



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:37 AM UTC

PDB ID : 2INV / pdb_00002inv
Title : Crystal structure of Inulin fructotransferase in the presence of di-fructose
Authors : Rhee, S.; Jung, W.S.
Deposited on : 2006-10-09
Resolution : 1.80 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

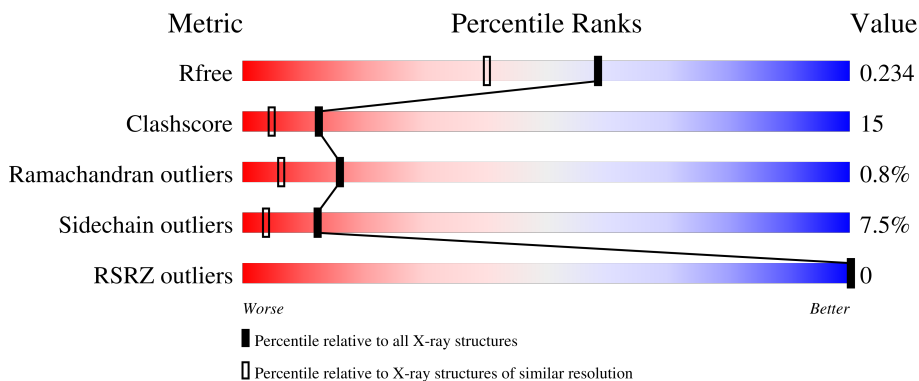
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	410	
1	B	410	
1	C	410	
2	D	2	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%

2 Entry composition [i](#)

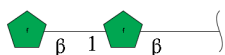
There are 4 unique types of molecules in this entry. The entry contains 9648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inulin fructotransferase.

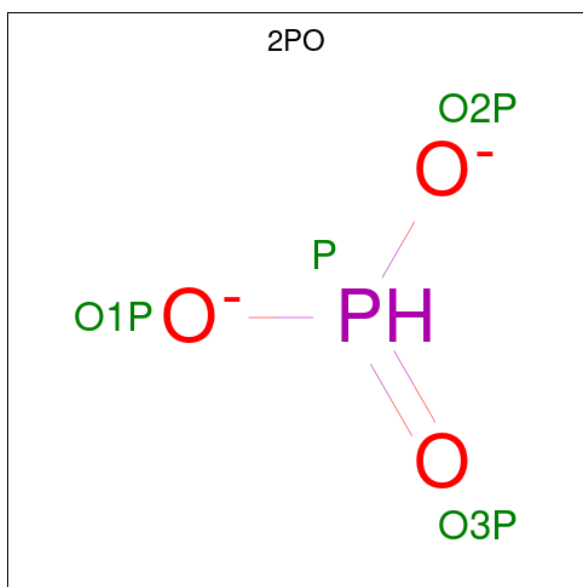
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	399	2982	1859	535	578	6	4	0	0	0
1	B	399	2982	1859	535	578	6	4	0	0	0
1	C	399	2982	1859	535	578	6	4	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is PHOSPHONATE (CCD ID: 2PO) (formula: HO₃P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 4 3 1	0	0
3	B	1	Total O P 4 3 1	0	0

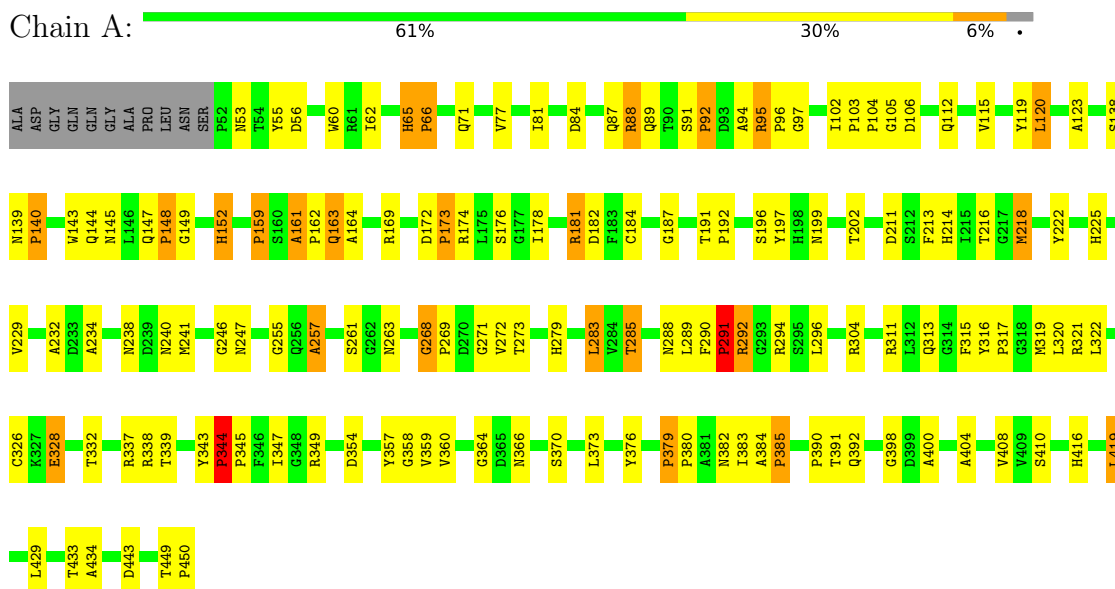
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	203	Total O 203 203	0	0
4	B	210	Total O 210 210	0	0
4	C	212	Total O 212 212	0	0

