



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:28 PM UTC

PDB ID : 1LFG / pdb_00001lfg
Title : Structure of diferric human lactoferrin
Authors : Baker, E.N.; Anderson, B.F.; Haridas, M.
Deposited on : 1992-02-05
Resolution : 2.20 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

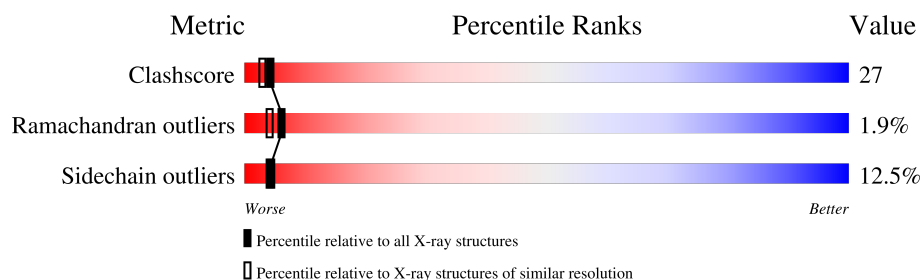
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	691	
2	B	2	
3	C	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	-	-	X	-
3	NAG	C	1	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5886 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	691	5322	3327	947	1011	37	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

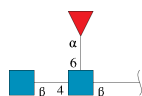
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	conflict	UNP P02788
A	200	LYS	ARG	conflict	UNP P02788
A	418	ALA	GLN	conflict	UNP P02788
A	500	ALA	ARG	conflict	UNP P02788
A	512	GLU	GLN	conflict	UNP P02788

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

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

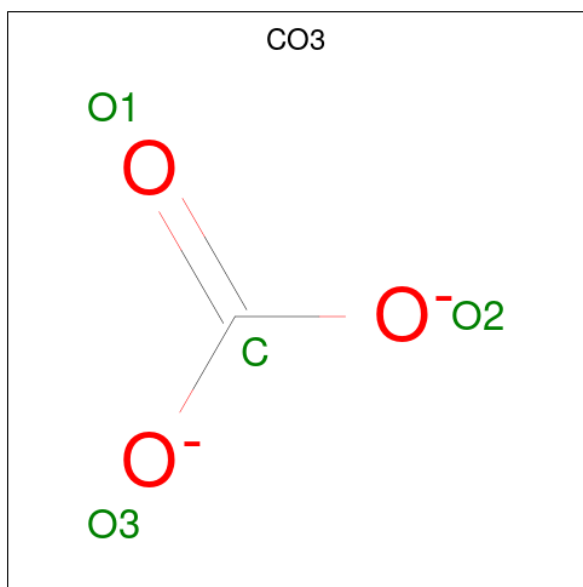


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			37	22	2	13			

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is water.

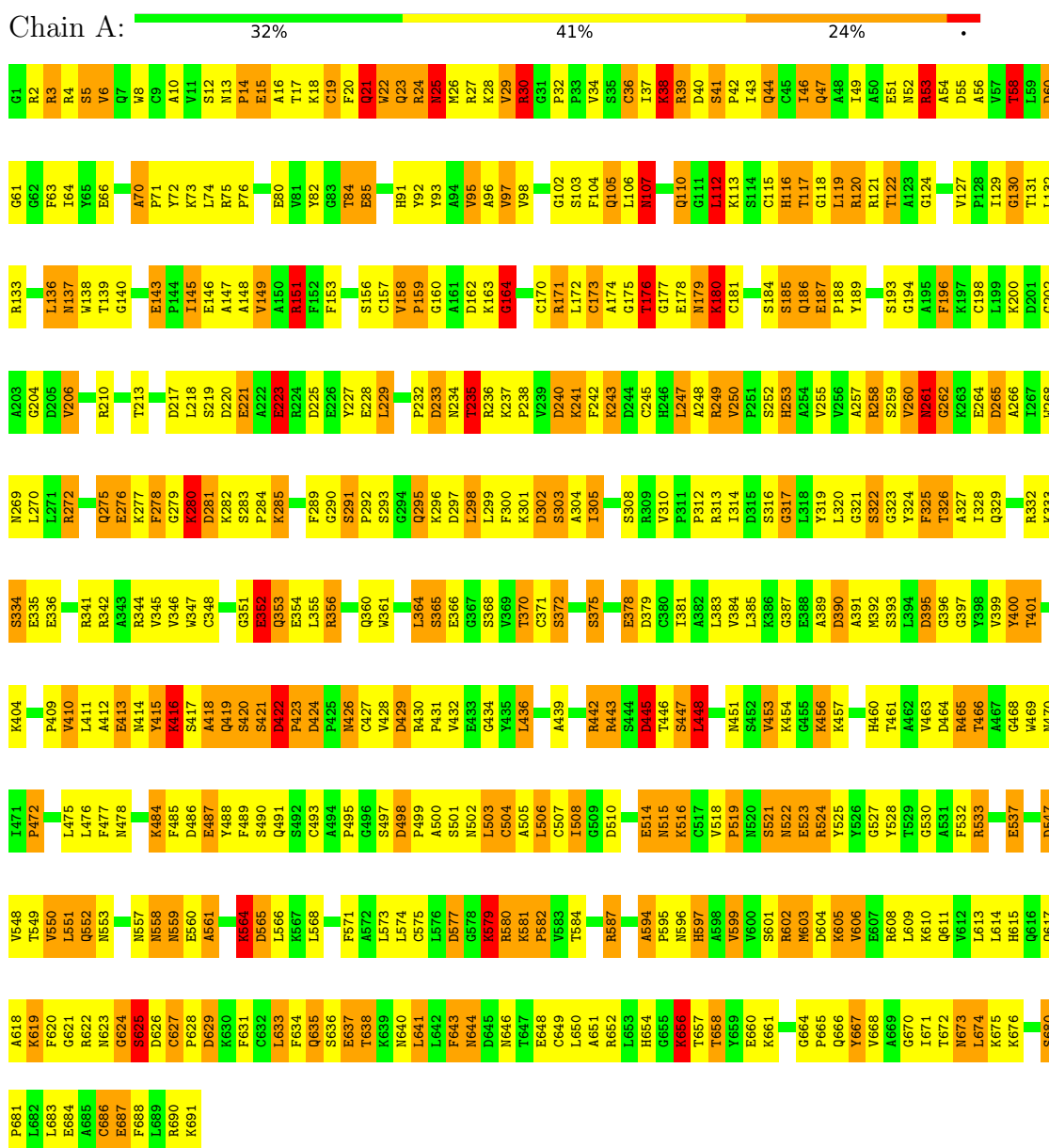
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	493	Total	O	0	0
			493	493		

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: LACTOFERRIN

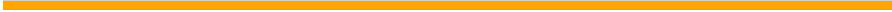


• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
FUC2

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

Chain C:  100%

MAG1
MAG2
FUC3

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	156.26Å 97.40Å 55.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5886	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: NAG, CO3, FE, FUC

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	1.19	10/5436 (0.2%)	2.82	555/7354 (7.5%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	VAL	C-N	-8.87	1.21	1.33
1	A	242	PHE	C-N	-8.31	1.22	1.33
1	A	204	GLY	N-CA	7.11	1.52	1.44
1	A	118	GLY	N-CA	6.21	1.52	1.45
1	A	102	GLY	N-CA	5.72	1.49	1.44
1	A	321	GLY	N-CA	5.72	1.52	1.45
1	A	113	LYS	N-CA	5.69	1.52	1.46
1	A	290	GLY	N-CA	5.56	1.51	1.45
1	A	434	GLY	N-CA	5.22	1.50	1.45
1	A	176	THR	CA-CB	5.12	1.60	1.53

