



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:35 PM UTC

PDB ID : 1G1Y / pdb_00001g1y
Title : CRYSTAL STRUCTURE OF ALPHA-AMYLASE II (TVAII) FROM THERMOACTINOMYCES VULGARIS R-47 AND BETA-CYCLODEXTRIN COMPLEX
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Deposited on : 2000-10-16
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

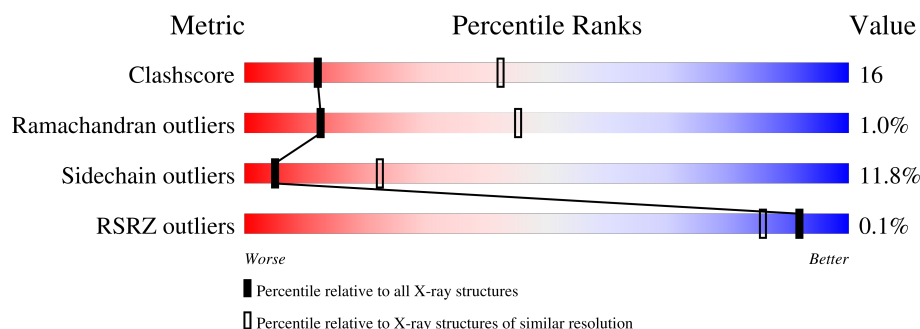
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	49% 38% 11% .
1	B	585	46% 39% 12% .
2	C	7	86% 14%
2	D	7	71% 29%

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	GLC	C	3	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10221 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.

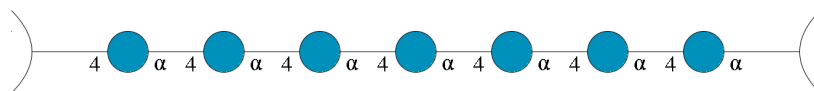
- Molecule 1 is a protein called ALPHA-AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4772	3054	831	872	15			
1	B	585	Total	C	N	O	S	0	0	0
			4772	3054	831	872	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	GLU	engineered mutation	UNP Q08751
B	354	ALA	GLU	engineered mutation	UNP Q08751

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	0	0
			77	42	35			
2	D	7	Total	C	O	0	0	0
			77	42	35			

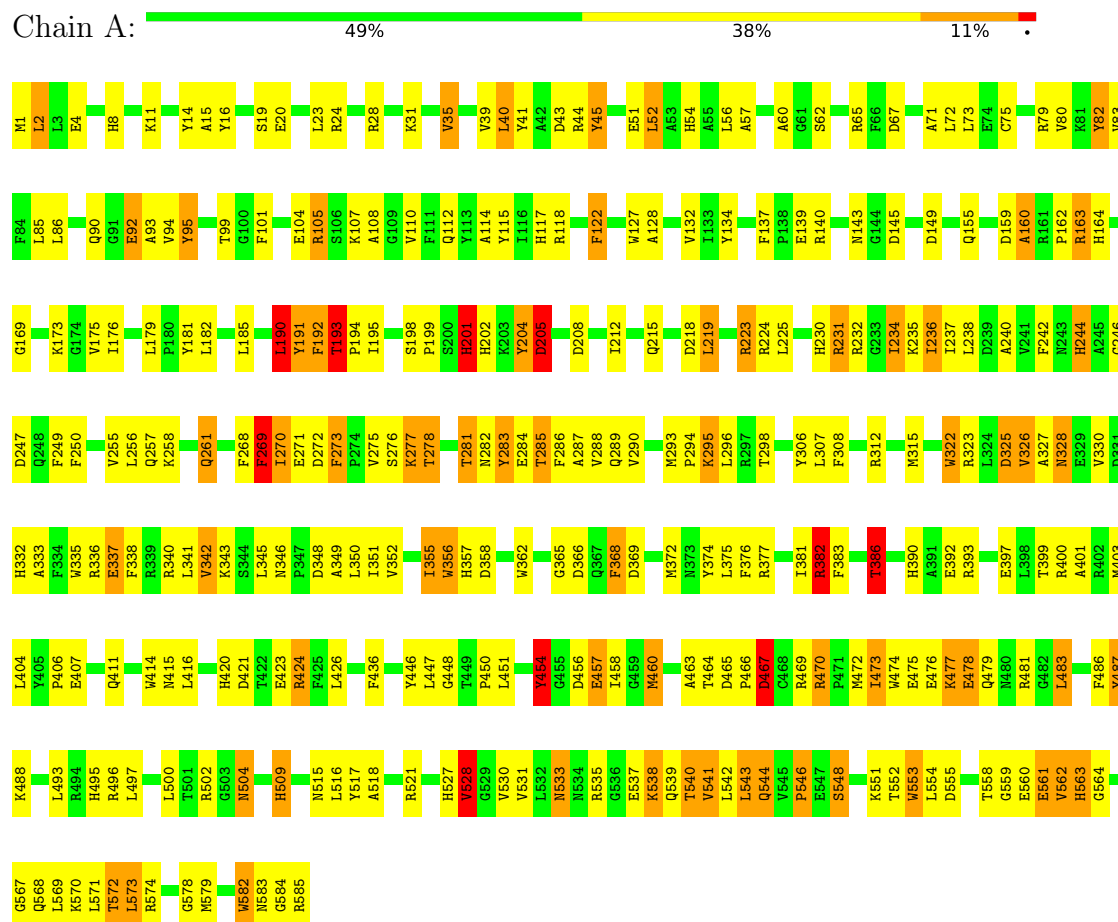
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	264	Total	O	0	0
			264	264		
3	B	259	Total	O	0	0
			259	259		

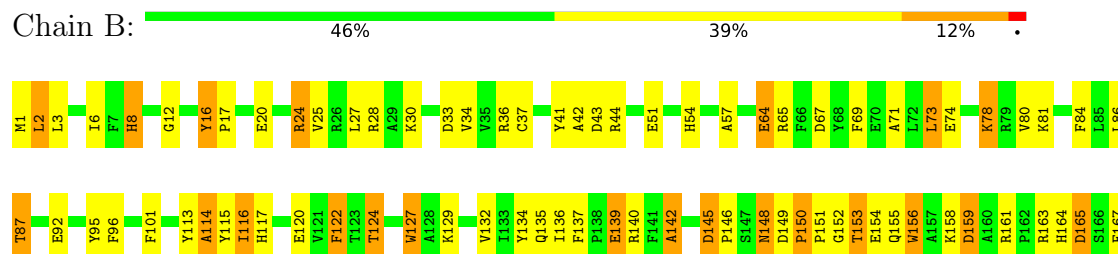
3 Residue-property plots

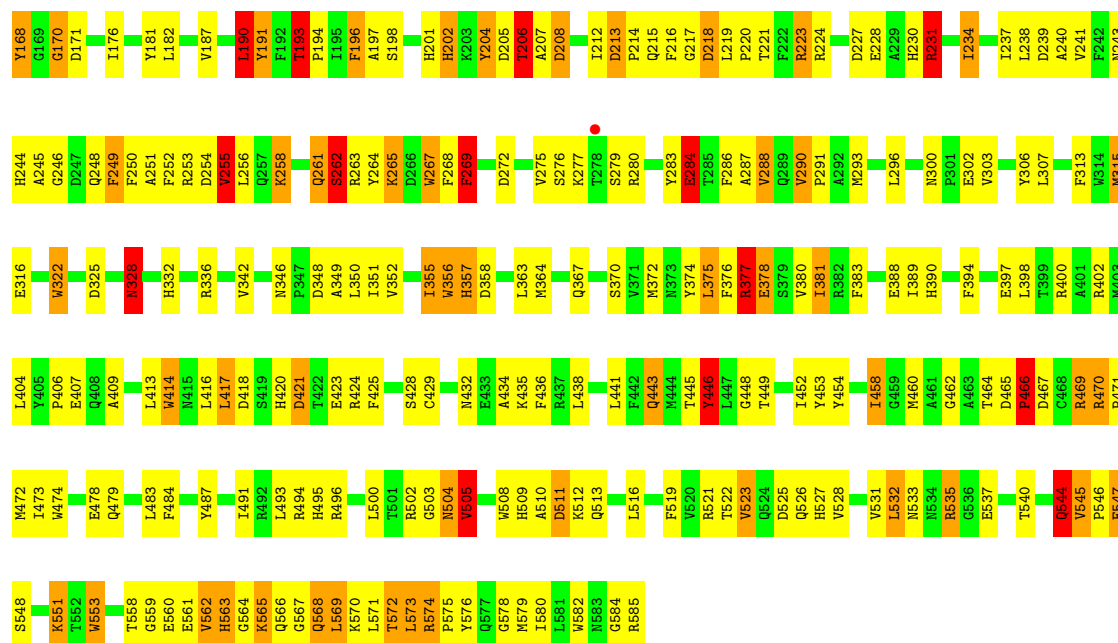
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ALPHA-AMYLASE II



• Molecule 1: ALPHA-AMYLASE II





- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C: 86% 14%



- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain D: 71% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.12Å 117.66Å 113.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.00) 87.1 (8.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.191 , 0.260 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 114.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10221	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

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	20/4902 (0.4%)	1.95	152/6636 (2.3%)
1	B	1.18	18/4902 (0.4%)	2.03	171/6636 (2.6%)
All	All	1.18	38/9804 (0.4%)	1.99	323/13272 (2.4%)

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	24
1	B	0	17
All	All	0	41

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	559	GLY	CA-C	7.79	1.59	1.51
1	B	545	VAL	C-N	7.55	1.42	1.33
1	A	390	HIS	CD2-NE2	-7.21	1.29	1.37
1	B	8	HIS	CD2-NE2	-7.18	1.29	1.37
1	B	54	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	164	HIS	CD2-NE2	-6.94	1.30	1.37
1	B	390	HIS	CD2-NE2	-6.88	1.30	1.37
1	B	332	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	332	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	563	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	509	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	357	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	8	HIS	CG-ND1	-6.49	1.31	1.38
1	B	527	HIS	CD2-NE2	-6.47	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	244	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	509	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	357	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	495	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	420	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	390	HIS	CG-ND1	-6.15	1.31	1.38
1	A	495	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	230	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	201	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	527	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	202	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	117	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	8	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	420	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	559	GLY	CA-C	5.31	1.58	1.52
1	A	230	HIS	CD2-NE2	-5.30	1.32	1.37
1	B	527	HIS	CG-ND1	-5.29	1.32	1.38
1	B	559	GLY	N-CA	5.23	1.50	1.45
1	B	563	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	562	VAL	CA-CB	5.09	1.59	1.53
1	A	39	VAL	CA-CB	-5.04	1.48	1.54
1	B	390	HIS	CG-ND1	-5.01	1.32	1.38
1	A	495	HIS	CG-ND1	-5.00	1.32	1.38

