



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:01 PM UTC

PDB ID : 1DED / pdb_00001ded
Title : CRYSTAL STRUCTURE OF ALKALOPHILIC ASPARAGINE 233-REPLACED CYCLODEXTRIN GLUCANOTRANSFERASE COMPLEXED WITH AN INHIBITOR, ACARBOSE, AT 2.0 Å RESOLUTION
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Deposited on : 1999-11-14
Resolution : 2.00 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

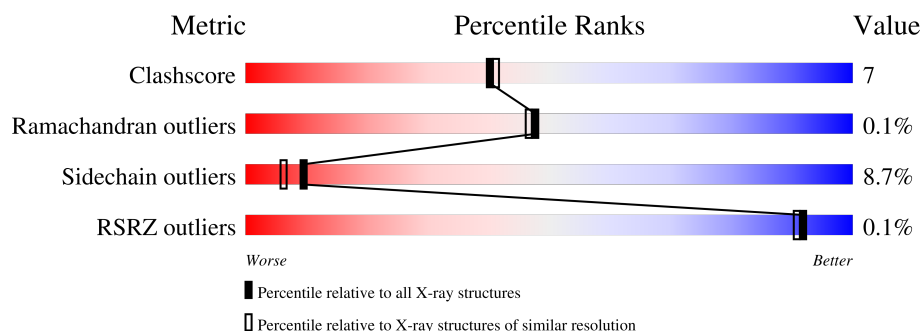
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

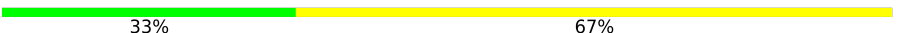
The reported resolution of this entry is 2.00 Å.

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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	686	
1	B	686	
2	C	3	
2	D	3	
2	E	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15555 atoms, of which 4040 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 CYCLODEXTRIN GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	686	Total	C	H	N	O	S	1195	0	0
			6505	3352	1195	905	1037	16			
1	B	686	Total	C	H	N	O	S	1195	0	0
			6505	3352	1195	905	1037	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	ASN	HIS	engineered mutation	UNP P05618
A	452	PRO	ARG	conflict	UNP P05618
A	454	GLY	ALA	conflict	UNP P05618
B	233	ASN	HIS	engineered mutation	UNP P05618
B	452	PRO	ARG	conflict	UNP P05618
B	454	GLY	ALA	conflict	UNP P05618

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O	44	1	0
			88	25	44	1	18			
2	D	3	Total	C	H	N	O	44	1	0
			88	25	44	1	18			
2	E	3	Total	C	H	N	O	44	1	0
			88	25	44	1	18			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		

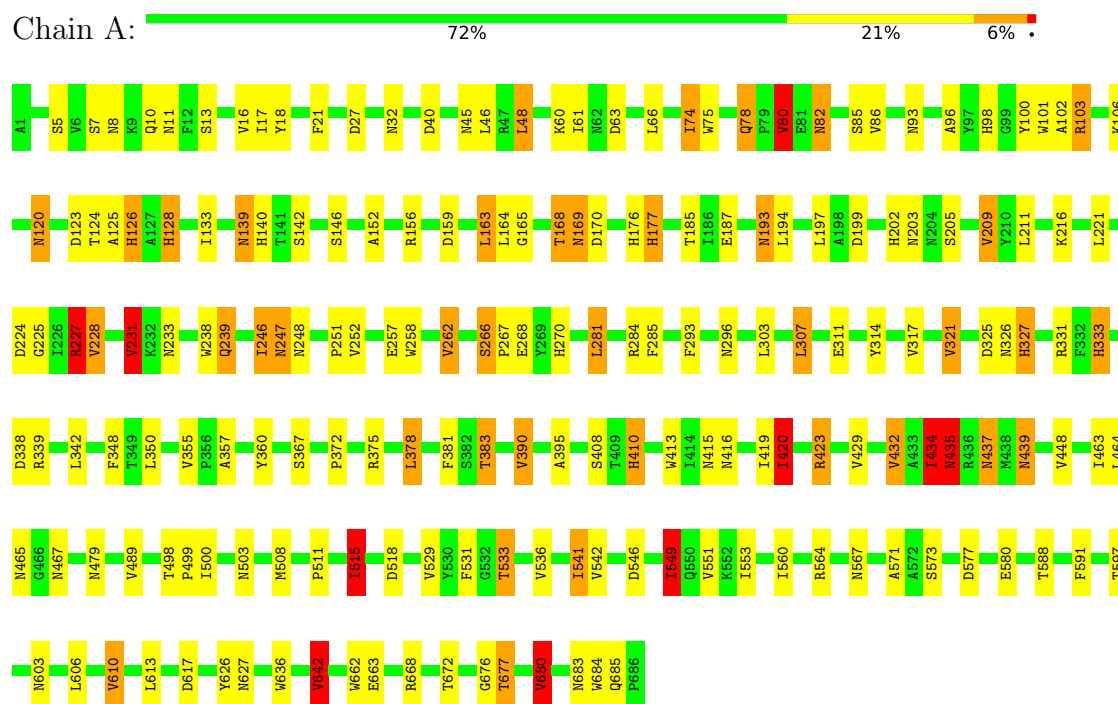
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	405	Total	H	O	810	0
			1215	810	405		
4	B	354	Total	H	O	708	0
			1062	708	354		

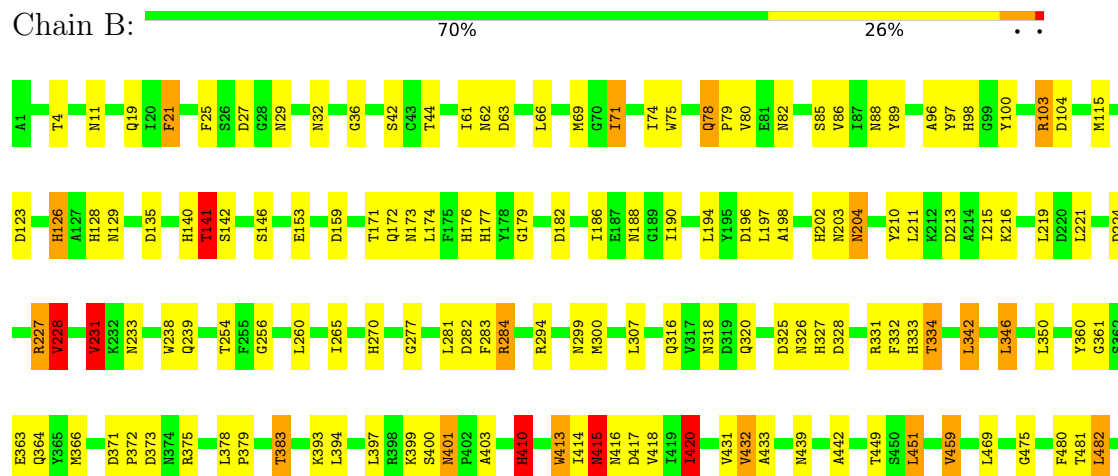
3 Residue-property plots

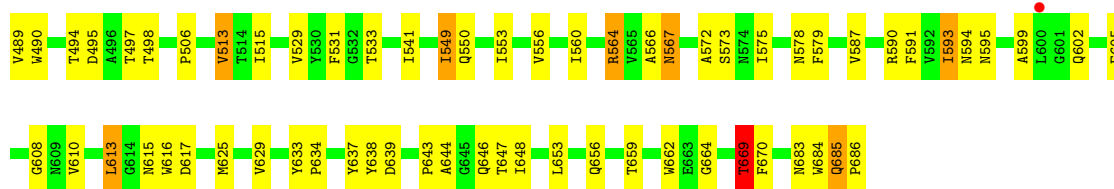
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: CYCLODEXTRIN GLUCANOTRANSFERASE