All (555) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ASN	CA-CB-CG	22.06	134.66	112.60
1	A	422	ASP	CA-CB-CG	19.73	132.33	112.60
1	A	342	ARG	CD-NE-CZ	17.67	149.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	GLU	CB-CG-CD	15.39	138.76	112.60
1	A	581	LYS	O-C-N	15.35	131.53	121.71
1	A	32	PRO	CB-CA-C	13.90	124.45	111.39
1	A	47	GLN	OE1-CD-NE2	13.21	135.81	122.60
1	A	465	ARG	NE-CZ-NH2	11.96	129.97	119.20
1	A	163	LYS	CA-C-O	11.85	133.43	120.63
1	A	443	ARG	CD-NE-CZ	-11.74	107.97	124.40
1	A	75	ARG	NE-CZ-NH2	11.46	129.51	119.20
1	A	434	GLY	CA-C-O	-11.42	112.06	122.57
1	A	53	ARG	NE-CZ-NH1	11.39	132.89	121.50
1	A	365	SER	CA-C-O	-11.16	105.77	119.28
1	A	559	ASN	CA-CB-CG	-11.01	101.59	112.60
1	A	233	ASP	CA-CB-CG	-10.89	101.71	112.60
1	A	326	THR	CA-CB-CG2	10.85	128.94	110.50
1	A	322	SER	O-C-N	10.78	134.44	122.15
1	A	687	GLU	CA-C-O	10.69	131.75	120.42
1	A	604	ASP	CA-CB-CG	10.62	123.22	112.60
1	A	21	GLN	N-CA-C	-10.41	99.94	111.07
1	A	420	SER	CA-C-N	10.33	136.01	120.82
1	A	420	SER	C-N-CA	10.33	136.01	120.82
1	A	310	VAL	O-C-N	10.11	129.35	121.46
1	A	372	SER	CA-C-O	-10.11	109.62	121.44
1	A	39	ARG	NE-CZ-NH2	-9.94	110.25	119.20
1	A	70	ALA	CB-CA-C	9.90	127.82	109.51
1	A	187	GLU	CB-CG-CD	9.88	129.40	112.60
1	A	672	THR	O-C-N	9.81	132.52	122.12
1	A	635	GLN	CB-CG-CD	9.74	129.16	112.60
1	A	504	CYS	CA-C-O	-9.74	107.69	119.18
1	A	18	LYS	N-CA-CB	9.67	124.44	110.13
1	A	27	ARG	CD-NE-CZ	9.63	137.89	124.40
1	A	260	VAL	N-CA-C	9.63	119.51	110.74
1	A	58	THR	CB-CA-C	9.52	126.11	110.22
1	A	63	PHE	CA-C-O	-9.46	108.20	119.27
1	A	46	ILE	CA-C-O	9.42	130.75	120.95
1	A	558	ASN	CA-C-O	9.42	131.95	120.27
1	A	348	CYS	CA-C-N	9.39	135.69	122.72
1	A	348	CYS	C-N-CA	9.39	135.69	122.72
1	A	261	ASN	CA-C-N	9.39	131.96	120.13
1	A	261	ASN	C-N-CA	9.39	131.96	120.13
1	A	445	ASP	CA-CB-CG	-9.29	103.31	112.60
1	A	186	GLN	N-CA-C	-9.29	101.05	112.38
1	A	565	ASP	CA-CB-CG	-9.24	103.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	GLU	CA-CB-CG	9.16	132.43	114.10
1	A	624	GLY	N-CA-C	9.15	126.00	111.64
1	A	229	LEU	CA-C-O	-9.14	110.83	121.16
1	A	392	MET	CA-CB-CG	-9.12	95.87	114.10
1	A	498	ASP	O-C-N	9.11	129.05	121.31
1	A	265	ASP	CA-CB-CG	-9.06	103.54	112.60
1	A	10	ALA	CA-C-O	-9.03	110.63	121.28
1	A	597	HIS	CA-CB-CG	-9.00	104.80	113.80
1	A	112	LEU	CA-C-N	-8.88	110.06	122.93
1	A	112	LEU	C-N-CA	-8.88	110.06	122.93
1	A	249	ARG	NE-CZ-NH1	-8.79	112.70	121.50
1	A	8	TRP	CA-C-O	-8.79	111.03	121.05
1	A	119	LEU	CA-C-O	-8.70	111.42	121.16
1	A	654	HIS	CA-CB-CG	-8.70	105.10	113.80
1	A	120	ARG	N-CA-C	8.68	125.63	113.56
1	A	242	PHE	CA-C-N	8.57	137.91	121.54
1	A	242	PHE	C-N-CA	8.57	137.91	121.54
1	A	527	GLY	CA-C-N	8.53	131.91	120.65
1	A	527	GLY	C-N-CA	8.53	131.91	120.65
1	A	493	CYS	N-CA-CB	8.49	124.72	110.87
1	A	258	ARG	CD-NE-CZ	-8.48	112.52	124.40
1	A	549	THR	CA-C-N	8.44	131.02	120.72
1	A	549	THR	C-N-CA	8.44	131.02	120.72
1	A	370	THR	CA-C-N	8.42	135.13	122.93
1	A	370	THR	C-N-CA	8.42	135.13	122.93
1	A	409	PRO	CA-C-O	-8.34	111.53	121.03
1	A	360	GLN	CA-C-O	8.33	130.25	120.92
1	A	426	ASN	CA-CB-CG	-8.31	104.29	112.60
1	A	635	GLN	OE1-CD-NE2	-8.25	114.35	122.60
1	A	396	GLY	CA-C-N	8.21	129.05	119.94
1	A	396	GLY	C-N-CA	8.21	129.05	119.94
1	A	395	ASP	CA-C-O	-8.21	112.85	121.55
1	A	151	ARG	NE-CZ-NH2	-8.20	111.82	119.20
1	A	217	ASP	CA-CB-CG	8.18	120.78	112.60
1	A	193	SER	CA-C-O	-8.12	111.82	120.42
1	A	611	GLN	OE1-CD-NE2	8.09	130.69	122.60
1	A	63	PHE	CA-CB-CG	-8.07	105.73	113.80
1	A	401	THR	CA-CB-OG1	-8.05	97.53	109.60
1	A	596	ASN	CA-CB-CG	8.04	120.64	112.60
1	A	644	ASN	CA-CB-CG	8.03	120.63	112.60
1	A	353	GLN	CA-C-O	-8.02	112.40	120.82
1	A	654	HIS	CA-C-N	-8.00	113.92	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	HIS	C-N-CA	-8.00	113.92	123.44
1	A	333	LYS	CA-C-O	-7.99	111.77	121.11
1	A	365	SER	O-C-N	7.95	133.33	122.37
1	A	304	ALA	N-CA-C	-7.94	100.05	110.53
1	A	656	LYS	CA-C-O	-7.92	112.83	122.41
1	A	84	THR	CA-C-O	-7.88	112.44	121.58
1	A	550	VAL	O-C-N	7.86	130.35	121.94
1	A	587	ARG	NE-CZ-NH2	-7.86	112.12	119.20
1	A	329	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	A	262	GLY	N-CA-C	7.77	123.61	113.27
1	A	319	TYR	O-C-N	7.76	130.99	122.15
1	A	426	ASN	OD1-CG-ND2	7.75	130.35	122.60
1	A	281	ASP	CA-C-N	7.74	134.99	121.52
1	A	281	ASP	C-N-CA	7.74	134.99	121.52
1	A	272	ARG	NE-CZ-NH2	-7.64	112.33	119.20
1	A	477	PHE	CA-C-O	7.63	128.51	120.42
1	A	75	ARG	CB-CG-CD	7.61	128.80	111.30
1	A	137	ASN	CA-C-O	-7.60	112.72	121.54
1	A	532	PHE	CA-C-O	7.58	128.51	120.70
1	A	39	ARG	NE-CZ-NH1	7.56	129.06	121.50
1	A	635	GLN	CB-CA-C	7.56	124.72	109.38
1	A	302	ASP	CA-C-N	-7.53	111.95	123.47
1	A	302	ASP	C-N-CA	-7.53	111.95	123.47
1	A	472	PRO	CA-C-N	7.53	130.98	120.29
1	A	472	PRO	C-N-CA	7.53	130.98	120.29
1	A	116	HIS	CA-CB-CG	-7.52	106.28	113.80
1	A	47	GLN	CG-CD-NE2	-7.52	105.12	116.40
1	A	356	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	A	187	GLU	CA-C-O	7.48	125.64	119.36
1	A	401	THR	CA-C-O	-7.46	112.98	120.82
1	A	234	ASN	CB-CA-C	7.45	122.46	111.89
1	A	242	PHE	O-C-N	-7.44	114.41	122.07
1	A	557	ASN	N-CA-C	-7.43	104.06	113.72
1	A	206	VAL	CA-C-O	-7.42	112.95	120.90
1	A	104	PHE	N-CA-C	-7.42	96.86	109.24
1	A	442	ARG	NE-CZ-NH1	-7.40	114.10	121.50
1	A	284	PRO	N-CA-C	-7.37	104.32	114.27
1	A	587	ARG	CD-NE-CZ	-7.35	114.11	124.40
1	A	448	LEU	CA-C-O	-7.35	112.06	120.58
1	A	602	ARG	NE-CZ-NH2	-7.33	112.60	119.20
1	A	383	LEU	CA-C-O	-7.31	112.80	120.55
1	A	163	LYS	CA-C-N	7.28	135.67	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	LYS	C-N-CA	7.28	135.67	121.41
1	A	620	PHE	O-C-N	7.28	130.99	122.19
1	A	255	VAL	CA-C-O	-7.26	112.58	120.85
1	A	264	GLU	CA-C-O	-7.26	112.79	120.63
1	A	143	GLU	O-C-N	7.23	127.90	121.18
1	A	484	LYS	O-C-N	7.23	132.03	122.56
1	A	495	PRO	CB-CA-C	7.21	120.72	111.56
1	A	432	VAL	O-C-N	7.21	131.46	122.59
1	A	27	ARG	NE-CZ-NH2	-7.20	112.72	119.20
1	A	47	GLN	CB-CG-CD	-7.20	100.37	112.60
1	A	249	ARG	CD-NE-CZ	-7.20	114.33	124.40
1	A	149	VAL	CB-CA-C	7.16	123.83	112.16
1	A	70	ALA	N-CA-C	-7.15	99.91	110.20
1	A	260	VAL	N-CA-CB	-7.14	102.07	110.64
1	A	360	GLN	CA-CB-CG	7.14	128.38	114.10
1	A	597	HIS	N-CA-C	-7.09	99.96	110.23
1	A	410	VAL	CB-CA-C	7.08	118.10	111.30
1	A	269	ASN	N-CA-C	-7.08	103.50	111.07
1	A	96	ALA	N-CA-CB	7.07	121.81	110.65
1	A	240	ASP	CA-C-O	7.07	127.59	119.18
1	A	196	PHE	CA-CB-CG	-7.06	106.74	113.80
1	A	49	ILE	N-CA-C	7.05	117.19	110.42
1	A	17	THR	CB-CA-C	7.04	124.18	110.67
1	A	270	LEU	N-CA-C	7.04	118.60	111.07
1	A	651	ALA	CA-C-N	7.04	131.48	121.42
1	A	651	ALA	C-N-CA	7.04	131.48	121.42
1	A	658	THR	CA-C-O	-7.02	112.89	121.11
1	A	465	ARG	CD-NE-CZ	-7.02	114.58	124.40
1	A	550	VAL	CA-C-O	-7.00	113.06	121.18
1	A	342	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	A	91	HIS	CA-C-O	-6.98	113.98	121.45
1	A	504	CYS	O-C-N	6.96	130.42	122.20
1	A	650	LEU	N-CA-C	-6.96	97.39	108.73
1	A	257	ALA	N-CA-C	-6.95	99.00	108.38
1	A	63	PHE	N-CA-C	-6.93	104.63	113.23
1	A	323	GLY	CA-C-N	6.93	129.45	120.44
1	A	323	GLY	C-N-CA	6.93	129.45	120.44
1	A	200	LYS	CG-CD-CE	6.92	127.22	111.30
1	A	503	LEU	O-C-N	6.91	131.63	122.43
1	A	611	GLN	N-CA-CB	6.91	120.09	110.07
1	A	159	PRO	CA-C-O	-6.91	113.79	121.32
1	A	553	ASN	O-C-N	6.89	131.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ILE	CB-CG1-CD1	6.89	128.27	113.80
1	A	491	GLN	OE1-CD-NE2	-6.89	115.71	122.60
1	A	673	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	413	GLU	CA-CB-CG	6.82	127.73	114.10
1	A	674	LEU	CA-C-O	6.81	127.72	120.70
1	A	325	PHE	O-C-N	-6.81	114.90	122.12
1	A	223	GLU	CA-C-N	6.81	130.08	120.28
1	A	223	GLU	C-N-CA	6.81	130.08	120.28
1	A	537	GLU	CG-CD-OE1	6.80	134.04	118.40
1	A	249	ARG	NH1-CZ-NH2	6.80	128.14	119.30
1	A	258	ARG	NE-CZ-NH2	6.76	125.28	119.20
1	A	391	ALA	N-CA-C	6.75	119.12	108.79
1	A	587	ARG	CB-CG-CD	-6.75	95.78	111.30
1	A	289	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	136	LEU	N-CA-C	6.73	121.51	113.16
1	A	411	LEU	O-C-N	6.72	131.07	123.27
