46
1:A:921:LYS:CE	1:A:946:LEU:HD12	2.45	0.46
1:A:569:ALA:O	1:A:573:GLY:HA2	2.15	0.46
2:B:411:GLU:HG3	2:B:413:SER:OG	2.15	0.46
1:A:5:VAL:HG12	1:A:5:VAL:O	2.16	0.46
1:A:390:ILE:HD12	1:A:392:GLU:HG2	1.98	0.46
1:A:575:GLN:HA	1:A:576:PRO:HD3	1.68	0.46
1:A:625:LEU:HD23	1:A:699:PHE:HB2	1.97	0.46
2:B:205:GLU:HG3	2:B:206:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:O	1:A:52:GLU:HG2	2.15	0.46
1:A:53:GLY:O	1:A:94:PHE:HB3	2.16	0.46
2:B:267:GLN:HE21	2:B:287:MET:HB2	1.81	0.46
2:B:538:GLY:O	2:B:539:HIS:HB2	2.14	0.46
1:A:42:LYS:HA	1:A:52:GLU:HB3	1.97	0.46
1:A:260:ASN:O	1:A:261:MET:HB3	2.16	0.46
2:B:148:ASN:HD22	2:B:149:LEU:N	2.13	0.46
1:A:232:ASN:O	1:A:233:GLY:C	2.59	0.46
1:A:260:ASN:ND2	6:A:2260:NAG:C6	2.79	0.46
1:A:674:ASN:O	1:A:676:THR:N	2.42	0.46
2:B:262:LEU:N	2:B:262:LEU:HD23	2.31	0.46
1:A:26:PHE:O	1:A:28:PRO:HD3	2.16	0.46
1:A:68:GLN:NE2	1:A:69:PRO:HD2	2.31	0.46
1:A:154:PHE:O	1:A:175:GLY:HA3	2.16	0.46
1:A:667:SER:HB2	1:A:682:ASP:HB2	1.97	0.46
1:A:647:ILE:HD11	1:A:670:PHE:HE2	1.81	0.46
2:B:82:GLN:HG2	2:B:107:VAL:HG23	1.98	0.46
2:B:378:GLU:O	2:B:379:VAL:HG22	2.15	0.46
2:B:621:ASP:O	2:B:626:MET:SD	2.74	0.46
1:A:271:GLN:HE22	1:A:301:MET:CB	2.29	0.45
1:A:606:LEU:CB	1:A:727:SER:HB3	2.46	0.45
2:B:169:PRO:CB	2:B:170:PRO:CD	2.93	0.45
2:B:333:LEU:HA	2:B:340:VAL:CG1	2.46	0.45
2:B:337:SER:O	2:B:338:SER:OG	2.27	0.45
2:B:354:LYS:HD2	2:B:354:LYS:C	2.41	0.45
1:A:74:ALA:O	1:A:75:THR:CG2	2.62	0.45
1:A:934:LYS:O	1:A:935:ASN:HB2	2.16	0.45
2:B:131:ILE:HG23	2:B:134:LEU:HG	1.98	0.45
2:B:269:ASN:ND2	2:B:290:PRO:HB3	2.30	0.45
2:B:417:LYS:HB3	2:B:424:SER:HB3	1.98	0.45
2:B:599:GLU:HG2	2:B:600:LYS:N	2.31	0.45
1:A:121:GLU:O	1:A:122:ARG:HB2	2.17	0.45
1:A:508:ILE:O	1:A:510:ARG:N	2.49	0.45
1:A:647:ILE:HG21	1:A:699:PHE:CE1	2.51	0.45
2:B:612:LYS:O	2:B:615:VAL:HG22	2.17	0.45
5:J:1:NAG:H62	5:J:1:NAG:O3	2.15	0.45
1:A:77:ASN:ND2	1:A:89:LYS:H	2.03	0.45
1:A:516:SER:O	1:A:518:SER:N	2.49	0.45
2:B:106:GLN:HB2	2:B:392:GLY:H	1.81	0.45
2:B:178:TYR:C	2:B:178:TYR:CD1	2.95	0.45
2:B:648:THR:O	2:B:650:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ASN:ND2	5:J:1:NAG:C6	2.79	0.45
1:A:756:PRO:HA	1:A:953:TRP:HZ3	1.82	0.45
2:B:366:LEU:HD23	2:B:366:LEU:H	1.81	0.45
1:A:903:LEU:HD13	1:A:905:THR:N	2.30	0.45
2:B:647:ASP:O	5:J:2:NDG:C1	2.64	0.45
1:A:301:MET:HG2	1:A:311:GLU:HA	1.98	0.45
1:A:347:LEU:CD2	1:A:422:LEU:HD12	2.46	0.45
1:A:552:LEU:CD2	1:A:592:ILE:H	2.29	0.45
1:A:644:ILE:HD12	1:A:680:VAL:HG22	1.99	0.45
2:B:64:LEU:HD22	2:B:86:GLN:CB	2.47	0.45
2:B:641:SER:OG	2:B:683:GLU:HB2	2.16	0.45
1:A:29:SER:HB2	1:A:103:ASP:OD1	2.17	0.45
2:B:244:HIS:O	2:B:245:LEU:HD23	2.16	0.45
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.99	0.45
1:A:61:TRP:CG	1:A:61:TRP:O	2.70	0.45
1:A:464:PRO:HG2	1:A:517:ARG:HE	1.80	0.45
2:B:281:TYR:HE1	2:B:283:ALA:HB3	1.82	0.45
2:B:365:GLU:HG3	2:B:407:PRO:HD3	1.99	0.45
1:A:61:TRP:C	1:A:63:SER:N	2.74	0.45
1:A:100:SER:CB	1:A:105:ILE:HG22	2.47	0.45
1:A:252:MET:CE	1:A:254:TYR:HE1	2.29	0.45
2:B:169:PRO:HD2	2:B:170:PRO:CD	2.47	0.45
1:A:445:ALA:HB1	1:A:559:MET:CE	2.47	0.44
1:A:685:ASN:HD22	1:A:685:ASN:C	2.25	0.44
1:A:252:MET:HA	1:A:267:PHE:O	2.17	0.44
1:A:284:ASP:O	1:A:356:ASN:HB2	2.17	0.44
1:A:796:HIS:O	1:A:924:ALA:HA	2.17	0.44
1:A:604:PRO:HD3	1:A:721:ASN:OD1	2.17	0.44
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.70	0.44
1:A:33:ARG:NH1	1:A:62:SER:HB2	2.32	0.44
1:A:487:LEU:H	1:A:488:PRO:CD	2.31	0.44
1:A:716:GLN:NE2	1:A:729:VAL:HG22	2.33	0.44
1:A:942:THR:O	1:A:943:ASN:HB2	2.16	0.44
2:B:173:LEU:HD11	2:B:176:PRO:HA	1.99	0.44
2:B:296:THR:HG22	2:B:297:GLU:N	2.32	0.44
2:B:607:ALA:O	2:B:609:THR:N	2.50	0.44
1:A:101:LYS:HB3	1:A:102:GLN:H	1.69	0.44
1:A:487:LEU:N	1:A:488:PRO:CD	2.81	0.44
2:B:58:VAL:O	2:B:98:LYS:HE2	2.18	0.44
2:B:58:VAL:HG12	2:B:92:LEU:HA	1.99	0.44
1:A:449:VAL:HG21	1:A:473:PHE:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLY:HA3	1:A:517:ARG:NH2	2.33	0.44
1:A:176:SER:CB	1:A:182:GLN:HE21	2.31	0.44
1:A:552:LEU:HD12	1:A:686:PRO:HG3	1.99	0.44
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.99	0.44
1:A:795:LEU:HD23	1:A:796:HIS:N	2.33	0.44
2:B:141:GLN:HB3	2:B:141:GLN:HE21	1.56	0.44
1:A:113:HIS:CD2	1:A:124:PRO:HD3	2.53	0.44
1:A:375:ILE:CD1	1:A:389:GLN:HB3	2.48	0.44
1:A:402:PRO:HA	1:A:428:GLY:HA3	2.00	0.44
1:A:906:GLU:C	1:A:908:PHE:H	2.26	0.44
2:B:71:ASP:HB3	2:B:108:GLU:CB	2.48	0.44
2:B:344:ILE:N	2:B:344:ILE:HD13	2.33	0.44
1:A:11:TYR:CE2	1:A:65:ARG:HA	2.51	0.44
1:A:15:GLU:HA	1:A:430:ASP:OD1	2.18	0.44
1:A:579:ASN:HB3	1:A:582:THR:CG2	2.48	0.44
2:B:62:ARG:CD	2:B:85:PRO:HB3	2.48	0.44
2:B:270:ASP:CG	2:B:272:GLN:HB2	2.43	0.44
2:B:295:MET:O	2:B:299:LEU:HB2	2.17	0.44
3:C:5001:ARG:N	3:C:5005:MVA:HN3	2.32	0.44
1:A:253:VAL:HG21	1:A:295:ILE:CG1	2.47	0.43
1:A:439:PRO:CB	1:A:487:LEU:HD13	2.48	0.43
2:B:215:ASN:O	3:C:5003:ASP:HB3	2.19	0.43
2:B:607:ALA:C	2:B:609:THR:N	2.76	0.43
1:A:526:THR:O	1:A:527:ILE:HG23	2.17	0.43
1:A:26:PHE:CZ	1:A:28:PRO:HG3	2.53	0.43
1:A:417:ASN:O	1:A:419:TYR:N	2.46	0.43
2:B:130:SER:HB3	2:B:338:SER:OG	2.17	0.43
2:B:132:GLN:O	2:B:204:ASN:ND2	2.50	0.43
2:B:182:THR:O	2:B:182:THR:HG22	2.18	0.43
1:A:222:LEU:HD12	1:A:223:GLY:N	2.32	0.43
1:A:410:GLY:O	1:A:411:ALA:CB	2.66	0.43
1:A:607:GLU:HG2	1:A:632:GLN:HB2	2.00	0.43
2:B:67:ARG:H	2:B:67:ARG:HD2	1.83	0.43
2:B:173:LEU:HD13	2:B:178:TYR:CG	2.53	0.43
2:B:620:PHE:HB3	2:B:622:ARG:NE	2.33	0.43
1:A:472:CYS:H	6:A:2458:NAG:H61	1.82	0.43
2:B:580:LYS:HB2	2:B:580:LYS:HZ2	1.79	0.43
1:A:440:VAL:HG22	1:A:577:ILE:CD1	2.49	0.43
2:B:127:ASP:HA	2:B:337:SER:HB3	2.00	0.43
2:B:133:ASN:O	2:B:134:LEU:C	2.62	0.43
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:CG2	1:A:473:PHE:HD1	2.32	0.43
1:A:451:PRO:HG2	1:A:473:PHE:HA	1.99	0.43
1:A:605:LYS:H	1:A:635:GLY:H	1.66	0.43
1:A:610:VAL:HG11	1:A:732:HIS:HB2	2.01	0.43
2:B:213:SER:O	2:B:214:ARG:HB2	2.17	0.43
1:A:271:GLN:HE22	1:A:301:MET:H	1.66	0.43
1:A:375:ILE:CG1	1:A:389:GLN:HB3	2.47	0.43
1:A:456:GLN:HE22	1:A:545:GLU:HB3	1.84	0.43
1:A:533:MET:HG3	1:A:533:MET:O	2.19	0.43
1:A:650:GLN:CB	1:A:701:VAL:HG23	2.45	0.43
1:A:755:LEU:C	1:A:757:ILE:N	2.74	0.43
2:B:83:VAL:HA	2:B:103:GLN:O	2.19	0.43
1:A:14:PRO:HG2	1:A:17:SER:OG	2.19	0.43
1:A:125:VAL:HG23	1:A:152:GLN:O	2.18	0.43
1:A:526:THR:HG22	1:A:527:ILE:N	2.34	0.43