- Molecule 2: 4,6-dideoxy-4-{\{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain C: 33% 67%



- Molecule 2: 4,6-dideoxy-4-{\{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D: 33% 67%



- Molecule 2: 4,6-dideoxy-4-{\{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.93Å 73.83Å 79.05Å 85.10° 105.40° 100.50°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	62.3 (10.00-2.00) 92.1 (10.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 1.85Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.163 , 0.222 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15555	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AC1, CA, GLC, BGC

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	1.00	21/5443 (0.4%)	1.79	115/7425 (1.5%)
1	B	0.97	18/5443 (0.3%)	1.79	119/7425 (1.6%)
All	All	0.98	39/10886 (0.4%)	1.79	234/14850 (1.6%)

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	B	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	ILE	CA-CB	10.51	1.67	1.54
1	B	228	VAL	CA-CB	9.44	1.65	1.54
1	A	228	VAL	CA-CB	8.45	1.64	1.54
1	B	126	HIS	CD2-NE2	-7.72	1.29	1.37
1	B	128	HIS	CD2-NE2	-7.42	1.29	1.37
1	B	420	ILE	CA-CB	7.39	1.64	1.54
1	A	333	HIS	CD2-NE2	-7.38	1.29	1.37
1	B	513	VAL	CA-CB	7.25	1.64	1.54
1	A	140	HIS	CD2-NE2	-7.22	1.29	1.37
1	A	202	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	128	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	98	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	176	HIS	CD2-NE2	-6.89	1.30	1.37
1	B	140	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.65	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	327	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	270	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	177	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	333	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	390	VAL	CA-CB	5.96	1.62	1.54
1	A	410	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	549	ILE	CA-CB	5.72	1.62	1.54
1	B	410	HIS	CD2-NE2	-5.69	1.31	1.37
1	B	202	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	176	HIS	CG-ND1	-5.46	1.32	1.38
1	B	549	ILE	CA-CB	5.36	1.64	1.54
1	A	419	ILE	CA-CB	5.29	1.61	1.54
1	A	270	HIS	CD2-NE2	-5.27	1.32	1.37
1	B	459	VAL	CA-CB	5.24	1.61	1.54
1	A	333	HIS	CG-ND1	-5.13	1.32	1.38
1	A	74	ILE	CA-CB	5.12	1.60	1.54
1	A	177	HIS	CG-ND1	-5.10	1.32	1.38
1	B	126	HIS	CG-ND1	-5.10	1.32	1.38
1	B	128	HIS	CG-ND1	-5.06	1.32	1.38
1	A	680	VAL	CA-CB	5.01	1.60	1.54