1	A	667	TYR	CA-C-O	6.71	128.08	120.90
1	A	680	SER	O-C-N	6.71	127.36	120.99
1	A	160	GLY	O-C-N	6.69	130.56	122.60
1	A	524	ARG	CA-C-O	-6.68	112.56	120.10
1	A	262	GLY	CA-C-N	6.66	132.08	122.35
1	A	262	GLY	C-N-CA	6.66	132.08	122.35
1	A	487	GLU	CA-C-O	-6.66	111.40	119.32
1	A	202	GLY	N-CA-C	-6.63	106.08	115.30
1	A	120	ARG	CB-CG-CD	6.63	126.55	111.30
1	A	171	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	A	210	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	A	29	VAL	O-C-N	6.61	128.55	122.14
1	A	409	PRO	CA-C-N	-6.60	116.25	122.66
1	A	409	PRO	C-N-CA	-6.60	116.25	122.66
1	A	584	THR	O-C-N	-6.59	113.37	122.46
1	A	686	CYS	CA-C-O	-6.58	112.67	120.10
1	A	485	PHE	CA-C-O	-6.57	111.54	119.49
1	A	321	GLY	N-CA-C	-6.57	103.38	112.18
1	A	660	GLU	O-C-N	6.55	128.81	122.07
1	A	223	GLU	CA-CB-CG	6.54	127.19	114.10
1	A	505	ALA	N-CA-C	6.53	120.35	112.38
1	A	38	LYS	O-C-N	6.51	131.70	123.23
1	A	490	SER	CA-C-O	-6.49	114.00	120.82
1	A	601	SER	CA-C-O	-6.49	114.48	121.36
1	A	352	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	355	LEU	CA-C-O	6.48	127.63	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	CG-CD-NE	6.47	126.24	112.00
1	A	58	THR	CA-C-O	6.47	127.67	120.43
1	A	366	GLU	CA-C-N	6.45	134.04	121.41
1	A	366	GLU	C-N-CA	6.45	134.04	121.41
1	A	322	SER	CA-C-O	-6.44	113.59	120.42
1	A	43	ILE	CA-C-O	6.44	127.65	120.95
1	A	461	THR	O-C-N	6.43	128.69	122.07
1	A	285	LYS	N-CA-CB	6.42	119.33	110.01
1	A	668	VAL	O-C-N	6.42	128.35	121.87
1	A	60	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	66	GLU	CA-C-O	-6.39	113.77	120.55
1	A	345	VAL	O-C-N	6.38	130.57	123.10
1	A	303	SER	N-CA-CB	-6.37	102.37	112.63
1	A	436	LEU	CA-C-O	-6.37	113.44	120.38
1	A	599	VAL	N-CA-CB	6.37	117.66	110.72
1	A	582	PRO	CB-CA-C	6.35	119.26	110.95
1	A	506	LEU	CA-C-O	-6.34	111.93	119.35
1	A	228	GLU	CA-CB-CG	6.34	126.77	114.10
1	A	105	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	A	177	GLY	O-C-N	6.32	130.91	122.70
1	A	234	ASN	N-CA-CB	-6.32	102.35	111.70
1	A	393	SER	CA-C-O	-6.30	113.42	120.54
1	A	466	THR	CA-C-N	-6.30	111.83	120.28
1	A	466	THR	C-N-CA	-6.30	111.83	120.28
1	A	36	CYS	CA-CB-SG	-6.30	99.90	114.40
1	A	667	TYR	O-C-N	-6.29	115.55	122.09
1	A	25	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	299	LEU	CA-C-O	-6.28	111.53	120.51
1	A	347	TRP	CA-C-N	-6.28	114.42	122.77
1	A	347	TRP	C-N-CA	-6.28	114.42	122.77
1	A	577	ASP	CA-C-O	-6.28	112.01	119.35
1	A	84	THR	CA-CB-OG1	-6.27	100.19	109.60
1	A	672	THR	N-CA-CB	6.27	119.34	110.12
1	A	63	PHE	O-C-N	6.24	131.01	122.46
1	A	503	LEU	CA-C-O	-6.23	111.25	119.10
1	A	217	ASP	CA-C-O	-6.23	112.29	119.14
1	A	131	THR	CA-CB-CG2	6.23	121.08	110.50
1	A	180	LYS	N-CA-CB	6.22	119.48	109.28
1	A	379	ASP	CA-C-O	-6.21	113.08	120.10
1	A	178	GLU	CA-C-N	6.20	129.73	120.31
1	A	178	GLU	C-N-CA	6.20	129.73	120.31
1	A	179	ASN	OD1-CG-ND2	6.20	128.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	CA-C-O	-6.18	111.86	120.21
1	A	24	ARG	CA-CB-CG	6.18	126.46	114.10
1	A	516	LYS	CA-CB-CG	6.18	126.46	114.10
1	A	514	GLU	CB-CG-CD	6.17	123.10	112.60
1	A	117	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	54	ALA	N-CA-CB	6.17	122.11	111.69
1	A	158	VAL	CA-C-O	6.17	128.21	119.95
1	A	277	LYS	N-CA-C	6.16	118.08	111.36
1	A	5	SER	N-CA-C	6.16	118.21	108.79
1	A	84	THR	N-CA-CB	-6.16	101.64	111.43
1	A	107	ASN	CB-CG-ND2	6.15	125.63	116.40
1	A	560	GLU	CA-C-N	6.15	133.28	121.54
1	A	560	GLU	C-N-CA	6.15	133.28	121.54
1	A	673	ASN	CA-C-O	6.14	126.93	120.42
1	A	519	PRO	N-CA-CB	6.14	106.88	102.28
1	A	133	ARG	CA-C-N	6.14	126.32	119.32
1	A	133	ARG	C-N-CA	6.14	126.32	119.32
1	A	372	SER	CA-CB-OG	-6.13	98.84	111.10
1	A	272	ARG	N-CA-CB	-6.13	101.11	110.12
1	A	41	SER	O-C-N	6.12	127.28	121.71
1	A	502	ASN	O-C-N	6.12	128.60	122.12
1	A	594	ALA	N-CA-CB	-6.09	97.84	110.45
1	A	650	LEU	CA-C-O	-6.09	113.84	120.36
1	A	656	LYS	O-C-N	6.07	130.39	122.38
1	A	47	GLN	CA-C-O	-6.06	114.46	120.70
1	A	378	GLU	CB-CG-CD	6.05	122.89	112.60
1	A	295	GLN	N-CA-C	6.04	119.02	110.14
1	A	332	ARG	CA-C-O	-6.03	112.60	119.78
1	A	615	HIS	N-CA-CB	6.02	118.69	109.91
1	A	58	THR	O-C-N	-6.01	116.21	123.13
1	A	253	HIS	ND1-CE1-NE2	6.01	114.41	108.40
1	A	561	ALA	O-C-N	6.01	130.58	122.59
1	A	381	ILE	CA-C-O	-6.00	114.48	120.85
1	A	596	ASN	OD1-CG-ND2	-6.00	116.59	122.60
1	A	234	ASN	O-C-N	-6.00	115.11	122.55
1	A	278	PHE	O-C-N	6.00	130.49	122.26
1	A	552	GLN	N-CA-C	6.00	120.14	112.34
1	A	103	SER	CB-CA-C	-6.00	101.84	111.86
1	A	132	LEU	CA-C-O	-6.00	112.25	119.27
1	A	478	ASN	CB-CG-ND2	-6.00	107.41	116.40
1	A	447	SER	N-CA-C	5.98	120.58	113.28
1	A	564	LYS	CA-C-N	5.98	132.58	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	LYS	C-N-CA	5.98	132.58	122.65
1	A	514	GLU	CA-CB-CG	5.98	126.06	114.10
1	A	399	VAL	N-CA-C	-5.98	103.67	112.04
1	A	76	PRO	CA-C-N	5.97	128.95	121.85
1	A	76	PRO	C-N-CA	5.97	128.95	121.85
1	A	276	GLU	O-C-N	5.96	128.23	122.03
1	A	670	GLY	N-CA-C	5.96	119.41	112.50
1	A	613	LEU	CA-C-N	5.96	128.18	120.44
1	A	613	LEU	C-N-CA	5.96	128.18	120.44
1	A	14	PRO	O-C-N	-5.95	115.75	122.18
1	A	522	ASN	CB-CG-ND2	-5.95	107.47	116.40
1	A	684	GLU	CG-CD-OE2	-5.95	104.71	118.40
1	A	461	THR	N-CA-C	-5.95	104.70	111.07
1	A	532	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	175	GLY	CA-C-N	5.95	131.94	123.14
1	A	175	GLY	C-N-CA	5.95	131.94	123.14
1	A	103	SER	CA-CB-OG	5.94	122.99	111.10
1	A	312	PRO	CA-C-O	-5.94	110.25	119.64
1	A	97	VAL	CA-C-O	5.94	127.73	120.84
1	A	424	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	643	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	163	LYS	O-C-N	-5.92	115.85	122.12
1	A	107	ASN	CA-C-O	5.91	126.22	119.18
1	A	594	ALA	CA-C-N	5.91	125.82	119.85
1	A	594	ALA	C-N-CA	5.91	125.82	119.85
1	A	596	ASN	O-C-N	5.91	130.08	122.81
1	A	594	ALA	CB-CA-C	5.90	116.85	108.76
1	A	104	PHE	CB-CA-C	5.90	121.03	109.35
1	A	579	LYS	N-CA-CB	-5.90	101.93	110.36
1	A	497	SER	CA-CB-OG	5.89	122.88	111.10
1	A	618	ALA	CA-C-O	5.89	126.76	120.10
1	A	434	GLY	CA-C-N	5.89	132.71	122.82
1	A	434	GLY	C-N-CA	5.89	132.71	122.82
1	A	53	ARG	NH1-CZ-NH2	-5.88	111.65	119.30
1	A	235	THR	CA-CB-OG1	5.88	118.41	109.60
1	A	688	PHE	CA-C-O	-5.87	114.65	120.82
1	A	378	GLU	CA-C-N	5.87	128.73	120.28
1	A	378	GLU	C-N-CA	5.87	128.73	120.28
1	A	673	ASN	CB-CA-C	5.87	120.82	110.85
1	A	250	VAL	O-C-N	5.87	127.79	121.10
1	A	21	GLN	CA-CB-CG	5.86	125.83	114.10
1	A	240	ASP	CA-CB-CG	-5.86	106.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLY	N-CA-C	-5.86	105.19	111.93
1	A	259	SER	CA-CB-OG	-5.85	99.41	111.10
1	A	528	TYR	O-C-N	5.84	128.11	122.03
1	A	650	LEU	O-C-N	5.84	129.88	123.22
1	A	506	LEU	O-C-N	5.84	129.64	122.34
1	A	52	ASN	OD1-CG-ND2	5.80	128.40	122.60
1	A	127	VAL	O-C-N	5.80	127.71	121.10
1	A	502	ASN	CA-CB-CG	-5.79	106.81	112.60
1	A	131	THR	CA-CB-OG1	-5.79	100.92	109.60
1	A	354	GLU	CA-C-O	-5.78	113.33	119.97
1	A	206	VAL	O-C-N	5.78	129.79	123.09
1	A	646	ASN	CA-C-O	-5.77	112.49	119.59
1	A	508	ILE	CB-CG1-CD1	5.77	125.91	113.80
1	A	74	LEU	CA-C-O	5.77	128.61	121.81
1	A	66	GLU	O-C-N	5.76	128.23	122.12
1	A	604	ASP	CB-CG-OD2	5.76	131.64	118.40
1	A	611	GLN	CA-C-O	-5.76	114.77	120.70
1	A	104	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	581	LYS	CA-C-O	-5.75	115.21	120.50
1	A	333	LYS	CA-CB-CG	-5.75	102.60	114.10
1	A	110	GLN	CA-C-O	-5.75	114.70	120.96
1	A	475	LEU	CA-C-N	5.75	127.98	120.28
1	A	475	LEU	C-N-CA	5.75	127.98	120.28
1	A	15	GLU	O-C-N	5.75	129.15	122.20
1	A	577	ASP	O-C-N	5.74	129.52	122.34
1	A	393	SER	O-C-N	5.73	129.76	123.22
1	A	151	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	302	ASP	CA-CB-CG	-5.73	106.87	112.60
1	A	129	ILE	CA-C-O	-5.72	114.70	121.05
1	A	606	VAL	CB-CA-C	5.72	120.67	111.29
1	A	672	THR	CA-C-O	-5.72	114.49	120.55
1	A	314	ILE	CA-C-O	5.71	127.36	120.85
1	A	453	VAL	CA-CB-CG1	5.71	120.10	110.40
1	A	198	CYS	O-C-N	-5.71	116.07	122.12
1	A	187	GLU	N-CA-CB	5.70	118.45	110.07
1	A	310	VAL	CA-C-O	-5.70	115.04	119.20
1	A	528	TYR	CA-C-O	-5.69	115.02	121.00