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	560	GLU	N-CA-C	16.85	133.42	109.15
1	B	258	LYS	N-CA-C	12.77	128.34	113.02
1	B	547	GLU	N-CA-C	12.16	124.08	111.07
1	B	367	GLN	N-CA-C	10.04	126.28	111.02
1	B	208	ASP	CA-CB-CG	9.96	122.56	112.60
1	B	558	THR	N-CA-C	9.86	127.03	114.31
1	B	269	PHE	N-CA-C	-9.71	94.88	110.32
1	B	511	ASP	CA-CB-CG	9.21	121.81	112.60
1	A	551	LYS	N-CA-C	-8.99	99.95	112.45
1	B	205	ASP	CA-CB-CG	8.88	121.48	112.60
1	A	288	VAL	N-CA-C	8.86	124.65	111.89
1	A	208	ASP	CA-CB-CG	8.62	121.22	112.60
1	B	149	ASP	N-CA-C	8.39	122.18	110.01
1	B	559	GLY	O-C-N	-8.36	114.72	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASP	CA-CB-CG	8.36	120.95	112.60
1	A	290	VAL	CA-C-O	-8.35	114.22	119.15
1	A	403	MET	N-CA-C	-8.34	102.66	113.17
1	B	522	THR	N-CA-C	8.32	123.46	108.48
1	B	267	TRP	N-CA-C	-8.29	103.16	113.28
1	B	249	PHE	CA-CB-CG	8.29	122.09	113.80
1	A	290	VAL	N-CA-C	-8.26	99.42	107.76
1	A	276	SER	N-CA-C	-8.16	93.54	107.99
1	A	553	TRP	NE1-CE2-CZ2	-8.07	118.00	130.10
1	A	558	THR	N-CA-C	7.89	127.62	110.80
1	B	545	VAL	CA-C-N	7.85	128.29	120.52
1	B	545	VAL	C-N-CA	7.85	128.29	120.52
1	B	207	ALA	N-CA-C	-7.75	102.37	112.68
1	A	467	ASP	N-CA-C	7.66	121.72	112.38
1	B	204	TYR	N-CA-C	-7.63	104.20	113.97
1	A	585	ARG	N-CA-C	-7.56	89.84	111.00
1	B	356	TRP	CB-CG-CD1	-7.55	115.57	126.90
1	A	356	TRP	CG-CD2-CE3	7.53	141.43	133.90
1	A	261	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	A	282	ASN	N-CA-C	7.48	121.84	112.87
1	A	559	GLY	O-C-N	-7.42	113.42	123.67
1	A	465	ASP	CA-CB-CG	7.42	120.02	112.60
1	B	156	TRP	NE1-CE2-CZ2	-7.40	119.00	130.10
1	B	511	ASP	N-CA-CB	-7.36	99.65	110.84
1	A	149	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	171	ASP	CA-CB-CG	7.33	119.93	112.60
1	B	252	PHE	N-CA-C	-7.30	103.33	112.90
1	B	566	GLN	N-CA-CB	7.25	122.43	111.70
1	B	221	THR	N-CA-C	-7.25	102.56	111.40
1	A	199	PRO	N-CA-C	7.20	127.30	112.47
1	B	469	ARG	N-CA-C	-7.17	102.79	112.26
1	A	195	ILE	N-CA-C	7.17	119.03	112.29
1	A	356	TRP	CB-CG-CD1	-7.17	116.15	126.90
1	B	156	TRP	CG-CD2-CE3	-7.16	126.74	133.90
1	A	325	ASP	O-C-N	7.13	131.34	123.22
1	A	218	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	502	ARG	N-CA-C	7.06	121.99	112.88
1	B	165	ASP	N-CA-C	-7.03	103.70	111.36
1	B	561	GLU	N-CA-C	7.02	119.08	109.11
1	B	33	ASP	CA-C-O	-7.02	113.11	120.55
1	B	291	PRO	N-CA-C	7.00	123.24	114.92
1	A	104	GLU	N-CA-C	-6.99	97.02	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	GLU	CA-C-O	-6.99	113.48	120.82
1	B	394	PHE	N-CA-C	-6.98	103.36	110.97
1	A	155	GLN	N-CA-C	-6.98	100.15	110.48
1	A	67	ASP	CA-CB-CG	6.98	119.58	112.60
1	B	558	THR	CA-C-O	-6.98	111.03	118.77
1	A	164	HIS	CB-CG-CD2	-6.93	122.18	131.20
1	A	244	HIS	CB-CG-CD2	-6.89	122.25	131.20
1	B	262	SER	N-CA-CB	-6.86	98.90	110.49
1	A	191	TYR	N-CA-C	-6.84	97.12	108.34
1	B	397	GLU	N-CA-C	-6.84	103.91	111.36
1	A	205	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	148	ASN	CA-CB-CG	6.83	119.43	112.60
1	B	404	LEU	N-CA-C	6.79	119.70	111.82
1	A	234	ILE	N-CA-CB	-6.79	103.13	110.53
1	B	288	VAL	N-CA-C	6.77	123.43	109.34
1	B	584	GLY	CA-C-O	-6.77	112.50	119.20
1	A	122	PHE	CA-CB-CG	6.74	120.54	113.80
1	B	544	GLN	CA-C-O	-6.73	113.07	120.81
1	A	40	LEU	N-CA-C	-6.72	97.94	108.90
1	B	428	SER	N-CA-C	-6.70	103.14	112.45
1	B	417	LEU	N-CA-C	-6.64	105.47	113.97
1	B	216	PHE	CA-CB-CG	6.61	120.41	113.80
1	B	569	LEU	N-CA-C	-6.61	97.50	108.34
1	A	43	ASP	CA-CB-CG	6.61	119.21	112.60
1	B	519	PHE	N-CA-C	6.60	118.97	109.14
1	A	90	GLN	N-CA-C	-6.59	105.11	113.02
1	B	78	LYS	CG-CD-CE	-6.58	96.16	111.30
1	A	269	PHE	O-C-N	-6.57	115.05	122.93
1	B	193	THR	O-C-N	-6.57	113.77	121.32
1	B	505	VAL	N-CA-C	6.53	117.66	107.28
1	A	563	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	A	179	LEU	CA-C-O	-6.51	111.24	120.16
1	A	454	TYR	CA-C-N	-6.49	115.71	123.44
1	A	454	TYR	C-N-CA	-6.49	115.71	123.44
1	A	582	TRP	CG-CD2-CE3	-6.49	127.41	133.90
1	A	337	GLU	N-CA-C	-6.49	104.14	111.14
1	A	368	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	261	GLN	CG-CD-NE2	6.44	126.06	116.40
1	B	269	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	399	THR	N-CA-C	6.43	118.28	111.28
1	B	114	ALA	N-CA-C	6.40	118.82	111.02
1	B	375	LEU	N-CA-C	-6.39	104.00	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	GLN	CA-C-O	6.38	127.30	119.97
1	A	569	LEU	N-CA-C	-6.35	98.84	109.07
1	B	268	PHE	N-CA-C	-6.34	99.41	109.23
1	A	198	SER	CA-C-N	6.34	127.76	119.84
1	A	198	SER	C-N-CA	6.34	127.76	119.84
1	A	60	ALA	N-CA-C	6.30	120.67	112.92
1	A	555	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	357	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	B	190	LEU	N-CA-C	-6.27	97.60	108.69
1	B	424	ARG	CB-CG-CD	-6.24	96.94	111.30
1	A	128	ALA	N-CA-C	-6.24	104.73	112.90
1	B	69	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	244	HIS	CA-CB-CG	6.19	119.99	113.80
1	A	212	ILE	N-CA-C	-6.18	101.60	109.58
1	B	155	GLN	N-CA-C	6.18	119.21	110.50
1	B	383	PHE	N-CA-C	-6.18	104.47	111.14
1	B	525	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	290	VAL	N-CA-C	6.16	114.67	107.77
1	A	35	VAL	N-CA-CB	-6.15	105.44	112.21
1	A	289	GLN	CA-C-N	-6.15	118.16	122.59
1	A	289	GLN	C-N-CA	-6.15	118.16	122.59
1	A	323	ARG	N-CA-C	-6.13	98.91	108.90
1	A	583	ASN	CA-CB-CG	6.13	118.73	112.60
1	B	332	HIS	CB-CG-CD2	-6.10	123.26	131.20
1	A	376	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	467	ASP	CA-CB-CG	-6.10	106.50	112.60
1	B	446	TYR	N-CA-C	6.07	118.38	110.43
1	A	579	MET	CA-C-O	-6.05	114.30	120.71
1	A	114	ALA	N-CA-C	6.05	121.35	111.37
1	B	243	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	470	ARG	CA-C-N	6.03	126.05	119.89
1	A	470	ARG	C-N-CA	6.03	126.05	119.89
1	A	527	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	B	532	LEU	N-CA-C	6.02	118.64	107.99
1	A	356	TRP	CE2-CD2-CG	-6.01	99.98	107.20
1	A	230	HIS	CA-CB-CG	6.01	119.81	113.80
1	A	333	ALA	CA-C-O	-6.01	114.51	120.70
1	B	388	GLU	N-CA-C	6.00	120.34	113.19
1	B	458	ILE	CB-CA-C	6.00	120.11	111.88
1	B	516	LEU	N-CA-C	-5.99	99.48	109.24
1	A	225	LEU	N-CA-C	5.98	117.47	111.07
1	A	269	PHE	CA-C-N	-5.98	115.12	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	PHE	C-N-CA	-5.98	115.12	123.13
1	A	54	HIS	CB-CG-CD2	-5.97	123.43	131.20
1	A	336	ARG	CB-CG-CD	-5.97	97.56	111.30
1	B	234	ILE	N-CA-C	-5.97	99.56	108.46
1	B	495	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	B	164	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	B	272	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	548	SER	CA-CB-OG	5.96	123.02	111.10
1	B	64	GLU	CA-CB-CG	5.95	125.99	114.10
1	B	356	TRP	CG-CD2-CE3	5.95	139.85	133.90
1	B	533	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	585	ARG	CA-CB-CG	5.92	125.95	114.10
1	A	215	GLN	N-CA-C	-5.92	106.10	113.38
1	B	580	ILE	N-CA-C	-5.92	96.07	106.61
1	A	390	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	A	190	LEU	N-CA-C	-5.92	100.25	109.72
1	B	443	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	392	GLU	CA-CB-CG	-5.88	102.34	114.10
1	A	107	LYS	N-CA-C	-5.88	106.06	113.18
1	B	16	TYR	O-C-N	-5.88	117.26	121.84
1	B	527	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	B	336	ARG	N-CA-C	-5.87	105.22	112.90
1	B	202	HIS	CA-C-N	-5.86	113.37	122.05
1	B	202	HIS	C-N-CA	-5.86	113.37	122.05
1	B	315	MET	CA-CB-CG	-5.86	102.39	114.10
1	B	513	GLN	N-CA-C	5.85	118.79	111.24
1	A	99	THR	CA-CB-OG1	-5.85	100.83	109.60
1	B	553	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	B	421	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	143	ASN	N-CA-C	-5.84	97.66	107.99
1	B	404	LEU	N-CA-CB	-5.84	101.23	110.28
1	B	462	GLY	O-C-N	-5.83	117.98	123.81
1	B	551	LYS	N-CA-C	-5.83	104.89	112.23
1	A	92	GLU	CB-CA-C	-5.82	101.11	109.84
1	B	572	THR	CA-C-O	-5.82	114.55	120.84
1	B	328	ASN	CA-CB-CG	5.82	118.42	112.60
1	B	389	ILE	N-CA-CB	5.81	120.98	111.45
1	B	127	TRP	CG-CD1-NE1	-5.81	102.65	110.20
1	A	159	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	526	GLN	N-CA-C	5.79	118.09	109.59
1	A	582	TRP	CG-CD1-NE1	-5.77	102.69	110.20
1	B	154	GLU	N-CA-C	5.76	118.63	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	PHE	CA-C-N	5.75	125.22	119.24
1	B	137	PHE	C-N-CA	5.75	125.22	119.24
1	A	118	ARG	N-CA-C	-5.75	104.99	112.23
1	A	193	THR	O-C-N	-5.75	114.71	121.32
1	A	202	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	B	510	ALA	N-CA-C	-5.72	97.66	107.61
1	A	164	HIS	N-CA-C	5.71	117.97	111.11
1	B	390	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	B	277	LYS	N-CA-C	-5.71	104.97	111.14
1	A	420	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	173	LYS	CA-CB-CG	5.71	125.51	114.10
1	A	356	TRP	CG-CD1-NE1	-5.70	102.79	110.20
1	B	41	TYR	N-CA-C	5.69	118.05	109.23
1	B	181	TYR	N-CA-C	-5.69	104.71	111.03
1	B	348	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	284	GLU	O-C-N	5.67	129.91	122.89
1	B	358	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	256	LEU	N-CA-C	-5.63	105.04	111.07
1	B	8	HIS	CB-CG-CD2	-5.63	123.89	131.20
1	A	348	ASP	N-CA-C	5.62	119.83	112.92
1	A	568	GLN	CA-CB-CG	5.62	125.33	114.10
1	B	512	LYS	N-CA-CB	-5.61	100.63	109.78
1	B	414	TRP	N-CA-C	5.61	117.36	108.67
1	A	582	TRP	NE1-CE2-CZ2	-5.60	121.69	130.10
1	B	217	GLY	O-C-N	-5.60	118.55	123.92
1	B	218	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	574	ARG	CA-CB-CG	5.59	125.27	114.10
1	A	362	TRP	CB-CG-CD1	-5.58	118.52	126.90
1	B	574	ARG	O-C-N	-5.58	114.90	121.32
1	B	466	PRO	N-CA-C	5.58	126.61	112.10
1	A	117	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	528	VAL	O-C-N	-5.58	117.18	122.98
1	B	54	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	B	159	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	99	THR	CA-C-O	5.54	126.29	120.42
1	A	232	ARG	O-C-N	-5.54	115.54	122.35
1	B	467	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	213	ASP	CA-C-N	5.51	126.72	119.84
1	B	213	ASP	C-N-CA	5.51	126.72	119.84
1	A	201	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	277	LYS	N-CA-C	-5.49	106.63	113.38
1	B	357	HIS	CB-CG-CD2	-5.48	124.07	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	GLU	CA-C-O	-5.48	114.98	120.96
1	B	367	GLN	O-C-N	-5.48	115.46	121.76
1	A	56	LEU	N-CA-C	5.47	118.46	109.76
1	A	561	GLU	CB-CG-CD	5.47	121.89	112.60
1	B	244	HIS	O-C-N	-5.46	116.10	123.19
1	A	237	ILE	O-C-N	-5.45	117.45	123.18
1	B	20	GLU	N-CA-C	5.44	117.97	111.71
1	A	377	ARG	N-CA-C	-5.43	105.27	111.14
1	B	425	PHE	CA-C-O	-5.43	114.12	120.20
1	B	243	ASN	CB-CG-ND2	5.43	124.55	116.40
1	B	239	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	386	THR	CA-CB-CG2	5.43	119.72	110.50
1	B	120	GLU	N-CA-C	-5.43	106.03	113.30
1	A	381	ILE	N-CA-C	-5.42	105.04	110.30
1	B	255	VAL	N-CA-C	-5.40	108.02	113.47
1	A	337	GLU	CA-CB-CG	-5.39	103.31	114.10
1	A	553	TRP	CB-CG-CD1	-5.39	118.81	126.90
1	B	545	VAL	N-CA-C	5.39	120.53	108.88
1	B	562	VAL	N-CA-CB	-5.39	102.34	111.23
1	B	116	ILE	O-C-N	-5.38	117.65	123.14
1	A	495	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	A	537	GLU	O-C-N	-5.38	118.13	123.46
1	B	122	PHE	CA-CB-CG	5.38	119.18	113.80
1	B	568	GLN	N-CA-C	-5.38	102.92	110.50
1	B	537	GLU	O-C-N	-5.37	117.92	123.29
1	A	546	PRO	N-CA-C	-5.36	102.81	111.77
1	A	382	ARG	CA-C-O	-5.36	115.37	121.00
1	A	509	HIS	CB-CG-CD2	-5.36	124.24	131.20
1	B	202	HIS	O-C-N	-5.36	116.28	122.87
1	A	244	HIS	CB-CG-ND1	5.35	130.73	122.70
1	A	287	ALA	CA-C-O	-5.33	115.74	121.45
1	B	33	ASP	N-CA-C	5.33	117.09	111.28
1	A	86	LEU	O-C-N	-5.33	116.97	123.10
1	B	206	THR	N-CA-C	-5.33	102.17	110.10
1	A	270	ILE	N-CA-CB	-5.32	105.20	111.90
1	B	508	TRP	N-CA-CB	-5.31	102.29	110.42
1	A	175	VAL	N-CA-C	-5.31	105.32	110.42
1	A	343	LYS	N-CA-C	-5.31	106.30	112.89
1	B	124	THR	CA-C-N	5.31	125.56	119.83
1	B	124	THR	C-N-CA	5.31	125.56	119.83
1	A	335	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	A	560	GLU	N-CA-CB	5.30	118.06	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	TRP	CD1-CG-CD2	5.30	114.78	106.30
1	A	366	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	346	ASN	CA-C-N	5.29	125.10	119.28
1	B	346	ASN	C-N-CA	5.29	125.10	119.28
1	B	2	LEU	N-CA-C	-5.29	100.11	108.73
1	A	247	ASP	N-CA-CB	-5.28	102.10	110.28
1	A	336	ARG	CA-CB-CG	-5.27	103.55	114.10
1	A	235	LYS	CA-C-O	-5.27	115.73	121.89
1	B	145	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	67	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	356	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	A	358	ASP	CA-CB-CG	5.24	117.83	112.60
1	B	572	THR	O-C-N	-5.23	116.44	122.87
1	B	509	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	101	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	108	ALA	CB-CA-C	-5.20	102.15	110.79
1	A	356	TRP	CD1-CG-CD2	5.20	114.61	106.30
1	B	202	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	B	87	THR	CA-CB-CG2	5.18	119.31	110.50
1	B	74	GLU	N-CA-C	-5.18	100.64	108.67
1	A	235	LYS	O-C-N	-5.17	116.63	122.68
1	A	127	TRP	CG-CD1-NE1	-5.17	103.48	110.20
1	B	441	LEU	N-CA-C	-5.17	105.83	111.82
1	B	142	ALA	O-C-N	-5.16	117.84	123.26
1	A	92	GLU	CA-CB-CG	5.16	124.42	114.10
1	B	176	ILE	N-CA-CB	5.16	116.58	110.55
1	B	146	PRO	N-CA-C	5.15	120.62	113.98
1	B	316	GLU	N-CA-C	-5.15	105.75	111.36
1	A	553	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	A	20	GLU	CA-CB-CG	-5.11	103.87	114.10
1	B	420	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	566	GLN	CG-CD-NE2	5.11	124.06	116.40
1	A	62	SER	N-CA-C	-5.10	99.35	108.13
1	B	484	PHE	CA-C-O	-5.10	115.44	120.90
1	A	362	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	A	322	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	B	92	GLU	CB-CA-C	-5.09	100.28	110.42
1	A	281	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	1	MET	N-CA-C	-5.07	96.81	111.00
1	A	35	VAL	CB-CA-C	5.07	117.17	110.84
1	A	278	THR	CA-CB-CG2	5.07	119.11	110.50
1	B	582	TRP	CG-CD1-NE1	-5.06	103.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ALA	N-CA-C	5.06	117.64	110.10
1	A	332	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	355	ILE	N-CA-C	-5.06	100.96	108.45
1	A	533	ASN	CA-C-O	-5.05	115.66	120.92
1	A	424	ARG	O-C-N	-5.05	117.25	122.96
1	B	381	ILE	CA-CB-CG1	-5.05	101.81	110.40
1	B	574	ARG	N-CA-CB	-5.05	101.38	110.37
1	A	335	TRP	CB-CG-CD1	-5.05	119.33	126.90
1	A	362	TRP	CG-CD1-NE1	-5.05	103.64	110.20
1	B	378	GLU	N-CA-C	5.04	118.59	112.23
1	A	460	MET	N-CA-C	5.04	116.96	109.25
1	B	356	TRP	CG-CD1-NE1	-5.04	103.65	110.20
1	A	343	LYS	CG-CD-CE	-5.03	99.73	111.30
1	B	153	THR	N-CA-CB	-5.02	102.82	110.45
1	B	322	TRP	CE2-CD2-CG	-5.01	101.19	107.20

