



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:58 PM UTC

PDB ID : 3VSU / pdb_00003vsu
Title : The complex structure of XylC with xylobiose
Authors : Huang, C.H.; Sun, Y.; Ko, T.P.; Ma, Y.; Chen, C.C.; Zheng, Y.; Chan, H.C.;
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Deposited on : 2012-05-09
Resolution : 2.05 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

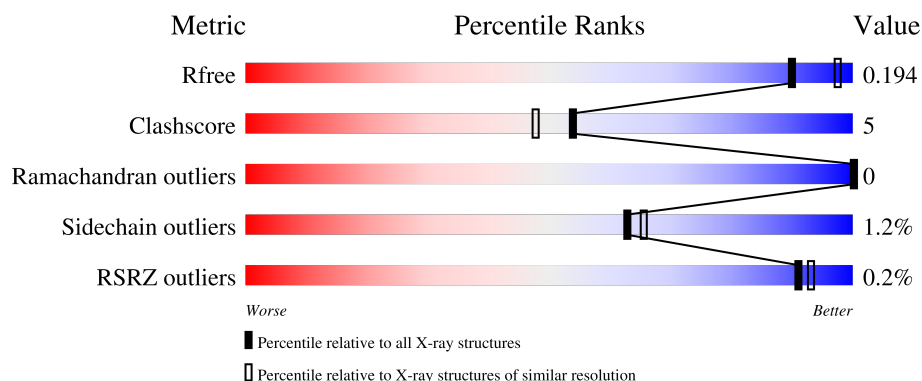
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

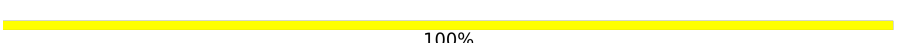
The reported resolution of this entry is 2.05 Å.

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))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	638	 84% 16% .
1	B	638	 84% 15% .
1	C	638	 84% 14% .
1	D	638	 86% 13% .
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23181 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 Xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5147	3275	877	983	12			
1	B	638	Total	C	N	O	S	0	0	0
			5147	3275	877	983	12			
1	C	638	Total	C	N	O	S	0	0	0
			5147	3275	877	983	12			
1	D	638	Total	C	N	O	S	0	0	0
			5147	3275	877	983	12			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			19	10	9			
2	F	2	Total	C	O	0	0	0
			19	10	9			
2	G	2	Total	C	O	0	0	0
			19	10	9			
2	H	2	Total	C	O	0	0	0
			19	10	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	626	Total	O	0	0
			626	626		
3	B	661	Total	O	0	0
			661	661		

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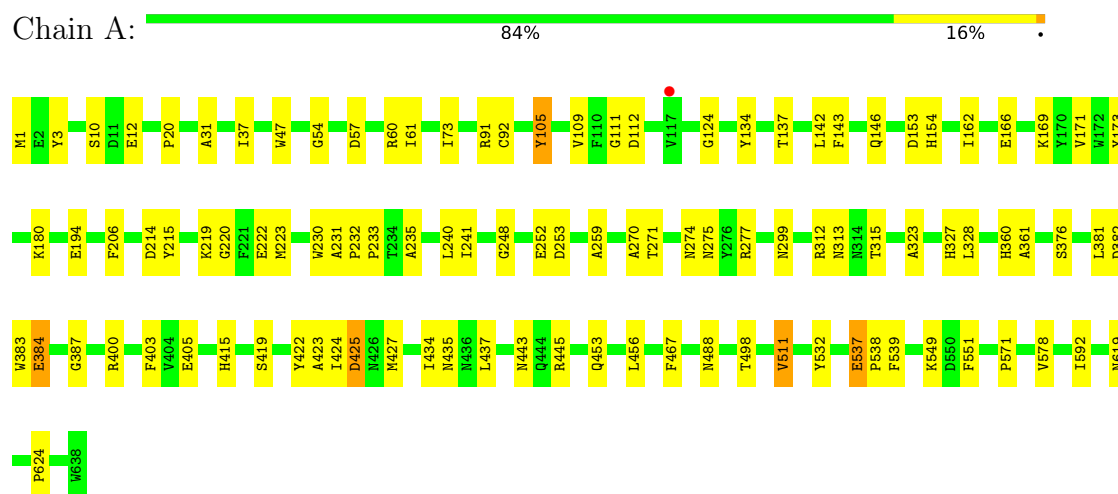
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	585	Total 585	O 585	0	0
3	D	645	Total 645	O 645	0	0