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	OD1-CG-ND2	-14.01	108.59	122.60
1	B	325	ASP	CA-CB-CG	11.65	124.25	112.60
1	B	415	ASN	OD1-CG-ND2	-10.34	112.26	122.60
1	A	415	ASN	CA-CB-CG	10.04	122.64	112.60
1	B	416	ASN	CA-CB-CG	9.89	122.49	112.60
1	A	577	ASP	CA-CB-CG	9.66	122.26	112.60
1	A	247	ASN	OD1-CG-ND2	-9.40	113.20	122.60
1	A	32	ASN	CA-CB-CG	9.02	121.62	112.60
1	B	326	ASN	CA-CB-CG	8.89	121.49	112.60
1	A	434	ILE	CB-CG1-CD1	-8.83	95.25	113.80
1	A	233	ASN	CB-CG-ND2	8.74	129.50	116.40
1	A	80	VAL	N-CA-CB	-8.72	98.31	110.26
1	B	233	ASN	OD1-CG-ND2	-8.69	113.91	122.60
1	B	196	ASP	CA-CB-CG	8.60	121.20	112.60
1	B	629	VAL	N-CA-C	8.43	118.34	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	B	331	ARG	NE-CZ-NH2	-8.30	111.73	119.20
1	B	415	ASN	CA-CB-CG	8.29	120.89	112.60
1	A	603	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	A	228	VAL	CA-C-O	8.23	129.37	120.57
1	B	88	ASN	N-CA-C	8.16	123.59	112.90
1	A	63	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	383	THR	N-CA-CB	-8.16	98.08	110.73
1	A	61	ILE	N-CA-C	-8.14	103.33	110.74
1	B	415	ASN	CB-CG-ND2	8.06	128.49	116.40
1	A	98	HIS	CB-CG-CD2	-8.05	120.73	131.20
1	A	676	GLY	O-C-N	7.88	129.68	122.90
1	B	480	PHE	CA-CB-CG	7.86	121.66	113.80
1	A	327	HIS	CB-CG-CD2	-7.81	121.04	131.20
1	A	642	VAL	N-CA-CB	-7.77	100.33	111.21
1	B	141	THR	N-CA-CB	-7.71	97.46	110.49
1	A	435	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	B	179	GLY	O-C-N	-7.59	116.37	122.90
1	A	325	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	541	ILE	N-CA-C	-7.54	95.97	107.73
1	B	172	GLN	N-CA-C	-7.47	96.39	108.41
1	A	610	VAL	N-CA-CB	-7.46	99.91	112.44
1	B	63	ASP	CA-CB-CG	7.41	120.00	112.60
1	A	333	HIS	CA-CB-CG	-7.40	106.40	113.80
1	B	126	HIS	CB-CG-CD2	-7.39	121.60	131.20
1	A	333	HIS	CB-CG-CD2	-7.38	121.60	131.20
1	B	11	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	A	139	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	B	216	LYS	CB-CG-CD	-7.32	94.46	111.30
1	B	495	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	98	HIS	CB-CG-CD2	-7.14	121.91	131.20
1	B	327	HIS	CB-CG-CD2	-7.12	121.94	131.20
1	B	320	GLN	OE1-CD-NE2	-7.11	115.49	122.60
1	A	164	LEU	N-CA-C	-7.10	103.48	112.93
1	A	610	VAL	CB-CA-C	7.09	121.33	110.55
1	A	126	HIS	CB-CG-CD2	-7.07	122.00	131.20
1	A	503	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	541	ILE	N-CA-C	-6.94	96.91	107.73
1	B	79	PRO	CA-C-N	6.92	129.97	120.35
1	B	79	PRO	C-N-CA	6.92	129.97	120.35
1	B	203	ASN	OD1-CG-ND2	-6.89	115.70	122.60
1	B	498	THR	CB-CA-C	6.87	118.23	108.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ASN	CA-CB-CG	6.85	119.45	112.60
1	B	61	ILE	N-CA-C	-6.84	104.19	110.82
1	B	204	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	98	HIS	CB-CG-ND1	6.81	132.91	122.70
1	B	219	LEU	N-CA-C	-6.81	103.94	111.36
1	A	202	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	A	479	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	227	ARG	CB-CG-CD	6.75	126.84	111.30
1	A	296	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	B	227	ARG	CA-C-N	-6.68	114.51	122.93
1	B	227	ARG	C-N-CA	-6.68	114.51	122.93
1	B	123	ASP	CA-C-O	-6.60	113.90	120.70
1	A	74	ILE	CA-CB-CG2	6.60	121.72	110.50
1	A	326	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	B	328	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	98	HIS	CB-CG-ND1	6.58	132.57	122.70
1	B	401	ASN	CB-CG-ND2	6.58	126.27	116.40
1	B	595	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	B	299	ASN	CA-CB-CG	6.58	119.18	112.60
1	A	156	ARG	N-CA-C	6.55	119.47	110.24
1	A	642	VAL	CA-C-N	6.54	126.49	119.76
1	A	642	VAL	C-N-CA	6.54	126.49	119.76
1	B	265	ILE	CA-C-O	6.52	126.70	120.25
1	A	103	ARG	N-CA-C	-6.49	106.57	114.75
1	B	182	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	123	ASP	CA-C-O	-6.47	113.69	120.55
1	A	327	HIS	N-CA-C	6.47	120.89	113.19
1	B	100	TYR	N-CA-C	6.46	121.01	113.20
1	B	202	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	B	413	TRP	CG-CD2-CE3	6.44	140.34	133.90
1	B	228	VAL	CA-C-O	6.42	127.44	120.57
1	A	102	ALA	N-CA-C	6.41	118.99	110.53
1	B	371	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	467	ASN	OD1-CG-ND2	-6.34	116.25	122.60
1	B	62	ASN	N-CA-C	6.31	118.24	111.36
1	A	503	ASN	CB-CG-ND2	6.28	125.83	116.40
1	B	416	ASN	CB-CG-ND2	6.26	125.80	116.40
1	A	338	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	27	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	141	THR	CB-CA-C	6.21	122.77	110.42
1	B	21	PHE	N-CA-C	-6.20	98.43	108.41
1	A	518	ASP	CA-CB-CG	6.20	118.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	B	129	ASN	N-CA-C	6.17	120.05	111.90
1	A	437	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	A	239	GLN	CA-CB-CG	-6.12	101.86	114.10
1	A	266	SER	CA-C-N	6.11	125.51	118.85
1	A	266	SER	C-N-CA	6.11	125.51	118.85
1	B	656	GLN	CA-CB-CG	6.11	126.32	114.10
1	A	231	VAL	N-CA-CB	-6.01	100.36	110.65
1	B	277	GLY	N-CA-C	-6.00	107.12	114.92
1	A	314	TYR	N-CA-C	-5.98	99.53	109.46
1	B	231	VAL	N-CA-CB	-5.97	98.51	111.05
1	A	177	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	B	578	ASN	CA-CB-CG	5.95	118.55	112.60
1	B	176	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	B	140	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	627	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	B	238	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	B	334	THR	N-CA-CB	-5.87	100.84	110.41
1	B	531	PHE	N-CA-C	-5.86	95.46	107.70
1	B	11	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	100	TYR	N-CA-C	5.84	120.25	113.18
1	B	413	TRP	CB-CG-CD1	-5.83	118.16	126.90
1	B	29	ASN	CA-C-N	5.83	125.69	119.28
1	B	29	ASN	C-N-CA	5.83	125.69	119.28
1	B	172	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	B	416	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	86	VAL	N-CA-C	-5.77	100.28	108.58
1	A	546	ASP	N-CA-C	5.74	118.31	111.71
1	A	326	ASN	CA-CB-CG	5.74	118.33	112.60
1	A	668	ARG	N-CA-C	-5.74	102.81	110.55
1	A	82	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	159	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	318	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	285	PHE	N-CA-C	-5.70	104.70	111.03
1	A	617	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	204	ASN	CB-CG-ND2	5.70	124.95	116.40
1	A	8	ASN	CB-CG-ND2	5.70	124.95	116.40
1	B	664	GLY	N-CA-C	-5.69	103.87	112.41
1	A	169	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	420	ILE	N-CA-C	-5.65	100.20	108.11
1	B	400	SER	N-CA-C	5.61	118.59	111.69
1	B	186	ILE	N-CA-C	-5.61	105.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	202	HIS	CB-CG-ND1	5.59	131.09	122.70
1	A	383	THR	CB-CA-C	5.58	120.14	110.72
1	B	141	THR	O-C-N	-5.57	115.18	122.59
1	A	684	TRP	CG-CD2-CE3	5.56	139.46	133.90
1	A	168	THR	N-CA-C	-5.55	101.43	110.20
1	A	515	ILE	CA-CB-CG2	5.55	119.93	110.50
1	A	262	VAL	N-CA-C	5.54	115.99	110.23
1	A	202	HIS	CB-CG-ND1	5.53	131.00	122.70
1	A	74	ILE	CA-CB-CG1	-5.52	101.01	110.40
1	A	410	HIS	CA-CB-CG	5.52	119.32	113.80
1	A	257	GLU	CB-CG-CD	5.52	121.98	112.60
1	A	258	TRP	N-CA-C	-5.52	98.20	108.02
1	B	270	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	A	85	SER	N-CA-C	5.48	118.23	110.50
1	A	120	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	B	567	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	683	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	553	ILE	CA-C-N	5.45	125.43	120.03
1	B	553	ILE	C-N-CA	5.45	125.43	120.03
1	A	216	LYS	CB-CG-CD	-5.45	98.76	111.30
1	A	247	ASN	CB-CG-ND2	5.44	124.56	116.40
1	A	415	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	86	VAL	N-CA-C	-5.43	99.41	107.51
1	B	413	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	A	531	PHE	N-CA-C	-5.40	98.44	107.99
1	B	383	THR	N-CA-CB	-5.38	102.53	110.49
1	A	416	ASN	N-CA-C	5.37	118.63	111.75
1	B	451	LEU	CA-C-N	5.35	125.30	119.78
1	B	451	LEU	C-N-CA	5.35	125.30	119.78
1	A	684	TRP	CE2-CD2-CG	-5.35	100.78	107.20
1	B	334	THR	CB-CA-C	5.35	118.66	109.51
1	A	10	GLN	CG-CD-NE2	5.35	124.42	116.40
1	B	104	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	193	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	662	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	B	646	GLN	OE1-CD-NE2	-5.33	117.28	122.60
1	A	152	ALA	CB-CA-C	-5.31	110.44	116.54
1	A	128	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	A	339	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	677	THR	N-CA-CB	-5.28	102.64	111.20
1	B	420	ILE	N-CA-C	-5.28	99.95	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASN	CB-CG-ND2	5.28	124.32	116.40
1	B	282	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	106	LYS	CA-CB-CG	-5.27	103.56	114.10
1	B	616	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	A	281	LEU	N-CA-C	-5.25	102.09	109.96
1	B	32	ASN	CA-CB-CG	5.25	117.85	112.60
1	B	327	HIS	CB-CG-ND1	5.23	130.55	122.70
1	B	331	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	A	564	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	B	188	ASN	CA-CB-CG	5.22	117.82	112.60
1	B	27	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	62	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	281	LEU	N-CA-C	-5.21	102.56	110.28
1	B	194	LEU	N-CA-C	-5.21	100.67	108.96
1	B	489	VAL	N-CA-C	-5.21	100.62	108.12
1	A	270	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	227	ARG	N-CA-C	-5.19	100.05	108.52
1	B	616	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	B	616	TRP	CB-CG-CD1	-5.19	119.12	126.90
1	A	126	HIS	CB-CG-ND1	5.18	130.47	122.70
1	B	662	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	B	326	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	465	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	423	ARG	N-CA-C	-5.16	101.28	109.59
1	A	248	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	668	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	A	227	ARG	CA-C-N	-5.12	116.48	122.93
1	A	227	ARG	C-N-CA	-5.12	116.48	122.93
1	A	10	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	78	GLN	CA-C-N	5.11	125.56	120.04
1	A	78	GLN	C-N-CA	5.11	125.56	120.04
1	B	190	ILE	N-CA-C	5.10	115.38	110.74
1	A	321	VAL	N-CA-CB	-5.09	105.19	111.00
1	B	373	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	125	ALA	N-CA-C	-5.08	105.82	111.36
1	B	213	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	556	VAL	CA-C-N	5.08	125.07	119.89
1	B	556	VAL	C-N-CA	5.08	125.07	119.89
1	B	227	ARG	N-CA-C	-5.07	99.52	108.20
1	A	467	ASN	CB-CG-ND2	5.06	124.00	116.40
1	B	669	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	228	VAL	CB-CA-C	5.04	117.70	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	N-CA-C	-5.04	106.47	113.18
1	B	617	ASP	CA-C-N	5.04	125.06	119.32
1	B	617	ASP	C-N-CA	5.04	125.06	119.32
1	A	603	ASN	CB-CG-ND2	5.03	123.95	116.40
1	A	140	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	B	529	VAL	N-CA-C	-5.03	100.88	108.12
1	B	300	MET	N-CA-C	5.01	117.47	111.71
1	B	393	LYS	CA-CB-CG	-5.01	104.08	114.10
1	B	363	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	97	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	5310	1195	5049	70	0
1	B	5310	1195	5049	66	0
2	C	44	44	20	0	0
2	D	44	44	20	3	0
2	E	44	44	20	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	405	810	0	8	0
4	B	354	708	0	7	0
All	All	11515	4040	10158	138	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 7.