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	LYS	Peptide
1	A	115	TYR	Sidechain
1	A	134	TYR	Sidechain
1	A	14	TYR	Sidechain
1	A	16	TYR	Sidechain
1	A	163	ARG	Sidechain
1	A	181	TYR	Sidechain
1	A	192	PHE	Sidechain
1	A	204	TYR	Sidechain
1	A	250	PHE	Sidechain
1	A	269	PHE	Peptide
1	A	28	ARG	Sidechain
1	A	283	TYR	Sidechain
1	A	374	TYR	Sidechain
1	A	382	ARG	Sidechain
1	A	400	ARG	Sidechain
1	A	45	TYR	Sidechain
1	A	454	TYR	Sidechain
1	A	487	TYR	Sidechain
1	A	502	ARG	Sidechain
1	A	548	SER	Peptide
1	A	65	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	82	TYR	Sidechain
1	A	95	TYR	Sidechain
1	B	113	TYR	Sidechain
1	B	165	ASP	Peptide
1	B	168	TYR	Sidechain
1	B	196	PHE	Sidechain
1	B	231	ARG	Sidechain
1	B	264	TYR	Sidechain
1	B	28	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	400	ARG	Sidechain
1	B	402	ARG	Sidechain
1	B	446	TYR	Sidechain
1	B	453	TYR	Sidechain
1	B	454	TYR	Sidechain
1	B	487	TYR	Sidechain
1	B	535	ARG	Sidechain
1	B	576	TYR	Sidechain
1	B	95	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4772	0	4606	140	0
1	B	4772	0	4606	159	0
2	C	77	0	63	10	0
2	D	77	0	63	5	0
3	A	264	0	0	2	0
3	B	259	0	0	4	0
All	All	10221	0	9338	296	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 16.