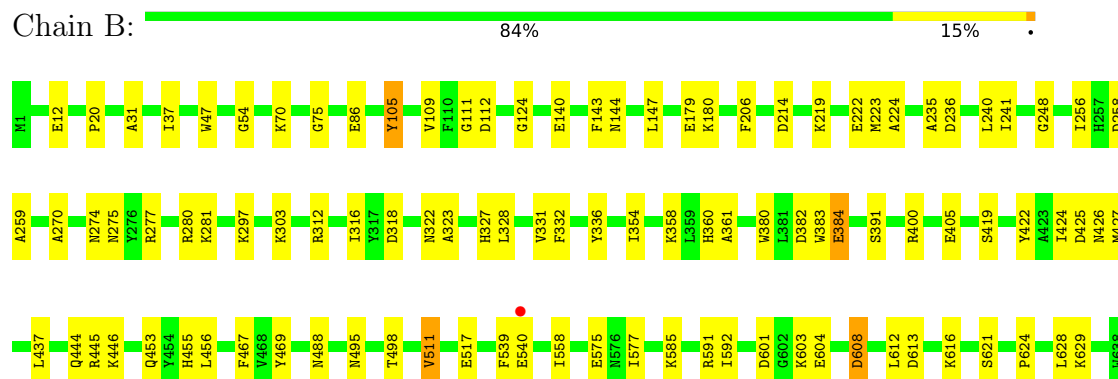
3 Residue-property plots

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

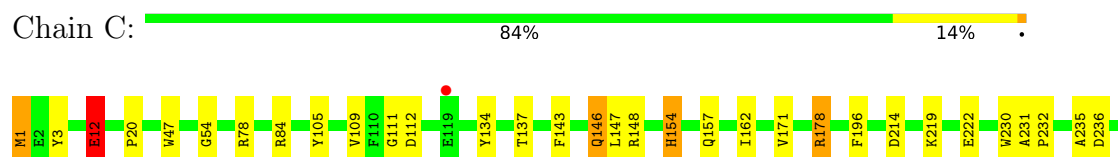
• Molecule 1: Xylosidase

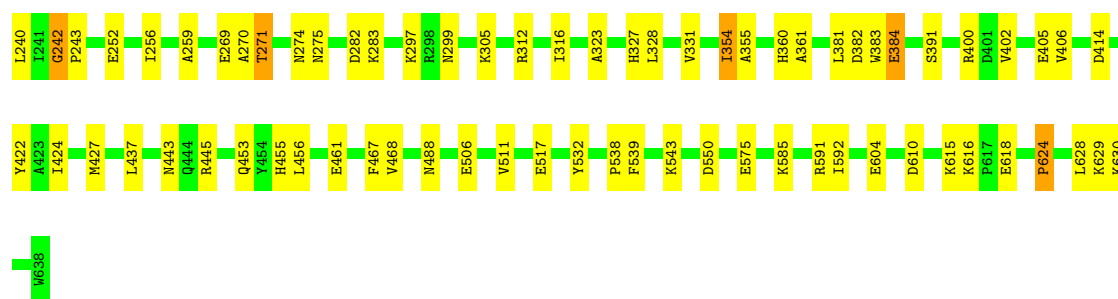


• Molecule 1: Xylosidase



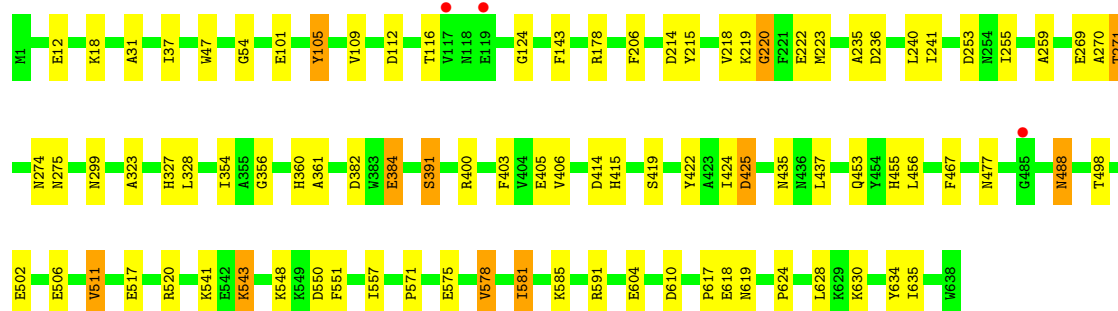
• Molecule 1: Xylosidase





- Molecule 1: Xylosidase

Chain D: 86% 13% •



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain E: 100%

XYP1
XYP2

- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain F: 100%

XYP1
XYP2

- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain G: 100%

XYP1
XYP2

- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain H: 100%

XYP1
XYP2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.68Å 202.31Å 100.40Å 90.00° 99.14° 90.00°	Depositor
Resolution (Å)	25.00 – 2.05 25.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.05) 90.6 (25.00-2.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.153 , 0.194 0.154 , 0.194	Depositor DCC
R_{free} test set	9835 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23181	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: XYP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/5276	1.13	42/7151 (0.6%)
1	B	0.82	1/5276 (0.0%)	1.14	37/7151 (0.5%)
1	C	0.78	2/5276 (0.0%)	1.14	36/7151 (0.5%)
1	D	0.81	1/5276 (0.0%)	1.14	32/7151 (0.4%)
All	All	0.80	4/21104 (0.0%)	1.14	147/28604 (0.5%)

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	VAL	CA-CB	6.44	1.60	1.54
1	C	331	VAL	CA-CB	5.71	1.60	1.54
1	C	1	MET	SD-CE	5.69	1.93	1.79
1	D	116	THR	CA-CB	5.66	1.60	1.52

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PHE	N-CA-C	11.78	124.20	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	VAL	N-CA-C	-11.15	94.12	108.84
1	C	109	VAL	N-CA-C	-10.11	93.57	108.54
1	B	270	ALA	N-CA-C	9.98	122.16	111.28
1	D	143	PHE	N-CA-C	9.91	122.16	111.36
1	A	270	ALA	N-CA-C	9.62	121.77	111.28
1	C	270	ALA	N-CA-C	8.94	121.02	111.28
1	B	111	GLY	N-CA-C	8.78	121.73	111.63
1	C	143	PHE	N-CA-C	8.78	120.93	111.36
1	D	54	GLY	N-CA-C	-8.78	100.70	112.82
1	A	54	GLY	N-CA-C	-8.63	100.90	112.82
1	A	109	VAL	N-CA-C	-8.52	95.93	108.54
1	D	270	ALA	N-CA-C	8.51	120.56	111.28
1	B	54	GLY	N-CA-C	-8.33	101.33	112.82
1	D	109	VAL	N-CA-C	-8.13	96.50	108.54
1	D	323	ALA	N-CA-C	-8.04	101.80	111.69
1	C	111	GLY	N-CA-C	7.95	120.77	111.63
1	A	323	ALA	N-CA-C	-7.29	102.73	111.69
1	C	54	GLY	N-CA-C	-7.25	102.81	112.82
1	D	222	GLU	N-CA-C	-6.95	97.91	109.24
1	C	453	GLN	N-CA-C	6.85	119.67	110.35
1	A	488	ASN	N-CA-C	6.84	120.98	111.74
1	C	236	ASP	N-CA-C	-6.81	101.08	110.35
1	D	424	ILE	N-CA-C	6.76	117.85	108.12
1	A	539	PHE	N-CA-C	-6.71	100.10	110.10
1	A	453	GLN	N-CA-C	6.69	119.45	110.35
1	B	222	GLU	N-CA-C	-6.66	98.84	109.76
1	B	12	GLU	N-CA-C	-6.64	104.41	113.30
1	A	222	GLU	N-CA-C	-6.63	98.88	109.76
1	A	111	GLY	N-CA-C	6.58	119.19	111.63
1	C	222	GLU	N-CA-C	-6.57	98.54	109.24
1	C	456	LEU	N-CA-C	-6.52	101.08	110.08
1	D	488	ASN	N-CA-C	6.49	120.50	112.58
1	A	437	LEU	N-CA-C	-6.41	98.08	108.52
1	B	437	LEU	N-CA-C	-6.40	98.08	108.52
1	C	323	ALA	N-CA-C	-6.40	103.81	111.69
1	A	456	LEU	N-CA-C	-6.28	101.41	110.08
1	D	12	GLU	N-CA-C	-6.24	105.31	113.17
1	B	455	HIS	N-CA-C	6.22	118.86	109.41
1	D	419	SER	N-CA-C	6.20	120.97	113.17
1	D	255	ILE	N-CA-C	-6.17	98.73	107.75
1	D	259	ALA	N-CA-C	-6.17	99.22	109.46
1	C	154	HIS	N-CA-C	6.15	117.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	GLY	N-CA-C	6.10	124.61	114.48
1	B	591	ARG	N-CA-C	6.07	117.76	111.03
1	B	219	LYS	N-CA-C	6.04	119.33	109.24
1	A	153	ASP	N-CA-C	-6.01	100.05	109.25
1	A	419	SER	N-CA-C	6.00	120.60	113.16
1	D	143	PHE	CA-C-N	-5.99	116.18	122.89
1	D	143	PHE	C-N-CA	-5.99	116.18	122.89
1	D	437	LEU	N-CA-C	-5.98	98.78	108.52
1	A	219	LYS	N-CA-C	5.97	118.86	108.76
1	D	384	GLU	N-CA-C	5.96	119.64	111.54
1	B	456	LEU	N-CA-C	-5.94	101.88	110.08
1	C	616	LYS	CA-C-N	5.92	126.38	120.52
1	C	616	LYS	C-N-CA	5.92	126.38	120.52
1	C	437	LEU	N-CA-C	-5.89	98.92	108.52
1	C	592	ILE	N-CA-C	5.88	116.06	110.42
1	B	498	THR	N-CA-C	-5.88	102.95	110.53
1	D	543	LYS	N-CA-C	5.88	118.57	111.40
1	B	179	GLU	N-CA-C	5.87	120.74	112.93
1	A	424	ILE	N-CA-C	5.87	116.74	108.17
1	C	219	LYS	N-CA-C	5.85	119.00	109.06
1	C	539	PHE	N-CA-C	-5.82	101.43	110.10
1	C	231	ALA	N-CA-C	5.82	119.56	108.97
1	C	591	ARG	N-CA-C	5.81	117.48	111.03
1	A	425	ASP	N-CA-C	-5.81	99.05	108.52
1	B	539	PHE	N-CA-C	-5.81	101.44	110.10
1	D	214	ASP	N-CA-C	5.80	117.55	110.41
1	B	143	PHE	N-CA-C	5.80	118.83	111.69
1	A	180	LYS	N-CA-C	5.79	117.59	108.96
1	D	591	ARG	N-CA-C	5.79	117.45	111.03
1	B	424	ILE	N-CA-C	5.77	116.60	108.17
1	B	236	ASP	N-CA-C	-5.77	102.37	110.50
1	A	137	THR	N-CA-C	5.77	118.51	111.82
1	C	259	ALA	N-CA-C	-5.76	99.90	109.46
1	A	434	ILE	N-CA-C	5.74	116.13	107.75
1	B	214	ASP	N-CA-C	5.73	117.46	110.41
1	D	453	GLN	N-CA-C	5.72	118.13	110.35
1	D	456	LEU	N-CA-C	-5.72	102.19	110.08
1	A	162	ILE	N-CA-C	-5.72	100.35	108.58
1	B	259	ALA	N-CA-C	-5.68	100.03	109.46
1	A	381	LEU	N-CA-C	-5.63	99.34	108.52
1	B	425	ASP	N-CA-C	-5.63	99.35	108.52
1	B	419	SER	N-CA-C	5.62	120.14	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	ALA	N-CA-C	-5.60	104.80	111.69
1	D	354	ILE	N-CA-C	5.59	116.63	108.58
1	A	387	GLY	N-CA-C	-5.54	107.99	115.36
1	A	220	GLY	N-CA-C	5.54	123.60	115.08
1	A	498	THR	N-CA-C	-5.54	103.39	110.53
1	C	488	ASN	N-CA-C	5.54	119.33	112.24
1	B	621	SER	N-CA-C	-5.53	103.39	110.53
1	A	214	ASP	N-CA-C	5.52	117.19	110.41
1	B	453	GLN	N-CA-C	5.51	117.85	110.35
1	A	384	GLU	N-CA-C	5.48	119.00	111.54
1	B	20	PRO	N-CA-C	5.48	119.63	111.41
1	B	624	PRO	N-CA-C	5.47	121.79	114.18
1	D	219	LYS	N-CA-C	5.47	118.37	108.69
1	C	424	ILE	N-CA-C	5.46	116.14	108.17
1	D	215	TYR	N-CA-C	5.46	118.77	111.24
1	B	488	ASN	N-CA-C	5.44	119.08	111.74
1	D	236	ASP	N-CA-C	-5.44	102.34	110.23
1	B	354	ILE	N-CA-C	5.43	116.40	108.58
1	A	376	SER	N-CA-C	-5.43	105.52	111.82
1	C	242	GLY	CA-C-N	5.42	125.51	119.87
1	C	242	GLY	C-N-CA	5.42	125.51	119.87
1	C	624	PRO	N-CA-C	5.42	121.59	114.27
1	B	384	GLU	N-CA-C	5.41	118.90	111.54
1	D	557	ILE	N-CA-C	-5.38	100.14	107.99
1	B	248	GLY	N-CA-C	5.35	123.36	114.48
1	A	20	PRO	N-CA-C	5.34	119.87	111.38
1	A	423	ALA	N-CA-C	5.32	118.23	111.69
1	C	12	GLU	N-CA-C	-5.31	106.48	113.17
1	B	608	ASP	N-CA-C	5.30	119.06	112.59
1	D	356	GLY	N-CA-C	-5.30	106.23	112.64
1	D	425	ASP	N-CA-C	-5.30	99.89	108.52
1	B	180	LYS	N-CA-C	5.29	118.20	109.85
1	D	220	GLY	N-CA-C	5.28	123.21	115.08
1	A	215	TYR	N-CA-C	5.26	118.50	111.24
1	A	315	THR	N-CA-C	-5.26	100.32	108.90
1	C	20	PRO	N-CA-C	5.26	119.30	111.41
1	C	162	ILE	N-CA-C	-5.26	101.01	108.58
1	A	624	PRO	N-CA-C	5.25	121.47	114.18
1	C	354	ILE	N-CA-C	5.25	116.13	108.58
1	C	455	HIS	N-CA-C	5.24	117.38	109.41
1	B	322	ASN	CB-CA-C	-5.23	100.89	110.62
1	C	402	VAL	N-CA-C	5.20	116.21	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	HIS	N-CA-C	5.20	116.63	111.07
1	D	455	HIS	N-CA-C	5.17	117.27	109.41
1	C	618	GLU	N-CA-C	5.16	116.90	111.28
1	A	231	ALA	N-CA-C	5.14	118.49	108.21
1	B	391	SER	N-CA-C	5.14	117.82	109.24
1	A	511	VAL	CA-C-N	5.13	125.12	119.89
1	A	511	VAL	C-N-CA	5.13	125.12	119.89
1	B	592	ILE	N-CA-C	5.09	115.31	110.42
1	C	137	THR	N-CA-C	5.09	118.65	112.23
1	D	391	SER	N-CA-C	5.09	117.72	109.06
1	A	271	THR	N-CA-C	5.09	118.59	112.38
1	C	384	GLU	N-CA-C	5.09	118.46	111.54
1	C	381	LEU	N-CA-C	-5.09	100.23	108.52
1	C	214	ASP	N-CA-C	5.06	116.64	110.41
1	A	592	ILE	N-CA-C	5.05	115.27	110.42
1	A	259	ALA	N-CA-C	-5.04	101.09	109.46
1	B	224	ALA	N-CA-C	5.03	115.95	108.60
1	D	498	THR	N-CA-C	-5.03	104.04	110.53
1	A	61	ILE	N-CA-C	-5.03	100.41	107.75
1	B	179	GLU	CB-CA-C	-5.01	102.22	110.08