1	A	604	ASP	OD1-CG-OD2	-5.69	109.25	122.90
1	A	553	ASN	CA-C-O	-5.68	113.66	120.65
1	A	23	GLN	O-C-N	5.68	128.14	122.12
1	A	178	GLU	CB-CA-C	5.67	121.23	109.95
1	A	519	PRO	CA-CB-CG	-5.67	93.73	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	SER	CA-C-O	-5.67	115.32	121.44
1	A	537	GLU	OE1-CD-OE2	-5.64	109.35	122.90
1	A	80	GLU	O-C-N	-5.64	116.20	122.86
1	A	519	PRO	CA-C-O	-5.63	115.35	121.77
1	A	258	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	A	364	LEU	O-C-N	5.62	129.08	122.34
1	A	351	GLY	CA-C-O	5.61	126.10	122.23
1	A	574	LEU	CA-C-O	-5.61	114.31	120.43
1	A	611	GLN	CB-CG-CD	-5.61	103.06	112.60
1	A	131	THR	CA-C-O	5.60	126.41	119.97
1	A	623	ASN	CA-C-N	5.59	127.02	120.71
1	A	623	ASN	C-N-CA	5.59	127.02	120.71
1	A	85	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	557	ASN	CA-C-N	5.58	130.31	121.72
1	A	557	ASN	C-N-CA	5.58	130.31	121.72
1	A	521	SER	O-C-N	-5.57	115.18	122.59
1	A	184	SER	O-C-N	5.57	128.83	123.04
1	A	320	LEU	N-CA-CB	-5.57	101.64	110.28
1	A	334	SER	CA-C-O	-5.57	115.64	121.99
1	A	52	ASN	CA-C-O	-5.56	112.56	120.51
1	A	151	ARG	N-CA-C	-5.56	106.34	113.23
1	A	308	SER	CA-CB-OG	-5.55	100.00	111.10
1	A	470	ASN	N-CA-C	5.55	117.77	111.11
1	A	200	LYS	CA-C-O	-5.54	114.98	121.07
1	A	319	TYR	CA-C-O	-5.54	114.55	120.42
1	A	530	GLY	CA-C-O	-5.54	114.79	120.66
1	A	17	THR	CA-CB-OG1	-5.52	101.33	109.60
1	A	423	PRO	CA-C-N	5.51	135.23	121.80
1	A	423	PRO	C-N-CA	5.51	135.23	121.80
1	A	17	THR	N-CA-C	-5.50	105.43	111.82
1	A	304	ALA	CA-C-O	-5.50	115.49	121.87
1	A	164	GLY	CA-C-N	5.50	130.02	120.68
1	A	164	GLY	C-N-CA	5.50	130.02	120.68
1	A	428	VAL	CA-C-O	-5.49	113.04	119.85
1	A	156	SER	CB-CA-C	-5.49	98.63	111.09
1	A	253	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
1	A	348	CYS	CB-CA-C	5.47	119.05	110.19
1	A	415	TYR	CA-C-O	-5.47	115.24	121.58
1	A	627	CYS	CB-CA-C	5.46	116.43	110.15
1	A	249	ARG	O-C-N	5.45	129.71	123.27
1	A	609	LEU	CA-C-O	5.45	126.33	120.55
1	A	130	GLY	CA-C-O	-5.45	115.14	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ILE	O-C-N	-5.43	116.60	121.87
1	A	240	ASP	CB-CA-C	5.43	120.15	109.72
1	A	304	ALA	N-CA-CB	5.43	118.13	110.36
1	A	552	GLN	CB-CG-CD	5.43	121.83	112.60
1	A	445	ASP	N-CA-CB	-5.43	101.31	110.49
1	A	36	CYS	N-CA-C	5.42	118.91	110.17
1	A	436	LEU	O-C-N	5.42	129.69	123.29
1	A	533	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	A	516	LYS	CA-C-O	5.42	127.15	121.19
1	A	557	ASN	CB-CG-ND2	5.42	124.52	116.40
1	A	668	VAL	CA-C-O	-5.41	114.78	120.57
1	A	148	ALA	CA-C-O	-5.41	114.69	120.42
1	A	463	VAL	CA-CB-CG1	5.40	119.59	110.40
1	A	140	GLY	N-CA-C	-5.40	101.33	112.34
1	A	173	CYS	CA-C-N	5.40	132.10	122.06
1	A	173	CYS	C-N-CA	5.40	132.10	122.06
1	A	247	LEU	N-CA-C	-5.40	106.70	113.28
1	A	314	ILE	N-CA-C	5.39	116.00	108.89
1	A	336	GLU	N-CA-CB	5.38	118.22	110.20
1	A	293	SER	N-CA-C	5.38	122.27	110.80
1	A	297	ASP	CA-C-O	-5.38	115.47	122.14
1	A	587	ARG	CA-C-O	-5.37	112.99	119.49
1	A	95	VAL	N-CA-CB	-5.36	105.68	112.60
1	A	127	VAL	CA-C-O	-5.36	112.77	119.95
1	A	137	ASN	CA-C-N	-5.36	112.49	121.39
1	A	137	ASN	C-N-CA	-5.36	112.49	121.39
1	A	18	LYS	CA-C-O	-5.36	114.82	120.55
1	A	22	TRP	N-CA-CB	5.36	119.54	110.49
1	A	24	ARG	CA-C-O	-5.36	115.20	120.82
1	A	91	HIS	O-C-N	5.35	129.25	123.10
1	A	278	PHE	CA-C-O	-5.35	113.58	119.78
1	A	389	ALA	N-CA-C	-5.35	100.94	109.07
1	A	664	GLY	CA-C-N	5.35	124.80	119.24
1	A	664	GLY	C-N-CA	5.35	124.80	119.24
1	A	55	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	122	THR	O-C-N	5.34	129.70	122.59
1	A	501	SER	CA-C-N	5.34	127.44	120.28
1	A	501	SER	C-N-CA	5.34	127.44	120.28
1	A	234	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	39	ARG	O-C-N	5.34	128.70	122.99
1	A	523	GLU	CA-C-O	5.34	126.41	120.43
1	A	550	VAL	N-CA-C	-5.33	105.41	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	LYS	N-CA-CB	-5.33	102.81	110.65
1	A	453	VAL	CB-CA-C	5.33	119.38	112.24
1	A	360	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	A	370	THR	CB-CA-C	5.32	121.78	110.07
1	A	608	ARG	CA-C-N	5.32	127.41	120.28
1	A	608	ARG	C-N-CA	5.32	127.41	120.28
1	A	291	SER	N-CA-CB	-5.31	99.97	110.70
1	A	243	LYS	CB-CA-C	-5.30	99.87	110.42
1	A	194	GLY	CA-C-N	5.30	127.64	120.38
1	A	194	GLY	C-N-CA	5.30	127.64	120.38
1	A	371	CYS	CA-C-O	5.30	126.33	120.71
1	A	451	ASN	CB-CG-ND2	-5.30	108.45	116.40
1	A	466	THR	CA-CB-CG2	5.28	119.48	110.50
1	A	533	ARG	CB-CG-CD	5.28	123.45	111.30
1	A	537	GLU	CA-C-O	5.27	125.73	119.56
1	A	565	ASP	N-CA-C	5.27	118.84	112.93
1	A	410	VAL	N-CA-C	5.27	116.17	111.90
1	A	14	PRO	N-CA-C	-5.27	105.25	113.78
1	A	486	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	680	SER	N-CA-CB	5.26	115.72	109.72
1	A	635	GLN	CG-CD-NE2	5.26	124.30	116.40
1	A	44	GLN	OE1-CD-NE2	5.26	127.86	122.60
1	A	571	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	275	GLN	CA-C-O	5.25	126.11	120.55
1	A	451	ASN	CA-C-O	-5.25	114.32	120.20
1	A	547	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	17	THR	N-CA-CB	-5.24	102.17	110.28
1	A	276	GLU	CA-CB-CG	5.22	124.55	114.10
1	A	240	ASP	N-CA-CB	-5.22	102.26	110.46
1	A	658	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	30	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	181	CYS	N-CA-CB	-5.20	104.39	112.30
1	A	283	SER	O-C-N	5.20	127.30	121.32
1	A	429	ASP	O-C-N	5.20	128.53	122.24
1	A	581	LYS	N-CA-CB	5.20	120.53	111.18
1	A	41	SER	N-CA-C	5.19	112.89	108.22
1	A	478	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	A	233	ASP	CB-CG-OD2	5.17	130.30	118.40
1	A	328	ILE	N-CA-CB	5.17	117.19	110.57
1	A	317	GLY	O-C-N	5.17	127.25	122.13
1	A	189	TYR	CA-C-N	5.16	128.80	121.42
1	A	189	TYR	C-N-CA	5.16	128.80	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ALA	N-CA-C	5.15	116.90	109.07
1	A	136	LEU	CA-C-O	-5.15	113.05	119.28
1	A	430	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	237	LYS	CA-CB-CG	5.15	124.40	114.10
1	A	345	VAL	CA-C-O	-5.15	115.02	120.53
1	A	19	CYS	N-CA-C	5.15	118.66	112.38
1	A	411	LEU	CA-C-O	-5.15	115.09	121.06
1	A	566	LEU	CA-C-O	5.14	126.35	120.54
1	A	465	ARG	NH1-CZ-NH2	-5.13	112.63	119.30
1	A	46	ILE	N-CA-CB	-5.13	103.57	110.54
1	A	414	ASN	N-CA-CB	5.12	118.53	110.23
1	A	24	ARG	N-CA-CB	5.12	117.44	110.01
1	A	157	CYS	CA-C-N	5.12	131.60	122.13
1	A	157	CYS	C-N-CA	5.12	131.60	122.13
1	A	98	VAL	CA-C-O	5.12	126.66	121.64
1	A	390	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	421	SER	O-C-N	5.11	129.36	122.82
1	A	219	SER	CA-C-N	5.11	128.10	120.95
1	A	219	SER	C-N-CA	5.11	128.10	120.95
1	A	565	ASP	N-CA-CB	-5.11	103.51	110.56
1	A	634	PHE	CA-C-N	-5.10	113.59	122.37
1	A	634	PHE	C-N-CA	-5.10	113.59	122.37
1	A	618	ALA	N-CA-C	-5.10	105.85	111.71
1	A	172	LEU	N-CA-C	5.09	119.25	113.19
1	A	375	SER	CA-CB-OG	-5.09	100.92	111.10
1	A	310	VAL	CA-CB-CG1	5.09	119.05	110.40
1	A	640	ASN	CB-CG-ND2	5.09	124.03	116.40
1	A	400	TYR	CA-C-O	5.09	125.94	120.70
1	A	547	ASP	CA-C-O	-5.08	115.04	120.42
1	A	595	PRO	N-CA-CB	5.08	108.05	103.33
1	A	277	LYS	CB-CG-CD	5.07	122.97	111.30
1	A	327	ALA	CA-C-O	-5.07	115.18	120.55
1	A	412	ALA	CA-C-O	-5.06	115.44	121.16
1	A	345	VAL	N-CA-CB	5.06	117.83	111.46
1	A	439	ALA	CA-C-N	5.06	129.62	123.10
1	A	439	ALA	C-N-CA	5.06	129.62	123.10
1	A	365	SER	N-CA-CB	5.05	118.17	110.44
1	A	657	THR	CA-CB-OG1	-5.04	102.05	109.60
1	A	515	ASN	N-CA-CB	-5.03	104.61	112.41
1	A	296	LYS	O-C-N	5.03	129.63	123.44
1	A	245	CYS	N-CA-CB	-5.03	101.99	110.49
1	A	478	ASN	CA-C-O	-5.03	112.51	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLY	N-CA-C	-5.03	103.89	112.64
1	A	335	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	6	VAL	CB-CA-C	-5.02	106.23	112.45
1	A	454	LYS	O-C-N	5.02	129.09	122.97
1	A	61	GLY	O-C-N	5.01	127.09	122.13
1	A	623	ASN	OD1-CG-ND2	5.00	127.60	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5322	0	5173	270	0
2	B	24	0	21	7	0
3	C	37	0	33	10	0
4	A	2	0	0	0	0
5	A	8	0	0	0	0
6	A	493	0	0	15	0
All	All	5886	0	5227	286	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 27.