All (296) 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:B:296:LEU:HD13	1:B:307:LEU:HD11	1.52	0.89
1:A:533:ASN:HB2	1:A:573:LEU:HD13	1.56	0.86
1:B:328:ASN:HB3	1:B:355:ILE:HG13	1.58	0.84
1:B:255:VAL:HG12	1:B:262:SER:HB2	1.59	0.83
2:D:3:GLC:O3	2:D:4:GLC:O2	1.96	0.83
1:B:548:SER:HB2	1:B:585:ARG:HH22	1.45	0.82
1:B:258:LYS:HB3	1:B:261:GLN:HB2	1.64	0.79
1:A:23:LEU:HD22	1:A:80:VAL:HG11	1.65	0.79
1:A:328:ASN:HB3	1:A:355:ILE:HG12	1.65	0.78
1:B:182:LEU:HD13	1:B:190:LEU:HD11	1.65	0.78
1:B:571:LEU:HD22	1:B:579:MET:SD	2.26	0.77
1:B:370:SER:HB2	1:B:413:LEU:HA	1.66	0.76
1:A:326:VAL:HG22	2:C:3:GLC:H61	1.67	0.76
1:B:500:LEU:HD23	1:B:521:ARG:HG3	1.68	0.75
1:A:312:ARG:HG2	1:A:345:LEU:HD11	1.70	0.72
1:A:269:PHE:HB2	1:A:284:GLU:HB2	1.70	0.72
1:A:132:VAL:HG13	1:A:450:PRO:HB2	1.72	0.71
1:B:42:ALA:HB3	1:B:81:LYS:HE2	1.72	0.71
1:A:475:GLU:HB2	1:A:478:GLU:HG3	1.70	0.71
1:B:300:ASN:HB3	1:B:303:VAL:HG23	1.71	0.71
1:A:286:PHE:CE1	2:C:4:GLC:H62	2.26	0.70
1:A:516:LEU:HD22	1:A:541:VAL:HG11	1.72	0.69
1:A:122:PHE:CD2	1:A:365:GLY:HA2	2.28	0.69
1:B:429:CYS:SG	1:B:435:LYS:HB2	2.33	0.69
1:A:85:LEU:HD13	1:A:95:TYR:CE1	2.28	0.68
1:A:355:ILE:HD11	1:A:368:PHE:HE1	1.57	0.67
1:B:142:ALA:O	1:B:170:GLY:HA2	1.93	0.67
1:B:139:GLU:O	1:B:170:GLY:HA3	1.95	0.67
1:A:268:PHE:HE2	1:A:296:LEU:HD23	1.60	0.67
1:A:52:LEU:HD11	1:A:105:ARG:NH2	2.10	0.67
1:A:272:ASP:HB2	1:A:283:TYR:HB3	1.77	0.66
1:A:283:TYR:CE1	1:A:294:PRO:HB3	2.31	0.66
1:B:148:ASN:HB2	1:B:215:GLN:O	1.96	0.66
1:A:454:TYR:OH	1:A:469:ARG:HA	1.95	0.65
1:B:267:TRP:HE1	1:B:302:GLU:HG3	1.61	0.64
1:B:249:PHE:CE1	1:B:306:TYR:HE1	2.15	0.64
1:B:573:LEU:HB3	1:B:579:MET:HE3	1.81	0.63
1:A:533:ASN:OD1	1:A:535:ARG:HB2	1.99	0.62
1:B:544:GLN:HE22	1:B:568:GLN:HE22	1.46	0.62
1:A:315:MET:HE1	1:A:342:VAL:HG22	1.79	0.62
1:A:257:GLN:HG3	1:A:258:LYS:HG3	1.81	0.61
1:B:132:VAL:HG21	1:B:491:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:TRP:HD1	1:B:449:THR:HB	1.66	0.61
1:B:269:PHE:HB2	1:B:284:GLU:HB2	1.83	0.61
1:A:538:LYS:HB2	1:A:574:ARG:HA	1.83	0.61
1:A:552:THR:O	1:A:553:TRP:HD1	1.82	0.61
1:B:156:TRP:CZ3	1:B:168:TYR:HB3	2.36	0.61
1:B:17:PRO:HB3	1:B:116:ILE:HG23	1.82	0.60
1:B:27:LEU:HD13	1:B:37:CYS:SG	2.42	0.60
1:A:44:ARG:HD2	1:A:112:GLN:OE1	2.03	0.59
1:A:356:TRP:HE1	2:C:3:GLC:C2	2.15	0.59
1:A:162:PRO:HD3	1:A:470:ARG:HG2	1.83	0.59
1:B:12:GLY:HA2	1:B:364:MET:HE1	1.84	0.59
1:B:286:PHE:HZ	2:D:3:GLC:H62	1.67	0.59
1:A:337:GLU:HG2	1:A:340:ARG:NH2	2.17	0.59
1:B:27:LEU:HD12	1:B:84:PHE:CD2	2.38	0.59
1:B:504:ASN:HD22	1:B:504:ASN:H	1.50	0.59
1:A:190:LEU:HD13	1:A:234:ILE:CG2	2.33	0.58
1:B:156:TRP:HZ3	1:B:168:TYR:HB3	1.67	0.58
1:A:244:HIS:HD2	1:A:293:MET:HB3	1.70	0.57
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.86	0.57
1:A:190:LEU:HD13	1:A:234:ILE:HG23	1.87	0.57
1:B:267:TRP:NE1	1:B:302:GLU:HG3	2.18	0.57
1:A:249:PHE:CZ	1:A:306:TYR:HE1	2.22	0.57
1:B:503:GLY:HA2	1:B:523:VAL:HG13	1.86	0.57
1:A:242:PHE:HE2	1:A:338:PHE:CE1	2.23	0.57
1:B:191:TYR:HA	1:B:237:ILE:O	2.05	0.56
1:B:241:VAL:HG12	1:B:325:ASP:HB3	1.87	0.56
1:B:372:MET:SD	1:B:414:TRP:HE3	2.29	0.56
1:A:372:MET:SD	1:A:414:TRP:HE3	2.29	0.56
1:A:479:GLN:OE1	1:A:481:ARG:NH2	2.38	0.56
1:B:148:ASN:HA	3:B:1385:HOH:O	2.04	0.56
1:B:1:MET:HE2	1:B:34:VAL:HG12	1.88	0.56
1:B:136:ILE:HD12	1:B:190:LEU:HG	1.88	0.56
1:A:122:PHE:CG	1:A:365:GLY:HA2	2.40	0.55
1:B:44:ARG:HA	1:B:81:LYS:HD3	1.87	0.55
1:A:268:PHE:O	1:A:270:ILE:HG12	2.06	0.55
1:B:245:ALA:O	1:B:293:MET:HA	2.07	0.55
1:B:460:MET:SD	1:B:473:ILE:HG13	2.46	0.55
1:B:356:TRP:HE1	2:D:3:GLC:H2	1.72	0.55
1:A:286:PHE:CZ	2:C:4:GLC:H62	2.42	0.55
1:A:24:ARG:HD2	1:A:407:GLU:OE2	2.07	0.54
1:A:295:LYS:HB2	1:A:295:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HD13	1:A:224:ARG:HD3	1.90	0.54
1:A:411:GLN:HG2	1:A:447:LEU:HD11	1.88	0.54
1:B:263:ARG:HD3	3:B:1411:HOH:O	2.06	0.54
1:A:483:LEU:O	1:A:486:PHE:HB3	2.07	0.54
1:B:228:GLU:HG3	1:B:231:ARG:HH21	1.73	0.54
1:B:544:GLN:NE2	1:B:568:GLN:HE22	2.05	0.54
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.43	0.53
1:B:255:VAL:HG12	1:B:262:SER:CB	2.36	0.53
1:A:240:ALA:HB2	1:A:322:TRP:HE3	1.72	0.53
1:A:249:PHE:HZ	1:A:306:TYR:HE1	1.54	0.53
1:B:44:ARG:CD	1:B:114:ALA:HA	2.39	0.53
1:B:122:PHE:HE2	1:B:363:LEU:O	1.92	0.53
1:A:415:ASN:HD21	1:A:448:GLY:HA3	1.74	0.52
1:B:250:PHE:CG	1:B:251:ALA:N	2.76	0.52
1:B:429:CYS:SG	1:B:435:LYS:CB	2.96	0.52
1:B:474:TRP:HA	1:B:479:GLN:HE21	1.73	0.52
1:A:286:PHE:HA	3:A:1521:HOH:O	2.09	0.52
1:B:521:ARG:HB2	1:B:528:VAL:HG13	1.91	0.52
1:B:458:ILE:HD12	1:B:460:MET:HG3	1.91	0.52
1:B:246:GLY:O	1:B:249:PHE:HB3	2.11	0.51
1:B:315:MET:HE1	1:B:342:VAL:HG22	1.91	0.51
1:B:531:VAL:HG21	1:B:571:LEU:HD13	1.93	0.51
1:A:193:THR:HB	1:A:194:PRO:HD2	1.93	0.51
1:B:24:ARG:HD2	1:B:407:GLU:OE2	2.11	0.51
1:B:140:ARG:HG3	1:B:469:ARG:O	2.10	0.51
1:B:342:VAL:HG12	1:B:349:ALA:HB3	1.92	0.51
1:B:356:TRP:CE3	1:B:374:TYR:HB3	2.46	0.51
1:B:423:GLU:CD	1:B:423:GLU:H	2.19	0.51
1:B:500:LEU:CD2	1:B:521:ARG:HG3	2.41	0.51
1:B:417:LEU:HG	1:B:443:GLN:NE2	2.26	0.50
1:A:327:ALA:HB1	1:A:368:PHE:HZ	1.75	0.50
1:B:134:TYR:HD1	1:B:187:VAL:HG11	1.76	0.50
1:B:545:VAL:HG13	1:B:567:GLY:O	2.11	0.50
1:A:182:LEU:HD13	1:A:190:LEU:HD11	1.94	0.50
1:A:185:LEU:HD22	1:A:457:GLU:HG2	1.92	0.50
1:B:140:ARG:NH1	1:B:168:TYR:HD2	2.10	0.50
1:B:167:PHE:CZ	1:B:201:HIS:HB2	2.46	0.50
1:A:249:PHE:HZ	1:A:306:TYR:CE1	2.30	0.50
1:A:493:LEU:HD12	1:A:496:ARG:HH11	1.77	0.50
1:A:140:ARG:HG2	1:A:469:ARG:O	2.13	0.49
1:A:382:ARG:HA	1:A:386:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HD11	1:A:539:GLN:NE2	2.27	0.49
1:A:2:LEU:HD23	1:B:2:LEU:HD11	1.95	0.49
1:B:445:THR:HB	1:B:500:LEU:HD22	1.94	0.49
1:B:446:TYR:HE1	1:B:505:VAL:HG21	1.77	0.49
1:A:350:LEU:HG	1:A:352:VAL:HG23	1.95	0.49
1:A:509:HIS:O	1:A:517:TYR:HA	2.12	0.49
1:B:249:PHE:CZ	1:B:306:TYR:HE1	2.31	0.49
1:A:242:PHE:HB3	1:A:307:LEU:HD13	1.93	0.49
1:A:421:ASP:O	1:A:464:THR:HG23	2.11	0.49
1:B:377:ARG:HG3	1:B:378:GLU:N	2.28	0.49
1:A:185:LEU:HD11	1:A:487:TYR:HB3	1.95	0.49
1:A:281:THR:HG22	1:A:285:THR:HG21	1.95	0.49
1:B:156:TRP:CZ2	1:B:471:PRO:HB3	2.48	0.49
1:B:521:ARG:HB2	1:B:528:VAL:CG1	2.42	0.49
1:B:153:THR:HA	1:B:167:PHE:O	2.14	0.48
1:B:432:ASN:OD1	1:B:434:ALA:HB3	2.13	0.48
1:B:8:HIS:CE1	1:B:25:VAL:HG13	2.48	0.48
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.95	0.48
1:A:24:ARG:HH11	1:A:72:LEU:HD13	1.77	0.48
1:A:326:VAL:CG2	2:C:3:GLC:H61	2.41	0.48
1:A:356:TRP:NE1	2:C:3:GLC:C2	2.77	0.48
1:B:300:ASN:OD1	1:B:302:GLU:HG2	2.13	0.48
1:B:127:TRP:HH2	1:B:237:ILE:HD11	1.78	0.48
1:A:356:TRP:HE1	2:C:3:GLC:C1	2.26	0.48
1:A:112:GLN:HE21	1:B:357:HIS:HB3	1.78	0.48