1:A:672:THR:HG22	1:A:677:ARG:CB	2.49	0.43
1:A:915:ASN:ND2	1:A:953:TRP:HE1	2.15	0.43
2:B:177:CYS:HB2	2:B:180:MET:SD	2.59	0.43
1:A:394:GLN:O	1:A:394:GLN:HG2	2.18	0.43
1:A:459:LYS:H	1:A:459:LYS:HG3	1.52	0.43
2:B:102:ILE:CG2	2:B:399:ILE:HD11	2.47	0.43
2:B:191:LYS:HD3	2:B:280:HIS:NE2	2.33	0.43
1:A:510:ARG:NH2	1:A:553:THR:O	2.45	0.42
1:A:781:GLU:HB2	1:A:896:ILE:HG23	1.99	0.42
1:A:523:LYS:HG2	1:A:536:GLU:OE2	2.19	0.42
1:A:704:GLN:HB3	1:A:707:MET:CB	2.49	0.42
1:A:783:ARG:NE	1:A:894:SER:OG	2.33	0.42
1:A:869:ILE:HG23	1:A:870:HIS:N	2.34	0.42
1:A:36:LEU:HB2	1:A:59:CYS:HB2	2.01	0.42
1:A:174:PRO:O	1:A:181:GLY:HA2	2.18	0.42
1:A:404:PHE:HA	1:A:426:ALA:HB2	2.01	0.42
1:A:17:SER:O	1:A:41:PRO:O	2.36	0.42
1:A:436:ARG:CZ	1:A:574:LEU:HD13	2.49	0.42
1:A:364:TYR:O	1:A:369:LYS:HG2	2.19	0.42
1:A:17:SER:HB2	1:A:43:ALA:HB2	2.02	0.42
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.83	0.42
1:A:60:ASP:C	1:A:62:SER:N	2.78	0.42
1:A:92:GLN:HG3	1:A:109:ALA:HB1	2.01	0.42
2:B:87:ARG:NH2	2:B:428:GLN:OE1	2.53	0.42
2:B:131:ILE:O	2:B:131:ILE:CG2	2.67	0.42
2:B:173:LEU:HD13	2:B:178:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:SER:OG	1:A:182:GLN:NE2	2.51	0.42
1:A:239:PHE:HD1	1:A:261:MET:SD	2.43	0.42
1:A:753:VAL:O	1:A:951:VAL:HA	2.19	0.42
2:B:65:GLU:O	2:B:66:ASP:C	2.61	0.42
2:B:187:MET:HE1	2:B:215:ASN:ND2	2.34	0.42
2:B:247:VAL:HG21	2:B:344:ILE:HD12	2.02	0.42
1:A:439:PRO:O	1:A:576:PRO:HB3	2.19	0.42
1:A:657:VAL:HG11	1:A:663:LEU:CD1	2.50	0.42
1:A:872:LEU:HD23	1:A:872:LEU:HA	1.76	0.42
1:A:907:THR:HG22	1:A:918:TYR:CD2	2.55	0.42
2:B:104:VAL:HG11	2:B:355:VAL:HG11	2.02	0.42
2:B:170:PRO:C	2:B:172:ALA:N	2.76	0.42
2:B:358:GLU:HG3	2:B:358:GLU:O	2.20	0.42
1:A:196:ASP:C	1:A:198:ASN:H	2.28	0.42
1:A:503:LYS:HE3	1:A:510:ARG:HD3	2.02	0.42
2:B:115:TYR:CD1	2:B:236:ILE:HG23	2.55	0.42
1:A:490:LYS:O	1:A:490:LYS:HG3	2.20	0.41
1:A:527:ILE:HB	1:A:528:SER:H	1.66	0.41
1:A:810:TYR:HE2	1:A:812:LEU:HD23	1.84	0.41
1:A:837:SER:HB3	1:A:838:LEU:H	1.53	0.41
1:A:916:HIS:HA	1:A:953:TRP:HD1	1.85	0.41
2:B:364:GLU:N	2:B:364:GLU:CD	2.78	0.41
2:B:379:VAL:O	2:B:379:VAL:HG23	2.20	0.41
2:B:643:LYS:C	2:B:645:LEU:H	2.28	0.41
1:A:260:ASN:HD22	6:A:2260:NAG:C6	2.33	0.41
1:A:455:ASN:HB3	6:A:2458:NAG:H4	2.02	0.41
1:A:552:LEU:HD11	1:A:591:HIS:CD2	2.51	0.41
1:A:785:ASN:O	1:A:786:GLY:C	2.63	0.41
2:B:55:GLU:O	2:B:56:PHE:HB2	2.20	0.41
2:B:120:LEU:HD22	2:B:155:ALA:CB	2.50	0.41
3:C:5004:PHE:HA	3:C:5005:MVA:HN1	1.57	0.41
4:D:2:NAG:N2	4:D:2:NAG:C5	2.81	0.41
1:A:295:ILE:HG22	1:A:296:GLY:N	2.34	0.41
1:A:808:LEU:O	1:A:809:LEU:HB2	2.20	0.41
2:B:62:ARG:CZ	2:B:85:PRO:HB3	2.50	0.41
2:B:173:LEU:HD11	2:B:176:PRO:C	2.45	0.41
2:B:571:ASN:HD21	2:B:573:LEU:CB	2.33	0.41
2:B:628:GLU:O	2:B:630:THR:HG23	2.20	0.41
1:A:50:ILE:HG23	1:A:90:SER:N	2.36	0.41
1:A:247:ALA:O	1:A:250:LEU:HB2	2.21	0.41
1:A:552:LEU:HD12	1:A:686:PRO:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:PRO:HG2	2:B:285:THR:HG22	2.02	0.41
1:A:243:VAL:HG12	1:A:246:ALA:HB2	2.01	0.41
1:A:486:VAL:O	1:A:487:LEU:HB3	2.19	0.41
2:B:221:GLY:C	2:B:223:PHE:H	2.28	0.41
2:B:679:LEU:HD12	2:B:679:LEU:N	2.35	0.41
1:A:61:TRP:O	1:A:61:TRP:CD2	2.73	0.41
1:A:113:HIS:CD2	1:A:122:ARG:O	2.74	0.41
1:A:119:LYS:HG2	1:A:120:GLN:H	1.86	0.41
1:A:463:LEU:HB3	1:A:466:THR:O	2.21	0.41
1:A:562:ARG:HG2	1:A:563:LEU:N	2.34	0.41
1:A:585:ASN:ND2	4:F:1:NAG:C6	2.74	0.41
2:B:62:ARG:NH1	2:B:85:PRO:HB3	2.36	0.41
1:A:108:CYS:SG	1:A:161:ILE:HD13	2.61	0.41
1:A:252:MET:HE2	1:A:254:TYR:CE1	2.55	0.41
1:A:480:LYS:HB3	1:A:533:MET:HB3	2.03	0.41
1:A:657:VAL:O	1:A:658:ARG:HB2	2.21	0.41
1:A:670:PHE:CD1	1:A:670:PHE:C	2.98	0.41
1:A:890:ASP:O	1:A:891:ARG:C	2.64	0.41
2:B:355:VAL:HG12	2:B:397:PHE:HZ	1.86	0.41
2:B:534:GLU:CB	2:B:544:CYS:SG	3.06	0.41
1:A:505:LYS:HE3	1:A:505:LYS:HB3	1.88	0.41
2:B:418:PRO:HG2	2:B:421:PHE:HB2	2.03	0.41
2:B:627:THR:HG22	2:B:627:THR:O	2.20	0.41
1:A:79:ASP:HB3	1:A:81:ALA:O	2.21	0.41
1:A:512:LEU:HD12	1:A:541:TYR:OH	2.21	0.41
1:A:514:LEU:HB3	1:A:515:TYR:H	1.71	0.41
1:A:617:ILE:HG13	1:A:617:ILE:O	2.21	0.41
1:A:656:VAL:HG23	1:A:657:VAL:N	2.30	0.41
1:A:765:ASN:HA	1:A:766:PRO:HD2	1.89	0.41
2:B:60:GLU:HB2	2:B:88:ILE:HD11	2.03	0.41
2:B:159:LYS:O	2:B:161:VAL:N	2.52	0.41
2:B:406:CYS:HB2	2:B:431:PHE:HB3	2.02	0.41
1:A:181:GLY:HA3	1:A:222:LEU:HB3	2.02	0.41
1:A:328:THR:CG2	1:A:329:THR:N	2.84	0.41
1:A:571:THR:C	1:A:573:GLY:N	2.78	0.41
1:A:614:GLN:HE21	1:A:616:LYS:NZ	2.19	0.41
1:A:749:SER:CB	1:A:750:PRO:CD	2.97	0.41
2:B:173:LEU:CD1	2:B:176:PRO:HA	2.51	0.41
1:A:292:ASP:O	1:A:294:PHE:CE1	2.74	0.40
1:A:459:LYS:HB3	1:A:469:LYS:HB3	2.01	0.40
1:A:571:THR:O	1:A:573:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ILE:HB	2:B:151:ILE:HG22	2.03	0.40
2:B:157:VAL:CG1	2:B:158:ASP:H	2.25	0.40
2:B:343:LEU:H	2:B:343:LEU:CD2	2.25	0.40
1:A:260:ASN:ND2	6:A:2260:NAG:H62	2.36	0.40
1:A:541:TYR:HE2	1:A:543:ARG:HA	1.87	0.40
1:A:618:TYR:CD2	1:A:737:ALA:HB3	2.56	0.40
1:A:652:ASP:O	1:A:699:PHE:HA	2.21	0.40
1:A:755:LEU:O	1:A:756:PRO:C	2.59	0.40
2:B:128:LEU:O	2:B:130:SER:N	2.55	0.40
2:B:278:ASP:OD1	2:B:280:HIS:HB2	2.21	0.40
1:A:365:GLY:O	1:A:369:LYS:HA	2.20	0.40
1:A:419:TYR:HA	1:A:420:PRO:HD3	1.83	0.40
1:A:552:LEU:HD21	1:A:591:HIS:HA	2.02	0.40
1:A:644:ILE:CD1	1:A:680:VAL:HG22	2.52	0.40
1:A:647:ILE:HG22	1:A:713:PHE:CE2	2.56	0.40
2:B:160:PRO:HG2	2:B:285:THR:CG2	2.51	0.40
2:B:624:PRO:O	2:B:627:THR:N	2.54	0.40
1:A:236:ILE:CD1	1:A:236:ILE:N	2.71	0.40
1:A:464:PRO:HD3	1:A:514:LEU:CD1	2.48	0.40
1:A:484:LYS:H	1:A:487:LEU:HD21	1.86	0.40
1:A:679:VAL:HG21	1:A:699:PHE:HZ	1.85	0.40
1:A:755:LEU:CD2	1:A:951:VAL:HB	2.51	0.40
1:A:766:PRO:O	1:A:767:GLU:HG3	2.21	0.40
2:B:590:GLN:C	2:B:592:GLY:N	2.80	0.40
1:A:62:SER:C	1:A:64:THR:N	2.80	0.40
1:A:190:GLU:OE2	1:A:205:ASN:HB2	2.22	0.40
1:A:688:LYS:HA	1:A:688:LYS:CE	2.51	0.40
1:A:812:LEU:HD21	1:A:902:LEU:CD2	2.49	0.40
1:A:936:LEU:HD13	1:A:936:LEU:HA	1.86	0.40
2:B:150:ARG:HA	2:B:197:THR:O	2.20	0.40
2:B:166:TYR:C	2:B:167:ILE:O	2.65	0.40
2:B:281:TYR:O	2:B:284:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	923/957 (96%)	743 (80%)	125 (14%)	55 (6%)	1	10
2	B	535/692 (77%)	392 (73%)	98 (18%)	45 (8%)	0	4
3	C	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
All	All	1461/1654 (88%)	1137 (78%)	223 (15%)	101 (7%)	1	7