All (286) 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:A:26:MET:HE2	1:A:278:PHE:CE2	1.72	1.22
1:A:36:CYS:C	1:A:37:ILE:HD12	1.69	1.16
1:A:138:TRP:CD2	1:A:145:ILE:HD13	1.90	1.06
1:A:422:ASP:HB3	1:A:423:PRO:HD3	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:FUC:C5	3:C:3:FUC:C1	2.30	1.05
1:A:110:GLN:NE2	2:B:1:NAG:O7	1.92	1.03
1:A:26:MET:HE2	1:A:278:PHE:HE2	0.85	1.01
3:C:1:NAG:H83	3:C:1:NAG:H3	1.47	0.95
1:A:26:MET:CE	1:A:278:PHE:HE2	1.80	0.94
1:A:686:CYS:O	1:A:690:ARG:HG2	1.69	0.91
1:A:38:LYS:O	1:A:39:ARG:HG2	1.70	0.91
1:A:302:ASP:O	1:A:303:SER:HB2	1.69	0.88
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.04	0.88
1:A:25:ASN:HA	1:A:28:LYS:HE3	1.56	0.87
1:A:622:ARG:HD3	1:A:622:ARG:C	1.99	0.87
3:C:1:NAG:C6	3:C:3:FUC:C1	2.52	0.87
1:A:564:LYS:NZ	1:A:565:ASP:OD2	2.08	0.86
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.58	0.84
1:A:417:SER:C	1:A:419:GLN:H	1.84	0.84
1:A:29:VAL:HG12	1:A:29:VAL:O	1.79	0.82
1:A:629:ASP:HB2	6:A:1037:HOH:O	1.80	0.81
1:A:295:GLN:CB	1:A:298:LEU:HD21	2.12	0.80
1:A:637:GLU:O	1:A:638:THR:HG23	1.82	0.79
1:A:241:LYS:HD2	1:A:241:LYS:N	1.97	0.79
1:A:26:MET:CE	1:A:278:PHE:CE2	2.61	0.79
1:A:422:ASP:CB	1:A:423:PRO:HD3	2.10	0.79
1:A:220:ASP:O	1:A:223:GLU:HG2	1.82	0.78
1:A:58:THR:HG21	1:A:300:PHE:CD1	2.20	0.77
1:A:581:LYS:HB3	1:A:582:PRO:HD2	1.64	0.77
1:A:279:GLY:HA3	1:A:282:LYS:NZ	2.00	0.77
1:A:279:GLY:HA3	1:A:282:LYS:HZ2	1.49	0.76
1:A:346:VAL:HG22	1:A:370:THR:HG23	1.68	0.76
1:A:637:GLU:C	1:A:638:THR:HG23	2.11	0.75
1:A:25:ASN:H	1:A:25:ASN:HD22	1.33	0.75
1:A:37:ILE:HD12	1:A:37:ILE:N	2.01	0.75
1:A:280:LYS:O	1:A:282:LYS:HE3	1.87	0.75
3:C:1:NAG:H82	3:C:1:NAG:C1	2.17	0.74
1:A:422:ASP:CB	1:A:423:PRO:CD	2.65	0.74
1:A:658:THR:HB	6:A:857:HOH:O	1.88	0.73
2:B:1:NAG:H5	2:B:2:FUC:H5	1.71	0.73
1:A:422:ASP:HB3	1:A:423:PRO:CD	2.15	0.72
6:A:1050:HOH:O	2:B:1:NAG:H82	1.89	0.72
1:A:107:ASN:H	1:A:107:ASN:HD22	1.35	0.72
1:A:295:GLN:HB2	1:A:298:LEU:HD21	1.70	0.71
1:A:577:ASP:OD1	1:A:579:LYS:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG21	1:A:300:PHE:CE1	2.25	0.71
1:A:176:THR:HG22	1:A:176:THR:O	1.90	0.71
1:A:260:VAL:HG13	1:A:261:ASN:N	2.05	0.71
1:A:515:ASN:O	1:A:518:VAL:HG12	1.91	0.70
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.27	0.70
2:B:1:NAG:C6	2:B:2:FUC:H5	2.22	0.69
1:A:13:ASN:N	1:A:14:PRO:HD2	2.07	0.69
1:A:28:LYS:HD2	1:A:285:LYS:HZ3	1.57	0.69
2:B:1:NAG:C5	2:B:2:FUC:H5	2.22	0.69
1:A:564:LYS:CE	1:A:565:ASP:OD2	2.41	0.69
1:A:6:VAL:O	1:A:34:VAL:HG23	1.93	0.69
1:A:28:LYS:HD2	1:A:285:LYS:NZ	2.08	0.68
1:A:36:CYS:O	1:A:37:ILE:HD12	1.93	0.68
1:A:322:SER:HB3	1:A:385:LEU:O	1.93	0.68
1:A:456:LYS:O	1:A:489:PHE:HB3	1.94	0.68
1:A:20:PHE:CE1	1:A:36:CYS:HB2	2.29	0.68
1:A:326:THR:HG22	6:A:999:HOH:O	1.95	0.67
1:A:138:TRP:CE3	1:A:145:ILE:HD13	2.29	0.67
1:A:233:ASP:OD2	1:A:235:THR:HG23	1.94	0.67
1:A:25:ASN:HD22	1:A:25:ASN:N	1.92	0.67
1:A:551:LEU:HD13	1:A:551:LEU:H	1.60	0.66
1:A:21:GLN:O	1:A:22:TRP:C	2.38	0.66
3:C:1:NAG:C1	3:C:1:NAG:C8	2.71	0.65
1:A:484:LYS:HB3	1:A:487:GLU:HG3	1.77	0.65
1:A:610:LYS:O	1:A:614:LEU:HG	1.95	0.65
1:A:47:GLN:O	1:A:51:GLU:HG2	1.95	0.64
1:A:176:THR:O	1:A:176:THR:CG2	2.45	0.64
1:A:147:ALA:O	1:A:151:ARG:HG3	1.98	0.64
1:A:421:SER:HB2	1:A:424:ASP:HB2	1.79	0.64
1:A:395:ASP:OD2	1:A:465:ARG:HA	1.97	0.64
1:A:138:TRP:CG	1:A:145:ILE:HD13	2.32	0.64
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.12	0.63
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.64	0.63
1:A:690:ARG:O	1:A:691:LYS:C	2.42	0.63
1:A:619:LYS:HE2	1:A:626:ASP:OD2	1.99	0.63
1:A:681:PRO:HD2	6:A:880:HOH:O	1.99	0.62
1:A:561:ALA:O	1:A:564:LYS:HG2	2.00	0.62
1:A:344:ARG:HD3	1:A:370:THR:HG21	1.82	0.61
1:A:260:VAL:HG13	1:A:261:ASN:H	1.64	0.61
1:A:218:LEU:HD11	1:A:227:TYR:CE2	2.34	0.61
1:A:573:LEU:O	1:A:580:ARG:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:HB3	1:A:223:GLU:OE2	2.01	0.60
1:A:220:ASP:O	1:A:223:GLU:CG	2.50	0.60
1:A:38:LYS:HD3	1:A:39:ARG:O	2.02	0.60
3:C:2:NAG:H83	3:C:2:NAG:H3	1.82	0.60
1:A:13:ASN:H	1:A:14:PRO:HD2	1.67	0.60
1:A:97:VAL:HG22	1:A:229:LEU:HD23	1.83	0.60
1:A:352:GLU:H	1:A:352:GLU:CD	2.05	0.60
1:A:240:ASP:C	1:A:241:LYS:HD2	2.26	0.59
3:C:1:NAG:H3	3:C:1:NAG:C8	2.18	0.59
1:A:38:LYS:O	1:A:39:ARG:NH1	2.24	0.59
1:A:130:GLY:HA3	6:A:934:HOH:O	2.02	0.59
1:A:581:LYS:HB3	1:A:582:PRO:CD	2.31	0.59
1:A:29:VAL:O	1:A:29:VAL:CG1	2.49	0.59
1:A:218:LEU:HD11	1:A:227:TYR:HE2	1.68	0.59
1:A:401:THR:HG23	1:A:683:LEU:HD13	1.85	0.59
1:A:13:ASN:N	1:A:14:PRO:CD	2.65	0.59
1:A:548:VAL:O	1:A:552:GLN:HG3	2.03	0.59
1:A:551:LEU:CD1	1:A:551:LEU:N	2.66	0.59
1:A:38:LYS:C	1:A:39:ARG:HG2	2.27	0.59
1:A:21:GLN:HA	1:A:24:ARG:CG	2.33	0.58
1:A:220:ASP:OD1	1:A:221:GLU:N	2.37	0.58
1:A:37:ILE:N	1:A:37:ILE:CD1	2.67	0.58
1:A:116:HIS:N	1:A:116:HIS:CD2	2.67	0.58
1:A:295:GLN:HB3	1:A:298:LEU:HD21	1.86	0.58
1:A:51:GLU:OE2	1:A:53:ARG:HD2	2.03	0.58
1:A:518:VAL:HG23	1:A:519:PRO:HD2	1.86	0.57
1:A:637:GLU:C	1:A:638:THR:CG2	2.76	0.57
1:A:280:LYS:O	1:A:282:LYS:HG3	2.05	0.56
1:A:361:TRP:CD1	1:A:361:TRP:O	2.58	0.56
1:A:70:ALA:CB	1:A:73:LYS:HE3	2.36	0.56
1:A:23:GLN:HB2	1:A:34:VAL:O	2.06	0.56
1:A:233:ASP:OD1	1:A:233:ASP:N	2.23	0.56
1:A:680:SER:HB2	1:A:681:PRO:CD	2.36	0.56
2:B:1:NAG:H62	2:B:2:FUC:H5	1.88	0.56
1:A:551:LEU:HD13	1:A:551:LEU:N	2.21	0.55
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.06	0.55
1:A:322:SER:O	1:A:326:THR:HG23	2.07	0.55
1:A:445:ASP:OD1	1:A:448:LEU:HD23	2.06	0.55
1:A:457:LYS:HB3	1:A:506:LEU:HD11	1.89	0.54
1:A:579:LYS:HD2	1:A:579:LYS:N	2.23	0.54
1:A:423:PRO:HB2	6:A:806:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TRP:HE1	1:A:143:GLU:HG2	1.73	0.53
1:A:3:ARG:HE	1:A:266:ALA:HB2	1.72	0.52
1:A:260:VAL:CG1	1:A:261:ASN:N	2.72	0.52
1:A:656:LYS:HE2	1:A:661:LYS:O	2.09	0.52
1:A:3:ARG:O	1:A:3:ARG:HG3	2.10	0.52
1:A:107:ASN:H	1:A:107:ASN:ND2	2.00	0.52
1:A:170:CYS:O	1:A:171:ARG:C	2.51	0.52
2:B:1:NAG:C6	2:B:2:FUC:C5	2.88	0.51
1:A:16:ALA:O	1:A:20:PHE:CD2	2.64	0.51
1:A:233:ASP:OD2	1:A:235:THR:CG2	2.58	0.51
1:A:445:ASP:OD1	1:A:448:LEU:CD2	2.59	0.51
1:A:13:ASN:HB3	1:A:14:PRO:HD3	1.93	0.51
1:A:279:GLY:O	1:A:280:LYS:C	2.53	0.50
1:A:105:GLN:HB2	1:A:107:ASN:ND2	2.26	0.50
3:C:2:NAG:H3	3:C:2:NAG:C8	2.31	0.50
1:A:633:LEU:HD22	1:A:643:PHE:CE2	2.46	0.50
1:A:136:LEU:O	1:A:137:ASN:C	2.54	0.50
1:A:21:GLN:O	1:A:24:ARG:N	2.44	0.50
1:A:51:GLU:HG3	1:A:53:ARG:HG3	1.92	0.50
1:A:185:SER:C	1:A:187:GLU:N	2.68	0.49
1:A:508:ILE:HD11	1:A:524:ARG:HB2	1.94	0.49
1:A:20:PHE:HE1	6:A:950:HOH:O	1.96	0.49
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.47	0.49
1:A:238:PRO:HB2	1:A:240:ASP:OD1	2.13	0.49
1:A:40:ASP:HB2	1:A:44:GLN:OE1	2.13	0.49
1:A:313:ARG:O	1:A:313:ARG:HG3	2.12	0.49
1:A:507:CYS:HB3	1:A:523:GLU:CD	2.37	0.49
1:A:352:GLU:CD	1:A:352:GLU:N	2.71	0.49
1:A:92:TYR:O	1:A:250:VAL:HG22	2.13	0.49
1:A:21:GLN:HA	1:A:24:ARG:HG2	1.93	0.49
1:A:424:ASP:OD1	1:A:424:ASP:C	2.53	0.49
1:A:625:SER:OG	1:A:626:ASP:OD1	2.30	0.49
1:A:138:TRP:CG	1:A:145:ILE:CD1	2.96	0.48
1:A:260:VAL:CG1	1:A:261:ASN:H	2.25	0.48
1:A:665:PRO:HG2	1:A:666:GLN:OE1	2.13	0.48
1:A:268:TRP:O	1:A:272:ARG:HB2	2.13	0.48
1:A:353:GLN:HG3	1:A:356:ARG:HH12	1.77	0.48
1:A:25:ASN:N	1:A:25:ASN:ND2	2.61	0.48
1:A:112:LEU:O	1:A:153:PHE:HB3	2.13	0.48
1:A:14:PRO:O	1:A:15:GLU:C	2.57	0.48
1:A:364:LEU:CD2	1:A:631:PHE:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:TYR:CE2	1:A:671:ILE:HD11	2.49	0.47
1:A:390:ASP:OD2	1:A:605:LYS:HE2	2.14	0.47
1:A:375:SER:HB3	6:A:938:HOH:O	2.14	0.47
1:A:429:ASP:O	1:A:431:PRO:HD3	2.14	0.47
1:A:472:PRO:O	1:A:476:LEU:HG	2.15	0.47
1:A:424:ASP:HB3	1:A:648:GLU:OE2	2.14	0.47
1:A:617:GLN:O	1:A:621:GLY:HA3	2.16	0.46
1:A:34:VAL:O	1:A:34:VAL:HG13	2.14	0.46
1:A:70:ALA:HA	1:A:73:LYS:HE3	1.97	0.46
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.81	0.46
1:A:238:PRO:HD2	1:A:241:LYS:HG2	1.98	0.46
1:A:221:GLU:H	1:A:221:GLU:HG2	1.32	0.46
1:A:341:ARG:O	1:A:341:ARG:HG3	2.16	0.46
1:A:499:PRO:HA	1:A:504:CYS:SG	2.56	0.46
1:A:20:PHE:O	1:A:24:ARG:HG2	2.14	0.46
1:A:93:TYR:CZ	1:A:243:LYS:HE2	2.51	0.46
1:A:38:LYS:O	1:A:39:ARG:CG	2.55	0.46
1:A:6:VAL:O	1:A:6:VAL:HG12	2.14	0.46
1:A:247:LEU:O	1:A:248:ALA:HB2	2.16	0.46
1:A:179:ASN:O	1:A:180:LYS:C	2.58	0.46
1:A:518:VAL:CG2	1:A:519:PRO:HD2	2.45	0.46
1:A:422:ASP:HB2	1:A:423:PRO:CD	2.46	0.45
1:A:624:GLY:O	1:A:626:ASP:N	2.49	0.45
1:A:51:GLU:HG3	1:A:53:ARG:HD2	1.98	0.45
1:A:498:ASP:OD1	1:A:500:ALA:HB3	2.15	0.45
1:A:3:ARG:O	1:A:3:ARG:CG	2.63	0.45
1:A:115:CYS:C	1:A:116:HIS:CD2	2.94	0.45
1:A:21:GLN:HA	1:A:24:ARG:HG3	1.97	0.45
1:A:220:ASP:OD1	1:A:220:ASP:C	2.60	0.45
1:A:415:TYR:C	1:A:416:LYS:O	2.56	0.45
1:A:417:SER:C	1:A:419:GLN:N	2.60	0.45
1:A:514:GLU:O	1:A:515:ASN:HB2	2.17	0.45
1:A:627:CYS:HA	1:A:628:PRO:HA	1.67	0.45
1:A:352:GLU:N	1:A:352:GLU:OE1	2.29	0.45
1:A:420:SER:OG	1:A:421:SER:N	2.35	0.45
1:A:258:ARG:HB2	1:A:262:GLY:HA2	1.98	0.45
1:A:624:GLY:O	1:A:625:SER:C	2.60	0.45
1:A:173:CYS:HB3	1:A:187:GLU:OE1	2.17	0.45
1:A:180:LYS:HE2	1:A:180:LYS:HB3	1.81	0.45
1:A:158:VAL:O	1:A:159:PRO:C	2.60	0.44
1:A:413:GLU:OE1	1:A:644:ASN:ND2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TYR:N	1:A:488:TYR:HD1	2.15	0.44
1:A:533:ARG:NE	1:A:537:GLU:OE2	2.48	0.44
1:A:279:GLY:H	1:A:282:LYS:HD2	1.83	0.44
1:A:533:ARG:HE	1:A:537:GLU:CD	2.24	0.44
1:A:41:SER:HB2	1:A:42:PRO:HD2	1.99	0.44
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.18	0.44
1:A:19:CYS:O	1:A:36:CYS:SG	2.75	0.44
1:A:365:SER:HB2	1:A:368:SER:OG	2.17	0.44
1:A:12:SER:C	1:A:38:LYS:HE2	2.43	0.44
1:A:13:ASN:O	1:A:14:PRO:C	2.60	0.44
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.83	0.44
1:A:443:ARG:HH11	1:A:443:ARG:HD3	1.25	0.44
1:A:558:ASN:OD1	1:A:558:ASN:C	2.60	0.44
1:A:42:PRO:O	1:A:46:ILE:HG13	2.17	0.44
1:A:427:CYS:C	1:A:649:CYS:SG	3.01	0.44
1:A:58:THR:CG2	1:A:300:PHE:CE1	2.98	0.44
1:A:525:TYR:CE1	1:A:533:ARG:HG2	2.53	0.43
1:A:84:THR:C	1:A:305:ILE:HD12	2.42	0.43
1:A:240:ASP:OD1	1:A:240:ASP:N	2.44	0.43
1:A:316:SER:O	1:A:317:GLY:C	2.61	0.43
1:A:442:ARG:HH11	1:A:442:ARG:HD3	1.60	0.43
1:A:70:ALA:HB1	1:A:73:LYS:HE3	2.01	0.43
1:A:258:ARG:HH11	1:A:258:ARG:HD2	1.50	0.43
1:A:390:ASP:CG	1:A:605:LYS:HE2	2.44	0.43
1:A:417:SER:O	1:A:419:GLN:N	2.50	0.43
1:A:603:MET:HE3	1:A:603:MET:HB2	1.62	0.43
1:A:105:GLN:HE22	1:A:236:ARG:HG3	1.83	0.43
1:A:162:ASP:OD1	1:A:164:GLY:HA3	2.19	0.43
1:A:275:GLN:O	1:A:279:GLY:HA3	2.19	0.43
1:A:378:GLU:HG3	6:A:1033:HOH:O	2.19	0.43
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.84	0.43
1:A:603:MET:HE2	6:A:824:HOH:O	2.18	0.43
1:A:119:LEU:HA	1:A:119:LEU:HD12	1.79	0.42
1:A:291:SER:HA	1:A:292:PRO:HD3	1.78	0.42
1:A:680:SER:HB2	1:A:681:PRO:HD2	2.00	0.42
1:A:233:ASP:OD1	1:A:233:ASP:C	2.56	0.42
1:A:397:GLY:O	1:A:400:TYR:HB3	2.19	0.42
3:C:1:NAG:C8	3:C:1:NAG:C3	2.89	0.42
1:A:488:TYR:N	1:A:488:TYR:CD1	2.87	0.42
3:C:1:NAG:O6	3:C:3:FUC:C5	2.67	0.42
1:A:122:THR:CG2	1:A:250:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:PRO:HG2	1:A:666:GLN:CD	2.44	0.42
1:A:395:ASP:HA	1:A:597:HIS:CD2	2.55	0.42
1:A:279:GLY:CA	1:A:282:LYS:NZ	2.78	0.42
1:A:499:PRO:HG3	6:A:1115:HOH:O	2.19	0.42
1:A:666:GLN:CD	1:A:666:GLN:H	2.23	0.42
1:A:466:THR:HG21	1:A:594:ALA:HB1	2.01	0.42
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.54	0.42
1:A:97:VAL:HG22	1:A:229:LEU:CD2	2.48	0.42
1:A:106:LEU:HD23	1:A:232:PRO:HA	2.02	0.42
1:A:346:VAL:HG22	1:A:370:THR:HG22	1.97	0.42
1:A:196:PHE:HB2	1:A:213:THR:HG21	2.02	0.41
1:A:279:GLY:N	1:A:282:LYS:HD2	2.35	0.41
1:A:179:ASN:ND2	1:A:186:GLN:OE1	2.54	0.41
1:A:510:ASP:HA	1:A:522:ASN:O	2.20	0.41
1:A:324:TYR:O	1:A:325:PHE:C	2.62	0.41
1:A:641:LEU:HD23	6:A:1239:HOH:O	2.20	0.41
1:A:419:GLN:HA	6:A:803:HOH:O	2.21	0.41
1:A:550:VAL:HG12	1:A:568:LEU:HD12	2.01	0.41
1:A:42:PRO:HG3	6:A:1204:HOH:O	2.20	0.41
1:A:418:ALA:C	1:A:419:GLN:HE21	2.28	0.41
1:A:508:ILE:HD11	1:A:524:ARG:CB	2.50	0.41
1:A:95:VAL:H	1:A:95:VAL:HG22	1.70	0.41
1:A:145:ILE:HD12	1:A:145:ILE:HA	1.82	0.41
1:A:249:ARG:HH11	1:A:249:ARG:HD3	1.52	0.41
1:A:276:GLU:O	1:A:282:LYS:HD3	2.21	0.41
1:A:285:LYS:HB2	1:A:285:LYS:HE3	1.80	0.41
1:A:460:HIS:ND1	1:A:468:GLY:O	2.51	0.41
1:A:387:GLY:HA2	1:A:602:ARG:NH1	2.36	0.41
1:A:448:LEU:O	1:A:580:ARG:HD2	2.21	0.41
1:A:464:ASP:H	1:A:469:TRP:CG	2.39	0.41
1:A:143:GLU:OE1	1:A:151:ARG:NH2	2.54	0.40
1:A:453:VAL:O	1:A:456:LYS:HB2	2.22	0.40
1:A:547:ASP:OD1	1:A:547:ASP:N	2.51	0.40
1:A:617:GLN:O	1:A:621:GLY:N	2.52	0.40
1:A:564:LYS:HG3	1:A:565:ASP:H	1.86	0.40
1:A:675:LYS:HD3	1:A:675:LYS:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	689/691 (100%)	618 (90%)	58 (8%)	13 (2%)	6 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	ASP
1	A	280	LYS
1	A	416	LYS
1	A	625	SER
1	A	637	GLU
1	A	418	ALA
1	A	564	LYS
1	A	281	ASP
1	A	164	GLY
1	A	446	THR
1	A	521	SER
1	A	606	VAL
1	A	636	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	570/572 (100%)	499 (88%)	71 (12%)	4 4