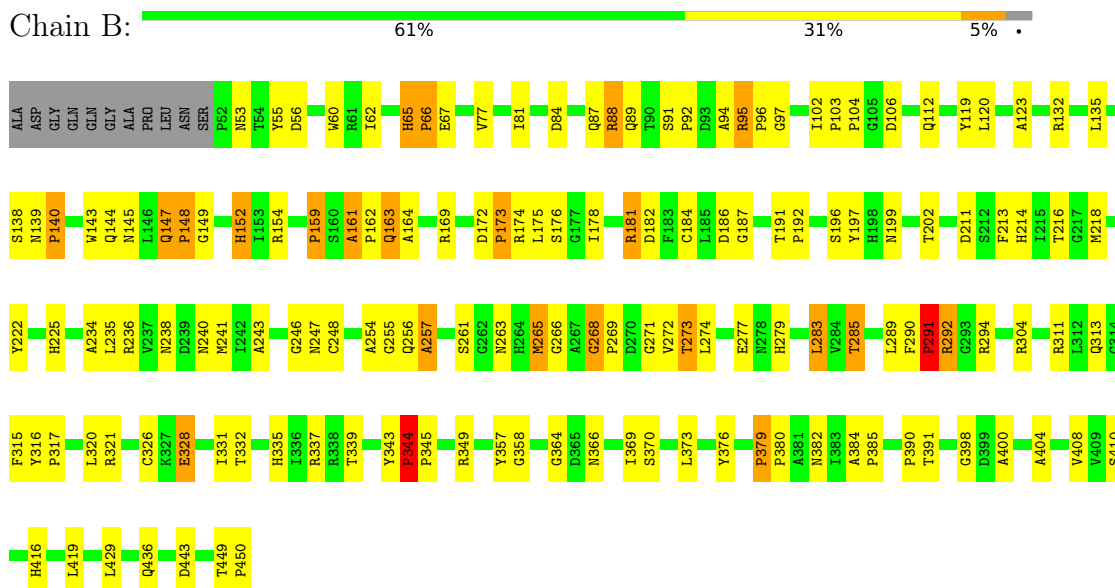
3 Residue-property plots

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: Inulin fructotransferase

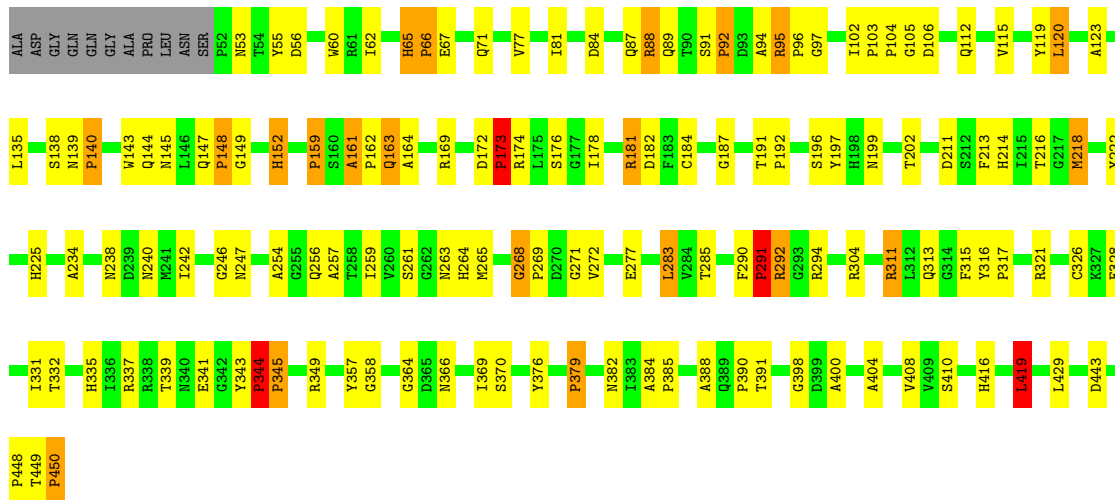


- Molecule 1: Inulin fructotransferase




- Molecule 1: Inulin fructotransferase

Chain C:  63% 28% 5% . . .