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	236	ILE
1	A	396	ALA
1	A	411	ALA
1	A	487	LEU
1	A	488	PRO
1	A	489	ARG
1	A	504	GLN
1	A	514	LEU
1	A	517	ARG
1	A	527	ILE
1	A	703	GLN
1	A	707	MET
1	A	749	SER
1	A	891	ARG
1	A	916	HIS
2	B	123	SER
2	B	129	TRP
2	B	162	SER
2	B	169	PRO
2	B	176	PRO
2	B	241	ASP
2	B	253	LYS
2	B	338	SER
2	B	339	ASN
2	B	546	ASP
3	C	5004	PHE
1	A	75	THR
1	A	82	LYS
1	A	167	ASP

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Mol	Chain	Res	Type
1	A	350	LEU
1	A	399	SER
1	A	416	LYS
1	A	509	ARG
1	A	528	SER
1	A	615	LYS
1	A	648	PRO
1	A	657	VAL
1	A	759	ASN
1	A	836	SER
1	A	837	SER
2	B	177	CYS
2	B	288	ASP
2	B	337	SER
2	B	341	LEU
2	B	376	ASN
2	B	410	LYS
2	B	537	SER
2	B	539	HIS
2	B	547	CYS
2	B	608	CYS
2	B	641	SER
2	B	643	LYS
2	B	649	GLY
2	B	672	ASP
2	B	682	VAL
2	B	684	GLU
1	A	205	ASN
1	A	552	LEU
1	A	621	ASP
1	A	656	VAL
1	A	680	VAL
1	A	705	SER
2	B	163	PRO
2	B	180	MET
2	B	182	THR
2	B	590	GLN
2	B	636	ARG
1	A	515	TYR
1	A	930	GLU
2	B	76	ASP
2	B	79	GLN