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	ARG
1	A	4	ARG
1	A	5	SER
1	A	21	GLN
1	A	25	ASN
1	A	30	ARG
1	A	38	LYS
1	A	53	ARG
1	A	58	THR
1	A	71	PRO
1	A	85	GLU
1	A	107	ASN
1	A	112	LEU
1	A	120	ARG
1	A	139	THR
1	A	145	ILE
1	A	146	GLU
1	A	149	VAL
1	A	176	THR
1	A	180	LYS
1	A	185	SER
1	A	206	VAL
1	A	221	GLU
1	A	223	GLU
1	A	225	ASP
1	A	235	THR
1	A	241	LYS
1	A	261	ASN
1	A	265	ASP
1	A	280	LYS
1	A	298	LEU
1	A	301	LYS
1	A	305	ILE
1	A	334	SER
1	A	352	GLU
1	A	372	SER
1	A	384	VAL
1	A	404	LYS
1	A	410	VAL
1	A	416	LYS
1	A	419	GLN
1	A	426	ASN

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Mol	Chain	Res	Type
1	A	436	LEU
1	A	445	ASP
1	A	447	SER
1	A	448	LEU
1	A	456	LYS
1	A	516	LYS
1	A	551	LEU
1	A	559	ASN
1	A	564	LYS
1	A	575	CYS
1	A	579	LYS
1	A	580	ARG
1	A	587	ARG
1	A	599	VAL
1	A	603	MET
1	A	619	LYS
1	A	625	SER
1	A	629	ASP
1	A	633	LEU
1	A	635	GLN
1	A	638	THR
1	A	641	LEU
1	A	652	ARG
1	A	656	LYS
1	A	673	ASN
1	A	674	LEU
1	A	676	LYS
1	A	687	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	23	GLN
1	A	25	ASN
1	A	47	GLN
1	A	91	HIS
1	A	105	GLN
1	A	107	ASN
1	A	295	GLN
1	A	329	GLN
1	A	353	GLN