1:A:518:ALA:HA	1:A:530:VAL:O	2.13	0.48
1:B:565:LYS:NZ	1:B:565:LYS:HB3	2.29	0.48
1:A:268:PHE:CE2	1:A:296:LEU:HD23	2.45	0.48
1:B:196:PHE:HB2	1:B:206:THR:HG22	1.96	0.47
1:A:415:ASN:ND2	1:A:448:GLY:HA3	2.30	0.47
1:A:544:GLN:HA	1:A:567:GLY:O	2.14	0.47
1:B:250:PHE:CE2	1:B:251:ALA:HB2	2.49	0.47
1:B:473:ILE:HG21	1:B:478:GLU:O	2.14	0.47
1:A:283:TYR:HE1	1:A:294:PRO:HB3	1.78	0.47
1:B:78:LYS:O	1:B:115:TYR:HA	2.14	0.47
1:A:458:ILE:HD13	1:A:473:ILE:HG12	1.95	0.47
1:A:95:TYR:CE2	1:A:105:ARG:HB2	2.50	0.47
1:B:202:HIS:O	1:B:202:HIS:ND1	2.48	0.47
1:B:458:ILE:HD13	1:B:473:ILE:HB	1.97	0.47
1:B:546:PRO:HG3	1:B:553:TRP:CH2	2.50	0.47
1:B:315:MET:HE2	1:B:322:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:TRP:HA	1:A:479:GLN:HE21	1.79	0.47
1:A:137:PHE:HD1	1:A:140:ARG:HB2	1.79	0.47
1:A:342:VAL:HG11	1:A:351:ILE:HD11	1.97	0.47
1:A:137:PHE:HB3	1:A:454:TYR:CE2	2.50	0.47
1:A:436:PHE:HZ	1:A:456:ASP:HB3	1.79	0.47
1:A:201:HIS:CE1	1:A:469:ARG:HH11	2.33	0.46
1:B:161:ARG:HA	1:B:161:ARG:HD3	1.76	0.46
1:B:540:THR:OG1	1:B:572:THR:HG23	2.15	0.46
1:A:185:LEU:HA	1:A:488:LYS:HG2	1.96	0.46
1:A:401:ALA:O	1:A:404:LEU:HB2	2.15	0.46
1:A:328:ASN:N	1:A:328:ASN:HD22	2.13	0.46
1:A:328:ASN:HD22	1:A:328:ASN:H	1.63	0.46
1:A:355:ILE:HD11	1:A:368:PHE:CE1	2.44	0.46
1:B:544:GLN:HE22	1:B:568:GLN:NE2	2.12	0.46
1:A:563:HIS:HD2	1:A:570:LYS:O	1.99	0.46
1:B:448:GLY:O	1:B:494:ARG:NH2	2.49	0.46
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.97	0.46
1:B:465:ASP:HA	1:B:466:PRO:HA	1.70	0.46
1:B:546:PRO:HG3	1:B:553:TRP:HH2	1.81	0.46
1:A:137:PHE:HA	1:A:193:THR:OG1	2.15	0.46
1:B:224:ARG:HA	1:B:224:ARG:NE	2.31	0.46
1:B:452:ILE:HD11	1:B:491:ILE:HD11	1.96	0.46
1:A:275:VAL:HG22	3:A:1330:HOH:O	2.14	0.46
1:B:376:PHE:O	1:B:380:VAL:HG22	2.16	0.46
1:B:531:VAL:O	1:B:578:GLY:HA2	2.15	0.45
1:A:41:TYR:CB	1:A:82:TYR:HB3	2.46	0.45
1:A:516:LEU:HD11	1:A:539:GLN:HE21	1.80	0.45
1:A:582:TRP:CZ2	1:A:584:GLY:HA2	2.51	0.45
1:B:124:THR:OG1	1:B:129:LYS:HE3	2.17	0.45
1:B:134:TYR:HB2	1:B:187:VAL:HG21	1.99	0.45
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.79	0.45
1:B:378:GLU:HG3	3:B:1471:HOH:O	2.17	0.45
1:A:112:GLN:NE2	1:B:357:HIS:HB3	2.31	0.45
1:B:3:LEU:HD13	1:B:101:PHE:CG	2.51	0.45
1:B:6:ILE:HD13	1:B:86:LEU:HD13	1.99	0.45
1:B:73:LEU:HD23	1:B:80:VAL:HG21	1.99	0.45
1:B:193:THR:HB	1:B:194:PRO:HD2	1.99	0.45
1:A:269:PHE:CD2	1:A:295:LYS:HG3	2.51	0.45
1:B:287:ALA:H	1:B:290:VAL:HG22	1.82	0.45
1:B:446:TYR:CE1	1:B:505:VAL:HG21	2.52	0.45
1:B:212:ILE:HG22	1:B:213:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:SER:HB2	1:B:585:ARG:NH2	2.23	0.45
1:A:244:HIS:CD2	1:A:293:MET:HB3	2.51	0.45
1:A:308:PHE:HB3	1:A:341:LEU:HD22	1.99	0.45
1:A:393:ARG:O	1:A:397:GLU:HG3	2.16	0.45
1:A:231:ARG:HH11	1:A:231:ARG:HD3	1.66	0.44
1:A:401:ALA:HA	1:A:404:LEU:HD13	1.99	0.44
1:B:197:ALA:HB3	1:B:208:ASP:HB3	1.99	0.44
1:A:205:ASP:C	1:A:246:GLY:HA3	2.41	0.44
1:A:500:LEU:HD21	1:A:528:VAL:HG21	2.00	0.44
1:B:470:ARG:HE	1:B:471:PRO:HG2	1.82	0.44
1:A:327:ALA:HB1	1:A:368:PHE:CZ	2.52	0.44
1:B:223:ARG:HH21	1:B:227:ASP:CG	2.25	0.44
1:A:75:CYS:SG	1:A:80:VAL:HB	2.57	0.44
1:A:223:ARG:HB3	1:A:223:ARG:NH1	2.32	0.44
1:A:504:ASN:O	1:A:521:ARG:HA	2.17	0.44
1:B:122:PHE:HB2	3:B:1120:HOH:O	2.17	0.44
1:B:429:CYS:SG	1:B:436:PHE:N	2.91	0.44
1:A:41:TYR:HB3	1:A:82:TYR:HB3	2.00	0.44
1:A:160:ALA:O	1:A:470:ARG:HD2	2.17	0.44
1:A:540:THR:HA	1:A:572:THR:HA	2.00	0.44
1:A:477:LYS:N	1:A:477:LYS:HD2	2.33	0.43
1:A:204:TYR:CZ	2:C:4:GLC:H2	2.54	0.43
1:A:356:TRP:HE1	2:C:3:GLC:H2	1.82	0.43
1:A:446:TYR:CG	1:A:447:LEU:N	2.86	0.43
1:B:315:MET:HE2	1:B:322:TRP:HZ2	1.83	0.43
1:A:242:PHE:HE2	1:A:338:PHE:HE1	1.64	0.43
1:A:424:ARG:HD3	1:A:460:MET:O	2.19	0.43
1:B:139:GLU:C	1:B:170:GLY:HA3	2.43	0.43
1:B:540:THR:HA	1:B:572:THR:HA	1.99	0.43
1:B:531:VAL:HG21	1:B:571:LEU:CD1	2.49	0.43
1:B:574:ARG:HG2	1:B:575:PRO:HD2	2.00	0.43
1:A:356:TRP:CE2	2:C:3:GLC:O2	2.66	0.43
1:B:553:TRP:CD1	1:B:553:TRP:N	2.85	0.43
1:A:15:ALA:HA	1:A:24:ARG:O	2.18	0.43
1:B:240:ALA:HB2	1:B:322:TRP:HE3	1.83	0.43
1:A:94:VAL:HG12	1:A:95:TYR:N	2.33	0.43
1:A:57:ALA:CA	1:A:71:ALA:HB2	2.49	0.43
1:A:325:ASP:CG	1:A:326:VAL:HG23	2.44	0.43
1:A:531:VAL:O	1:A:578:GLY:HA2	2.18	0.43
1:B:16:TYR:CE2	1:B:406:PRO:HA	2.53	0.42
1:B:276:SER:O	1:B:283:TYR:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:HIS:O	1:B:202:HIS:CG	2.73	0.42
1:B:363:LEU:HD22	1:B:409:ALA:HB1	2.01	0.42
1:B:350:LEU:HG	1:B:352:VAL:HG23	2.01	0.42
1:A:45:TYR:HD1	1:A:79:ARG:NH2	2.17	0.42
1:A:95:TYR:CD2	1:A:105:ARG:HA	2.55	0.42
1:B:44:ARG:HD2	1:B:114:ALA:HA	2.02	0.42
1:A:192:PHE:HE2	1:A:236:ILE:HG13	1.85	0.42
1:A:372:MET:HE1	1:A:451:LEU:CD2	2.50	0.42
1:A:463:ALA:H	1:A:467:ASP:HB3	1.84	0.42
1:B:36:ARG:HB3	1:B:87:THR:HB	2.02	0.42
1:A:460:MET:HE2	1:A:460:MET:HB3	1.86	0.42
1:B:438:LEU:HD12	1:B:438:LEU:HA	1.84	0.42
1:A:497:LEU:HD13	1:A:528:VAL:HG11	2.01	0.41
1:B:249:PHE:HE1	1:B:306:TYR:HE1	1.65	0.41
1:A:546:PRO:HG2	1:A:553:TRP:CZ2	2.55	0.41
1:B:27:LEU:HD12	1:B:84:PHE:CE2	2.55	0.41
1:B:150:PRO:O	1:B:151:PRO:C	2.64	0.41
1:B:219:LEU:HD21	1:B:313:PHE:HZ	1.85	0.41
1:B:84:PHE:HB2	1:B:96:PHE:HB3	2.01	0.41
1:B:573:LEU:HD23	1:B:573:LEU:H	1.84	0.41
1:A:542:LEU:C	1:A:543:LEU:HD12	2.45	0.41
1:B:148:ASN:O	1:B:215:GLN:HA	2.20	0.41
1:B:573:LEU:HD23	1:B:573:LEU:N	2.35	0.41
1:B:27:LEU:HD11	1:B:86:LEU:HD21	2.02	0.41
1:B:213:ASP:OD1	1:B:215:GLN:HG2	2.19	0.41
1:B:254:ASP:O	1:B:258:LYS:HB2	2.20	0.41
1:B:262:SER:O	1:B:265:LYS:HG3	2.21	0.41
1:A:85:LEU:HD11	1:A:93:ALA:HB1	2.03	0.41
1:A:273:PHE:HD1	1:A:273:PHE:HA	1.62	0.41
1:B:249:PHE:O	1:B:253:ARG:HG3	2.20	0.41
1:B:218:ASP:CG	1:B:220:PRO:HD2	2.46	0.41
1:B:250:PHE:CD2	1:B:251:ALA:N	2.89	0.41
1:B:351:ILE:HD13	1:B:351:ILE:HG21	1.87	0.41
1:A:219:LEU:HD13	1:A:219:LEU:HA	1.87	0.41
1:B:563:HIS:ND1	1:B:570:LYS:O	2.54	0.41
1:A:23:LEU:HD23	1:A:73:LEU:HD12	2.02	0.40
1:B:17:PRO:HB3	1:B:116:ILE:CG2	2.51	0.40
1:A:346:ASN:HB3	1:A:349:ALA:HB2	2.02	0.40
1:B:204:TYR:CD2	2:D:4:GLC:H4	2.56	0.40
1:B:267:TRP:HE1	1:B:302:GLU:CG	2.33	0.40
1:A:40:LEU:HD12	1:A:83:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD12	1:A:369:ASP:OD2	2.22	0.40
1:A:383:PHE:HE1	1:A:515:ASN:OD1	2.03	0.40
1:B:64:GLU:HG3	1:B:65:ARG:HG3	2.03	0.40
1:B:356:TRP:CD1	2:D:3:GLC:C1	3.04	0.40
1:B:574:ARG:HG2	1:B:574:ARG:HH11	1.86	0.40
1:A:4:GLU:HG2	1:B:65:ARG:HB3	2.03	0.40
1:A:285:THR:OG1	1:A:286:PHE:N	2.54	0.40
1:B:574:ARG:CG	1:B:575:PRO:HD2	2.52	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	583/585 (100%)	533 (91%)	47 (8%)	3 (0%)	24	60
1	B	583/585 (100%)	533 (91%)	41 (7%)	9 (2%)	8	35
All	All	1166/1170 (100%)	1066 (91%)	88 (8%)	12 (1%)	12	45