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Mol	Chain	Res	Type
2	B	122	TYR
2	B	258	LEU
2	B	335	MET
2	B	407	PRO
2	B	647	ASP
2	B	651	ASP
1	A	62	SER
1	A	550	ASP
1	A	572	THR
1	A	685	ASN
1	A	687	MET
1	A	708	ASP
1	A	757	ILE
1	A	954	GLY
2	B	379	VAL
1	A	126	GLY
1	A	418	GLY
1	A	554	PRO
2	B	56	PHE
2	B	168	SER
2	B	405	GLY
2	B	541	GLN
1	A	348	GLY
1	A	450	TYR
1	A	464	PRO
1	A	508	ILE
1	A	197	PRO
1	A	573	GLY
2	B	167	ILE

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	787/812 (97%)	699 (89%)	88 (11%)	6	25
2	B	484/616 (79%)	401 (83%)	83 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	3/3 (100%)	3 (100%)	0	100	100
All	All	1274/1431 (89%)	1103 (87%)	171 (13%)	4	19

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	ASP
1	A	10	GLU
1	A	24	ASP
1	A	29	SER
1	A	34	MET
1	A	51	VAL
1	A	71	GLU
1	A	86	LEU
1	A	90	SER
1	A	101	LYS
1	A	102	GLN
1	A	119	LYS
1	A	120	GLN
1	A	125	VAL
1	A	134	THR
1	A	145	GLN
1	A	162	ASP
1	A	169	VAL
1	A	170	LEU
1	A	187	GLN
1	A	219	ASP
1	A	226	VAL
1	A	234	ASP
1	A	236	ILE
1	A	264	LEU
1	A	275	TYR
1	A	303	ARG
1	A	311	GLU
1	A	318	SER
1	A	321	ARG
1	A	339	ARG
1	A	390	ILE
1	A	394	GLN
1	A	408	MET
1	A	459	LYS

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Mol	Chain	Res	Type
1	A	477	PHE
1	A	488	PRO
1	A	489	ARG
1	A	494	GLN
1	A	495	VAL
1	A	514	LEU
1	A	527	ILE
1	A	539	ILE
1	A	549	ARG
1	A	551	LYS
1	A	552	LEU
1	A	574	LEU
1	A	577	ILE
1	A	578	LEU
1	A	585	ASN
1	A	598	GLU
1	A	607	GLU
1	A	616	LYS
1	A	634	GLN
1	A	652	ASP
1	A	676	THR
1	A	685	ASN
1	A	701	VAL
1	A	712	LYS
1	A	735	ASP
1	A	753	VAL
1	A	755	LEU
1	A	756	PRO
1	A	768	THR
1	A	770	GLU
1	A	782	LEU
1	A	813	HIS
1	A	835	ILE
1	A	878	GLN
1	A	880	LEU
1	A	881	LYS
1	A	885	GLN
1	A	896	ILE
1	A	897	LEU
1	A	902	LEU
1	A	903	LEU
1	A	904	TRP

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Mol	Chain	Res	Type
1	A	905	THR
1	A	906	GLU
1	A	907	THR
1	A	908	PHE
1	A	916	HIS
1	A	931	PHE
1	A	936	LEU
1	A	938	ILE
1	A	946	LEU
1	A	956	GLN
2	B	58	VAL
2	B	60	GLU
2	B	64	LEU
2	B	67	ARG
2	B	68	PRO
2	B	81	THR
2	B	88	ILE
2	B	99	ASN
2	B	102	ILE
2	B	113	ASP
2	B	116	TYR
2	B	120	LEU
2	B	126	ASP
2	B	127	ASP
2	B	129	TRP
2	B	131	ILE
2	B	132	GLN
2	B	141	GLN
2	B	145	LEU
2	B	161	VAL
2	B	162	SER
2	B	167	ILE
2	B	174	GLU
2	B	176	PRO
2	B	178	TYR
2	B	183	THR
2	B	185	LEU
2	B	188	PHE
2	B	193	VAL
2	B	212	VAL
2	B	216	ARG
2	B	217	ASP

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Mol	Chain	Res	Type
2	B	220	GLU
2	B	224	ASP
2	B	240	ASN
2	B	251	ASP
2	B	254	THR
2	B	261	ARG
2	B	262	LEU
2	B	272	GLN
2	B	296	THR
2	B	300	SER
2	B	307	ILE
2	B	316	ASN
2	B	329	THR
2	B	336	ASP
2	B	343	LEU
2	B	346	ASP
2	B	357	LEU
2	B	360	ARG
2	B	364	GLU
2	B	366	LEU
2	B	373	THR
2	B	375	LEU
2	B	376	ASN
2	B	379	VAL
2	B	387	MET
2	B	397	PHE
2	B	400	GLU
2	B	415	THR
2	B	429	VAL
2	B	430	THR
2	B	433	CYS
2	B	539	HIS
2	B	544	CYS
2	B	561	THR
2	B	568	MET
2	B	573	LEU
2	B	580	LYS
2	B	596	ASP
2	B	603	THR
2	B	617	CYS
2	B	619	LYS
2	B	622	ARG

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Mol	Chain	Res	Type
2	B	623	GLU
2	B	624	PRO
2	B	626	MET
2	B	640	GLU
2	B	643	LYS
2	B	651	ASP
2	B	671	GLU
2	B	673	SER
2	B	674	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	77	ASN
1	A	102	GLN
1	A	113	HIS
1	A	180	GLN
1	A	182	GLN
1	A	187	GLN
1	A	206	ASN
1	A	271	GLN
1	A	314	GLN
1	A	320	GLN
1	A	377	ASN
1	A	394	GLN
1	A	492	ASN
1	A	494	GLN
1	A	589	GLN
1	A	591	HIS
1	A	614	GLN
1	A	685	ASN
1	A	716	GLN
1	A	718	GLN
1	A	759	ASN
1	A	765	ASN
1	A	778	HIS
1	A	785	ASN
1	A	804	ASN
1	A	870	HIS
1	A	914	GLN
1	A	927	ASN