All (138) 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:238:TRP:HD1	1:A:588:THR:HG21	1.50	0.77
1:A:231:VAL:HG22	1:A:239:GLN:HE22	1.51	0.76
1:A:293:PHE:HE2	1:A:434:ILE:HD11	1.49	0.76
1:A:434:ILE:HG21	4:A:3075:HOH:O	1.88	0.74
1:B:431:VAL:HG23	1:B:490:TRP:HE3	1.56	0.71
1:A:515:ILE:HD13	1:A:553:ILE:HD11	1.72	0.70
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.77	0.65
1:B:433:ALA:HB1	1:B:482:LEU:HD11	1.76	0.65
1:A:410:HIS:HB2	4:A:3081:HOH:O	1.97	0.65
1:A:549:ILE:HD11	1:A:551:VAL:HB	1.80	0.64
1:B:449:THR:HG23	1:B:451:LEU:H	1.63	0.63
1:A:463:ILE:HG13	1:A:464:LEU:HD12	1.81	0.63
1:A:203:ASN:O	1:A:677:THR:HG21	1.99	0.62
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.82	0.61
1:A:120:ASN:O	1:A:124:THR:HG23	2.01	0.61
1:B:342:LEU:HD22	1:B:346:LEU:HD22	1.83	0.59
1:B:410:HIS:HB3	4:B:3076:HOH:O	2.03	0.59
1:B:171:THR:HB	4:B:874:HOH:O	2.02	0.58
1:A:231:VAL:HG22	1:A:239:GLN:NE2	2.17	0.58
1:A:82:ASN:HD22	1:A:96:ALA:HB1	1.70	0.57
1:B:590:ARG:HD3	1:B:639:ASP:OD2	2.05	0.57
1:B:4:THR:HB	1:B:399:LYS:HD2	1.86	0.56
1:A:246:ILE:HG21	4:A:3050:HOH:O	2.04	0.56
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.40	0.56
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.88	0.56
1:B:78:GLN:HG2	1:B:80:VAL:HB	1.87	0.56
1:B:361:GLY:HA3	1:B:366:MET:SD	2.46	0.56
1:A:238:TRP:CD1	1:A:588:THR:HG21	2.36	0.55
1:A:205:SER:O	1:A:209:VAL:HG13	2.07	0.55
1:A:529:VAL:HB	1:A:536:VAL:CG2	2.37	0.54
1:B:82:ASN:OD1	1:B:96:ALA:HB1	2.08	0.54
1:B:231:VAL:HG21	1:B:256:GLY:HA3	1.87	0.54
1:B:633:TYR:CD1	1:B:634:PRO:HA	2.43	0.54
1:A:124:THR:O	1:A:128:HIS:HD2	1.91	0.54
1:B:141:THR:HG22	1:B:198:ALA:HB3	1.90	0.54
1:B:413:TRP:HB3	1:B:420:ILE:HG23	1.90	0.53
1:A:413:TRP:HB3	1:A:420:ILE:HG23	1.90	0.53
1:B:228:VAL:HG22	1:B:231:VAL:HG23	1.91	0.53
1:A:567:ASN:HD21	1:A:571:ALA:HB3	1.74	0.53
1:A:536:VAL:HG21	1:A:551:VAL:HG21	1.90	0.53
1:A:185:THR:HG22	1:A:187:GLU:H	1.73	0.52
1:B:231:VAL:HG22	1:B:239:GLN:HE22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:O	1:A:307:LEU:HD22	2.09	0.52
1:B:394:LEU:HA	1:B:397:LEU:HD13	1.93	0.51
1:A:82:ASN:ND2	1:A:101:TRP:H	2.08	0.50
1:A:529:VAL:HB	1:A:536:VAL:HG23	1.92	0.50
1:B:69:MET:HB3	1:B:71:ILE:HD13	1.92	0.50
1:A:139:ASN:ND2	1:A:194:LEU:HD12	2.27	0.50
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.47	0.50
1:B:415:ASN:HD22	1:B:418:VAL:H	1.59	0.49
1:B:594:ASN:HB2	1:B:683:ASN:OD1	2.12	0.49
1:A:18:TYR:CZ	1:A:360:TYR:HA	2.47	0.49
1:A:78:GLN:HG2	1:A:80:VAL:HB	1.94	0.49
1:A:348:PHE:HB2	4:A:3075:HOH:O	2.12	0.49
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.96	0.49
1:B:75:TRP:CZ2	1:B:227:ARG:HG3	2.48	0.49
1:A:327:HIS:H	1:A:327:HIS:HD1	1.61	0.48
1:A:533:THR:HG22	1:B:533:THR:HG22	1.96	0.48
1:B:593:ILE:HD11	1:B:684:TRP:HA	1.96	0.48
1:B:115:MET:HE1	1:B:221:LEU:HD11	1.95	0.48
1:B:560:ILE:HA	1:B:579:PHE:O	2.13	0.48
1:B:364:GLN:CG	1:B:378:LEU:HD11	2.43	0.48
1:A:11:ASN:ND2	4:A:3005:HOH:O	2.46	0.48
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.96	0.47
1:A:331:ARG:HG2	4:A:3086:HOH:O	2.13	0.47
1:A:408:SER:O	1:A:423:ARG:HA	2.14	0.47
1:B:316:GLN:HG2	4:B:706:HOH:O	2.14	0.47
1:A:185:THR:HG22	1:A:187:GLU:N	2.29	0.47
1:A:420:ILE:HA	1:A:432:VAL:O	2.14	0.47
1:B:85:SER:OG	1:B:153:GLU:HG3	2.15	0.47
1:B:401:ASN:HD22	1:B:403:ALA:H	1.62	0.47
1:B:231:VAL:HG22	1:B:239:GLN:NE2	2.30	0.47
1:A:60:LYS:HE2	1:A:381:PHE:CD1	2.50	0.47
1:B:284:ARG:HD3	4:B:3539:HOH:O	2.15	0.47
1:B:415:ASN:ND2	1:B:417:ASP:H	2.12	0.46
1:B:599:ALA:H	1:B:602:GLN:HB3	1.80	0.46
1:B:364:GLN:HG3	1:B:378:LEU:HD11	1.95	0.46
1:B:610:VAL:HG22	1:B:613:LEU:HD22	1.98	0.46
2:D:1:BGC:H6C2	2:D:2:GLC:O5	2.15	0.46
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.16	0.45
1:A:40:ASP:HB2	1:A:48:LEU:HD23	1.98	0.45
1:B:605:PHE:HB2	1:B:653:LEU:HG	1.99	0.45
1:A:224:ASP:O	1:A:252:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:CD1	1:A:553:ILE:HD11	2.46	0.45
1:B:564:ARG:HD2	1:B:573:SER:O	2.17	0.45
1:A:45:ASN:HD22	1:A:48:LEU:HD22	1.82	0.45
1:B:420:ILE:HA	1:B:432:VAL:O	2.17	0.44
1:A:146:SER:HA	1:A:168:THR:OG1	2.17	0.44
1:A:591:PHE:HA	1:A:680:VAL:HG22	1.99	0.44
1:A:432:VAL:HB	1:A:489:VAL:HG22	2.00	0.43
1:B:414:ILE:HG12	1:B:415:ASN:N	2.33	0.43
1:A:311:GLU:HG3	1:A:317:VAL:HG11	2.00	0.43
1:A:82:ASN:HD21	1:A:101:TRP:H	1.66	0.43
1:A:435:ASN:ND2	1:A:437:ASN:H	2.17	0.43
1:A:126:HIS:HE1	1:A:224:ASP:OD2	2.01	0.43
1:A:247:ASN:HA	1:A:251:PRO:HB3	2.01	0.43
1:B:260:LEU:HB3	1:B:283:PHE:HB3	2.01	0.42
1:B:564:ARG:HD3	1:B:575:ILE:HG13	2.01	0.42
1:B:591:PHE:O	1:B:637:TYR:HA	2.19	0.42
1:A:508:MET:HA	1:A:580:GLU:O	2.19	0.42
1:B:401:ASN:ND2	1:B:403:ALA:H	2.18	0.42
1:B:648:ILE:O	1:B:669:THR:HA	2.20	0.42
1:A:133:ILE:HG12	1:A:225:GLY:HA3	2.01	0.42
1:A:663:GLU:HB2	1:A:685:GLN:O	2.19	0.42
1:B:294:ARG:HB2	1:B:332:PHE:CZ	2.55	0.42
1:A:17:ILE:HB	1:A:357:ALA:HA	2.02	0.42
1:B:587:VAL:HG13	1:B:644:ALA:HB2	2.02	0.42
1:A:266:SER:HA	1:A:267:PRO:HD3	1.70	0.42
1:B:19:GLN:O	1:B:360:TYR:HB3	2.20	0.42
1:B:647:THR:HA	1:B:670:PHE:O	2.20	0.42
1:A:498:THR:HG22	1:A:499:PRO:O	2.20	0.42
1:B:159:ASP:HA	1:B:210:TYR:HE1	1.84	0.42
1:A:163:LEU:HD22	1:A:165:GLY:N	2.35	0.41
1:A:268:GLU:H	1:A:268:GLU:CD	2.27	0.41
1:B:141:THR:HG23	1:B:142:SER:H	1.85	0.41
1:B:567:ASN:HB2	4:B:3573:HOH:O	2.20	0.41
2:D:1:BGC:H5	2:D:2:GLC:O5	2.21	0.41
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.81	0.41
1:B:515:ILE:O	1:B:550:GLN:HA	2.20	0.41
1:A:321:VAL:HA	1:A:355:VAL:O	2.21	0.41
1:B:442:ALA:O	1:B:481:THR:HA	2.21	0.41
1:A:567:ASN:ND2	1:A:571:ALA:HB3	2.36	0.41
1:B:25:PHE:HB3	4:B:696:HOH:O	2.21	0.41
1:B:469:LEU:HA	1:B:469:LEU:HD12	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:PRO:HB2	4:B:879:HOH:O	2.20	0.41
1:B:685:GLN:HA	1:B:686:PRO:HD3	1.89	0.41
1:A:16:VAL:HG21	1:A:395:ALA:CB	2.51	0.41
1:A:626:TYR:O	1:A:636:TRP:HA	2.21	0.41
1:B:647:THR:HG22	1:B:669:THR:OG1	2.21	0.41
1:A:93:ASN:HB2	4:A:964:HOH:O	2.21	0.40
1:A:124:THR:O	1:A:128:HIS:CD2	2.73	0.40
1:A:333:HIS:HD2	4:A:968:HOH:O	2.04	0.40
1:A:642:VAL:HG13	1:A:672:THR:HG21	2.02	0.40
1:A:541:ILE:HG23	1:A:549:ILE:CD1	2.51	0.40
1:B:449:THR:HG22	1:B:475:GLY:O	2.21	0.40
1:B:566:ALA:HA	1:B:572:ALA:HA	2.03	0.40
1:B:608:GLY:N	1:B:613:LEU:HB3	2.36	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	684/686 (100%)	662 (97%)	22 (3%)	0	100	100
1	B	684/686 (100%)	657 (96%)	25 (4%)	2 (0%)	36	35
All	All	1368/1372 (100%)	1319 (96%)	47 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	GLY
1	B	89	TYR