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	B	105	TYR	Sidechain
1	C	105	TYR	Sidechain
1	D	105	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	5147	0	4962	47	0
1	B	5147	0	4962	49	0
1	C	5147	0	4962	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5147	0	4962	60	0
2	E	19	0	0	2	0
2	F	19	0	0	1	0
2	G	19	0	0	1	0
2	H	19	0	0	1	0
3	A	626	0	0	1	0
3	B	661	0	0	3	0
3	C	585	0	0	3	0
3	D	645	0	0	7	0
All	All	23181	0	19848	198	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 5.

All (198) 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:C:178:ARG:HH11	1:C:178:ARG:HB2	1.10	1.13
1:C:146:GLN:HE21	1:C:146:GLN:HA	1.31	0.94
1:A:443:ASN:HD21	1:A:445:ARG:HH11	1.01	0.94
1:C:178:ARG:HH11	1:C:178:ARG:CB	1.81	0.92
1:D:543:LYS:HE2	3:D:1258:HOH:O	1.70	0.91
1:B:467:PHE:CZ	1:C:467:PHE:HE1	1.90	0.88
1:D:575:GLU:HG3	1:D:630:LYS:HD3	1.54	0.88
1:A:467:PHE:CZ	1:D:467:PHE:HE1	1.96	0.82
1:C:178:ARG:HB2	1:C:178:ARG:NH1	1.93	0.80
1:C:575:GLU:HG3	1:C:630:LYS:HD3	1.62	0.80
1:A:443:ASN:ND2	1:A:445:ARG:HH11	1.78	0.79
1:A:443:ASN:HD21	1:A:445:ARG:NH1	1.80	0.79
1:B:467:PHE:HZ	1:C:467:PHE:HE1	1.29	0.78
1:B:427:MET:HE2	1:B:445:ARG:NH1	2.00	0.77
1:C:443:ASN:HD21	1:C:445:ARG:HH11	1.33	0.77
1:B:144:ASN:HB2	3:B:1316:HOH:O	1.83	0.77
1:D:269:GLU:OE1	1:D:271:THR:HB	1.85	0.76
1:B:467:PHE:CZ	1:C:467:PHE:CE1	2.76	0.73
1:D:327:HIS:CD2	1:D:328:LEU:HG	2.25	0.72
1:D:575:GLU:CG	1:D:630:LYS:HD3	2.20	0.71
1:D:541:LYS:O	1:D:543:LYS:HE3	1.90	0.70
1:A:467:PHE:HE1	1:D:467:PHE:CZ	2.09	0.70
1:C:443:ASN:HD21	1:C:445:ARG:NH1	1.89	0.70
1:D:634:TYR:C	1:D:635:ILE:HD12	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:HE2	1:A:445:ARG:NH1	2.08	0.69
1:D:581:ILE:HD11	1:D:617:PRO:O	1.94	0.67
1:C:269:GLU:OE1	1:C:271:THR:HB	1.94	0.67
1:B:112:ASP:H	1:B:275:ASN:ND2	1.93	0.66
1:A:467:PHE:CE1	1:D:467:PHE:CE1	2.83	0.66
1:B:467:PHE:HE1	1:C:467:PHE:CZ	2.12	0.66
1:B:223:MET:HE1	1:B:241:ILE:HD12	1.76	0.66
1:D:578:VAL:HG11	1:D:619:ASN:HB3	1.79	0.65
1:A:467:PHE:HZ	1:D:467:PHE:HE1	1.40	0.65
1:C:575:GLU:CG	1:C:630:LYS:HD3	2.28	0.63
1:A:327:HIS:CD2	1:A:328:LEU:HG	2.34	0.63
1:B:467:PHE:HZ	1:C:467:PHE:CE1	2.14	0.63
1:B:467:PHE:CE1	1:C:467:PHE:CE1	2.87	0.62
1:C:443:ASN:ND2	1:C:445:ARG:HH11	1.95	0.61
1:C:146:GLN:HE21	1:C:146:GLN:CA	2.07	0.61
1:C:299:ASN:OD1	1:D:299:ASN:ND2	2.34	0.61
1:C:146:GLN:HA	1:C:146:GLN:NE2	2.11	0.60
1:A:467:PHE:CE1	1:D:467:PHE:HE1	2.20	0.60
1:C:178:ARG:HH11	1:C:178:ARG:CG	2.15	0.60
1:C:610:ASP:HB2	1:C:624:PRO:O	2.05	0.57
1:C:112:ASP:H	1:C:275:ASN:ND2	2.02	0.57
1:B:277:ARG:C	1:B:277:ARG:HD3	2.30	0.56
1:D:581:ILE:HD13	1:D:618:GLU:HA	1.86	0.56
1:D:405:GLU:OE2	2:H:1:XYP:C4	2.53	0.56
1:B:467:PHE:HE1	1:C:467:PHE:HZ	1.53	0.56
1:C:361:ALA:HA	1:C:384:GLU:HB2	1.86	0.56
1:D:18:LYS:HE2	1:D:18:LYS:HA	1.88	0.56
1:A:467:PHE:CZ	1:D:467:PHE:CE1	2.87	0.56
1:B:405:GLU:OE2	2:F:1:XYP:C4	2.54	0.56
1:D:112:ASP:H	1:D:275:ASN:ND2	2.04	0.56
1:A:467:PHE:HE1	1:D:467:PHE:CE1	2.24	0.55
1:C:327:HIS:CD2	1:C:328:LEU:HG	2.41	0.55
1:D:391:SER:HB2	1:D:414:ASP:OD1	2.07	0.55
1:B:467:PHE:CE1	1:C:467:PHE:CZ	2.94	0.55
1:C:532:TYR:CE1	1:C:538:PRO:HB3	2.42	0.54
1:A:361:ALA:HA	1:A:384:GLU:HB2	1.88	0.54
1:A:112:ASP:H	1:A:275:ASN:ND2	2.06	0.54
1:B:361:ALA:HA	1:B:384:GLU:HB2	1.90	0.53
1:C:405:GLU:OE2	2:G:1:XYP:C4	2.56	0.53
1:B:608:ASP:C	1:B:616:LYS:HG3	2.34	0.53
1:B:467:PHE:CE1	1:C:467:PHE:HE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:LYS:HG3	1:D:604:GLU:OE2	2.09	0.53
1:A:467:PHE:HE1	1:D:467:PHE:HZ	1.58	0.52
1:A:91:ARG:HG2	1:A:92:CYS:N	2.24	0.52
1:D:235:ALA:HA	1:D:274:ASN:HA	1.90	0.52
1:B:235:ALA:HA	1:B:274:ASN:HA	1.92	0.52
1:A:166:GLU:OE2	1:A:169:LYS:HD3	2.10	0.51
1:C:12:GLU:CD	1:D:178:ARG:HH11	2.17	0.51
1:C:134:TYR:O	1:C:171:VAL:HA	2.10	0.51
1:B:223:MET:HE1	1:B:241:ILE:CD1	2.41	0.51
1:D:405:GLU:HG2	1:D:406:VAL:HG22	1.91	0.51
1:C:628:LEU:HD12	3:C:1281:HOH:O	2.09	0.51
1:C:235:ALA:HA	1:C:274:ASN:HA	1.92	0.51
1:A:405:GLU:OE2	2:E:1:XYP:C4	2.59	0.51
1:A:537:GLU:OE1	1:A:549:LYS:HE2	2.10	0.51
1:A:427:MET:HE2	1:A:445:ARG:CZ	2.40	0.50
1:D:361:ALA:HA	1:D:384:GLU:HB2	1.93	0.50
1:B:240:LEU:C	1:B:240:LEU:HD23	2.36	0.50
1:B:206:PHE:O	1:B:241:ILE:HA	2.12	0.50
1:C:427:MET:HE2	1:C:445:ARG:CZ	2.42	0.50
1:D:488:ASN:ND2	3:D:1174:HOH:O	2.37	0.50
1:B:327:HIS:CD2	1:B:328:LEU:HG	2.47	0.50
1:B:303:LYS:HB2	1:B:332:PHE:CE2	2.47	0.50
1:B:601:ASP:OD2	1:B:603:LYS:HD2	2.12	0.50
1:B:495:ASN:OD1	1:B:540:GLU:HG2	2.11	0.50
1:A:105:TYR:CE1	1:A:124:GLY:HA3	2.46	0.50
1:B:558:ILE:HD12	1:B:558:ILE:N	2.27	0.49
1:B:446:LYS:HE2	1:B:469:TYR:O	2.11	0.49
1:D:220:GLY:HA2	1:D:253:ASP:O	2.12	0.49
1:D:551:PHE:CE1	1:D:571:PRO:HD3	2.48	0.49
1:B:382:ASP:O	1:B:383:TRP:HB2	2.13	0.49
1:B:105:TYR:CE1	1:B:124:GLY:HA3	2.48	0.49
1:B:280:ARG:O	1:B:281:LYS:HB2	2.13	0.49
1:A:57:ASP:O	1:A:60:ARG:HG3	2.12	0.49
1:A:532:TYR:CE1	1:A:538:PRO:HB3	2.48	0.49
1:C:585:LYS:HG3	1:C:604:GLU:OE2	2.13	0.48
1:B:297:LYS:NZ	3:B:1323:HOH:O	2.44	0.48
1:B:628:LEU:O	1:B:629:LYS:HD2	2.12	0.48
1:D:511:VAL:HG22	1:D:517:GLU:OE1	2.13	0.48
1:D:517:GLU:O	1:D:520:ARG:HG2	2.13	0.48
1:D:360:HIS:HA	1:D:382:ASP:O	2.14	0.48
1:C:12:GLU:CD	1:D:178:ARG:HD3	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:HIS:HA	1:C:382:ASP:O	2.14	0.48