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Mol	Chain	Res	Type
1	A	419	GLN
1	A	552	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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	B	1	1,2	14,14,15	2.25	4 (28%)	17,19,21	4.96	13 (76%)
2	FUC	B	2	2	10,10,11	1.14	1 (10%)	14,14,16	1.33	2 (14%)
3	NAG	C	1	1,3	14,14,15	2.11	3 (21%)	17,19,21	3.72	9 (52%)
3	NAG	C	2	3	14,14,15	1.37	2 (14%)	17,19,21	6.23	8 (47%)
3	FUC	C	3	3	8,8,11	0.35	0	10,10,16	1.86	3 (30%)

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	B	1	1,2	-	5/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	6/6/23/26	0/1/1/1
3	FUC	C	3	3	-	0/10/10/20	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O6-C6	-6.57	1.14	1.42
2	B	1	NAG	C2-N2	-5.78	1.36	1.46
2	B	1	NAG	O7-C7	-3.74	1.14	1.23
3	C	2	NAG	O7-C7	-3.39	1.15	1.23
2	B	1	NAG	C6-C5	-3.09	1.41	1.51
2	B	1	NAG	O5-C1	2.65	1.48	1.43
3	C	1	NAG	C1-C2	2.62	1.55	1.52
3	C	1	NAG	O7-C7	-2.46	1.17	1.23
3	C	2	NAG	C1-C2	2.41	1.55	1.52
2	B	2	FUC	O5-C5	-2.01	1.39	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C8-C7-N2	14.18	139.64	116.12
3	C	2	NAG	C1-O5-C5	13.53	130.32	112.19
3	C	2	NAG	O7-C7-N2	-13.19	98.67	121.98
3	C	1	NAG	O6-C6-C5	8.43	140.04	111.33
2	B	1	NAG	C1-O5-C5	-7.57	102.04	112.19
2	B	1	NAG	O3-C3-C2	7.52	125.03	109.40
2	B	1	NAG	C1-C2-N2	7.50	122.26	110.43
2	B	1	NAG	C2-N2-C7	7.09	132.41	122.90
3	C	1	NAG	C2-N2-C7	-6.97	113.56	122.90
3	C	1	NAG	C8-C7-N2	6.42	126.76	116.12
3	C	2	NAG	C1-C2-N2	-6.30	100.51	110.43
2	B	1	NAG	C6-C5-C4	-6.19	97.83	113.02
2	B	1	NAG	O7-C7-N2	-5.82	111.69	121.98
2	B	1	NAG	O5-C1-C2	-5.76	102.38	111.29
3	C	1	NAG	C1-O5-C5	5.12	119.04	112.19
2	B	1	NAG	C8-C7-N2	5.08	124.54	116.12
3	C	3	FUC	C1-C2-C3	-4.31	106.84	112.11
2	B	1	NAG	O4-C4-C5	-4.26	98.84	109.32
3	C	2	NAG	O5-C1-C2	-4.20	104.79	111.29
3	C	2	NAG	C3-C4-C5	-4.16	102.70	110.23
2	B	1	NAG	O6-C6-C5	4.12	125.36	111.33
3	C	1	NAG	O7-C7-N2	-3.38	116.00	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	FUC	O4-C4-C3	3.33	118.21	110.38
2	B	1	NAG	C4-C3-C2	-3.22	106.31	111.02
3	C	1	NAG	C1-C2-N2	-3.18	105.42	110.43
2	B	1	NAG	O3-C3-C4	-3.13	102.99	110.38
3	C	2	NAG	C6-C5-C4	-2.78	106.20	113.02
3	C	1	NAG	C4-C3-C2	2.74	115.04	111.02
3	C	2	NAG	O5-C5-C6	2.72	112.96	107.66
3	C	1	NAG	O7-C7-C8	-2.71	117.23	122.05
3	C	1	NAG	O3-C3-C2	-2.52	104.17	109.40
2	B	1	NAG	C3-C4-C5	-2.42	105.84	110.23
2	B	2	FUC	C1-C2-C3	-2.40	106.15	109.64
3	C	3	FUC	C4-C3-C2	-2.21	109.08	112.48
3	C	3	FUC	C5-C4-C3	-2.08	110.68	113.97