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	564/564 (100%)	511 (91%)	53 (9%)	8	5
1	B	564/564 (100%)	519 (92%)	45 (8%)	11	8
All	All	1128/1128 (100%)	1030 (91%)	98 (9%)	9	6

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	7	SER
1	A	13	SER
1	A	21	PHE
1	A	46	LEU
1	A	48	LEU
1	A	66	LEU
1	A	74	ILE
1	A	80	VAL
1	A	103	ARG
1	A	142	SER
1	A	163	LEU
1	A	169	ASN
1	A	197	LEU
1	A	209	VAL
1	A	211	LEU
1	A	221	LEU
1	A	227	ARG
1	A	228	VAL
1	A	231	VAL
1	A	246	ILE
1	A	262	VAL
1	A	281	LEU
1	A	284	ARG
1	A	307	LEU
1	A	342	LEU
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	367	SER
1	A	372	PRO
1	A	375	ARG
1	A	378	LEU
1	A	383	THR
1	A	390	VAL
1	A	420	ILE
1	A	429	VAL
1	A	432	VAL
1	A	434	ILE
1	A	435	ASN
1	A	439	ASN
1	A	448	VAL
1	A	500	ILE
1	A	511	PRO
1	A	515	ILE
1	A	533	THR
1	A	542	VAL
1	A	549	ILE
1	A	560	ILE
1	A	597	THR
1	A	606	LEU
1	A	610	VAL
1	A	613	LEU
1	A	642	VAL
1	A	680	VAL
1	B	21	PHE
1	B	42	SER
1	B	44	THR
1	B	66	LEU
1	B	71	ILE
1	B	74	ILE
1	B	103	ARG
1	B	135	ASP
1	B	141	THR
1	B	146	SER
1	B	173	ASN
1	B	174	LEU
1	B	197	LEU
1	B	204	ASN
1	B	211	LEU
1	B	228	VAL