1:B:585:LYS:HE2	1:B:604:GLU:OE2	2.14	0.47
1:C:511:VAL:CG2	1:C:517:GLU:OE1	2.62	0.47
1:D:550:ASP:HB2	3:D:1412:HOH:O	2.15	0.47
1:A:31:ALA:CB	1:A:37:ILE:HD11	2.45	0.47
1:A:73:ILE:HD12	1:A:223:MET:HE2	1.96	0.47
1:C:78:ARG:HD2	1:C:196:PHE:CE1	2.49	0.47
1:A:253:ASP:HA	1:A:313:ASN:O	2.15	0.47
1:A:382:ASP:O	1:A:383:TRP:HB2	2.15	0.47
1:C:391:SER:HA	1:C:414:ASP:O	2.15	0.47
1:B:47:TRP:C	1:B:47:TRP:CD1	2.92	0.47
1:D:47:TRP:C	1:D:47:TRP:CD1	2.93	0.47
1:D:610:ASP:HB2	1:D:624:PRO:O	2.15	0.46
1:B:140:GLU:H	1:B:140:GLU:CD	2.22	0.46
1:B:360:HIS:HA	1:B:382:ASP:O	2.15	0.46
1:A:240:LEU:C	1:A:240:LEU:HD23	2.41	0.46
1:A:578:VAL:HG11	1:A:619:ASN:HB3	1.97	0.46
1:A:252:GLU:HA	1:A:312:ARG:O	2.16	0.46
1:B:612:LEU:O	1:B:613:ASP:HB2	2.15	0.45
1:D:517:GLU:OE1	1:D:520:ARG:NE	2.39	0.45
1:B:400:ARG:HG2	1:B:422:TYR:CG	2.51	0.45
1:B:427:MET:CE	1:B:445:ARG:NH1	2.74	0.45
1:C:178:ARG:NH1	1:C:178:ARG:CG	2.78	0.45
1:C:382:ASP:O	1:C:383:TRP:HB2	2.16	0.45
1:C:406:VAL:HA	1:C:468:VAL:HG21	1.99	0.45
1:D:581:ILE:CD1	3:D:1445:HOH:O	2.64	0.45
1:D:403:PHE:CE1	1:D:405:GLU:HB2	2.52	0.45
1:B:400:ARG:HA	1:B:422:TYR:O	2.17	0.45
1:D:578:VAL:CG1	1:D:619:ASN:HB3	2.46	0.45
1:D:31:ALA:CB	1:D:37:ILE:HD11	2.47	0.44
1:D:435:ASN:HA	1:D:477:ASN:O	2.17	0.44
3:A:1070:HOH:O	2:E:1:XYP:C1	2.64	0.44
1:B:358:LYS:HE3	1:B:380:TRP:CD2	2.53	0.44
1:D:206:PHE:O	1:D:241:ILE:HA	2.16	0.44
1:D:543:LYS:HA	1:D:543:LYS:HD3	1.85	0.44
1:A:142:LEU:HD21	1:A:173:TYR:HB3	1.99	0.44
1:D:105:TYR:CE1	1:D:124:GLY:HA3	2.53	0.44
1:C:47:TRP:CD1	1:C:47:TRP:C	2.96	0.44
1:C:443:ASN:HD21	1:C:445:ARG:HD3	1.82	0.44
1:C:1:MET:HG2	1:C:3:TYR:CZ	2.52	0.44
1:A:47:TRP:C	1:A:47:TRP:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:HIS:HA	1:A:435:ASN:O	2.18	0.43
1:D:506:GLU:HG3	3:D:1144:HOH:O	2.18	0.43
1:A:403:PHE:CD1	1:A:425:ASP:HB3	2.52	0.43
1:A:1:MET:HG2	1:A:3:TYR:CZ	2.54	0.43
1:D:400:ARG:HG2	1:D:422:TYR:CG	2.53	0.43
1:A:134:TYR:O	1:A:171:VAL:HA	2.18	0.43
1:A:551:PHE:CE1	1:A:571:PRO:HD3	2.54	0.43
1:A:277:ARG:HD3	1:A:277:ARG:C	2.44	0.43
1:A:206:PHE:O	1:A:241:ILE:HA	2.19	0.43
1:B:256:ILE:O	1:B:316:ILE:HA	2.19	0.43
1:B:258:ASP:HA	1:B:318:ASP:O	2.19	0.43
1:A:400:ARG:HG2	1:A:422:TYR:CG	2.54	0.42
1:D:218:VAL:HG11	1:D:223:MET:HE1	2.01	0.42
1:A:235:ALA:HA	1:A:274:ASN:HA	1.99	0.42
1:D:240:LEU:C	1:D:240:LEU:HD23	2.45	0.42
1:D:628:LEU:HD12	3:D:917:HOH:O	2.19	0.42
1:C:240:LEU:HD23	1:C:240:LEU:C	2.44	0.42
1:B:31:ALA:CB	1:B:37:ILE:HD11	2.49	0.42
1:B:75:GLY:HA2	3:B:1320:HOH:O	2.19	0.42
1:C:256:ILE:O	1:C:316:ILE:HA	2.20	0.42
1:C:443:ASN:ND2	1:C:445:ARG:HD3	2.35	0.42
1:A:146:GLN:NE2	1:A:146:GLN:HA	2.35	0.42
1:C:252:GLU:HA	1:C:312:ARG:O	2.20	0.42
1:C:443:ASN:ND2	1:C:445:ARG:NH1	2.58	0.42
1:D:327:HIS:HA	1:D:360:HIS:HB2	2.02	0.42
1:C:154:HIS:O	1:C:157:GLN:NE2	2.51	0.41
1:C:400:ARG:HG2	1:C:422:TYR:CG	2.55	0.41
1:D:502:GLU:O	1:D:506:GLU:HG3	2.21	0.41
1:A:230:TRP:CD1	1:A:232:PRO:HD3	2.56	0.41
1:C:354:ILE:O	1:C:355:ALA:HB2	2.21	0.41
1:D:581:ILE:HD12	3:D:1445:HOH:O	2.21	0.41
1:B:511:VAL:HG22	1:B:517:GLU:OE1	2.21	0.41
1:C:282:ASP:C	1:C:283:LYS:HG3	2.46	0.41
1:C:297:LYS:HE2	1:C:461:GLU:HA	2.03	0.41
1:D:415:HIS:HA	1:D:435:ASN:O	2.21	0.41
1:C:391:SER:HB2	1:C:414:ASP:OD1	2.21	0.41
1:D:502:GLU:CD	1:D:502:GLU:H	2.29	0.41
1:C:242:GLY:HA2	1:C:243:PRO:HD3	1.86	0.41
1:D:548:LYS:HE3	1:D:548:LYS:HB3	1.91	0.41
1:D:635:ILE:HD12	1:D:635:ILE:N	2.35	0.41
1:A:91:ARG:HE	1:A:91:ARG:HB3	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SER:C	1:A:12:GLU:H	2.30	0.40
1:C:230:TRP:CD1	1:C:232:PRO:HD3	2.56	0.40
1:D:403:PHE:CD1	1:D:425:ASP:HB3	2.56	0.40
1:B:140:GLU:CD	1:B:140:GLU:N	2.79	0.40
1:C:305:LYS:NZ	3:C:1261:HOH:O	2.54	0.40
1:A:232:PRO:HB2	1:A:233:PRO:HD2	2.03	0.40
1:A:360:HIS:CD2	1:A:382:ASP:HB3	2.56	0.40
1:B:426:ASN:O	1:B:444:GLN:HA	2.21	0.40
1:C:148:ARG:HD2	3:C:979:HOH:O	2.20	0.40
1:B:312:ARG:HA	1:B:336:TYR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/638 (100%)	603 (95%)	33 (5%)	0	100	100
1	B	636/638 (100%)	607 (95%)	29 (5%)	0	100	100
1	C	636/638 (100%)	607 (95%)	29 (5%)	0	100	100
1	D	636/638 (100%)	604 (95%)	32 (5%)	0	100	100
All	All	2544/2552 (100%)	2421 (95%)	123 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	550/550 (100%)	546 (99%)	4 (1%)	76	80
1	B	550/550 (100%)	544 (99%)	6 (1%)	65	68
1	C	550/550 (100%)	539 (98%)	11 (2%)	48	48
1	D	550/550 (100%)	545 (99%)	5 (1%)	70	75
All	All	2200/2200 (100%)	2174 (99%)	26 (1%)	63	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	299	ASN
1	A	511	VAL
1	A	537	GLU
1	B	70	LYS
1	B	86	GLU
1	B	147	LEU
1	B	511	VAL
1	B	575	GLU
1	B	577	ILE
1	C	12	GLU
1	C	84	ARG
1	C	146	GLN
1	C	147	LEU
1	C	178	ARG
1	C	271	THR
1	C	506	GLU
1	C	543	LYS
1	C	550	ASP
1	C	615	LYS
1	C	629	LYS
1	D	101	GLU
1	D	271	THR
1	D	511	VAL
1	D	578	VAL
1	D	581	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	88	ASN
1	A	93	GLN
1	A	146	GLN
1	A	275	ASN
1	A	443	ASN
1	A	444	GLN
1	A	477	ASN
1	B	83	GLN
1	B	93	GLN
1	B	144	ASN
1	B	146	GLN
1	B	275	ASN
1	B	443	ASN
1	B	444	GLN
1	B	477	ASN
1	B	569	GLN
1	B	632	ASN
1	C	93	GLN
1	C	146	GLN
1	C	275	ASN
1	C	289	GLN
1	C	443	ASN
1	C	477	ASN
1	D	93	GLN
1	D	146	GLN
1	D	275	ASN
1	D	295	ASN
1	D	299	ASN
1	D	477	ASN
1	D	496	ASN
1	D	569	GLN
1	D	632	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 ⓘ