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Mol	Chain	Res	Type
1	A	935	ASN
2	B	99	ASN
2	B	133	ASN
2	B	141	GLN
2	B	148	ASN
2	B	175	ASN
2	B	215	ASN
2	B	240	ASN
2	B	255	HIS
2	B	267	GLN
2	B	269	ASN
2	B	272	GLN
2	B	303	ASN
2	B	305	ASN
2	B	316	ASN
2	B	339	ASN
2	B	342	GLN
2	B	541	GLN
2	B	571	ASN
2	B	629	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MVA	C	5005	3	6,7,8	1.37	1 (16%)	6,8,10	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MVA	C	5005	3	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5005	MVA	CN-N	-2.70	1.40	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5005	MVA	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5005	MVA	3	0

5.5 Carbohydrates

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.47	0	17,19,21	0.68	0
4	NAG	D	2	4	14,14,15	0.41	0	17,19,21	0.82	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.51	0	17,19,21	0.83	0
4	NAG	E	2	4	14,14,15	0.41	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	1,4	14,14,15	0.78	0	17,19,21	0.68	0
4	NAG	F	2	4	14,14,15	0.55	0	17,19,21	0.75	0
5	NAG	G	1	1,5	14,14,15	0.49	0	17,19,21	0.74	1 (5%)
5	NDG	G	2	5	14,14,15	0.70	0	17,19,21	0.55	0
4	NAG	H	1	1,4	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.59	0
5	NAG	I	1	5,2	14,14,15	0.82	0	17,19,21	0.72	0
5	NDG	I	2	5	14,14,15	0.82	1 (7%)	17,19,21	1.07	2 (11%)
5	NAG	J	1	5,2	14,14,15	0.63	0	17,19,21	0.74	0
5	NDG	J	2	5	14,14,15	0.49	0	17,19,21	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NDG	G	2	5	-	4/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,2	-	2/6/23/26	0/1/1/1
5	NDG	I	2	5	-	1/6/23/26	0/1/1/1
5	NAG	J	1	5,2	-	2/6/23/26	0/1/1/1
5	NDG	J	2	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	NDG	C1-C2	2.37	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C3-C4-C5	3.20	116.04	110.23
4	H	1	NAG	C4-C3-C2	3.09	115.55	111.02
5	I	2	NDG	C1-O5-C5	2.73	115.84	112.19
5	I	2	NDG	C2-N2-C7	-2.36	119.73	122.90
4	D	2	NAG	C2-N2-C7	-2.32	119.79	122.90
5	G	1	NAG	C2-N2-C7	-2.08	120.11	122.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	G	2	NDG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	I	2	NDG	O5-C5-C6-O6
5	G	2	NDG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6
5	G	2	NDG	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
5	G	2	NDG	C1-C2-N2-C7
4	F	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C3-C2-N2-C7
5	I	1	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 26 short contacts:

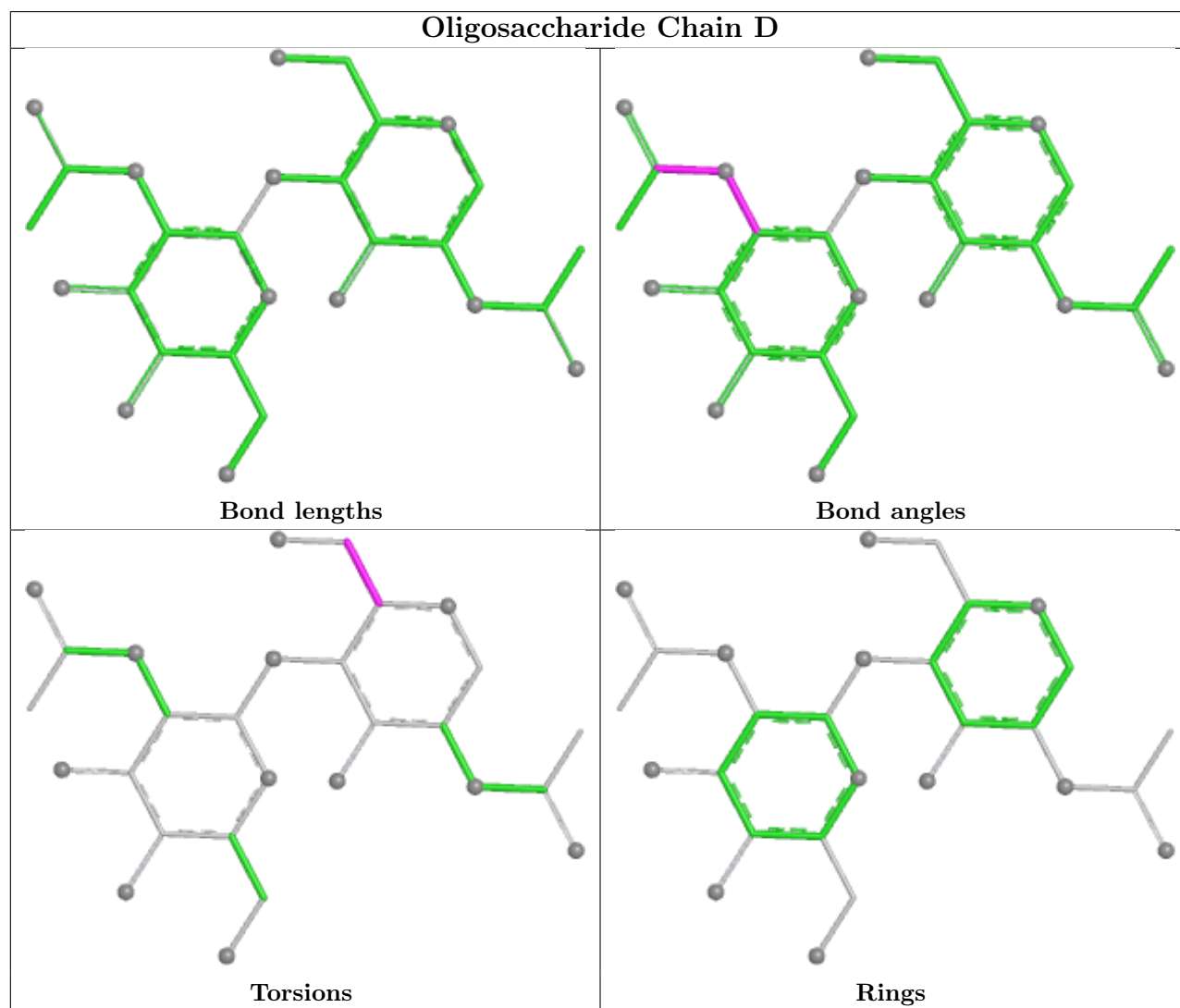
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NDG	4	0
4	F	1	NAG	3	0
5	G	1	NAG	3	0
5	J	1	NAG	4	0
4	D	2	NAG	5	0