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Mol	Chain	Res	Type
1	B	231	VAL
1	B	254	THR
1	B	284	ARG
1	B	307	LEU
1	B	334	THR
1	B	342	LEU
1	B	346	LEU
1	B	350	LEU
1	B	372	PRO
1	B	375	ARG
1	B	383	THR
1	B	410	HIS
1	B	415	ASN
1	B	420	ILE
1	B	432	VAL
1	B	459	VAL
1	B	482	LEU
1	B	494	THR
1	B	497	THR
1	B	506	PRO
1	B	513	VAL
1	B	549	ILE
1	B	564	ARG
1	B	593	ILE
1	B	613	LEU
1	B	615	ASN
1	B	659	THR
1	B	669	THR
1	B	685	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	ASN
1	A	19	GLN
1	A	45	ASN
1	A	82	ASN
1	A	116	GLN
1	A	126	HIS
1	A	128	HIS
1	A	129	ASN

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Mol	Chain	Res	Type
1	A	140	HIS
1	A	160	ASN
1	A	162	ASN
1	A	177	HIS
1	A	239	GLN
1	A	271	GLN
1	A	316	GLN
1	A	333	HIS
1	A	435	ASN
1	A	503	ASN
1	A	550	GLN
1	A	578	ASN
1	A	594	ASN
1	A	595	ASN
1	A	602	GLN
1	A	615	ASN
1	A	632	GLN
1	A	646	GLN
1	B	19	GLN
1	B	62	ASN
1	B	126	HIS
1	B	129	ASN
1	B	160	ASN
1	B	162	ASN
1	B	173	ASN
1	B	177	HIS
1	B	204	ASN
1	B	239	GLN
1	B	364	GLN
1	B	401	ASN
1	B	415	ASN
1	B	416	ASN
1	B	467	ASN
1	B	479	ASN
1	B	603	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	BGC	C	1	2	12,12,12	0.74	0	17,17,17	1.08	2 (11%)
2	GLC	C	2	2	11,11,12	1.08	1 (9%)	15,15,17	2.63	5 (33%)
2	BGC	D	1	2	12,12,12	1.30	1 (8%)	17,17,17	1.15	1 (5%)
2	GLC	D	2	2	11,11,12	1.57	2 (18%)	15,15,17	2.26	6 (40%)
2	BGC	E	1	2	12,12,12	0.97	1 (8%)	17,17,17	1.18	2 (11%)
2	GLC	E	2	2	11,11,12	0.94	0	15,15,17	1.21	1 (6%)

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	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C2-C3	3.58	1.58	1.52
2	D	1	BGC	C4-C5	3.17	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	BGC	C4-C5	2.57	1.58	1.53
2	D	2	GLC	C1-C2	2.35	1.57	1.52
2	C	2	GLC	C4-C5	2.32	1.58	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C1-O5-C5	7.91	122.79	112.19
2	D	2	GLC	C1-O5-C5	4.81	118.64	112.19
2	D	2	GLC	O5-C5-C4	-3.43	102.49	110.83
2	D	2	GLC	C3-C4-C5	-3.29	104.26	110.23
2	D	2	GLC	O5-C5-C6	3.06	113.62	107.66
2	C	2	GLC	O5-C5-C6	-2.99	101.85	107.66
2	C	2	GLC	C1-C2-C3	-2.86	105.47	109.64
2	D	1	BGC	O4-C4-C3	-2.85	103.66	110.38
2	C	2	GLC	O2-C2-C1	2.76	115.55	109.22
2	C	1	BGC	C6-C5-C4	2.73	119.72	113.02
2	C	1	BGC	O4-C4-C3	-2.67	104.07	110.38
2	C	2	GLC	O5-C5-C4	2.57	117.08	110.83
2	E	1	BGC	O4-C4-C3	-2.55	104.36	110.38
2	E	1	BGC	C4-C3-C2	-2.51	106.42	110.83
2	D	2	GLC	C1-C2-C3	2.38	113.11	109.64
2	E	2	GLC	C1-C2-C3	2.27	112.95	109.64
2	D	2	GLC	O4-C4-C5	2.24	114.83	109.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6