8 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	XYP	E	1	2	10,10,10	0.56	0	14,14,14	0.57	0
2	XYP	E	2	2	9,9,10	0.39	0	10,12,14	1.55	3 (30%)
2	XYP	F	1	2	10,10,10	0.55	0	14,14,14	0.54	0
2	XYP	F	2	2	9,9,10	0.35	0	10,12,14	1.66	1 (10%)
2	XYP	G	1	2	10,10,10	0.56	0	14,14,14	0.64	0
2	XYP	G	2	2	9,9,10	0.39	0	10,12,14	1.74	2 (20%)
2	XYP	H	1	2	10,10,10	0.58	0	14,14,14	0.56	0
2	XYP	H	2	2	9,9,10	0.36	0	10,12,14	1.52	2 (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	XYP	E	1	2	-	-	0/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	F	1	2	-	-	0/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	XYP	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	H	1	2	-	-	0/1/1/1
2	XYP	H	2	2	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	XYP	C1-C2-C3	4.08	115.58	109.64
2	F	2	XYP	C1-C2-C3	4.03	115.52	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	XYP	C1-C2-C3	3.46	114.68	109.64
2	E	2	XYP	C1-C2-C3	3.33	114.50	109.64
2	G	2	XYP	C5-O5-C1	-2.31	107.68	111.42
2	E	2	XYP	C5-O5-C1	-2.27	107.74	111.42
2	E	2	XYP	C4-C3-C2	2.25	113.59	110.92
2	H	2	XYP	C5-O5-C1	-2.22	107.83	111.42

There are no chirality outliers.