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	PRO
1	B	170	GLY
1	B	193	THR
1	B	262	SER
1	B	562	VAL
1	A	169	GLY
1	A	298	THR
1	B	275	VAL
1	B	288	VAL
1	B	564	GLY

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Mol	Chain	Res	Type
1	B	152	GLY
1	A	564	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/492 (100%)	429 (87%)	63 (13%)	4	19
1	B	492/492 (100%)	439 (89%)	53 (11%)	6	26
All	All	984/984 (100%)	868 (88%)	116 (12%)	5	22

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	19	SER
1	A	31	LYS
1	A	35	VAL
1	A	51	GLU
1	A	52	LEU
1	A	92	GLU
1	A	105	ARG
1	A	110	VAL
1	A	139	GLU
1	A	145	ASP
1	A	163	ARG
1	A	190	LEU
1	A	191	TYR
1	A	193	THR
1	A	201	HIS
1	A	205	ASP
1	A	219	LEU
1	A	223	ARG
1	A	231	ARG
1	A	236	ILE

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	255	VAL
1	A	256	LEU
1	A	261	GLN
1	A	271	GLU
1	A	273	PHE
1	A	277	LYS
1	A	278	THR
1	A	285	THR
1	A	295	LYS
1	A	326	VAL
1	A	328	ASN
1	A	330	VAL
1	A	342	VAL
1	A	375	LEU
1	A	386	THR
1	A	406	PRO
1	A	416	LEU
1	A	423	GLU
1	A	426	LEU
1	A	457	GLU
1	A	466	PRO
1	A	467	ASP
1	A	472	MET
1	A	473	ILE
1	A	476	GLU
1	A	477	LYS
1	A	478	GLU
1	A	483	LEU
1	A	504	ASN
1	A	528	VAL
1	A	538	LYS
1	A	540	THR
1	A	541	VAL
1	A	543	LEU
1	A	544	GLN
1	A	554	LEU
1	A	561	GLU
1	A	562	VAL
1	A	571	LEU
1	A	572	THR
1	A	573	LEU