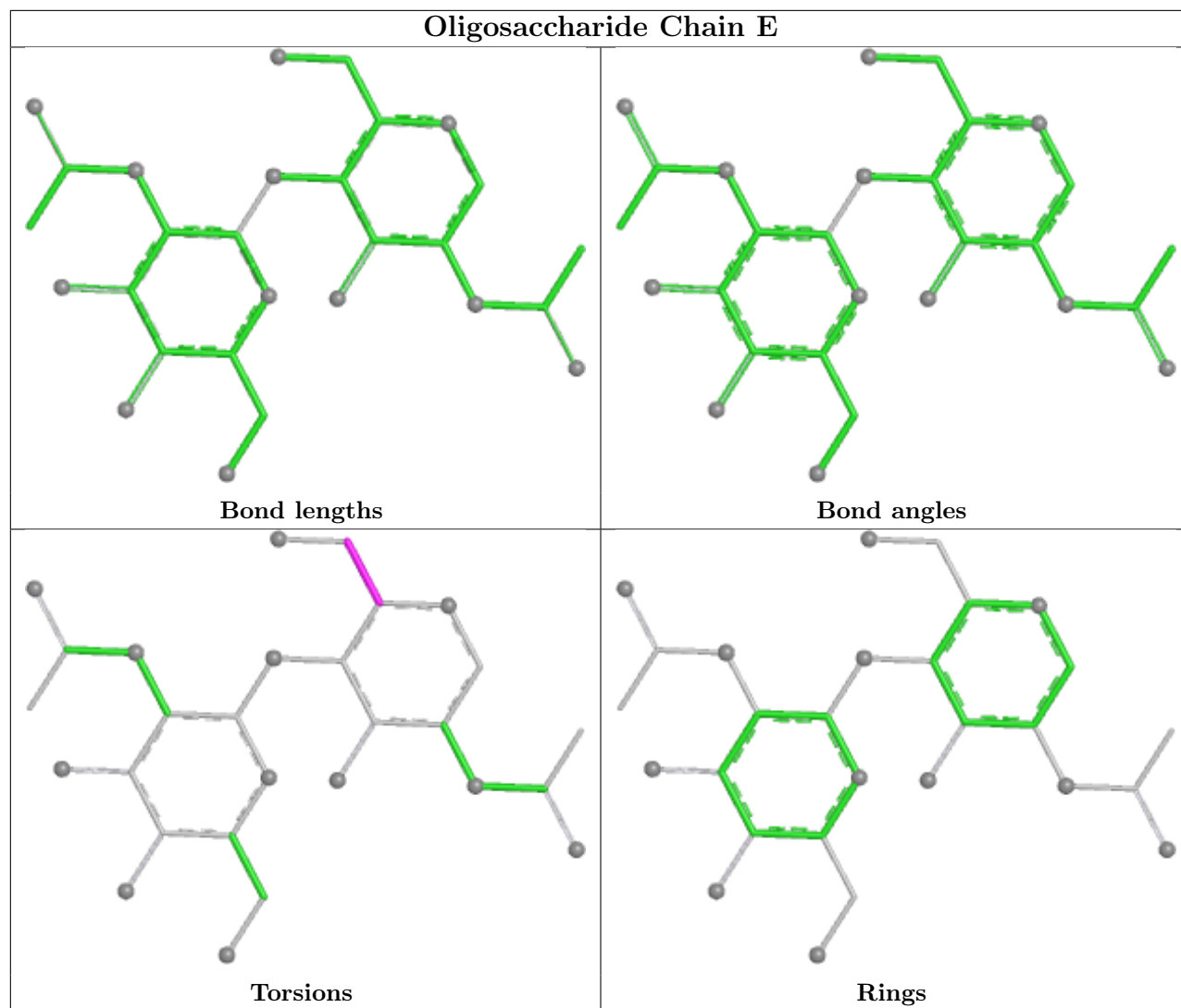
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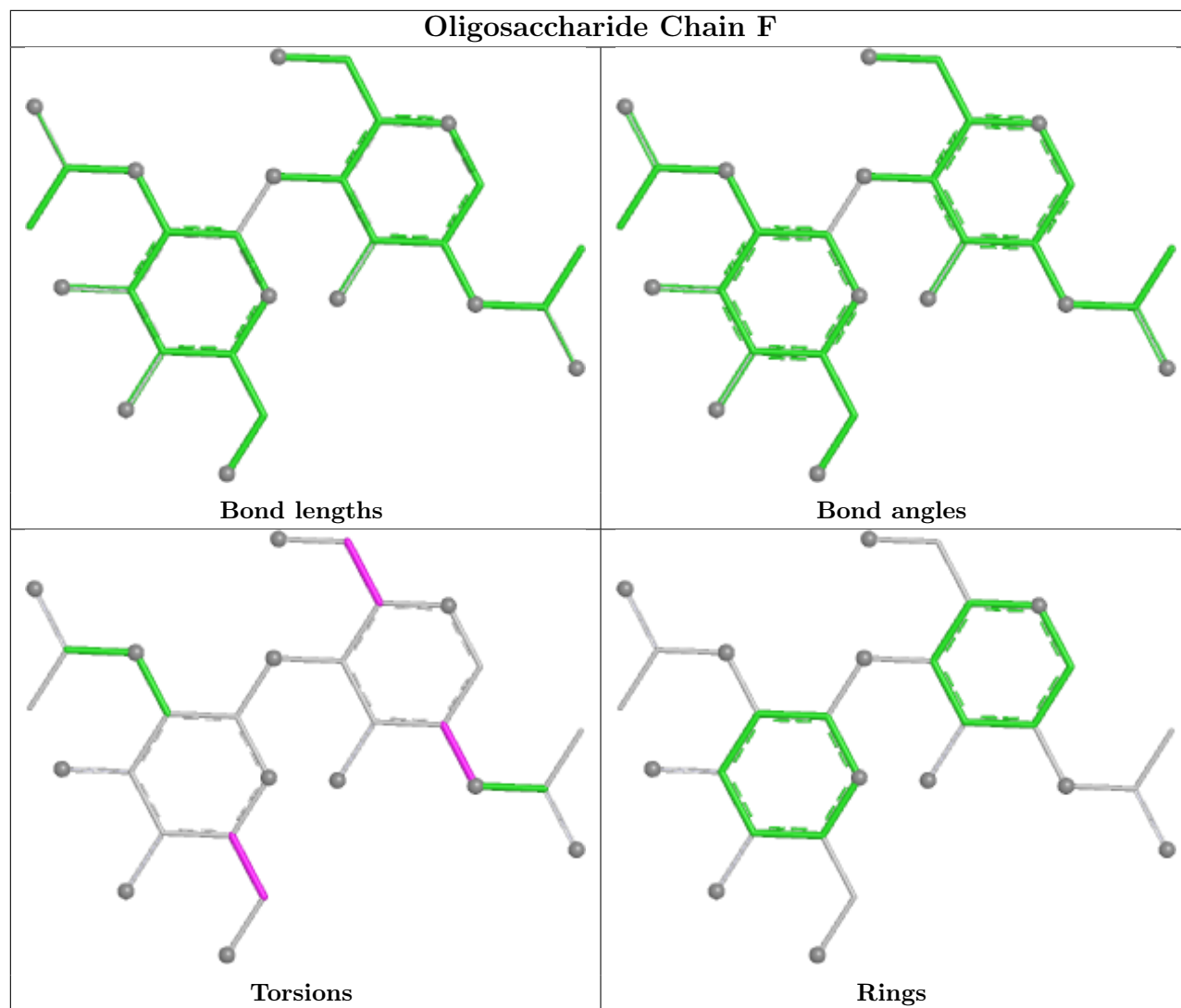
Continued from previous page...