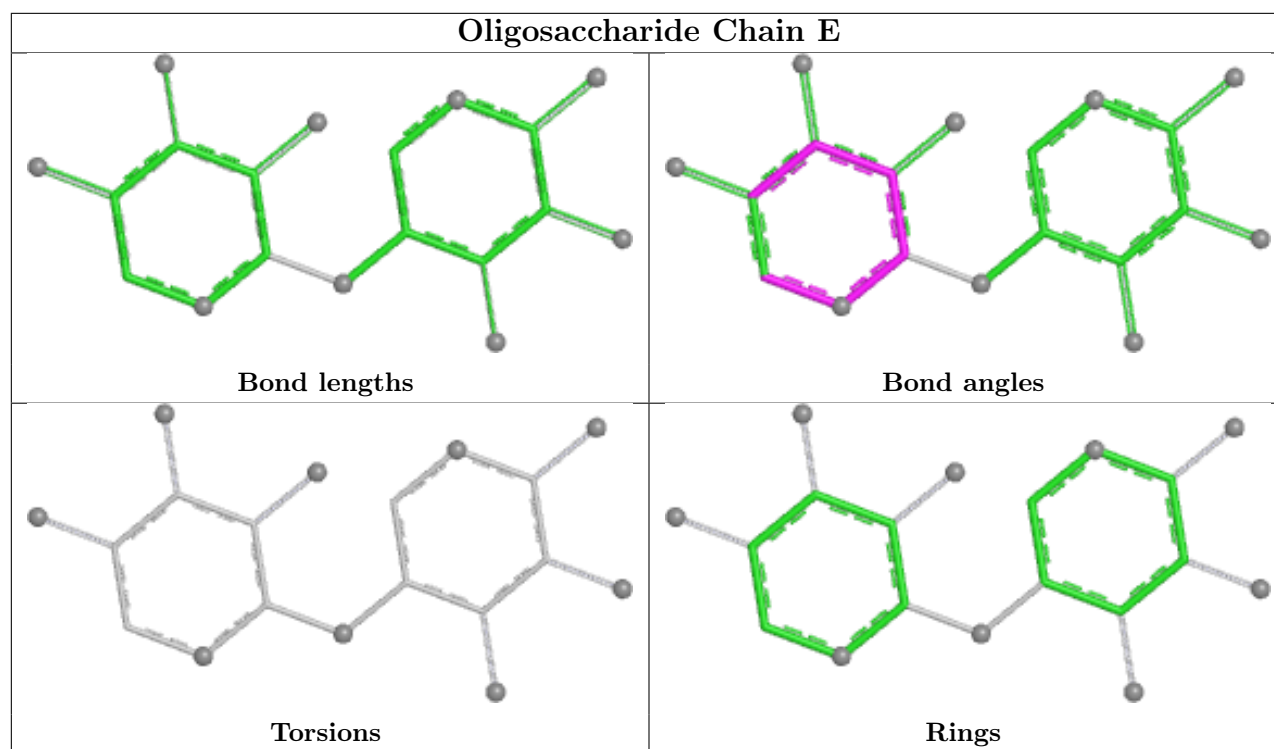
There are no torsion outliers.

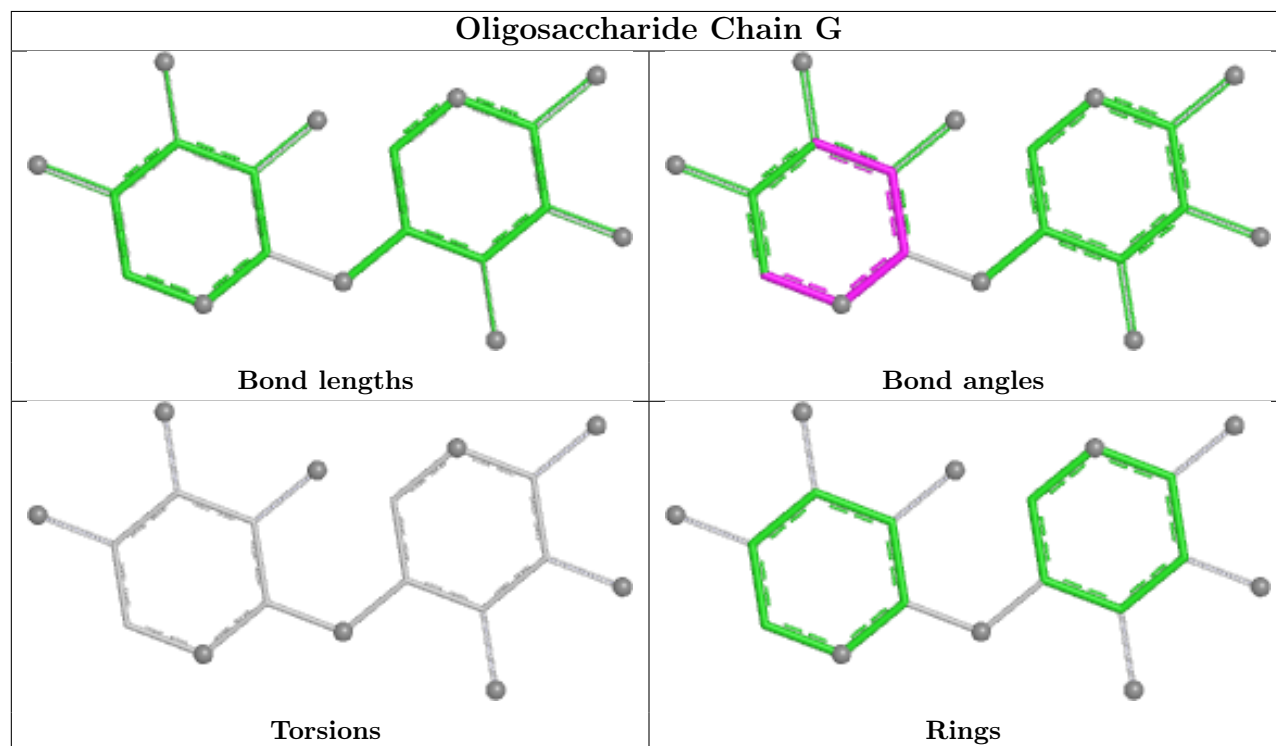
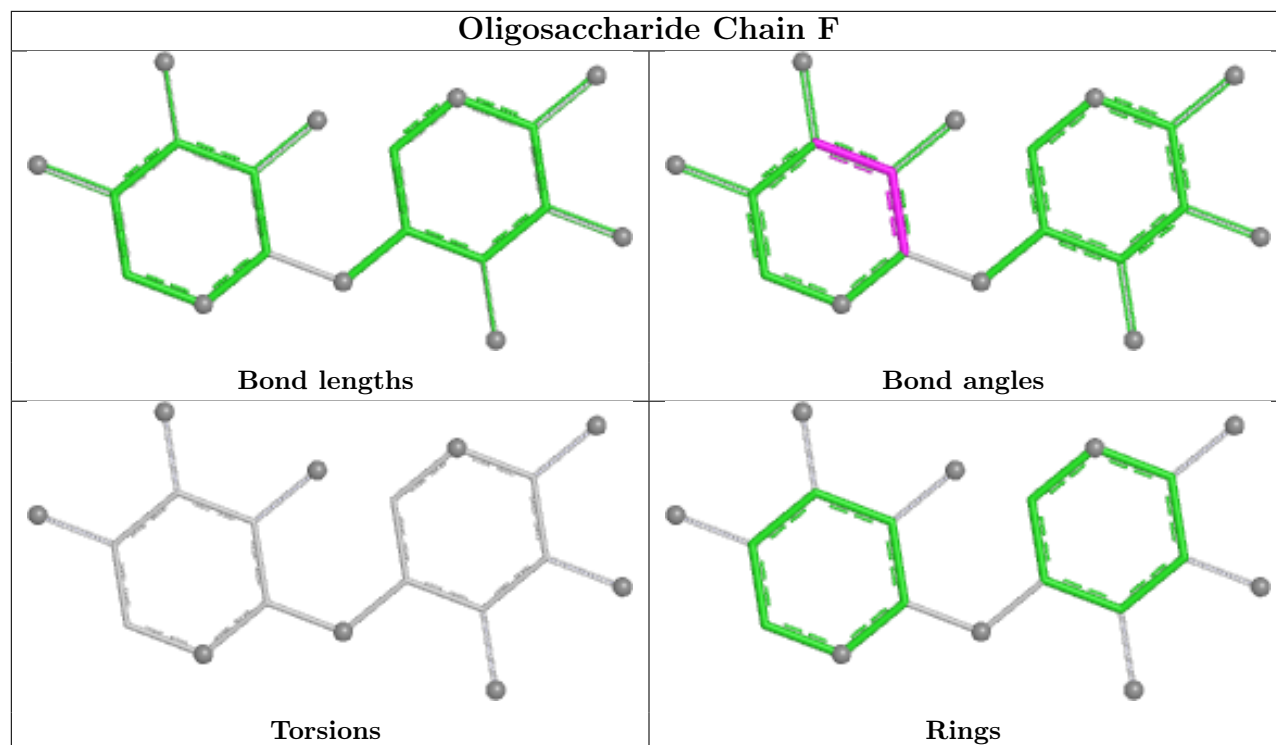
There are no ring outliers.