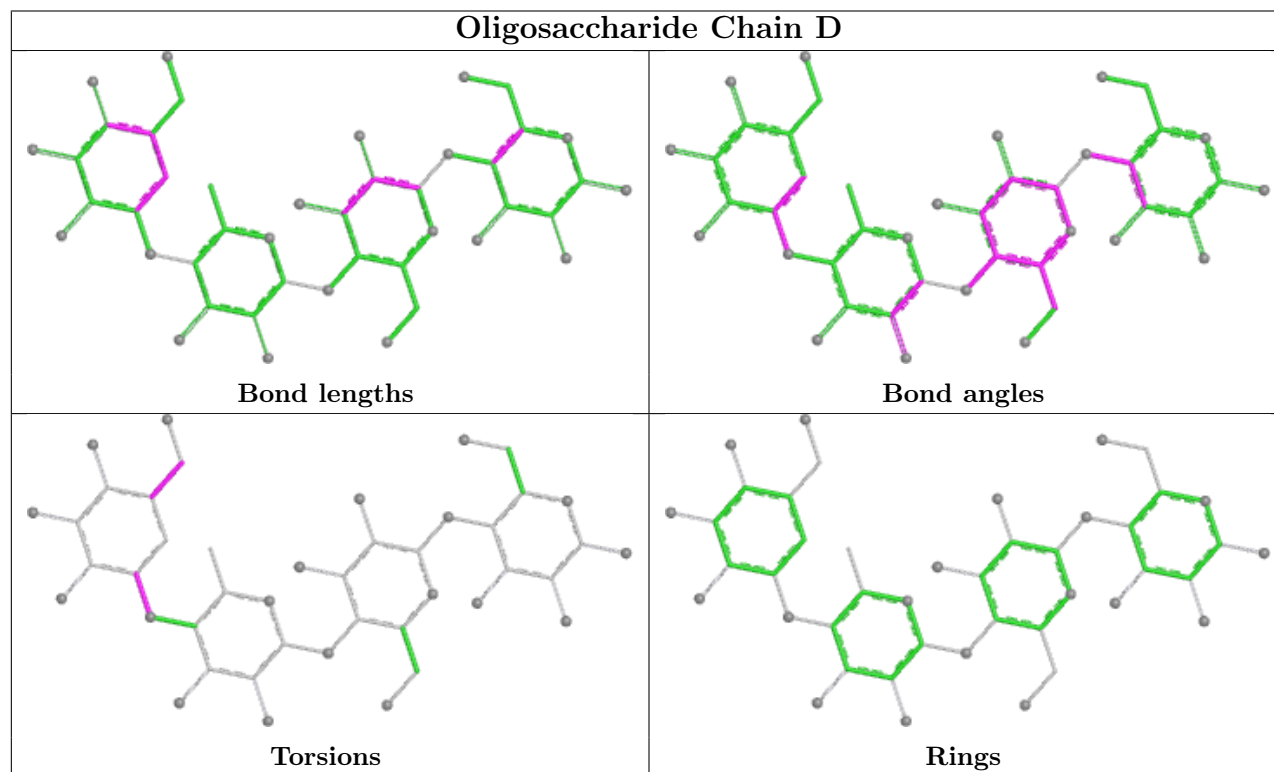
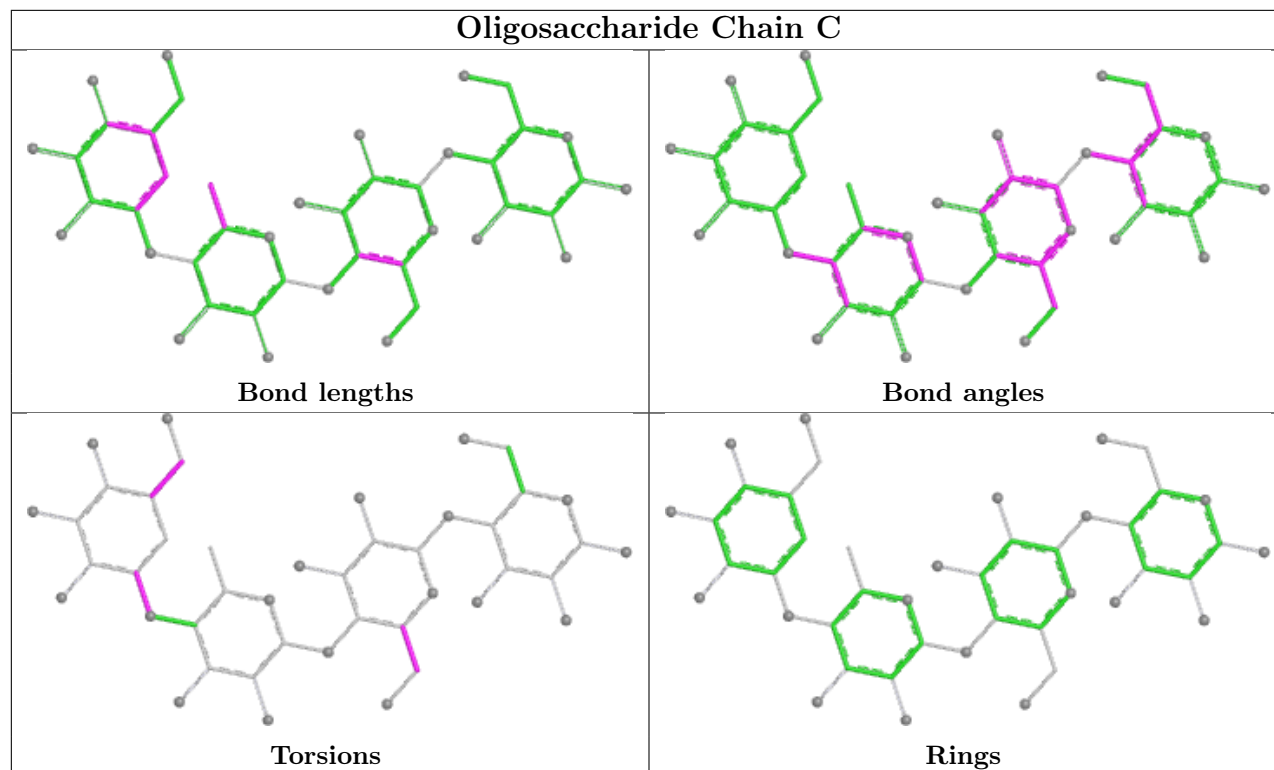
There are no ring outliers.

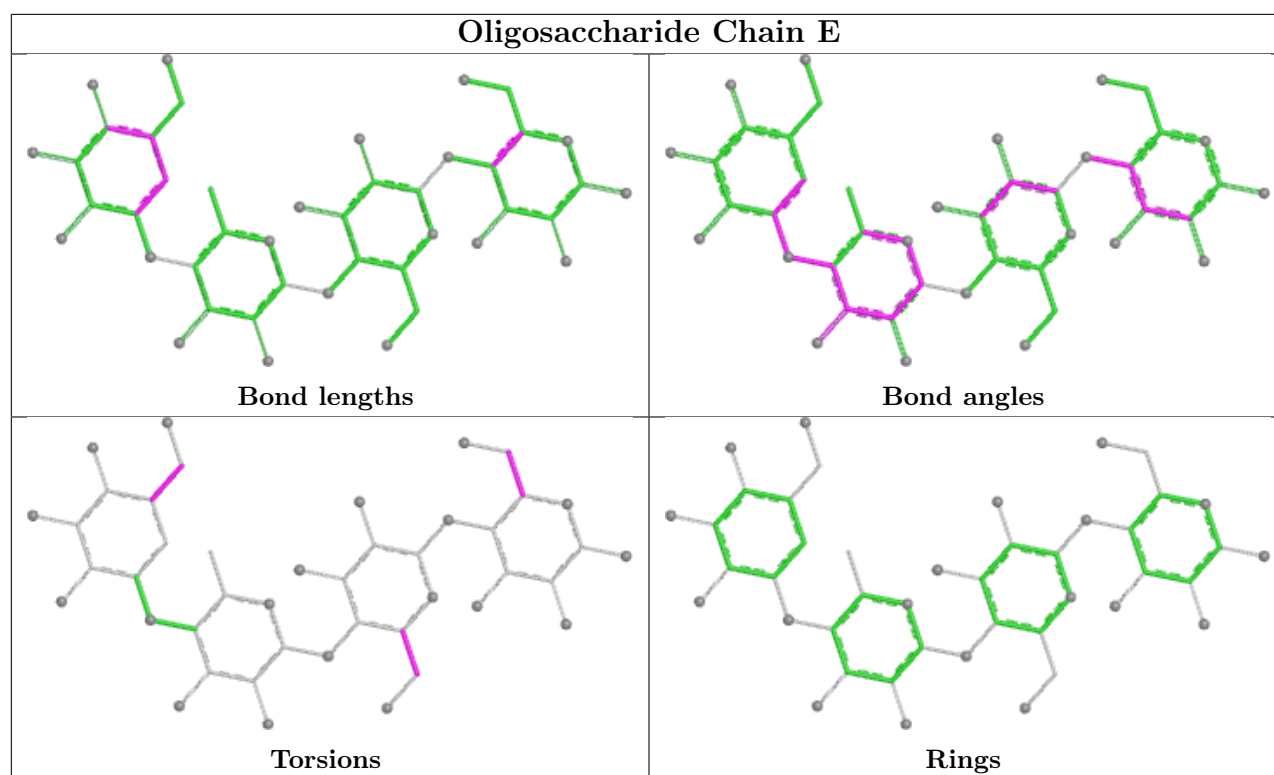
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	3	0
2	D	1	BGC	2	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, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	686/686 (100%)	-0.31	0 100 100	5, 13, 26, 55	0
1	B	686/686 (100%)	-0.11	1 (0%) 92 91	5, 17, 35, 55	0
All	All	1372/1372 (100%)	-0.21	1 (0%) 92 91	5, 15, 31, 55	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	2.0