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Mol	Chain	Res	Type
1	B	24	ARG
1	B	30	LYS
1	B	43	ASP
1	B	51	GLU
1	B	73	LEU
1	B	135	GLN
1	B	139	GLU
1	B	145	ASP
1	B	158	LYS
1	B	159	ASP
1	B	163	ARG
1	B	190	LEU
1	B	191	TYR
1	B	198	SER
1	B	206	THR
1	B	214	PRO
1	B	223	ARG
1	B	231	ARG
1	B	238	LEU
1	B	248	GLN
1	B	255	VAL
1	B	265	LYS
1	B	269	PHE
1	B	279	SER
1	B	280	ARG
1	B	284	GLU
1	B	328	ASN
1	B	355	ILE
1	B	375	LEU
1	B	377	ARG
1	B	381	ILE
1	B	398	LEU
1	B	416	LEU
1	B	418	ASP
1	B	421	ASP
1	B	464	THR
1	B	466	PRO
1	B	470	ARG
1	B	472	MET
1	B	483	LEU
1	B	496	ARG
1	B	504	ASN

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Mol	Chain	Res	Type
1	B	505	VAL
1	B	511	ASP
1	B	523	VAL
1	B	532	LEU
1	B	535	ARG
1	B	544	GLN
1	B	547	GLU
1	B	551	LYS
1	B	565	LYS
1	B	569	LEU
1	B	573	LEU

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

Mol	Chain	Res	Type
1	A	148	ASN
1	A	164	HIS
1	A	201	HIS
1	A	244	HIS
1	A	248	GLN
1	A	328	ASN
1	A	373	ASN
1	A	415	ASN
1	A	443	GLN
1	A	509	HIS
1	A	539	GLN
1	A	563	HIS
1	B	22	GLN
1	B	143	ASN
1	B	148	ASN
1	B	164	HIS
1	B	243	ASN
1	B	257	GLN
1	B	261	GLN
1	B	328	ASN
1	B	367	GLN
1	B	411	GLN
1	B	443	GLN
1	B	504	ASN
1	B	544	GLN
1	B	566	GLN
1	B	568	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 ⓘ

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	$\# Z > 2$
2	GLC	C	1	2	11,11,12	0.80	0	15,15,17	0.86	1 (6%)
2	GLC	C	2	2	11,11,12	0.89	1 (9%)	15,15,17	1.96	2 (13%)
2	GLC	C	3	2	11,11,12	0.76	0	15,15,17	2.04	2 (13%)
2	GLC	C	4	2	11,11,12	0.60	0	15,15,17	0.63	0
2	GLC	C	5	2	11,11,12	0.68	0	15,15,17	0.88	1 (6%)
2	GLC	C	6	2	11,11,12	0.89	0	15,15,17	0.81	1 (6%)
2	GLC	C	7	2	11,11,12	0.84	0	15,15,17	1.21	3 (20%)
2	GLC	D	1	2	11,11,12	0.75	0	15,15,17	1.23	2 (13%)
2	GLC	D	2	2	11,11,12	0.69	0	15,15,17	1.03	1 (6%)
2	GLC	D	3	2	11,11,12	0.77	0	15,15,17	1.46	2 (13%)
2	GLC	D	4	2	11,11,12	0.53	0	15,15,17	1.59	2 (13%)
2	GLC	D	5	2	11,11,12	0.61	0	15,15,17	2.17	3 (20%)
2	GLC	D	6	2	11,11,12	0.80	0	15,15,17	0.94	1 (6%)
2	GLC	D	7	2	11,11,12	0.73	0	15,15,17	1.64	3 (20%)

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	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	2/2/19/22	0/1/1/1
2	GLC	C	7	2	-	1/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	5	2	-	2/2/19/22	0/1/1/1
2	GLC	D	6	2	-	1/2/19/22	0/1/1/1
2	GLC	D	7	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O4-C4	2.02	1.48	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	GLC	O4-C4-C3	-7.22	93.35	110.38
2	C	3	GLC	O4-C4-C5	-6.85	92.44	109.32
2	C	2	GLC	O4-C4-C3	-5.85	96.58	110.38
2	D	7	GLC	O4-C4-C3	-4.76	99.16	110.38
2	D	4	GLC	O4-C4-C3	-4.53	99.71	110.38
2	D	3	GLC	O4-C4-C3	-4.14	100.61	110.38
2	C	2	GLC	O4-C4-C5	4.02	119.24	109.32
2	D	4	GLC	O4-C4-C5	-3.43	100.88	109.32
2	D	5	GLC	O4-C4-C5	-3.34	101.10	109.32
2	D	1	GLC	O4-C4-C5	3.07	116.87	109.32
2	C	7	GLC	O4-C4-C5	-2.69	102.71	109.32
2	D	7	GLC	C1-O5-C5	2.68	115.77	112.19
2	C	7	GLC	C1-O5-C5	2.66	115.76	112.19
2	D	2	GLC	O4-C4-C3	-2.66	104.11	110.38
2	C	5	GLC	C1-O5-C5	2.61	115.68	112.19
2	C	6	GLC	C1-O5-C5	2.58	115.64	112.19
2	D	7	GLC	O4-C4-C5	-2.58	102.98	109.32
2	D	6	GLC	C1-O5-C5	2.55	115.61	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	GLC	C1-O5-C5	2.53	115.58	112.19
2	C	1	GLC	C1-O5-C5	2.34	115.32	112.19
2	D	1	GLC	C1-O5-C5	2.29	115.26	112.19
2	C	7	GLC	O4-C4-C3	-2.13	105.34	110.38
2	C	3	GLC	C1-O5-C5	2.08	114.97	112.19
2	D	3	GLC	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	GLC	C4-C5-C6-O6
2	C	6	GLC	O5-C5-C6-O6
2	D	7	GLC	C4-C5-C6-O6
2	D	7	GLC	O5-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	7	GLC	C4-C5-C6-O6
2	D	5	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	D	6	GLC	C4-C5-C6-O6
2	D	5	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6

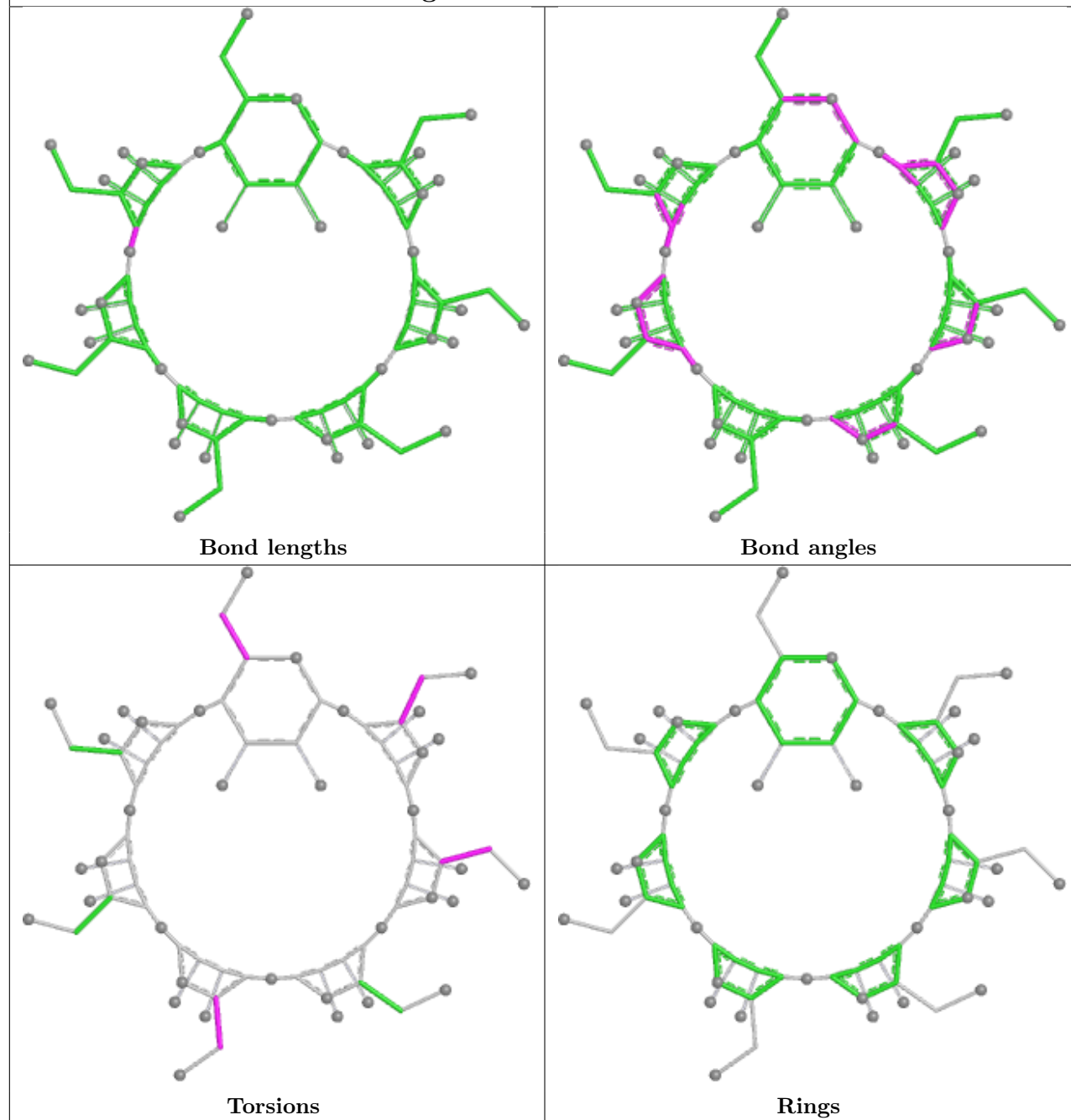
There are no ring outliers.