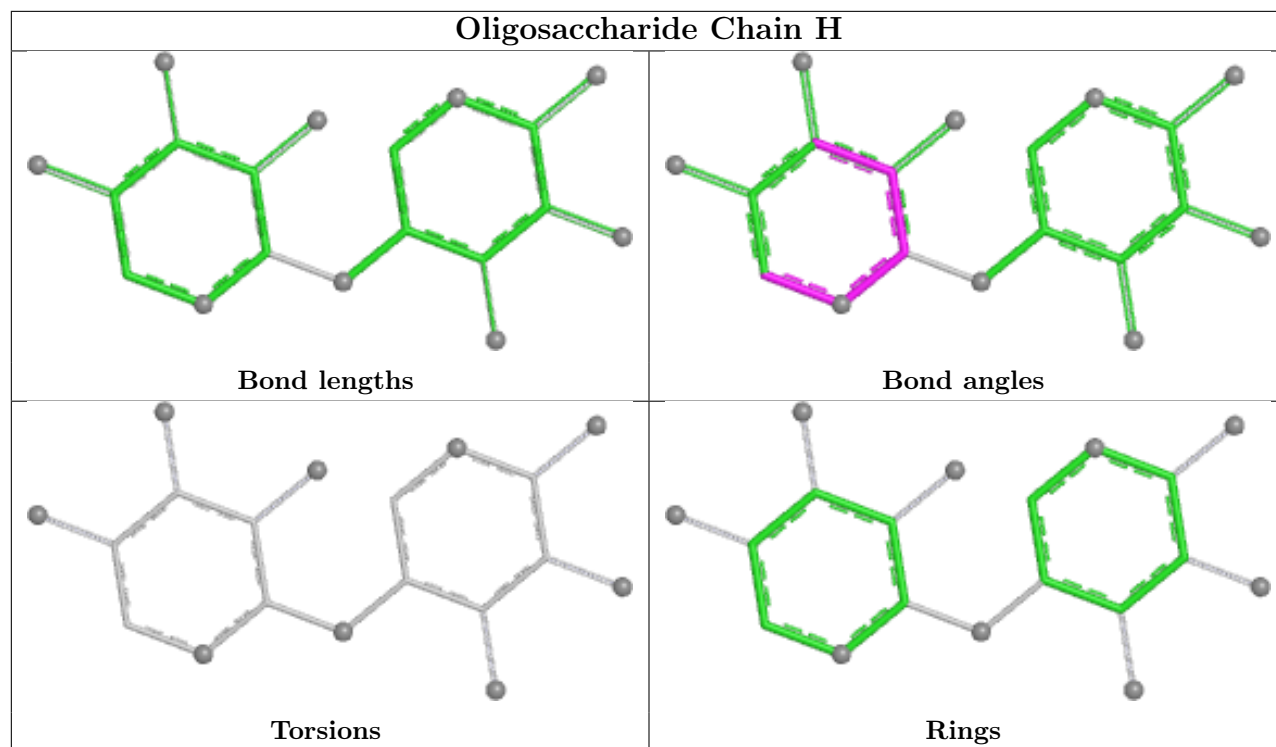
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	XYP	1	0
2	H	1	XYP	1	0
2	F	1	XYP	1	0
2	E	1	XYP	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](#)

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 [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	638/638 (100%)	-0.63	1 (0%) 91 93	7, 15, 31, 52	0
1	B	638/638 (100%)	-0.66	1 (0%) 91 93	8, 14, 30, 49	0
1	C	638/638 (100%)	-0.56	1 (0%) 91 93	8, 16, 33, 50	0
1	D	638/638 (100%)	-0.66	3 (0%) 87 89	7, 15, 30, 51	0
All	All	2552/2552 (100%)	-0.63	6 (0%) 91 93	7, 15, 32, 52	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	VAL	2.4
1	D	117	VAL	2.4
1	B	540	GLU	2.3
1	D	119	GLU	2.2
1	C	119	GLU	2.1
1	D	485	GLY	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.

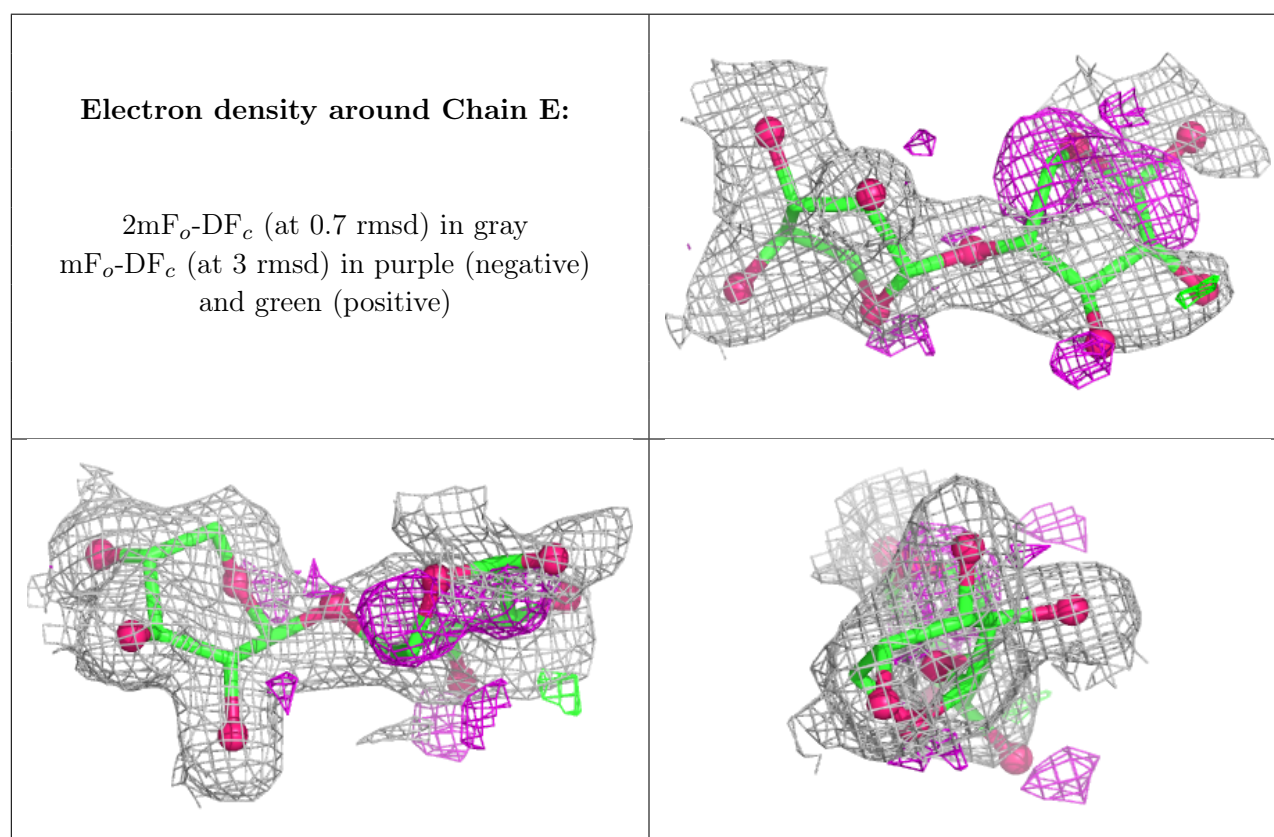
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XYP	E	1	10/10	0.77	0.17	41,53,55,55	0