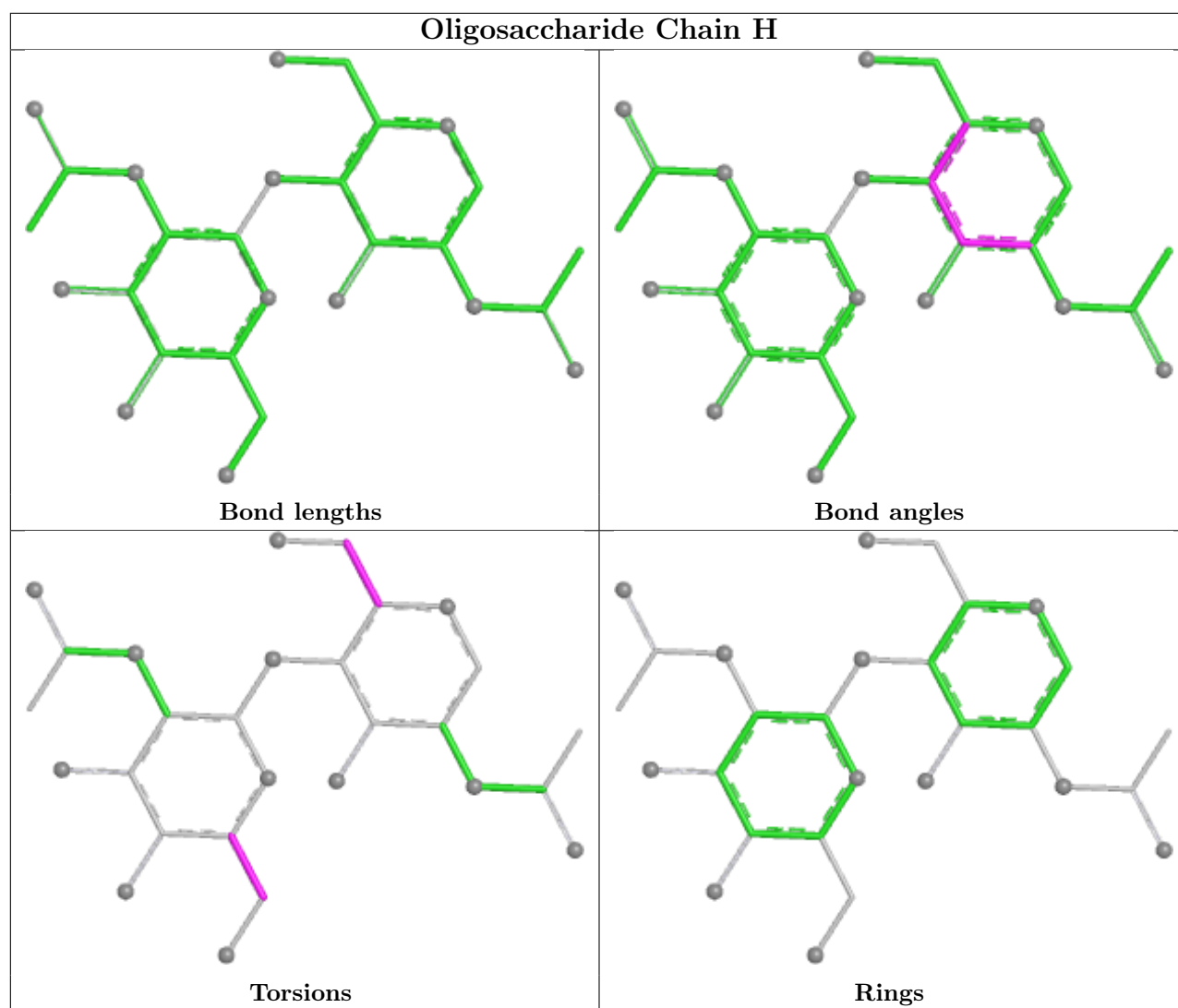
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
5	J	2	NDG	4	0
4	H	1	NAG	3	0

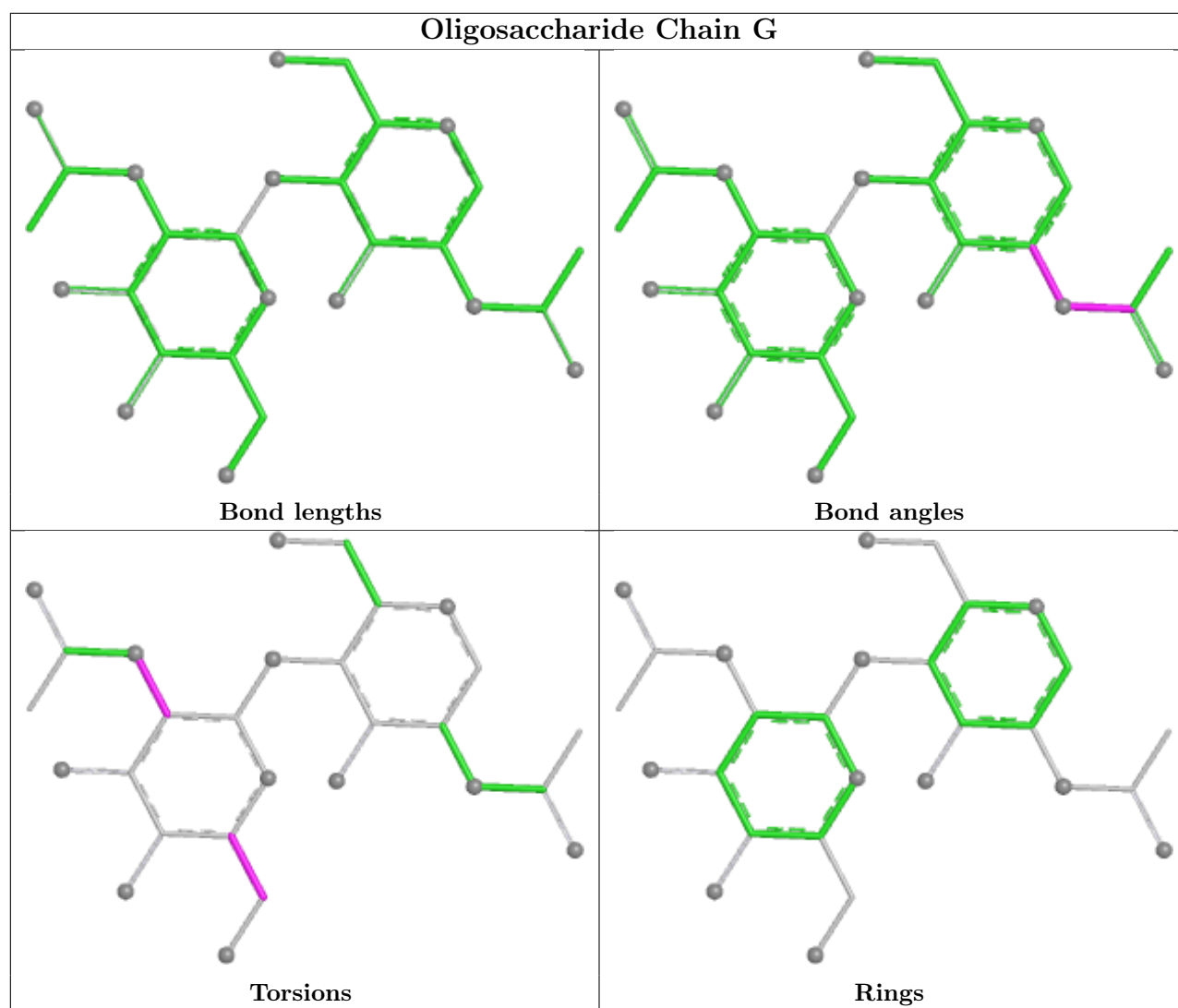
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