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	0.44	0.17	0,0,97,99	10
2	AC1	D	3[A]	21/22	0.46	0.20	0,0,101,102	22
2	AC1	D	3[B]	21/22	0.46	0.20	0,0,101,102	22
2	GLC	C	2	11/12	0.47	0.23	0,0,68,76	10
2	AC1	E	3[A]	21/22	0.57	0.15	0,0,59,60	22
2	AC1	E	3[B]	21/22	0.57	0.15	0,0,59,60	22
2	AC1	C	3[B]	21/22	0.60	0.14	0,0,61,63	22
2	AC1	C	3[A]	21/22	0.60	0.14	0,0,61,63	22

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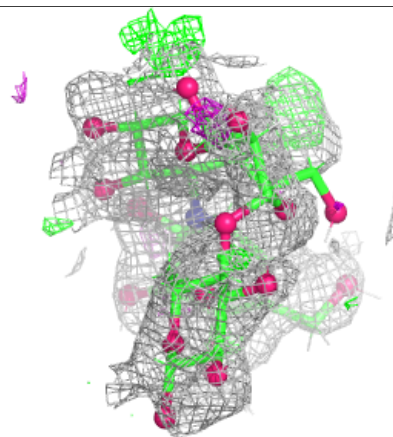
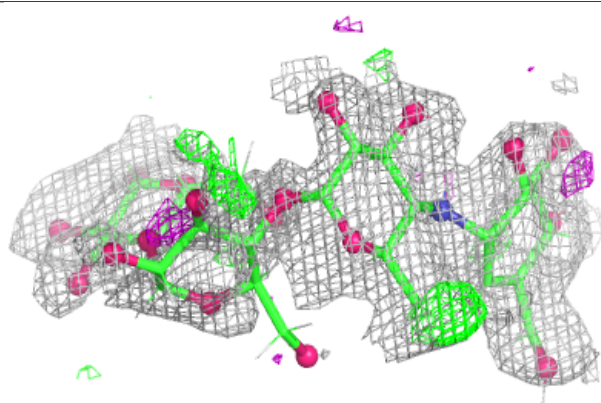
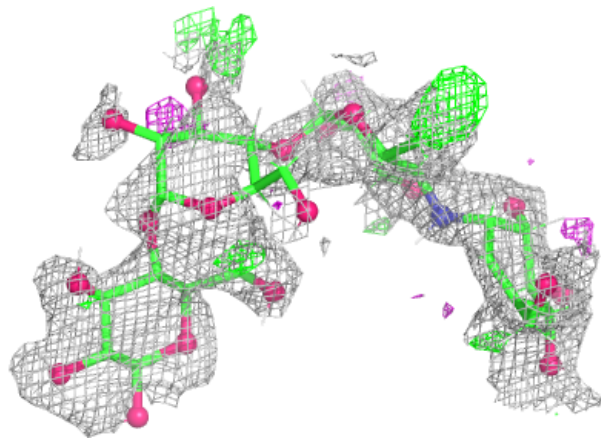
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	C	1	12/12	0.61	0.17	0,0,73,76	11
2	BGC	E	1	12/12	0.68	0.14	0,0,71,73	11
2	BGC	D	1	12/12	0.71	0.16	0,0,92,94	11
2	GLC	E	2	11/12	0.77	0.16	0,0,62,68	10

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.

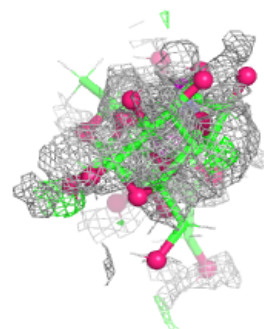
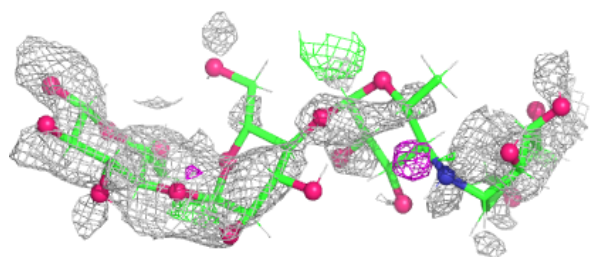
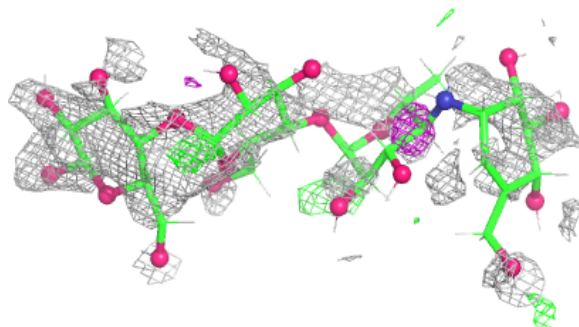
Electron density around Chain C:

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

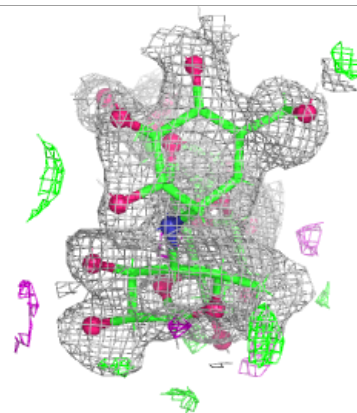
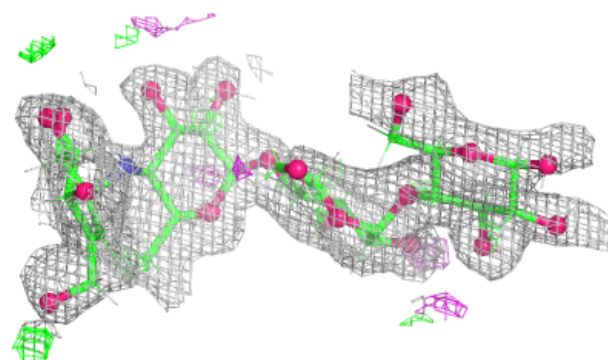
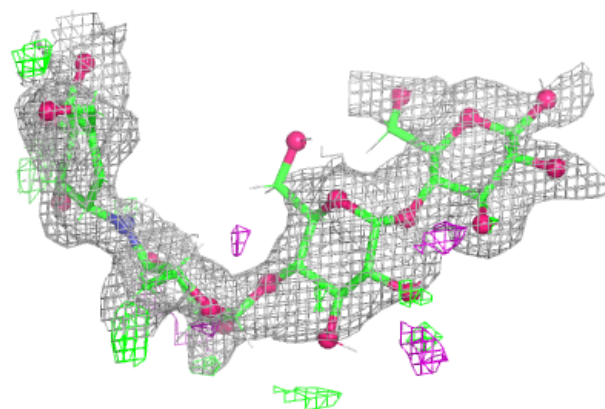


Electron density around Chain D:

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

**Electron density around Chain E:**

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



6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	CA	B	5002	1/1	0.53	0.12	27,27,27,27	0
3	CA	A	5003	1/1	0.82	0.11	36,36,36,36	0
3	CA	B	5004	1/1	0.87	0.06	32,32,32,32	0
3	CA	A	5001	1/1	0.89	0.06	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.