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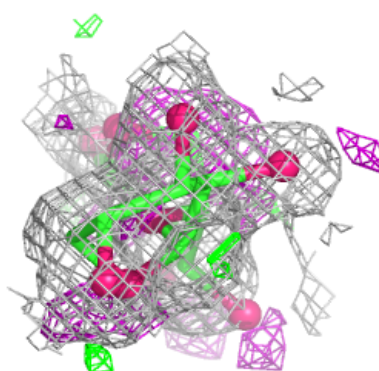
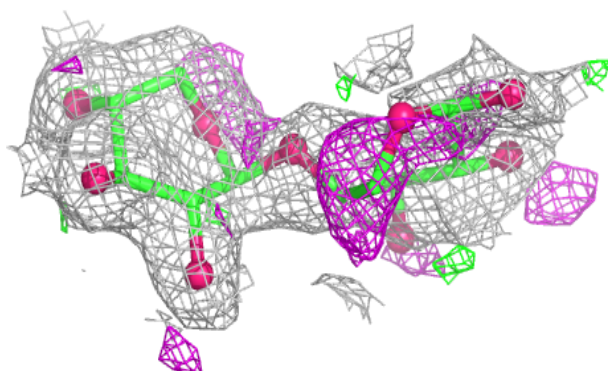
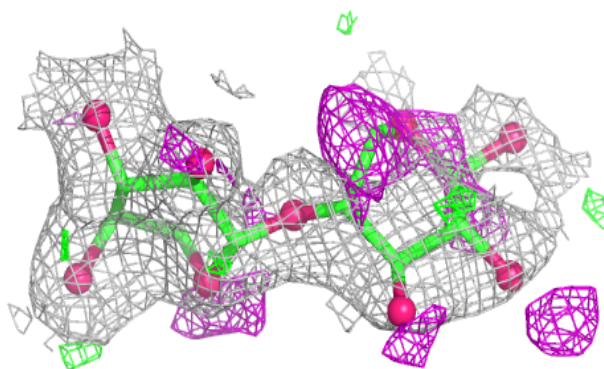
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYP	F	1	10/10	0.79	0.17	37,51,54,54	0
2	XYP	G	1	10/10	0.81	0.16	39,52,55,56	0
2	XYP	H	1	10/10	0.81	0.17	40,54,55,56	0
2	XYP	F	2	9/10	0.92	0.09	17,22,27,28	0
2	XYP	E	2	9/10	0.93	0.09	17,23,32,32	0
2	XYP	G	2	9/10	0.94	0.09	11,21,27,28	0
2	XYP	H	2	9/10	0.96	0.07	16,24,28,31	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.

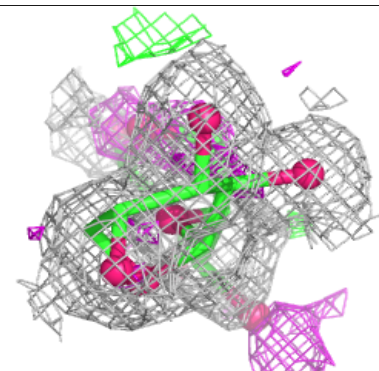
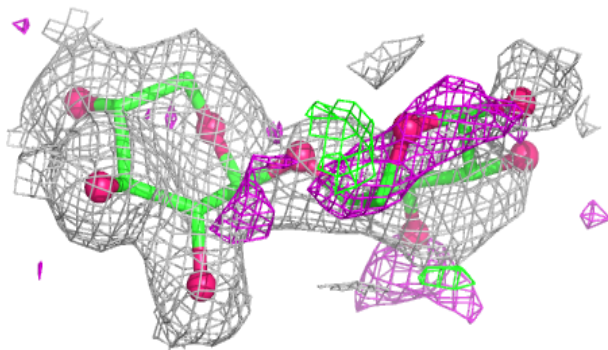
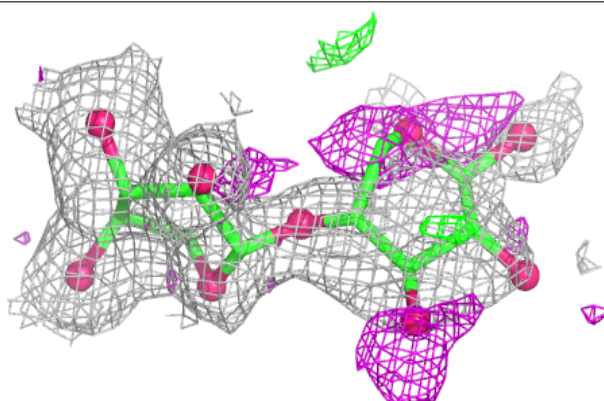


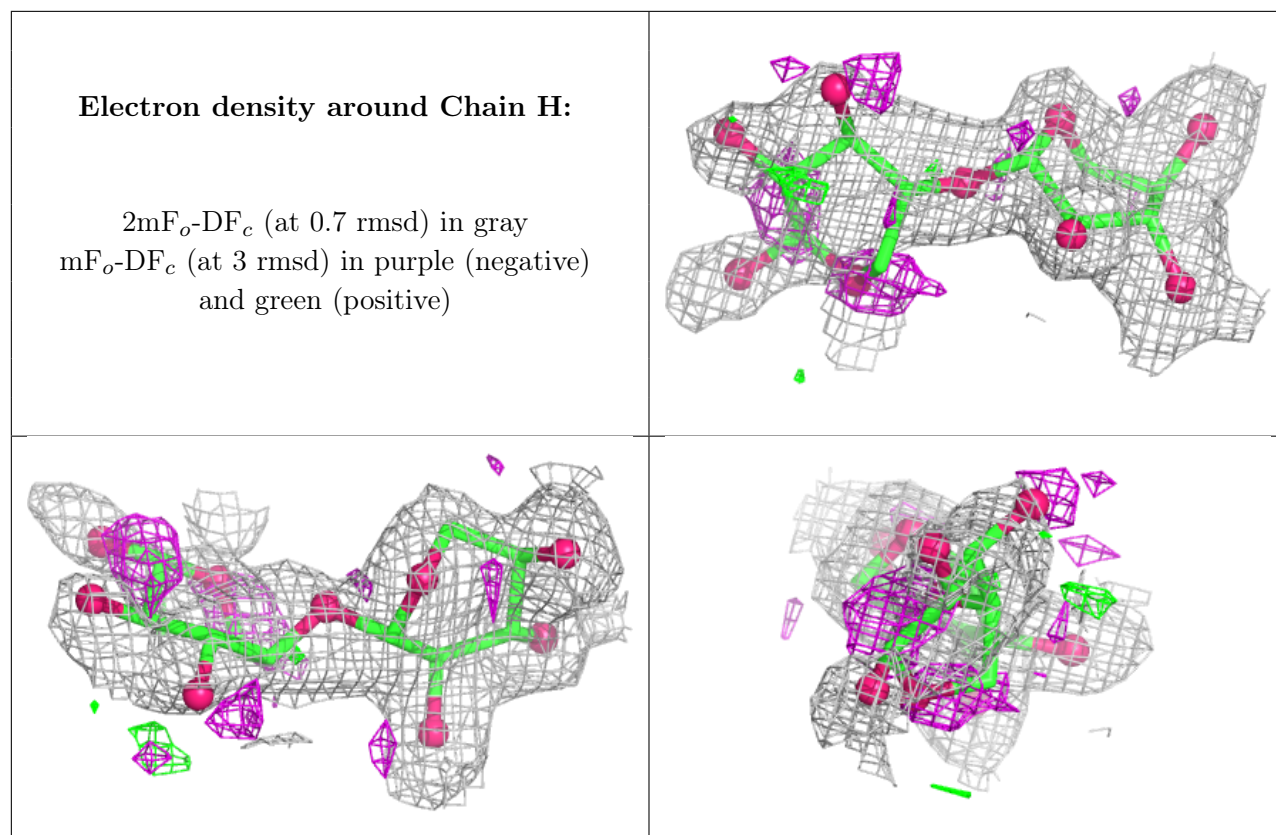
Electron density around Chain F:

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

**Electron density around Chain G:**

$2mF_o-DF_c$ (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.