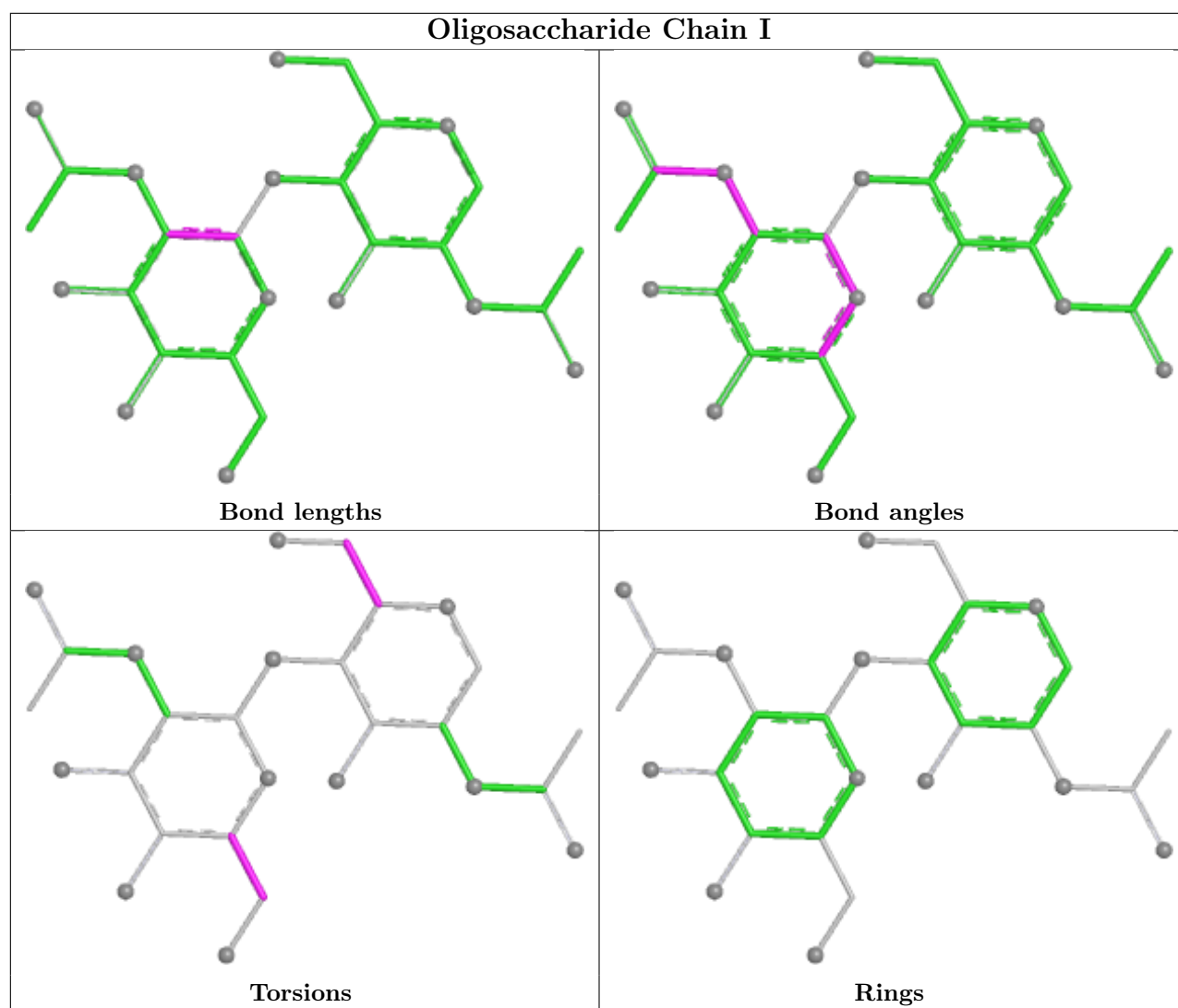


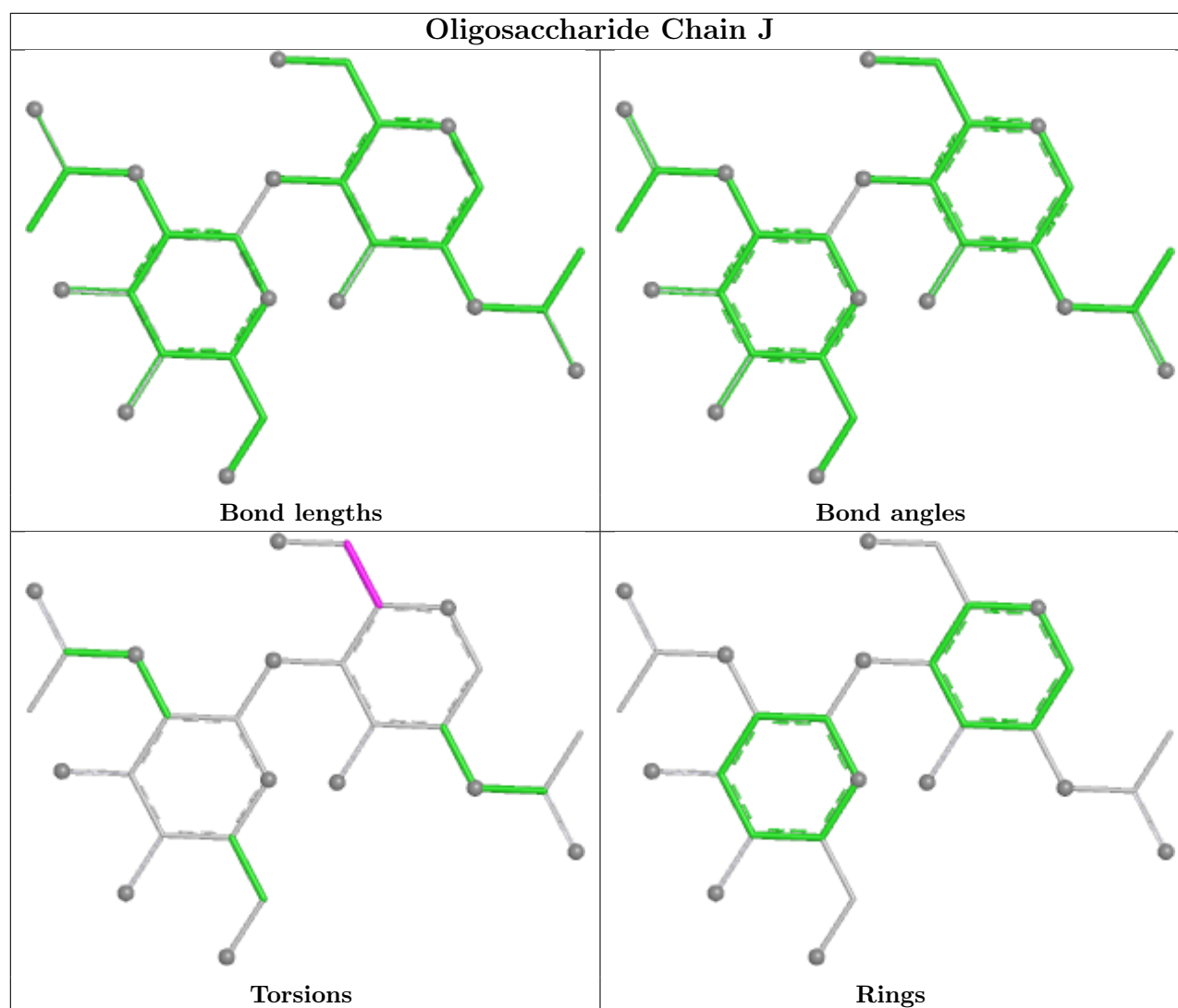












5.6 Ligand geometry [i](#)

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	A	2260	1	14,14,15	0.69	0	17,19,21	0.72	0
6	NAG	A	2458	1	14,14,15	0.47	0	17,19,21	0.82	0
6	NAG	B	3320	2	14,14,15	0.56	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	3371	2	14,14,15	0.52	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	2260	1	-	4/6/23/26	0/1/1/1
6	NAG	A	2458	1	-	1/6/23/26	0/1/1/1
6	NAG	B	3320	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3371	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3320	NAG	C2-N2-C7	-2.14	120.03	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2260	NAG	C1-C2-N2-C7
6	A	2260	NAG	C4-C5-C6-O6
6	A	2260	NAG	O5-C5-C6-O6
6	B	3371	NAG	O5-C5-C6-O6
6	A	2458	NAG	O5-C5-C6-O6
6	B	3371	NAG	C3-C2-N2-C7
6	B	3371	NAG	C4-C5-C6-O6
6	A	2260	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2260	NAG	3	0
6	A	2458	NAG	5	0
6	B	3320	NAG	1	0
6	B	3371	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.