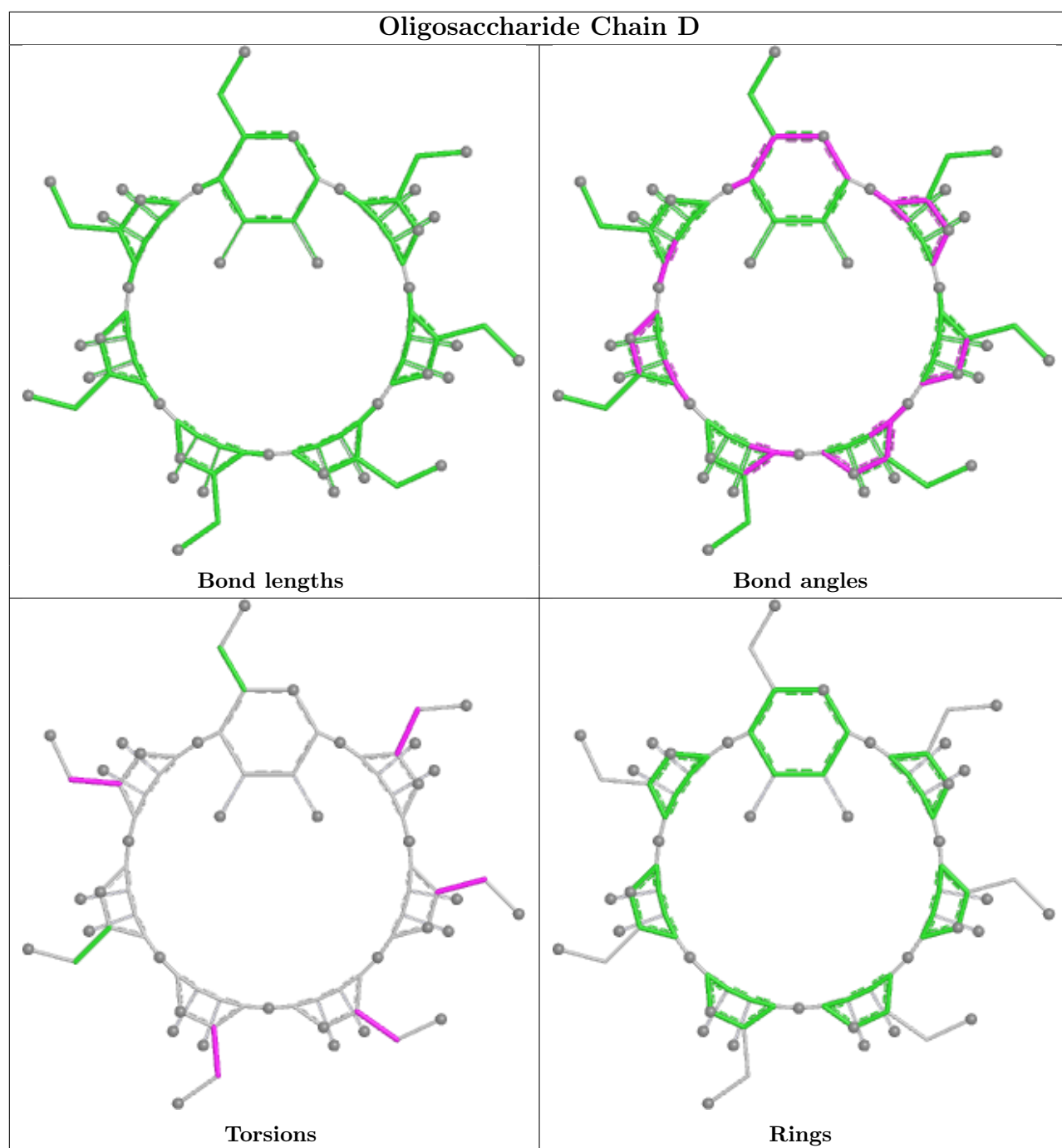
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	GLC	4	0
2	C	4	GLC	3	0
2	D	4	GLC	2	0
2	C	3	GLC	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.

Oligosaccharide Chain C





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/585 (100%)	-0.78	0 100 100	7, 22, 39, 50	0
1	B	585/585 (100%)	-0.72	1 (0%) 91 83	6, 23, 39, 50	0
All	All	1170/1170 (100%)	-0.75	1 (0%) 92 86	6, 22, 39, 50	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	2	11/12	0.68	0.10	43,47,49,49	0
2	GLC	D	6	11/12	0.69	0.11	49,50,51,53	0
2	GLC	D	5	11/12	0.70	0.10	47,50,53,56	0
2	GLC	D	1	11/12	0.71	0.10	47,48,50,51	0
2	GLC	D	7	11/12	0.73	0.10	46,50,52,52	0
2	GLC	C	6	11/12	0.75	0.09	44,49,52,53	0
2	GLC	D	4	11/12	0.76	0.11	43,46,48,49	0
2	GLC	C	7	11/12	0.77	0.10	40,49,50,51	0

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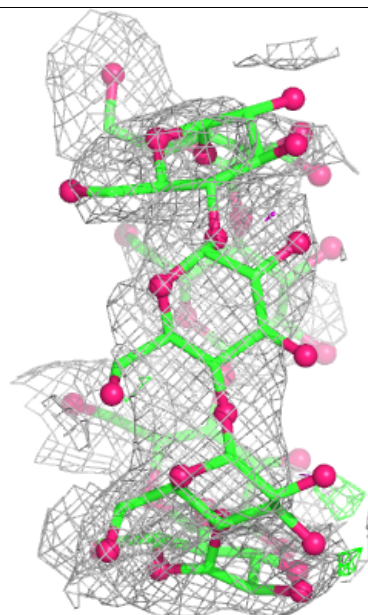
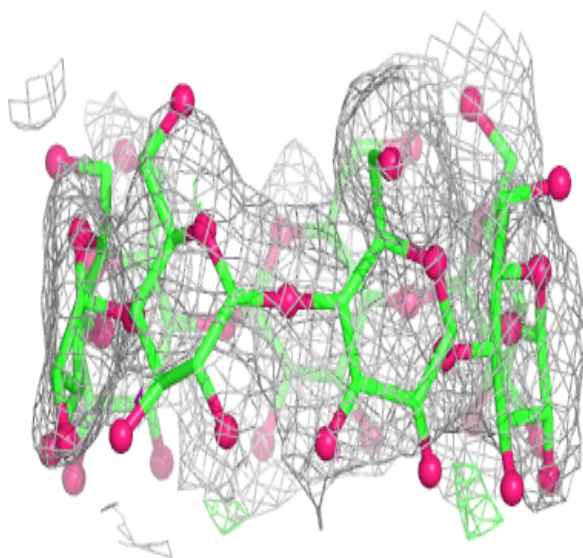
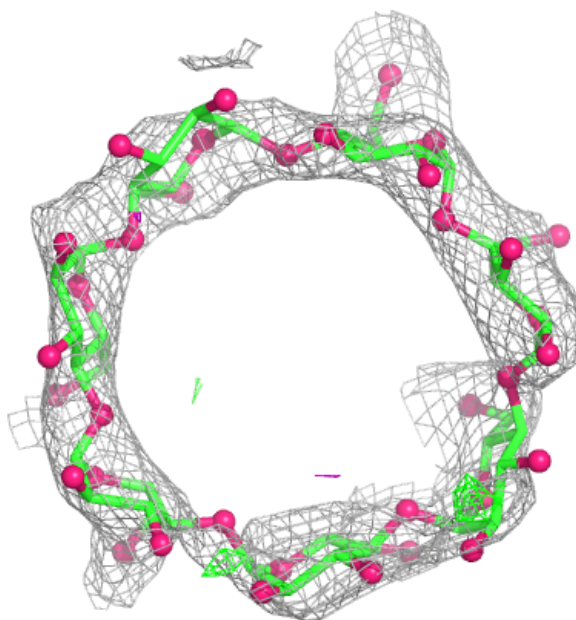
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	2	11/12	0.78	0.09	36,49,51,53	0
2	GLC	D	3	11/12	0.81	0.09	45,50,51,51	0
2	GLC	C	5	11/12	0.82	0.10	36,38,42,47	0
2	GLC	C	3	11/12	0.83	0.11	45,49,53,55	0
2	GLC	C	4	11/12	0.87	0.11	33,38,44,46	0
2	GLC	C	1	11/12	0.88	0.08	46,48,50,53	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

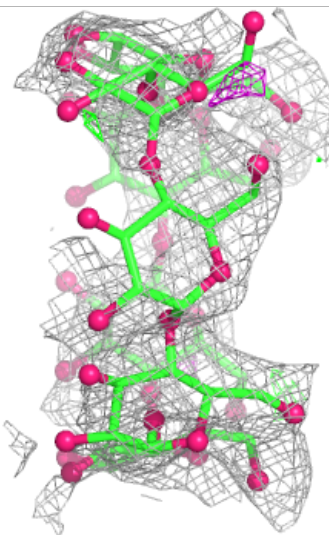
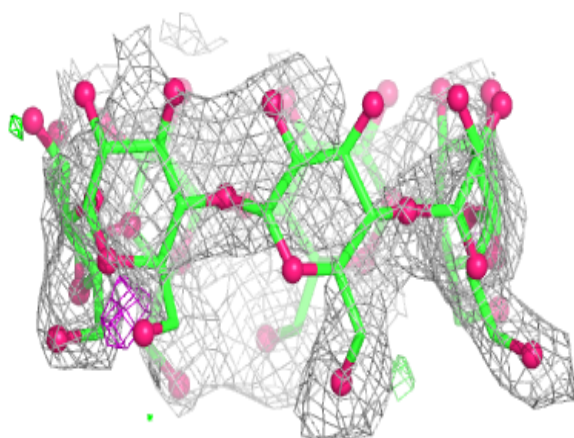
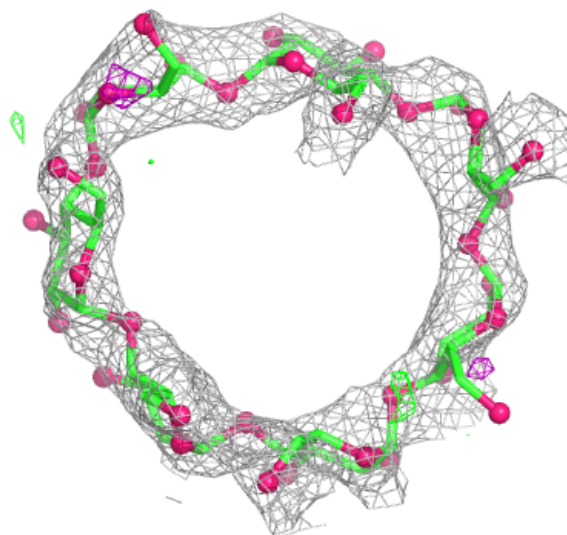
Electron density around Chain C:

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



Electron density around Chain D:

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

**6.4 Ligands** [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.