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C1-C2-N2-C7
3	C	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
2	B	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 17 short contacts:

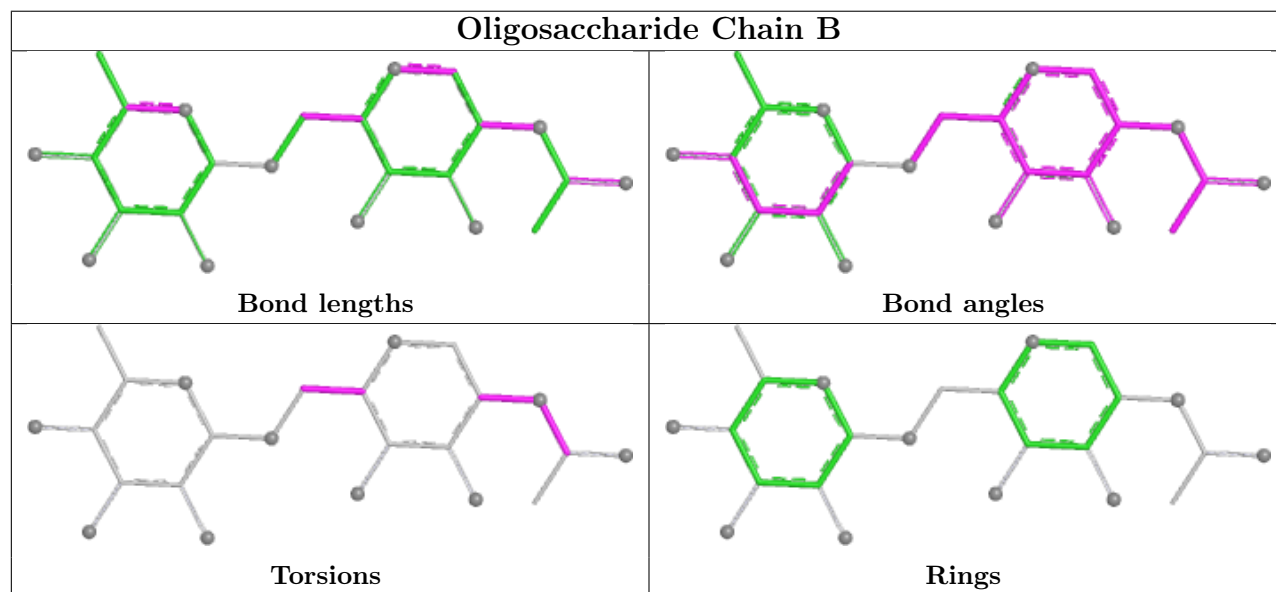
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	7	0

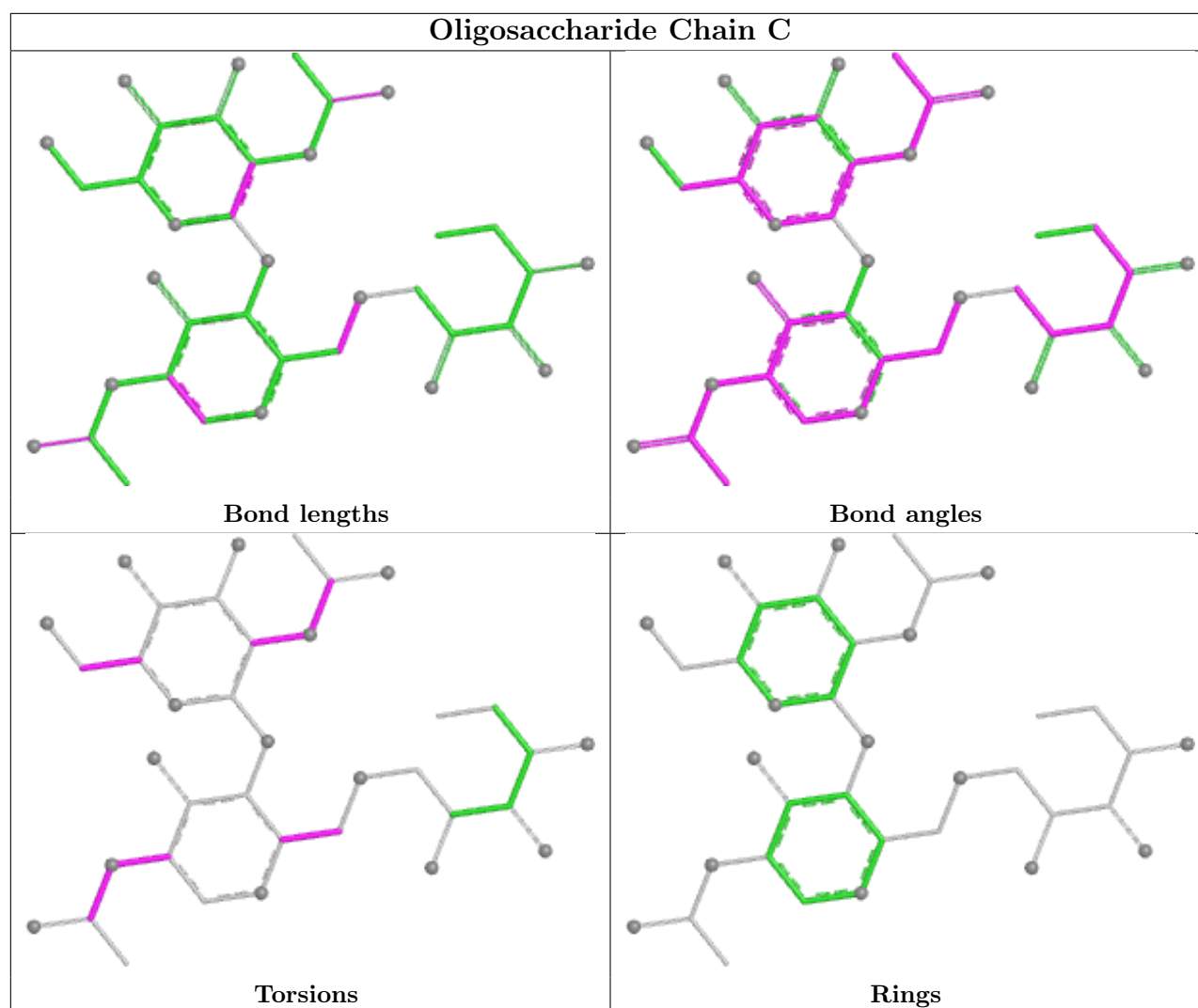
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	2	0
3	C	3	FUC	3	0
2	B	2	FUC	5	0
3	C	1	NAG	7	0

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	CO3	A	704	4	3,3,3	0.61	0	2,3,3	1.12	0
5	CO3	A	703	4	3,3,3	0.95	0	2,3,3	1.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.