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain D:  50% 50%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain E:  100%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain F:  50% 50%

FRU1
FRU2

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.17Å 91.90Å 92.92Å 90.00° 124.82° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	82.4 (50.00-1.80) 98.1 (50.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.227 0.214 , 0.234	Depositor DCC
R_{free} test set	10154 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.012 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.013 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.019 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.019 for $-h+k-l, -l, -k$ 0.005 for $-h-k-l, l, k$ 0.019 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.005 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.487 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.487 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.013 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FRU, 2PO

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	0.69	9/3042 (0.3%)	1.49	49/4143 (1.2%)
1	B	0.66	5/3042 (0.2%)	1.51	51/4143 (1.2%)
1	C	0.64	5/3042 (0.2%)	1.76	53/4143 (1.3%)
All	All	0.66	19/9126 (0.2%)	1.59	153/12429 (1.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	C-N	19.16	1.60	1.33
1	B	291	PRO	C-N	18.08	1.58	1.33
1	C	291	PRO	C-N	16.81	1.56	1.33
1	B	285	THR	CB-OG1	8.87	1.57	1.43
1	A	285	THR	CB-OG1	8.78	1.57	1.43
1	C	331	ILE	CG1-CD1	-7.96	1.20	1.51
1	A	320	LEU	CB-CG	6.68	1.66	1.53
1	A	289	LEU	CG-CD2	-6.33	1.31	1.52
1	A	292	ARG	C-N	6.26	1.42	1.33
1	A	419	LEU	CG-CD1	-5.26	1.35	1.52
1	B	240	ASN	CG-OD1	5.25	1.33	1.23
1	A	240	ASN	CG-OD1	5.25	1.33	1.23
1	A	292	ARG	N-CA	5.22	1.56	1.46
1	B	292	ARG	N-CA	5.20	1.56	1.46
1	C	292	ARG	N-CA	5.19	1.56	1.46
1	B	263	ASN	CG-OD1	5.12	1.33	1.23
1	C	240	ASN	CG-OD1	5.11	1.33	1.23
1	A	263	ASN	CG-OD1	5.11	1.33	1.23
1	C	263	ASN	CG-OD1	5.06	1.33	1.23

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	ASP	CA-C-N	47.90	179.72	119.84
1	C	172	ASP	C-N-CA	47.90	179.72	119.84
1	B	291	PRO	O-C-N	-34.65	75.86	122.64
1	C	291	PRO	O-C-N	-33.80	77.02	122.64
1	A	291	PRO	O-C-N	-33.23	77.78	122.64
1	B	172	ASP	CA-C-N	20.95	177.28	127.00
1	B	172	ASP	C-N-CA	20.95	177.28	127.00
1	A	172	ASP	CA-C-N	20.57	176.38	127.00
1	A	172	ASP	C-N-CA	20.57	176.38	127.00
1	B	172	ASP	C-N-CD	-20.41	75.70	120.60
1	A	172	ASP	C-N-CD	-20.02	76.55	120.60
1	B	449	THR	N-CA-C	-12.62	90.96	109.50
1	A	449	THR	N-CA-C	-12.61	90.76	109.42
1	C	449	THR	N-CA-C	-12.44	91.02	109.42
1	C	172	ASP	C-N-CD	-12.19	75.03	125.00
1	C	95	ARG	CA-C-N	11.85	132.20	119.05
1	C	95	ARG	C-N-CA	11.85	132.20	119.05
1	A	95	ARG	CA-C-N	11.80	132.26	119.28
1	A	95	ARG	C-N-CA	11.80	132.26	119.28
1	B	95	ARG	CA-C-N	11.61	131.93	119.05
1	B	95	ARG	C-N-CA	11.61	131.93	119.05
1	B	147	GLN	N-CA-C	11.48	118.56	108.22
1	C	147	GLN	N-CA-C	8.96	118.64	108.25
1	A	147	GLN	N-CA-C	8.82	118.48	108.25
1	B	331	ILE	CB-CG1-CD1	8.73	132.13	113.80
1	A	384	ALA	C-N-CD	-8.55	101.79	120.60
1	A	291	PRO	N-CA-C	8.51	130.00	112.47
1	C	291	PRO	N-CA-C	8.45	129.87	112.47
1	B	291	PRO	N-CA-C	8.44	129.86	112.47
1	C	384	ALA	C-N-CD	-8.43	102.06	120.60
1	B	384	ALA	C-N-CD	-8.43	102.06	120.60
1	C	294	ARG	N-CA-C	-8.02	102.52	111.82
1	B	294	ARG	N-CA-C	-7.97	102.57	111.82
1	A	294	ARG	N-CA-C	-7.86	102.70	111.82
1	A	191	THR	C-N-CD	-7.62	103.83	120.60
1	C	191	THR	C-N-CD	-7.36	104.41	120.60
1	B	191	THR	C-N-CD	-7.21	104.74	120.60
1	A	343	TYR	CA-C-N	7.19	127.78	120.38
1	A	343	TYR	C-N-CA	7.19	127.78	120.38
1	C	331	ILE	CB-CG1-CD1	7.11	128.74	113.80
1	A	191	THR	CA-C-N	7.09	144.01	127.00
1	A	191	THR	C-N-CA	7.09	144.01	127.00
1	C	65	HIS	CA-C-N	7.04	127.34	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	HIS	C-N-CA	7.04	127.34	119.32
1	B	343	TYR	CA-C-N	7.01	127.60	120.38
1	B	343	TYR	C-N-CA	7.01	127.60	120.38
1	C	343	TYR	CA-C-N	7.01	127.60	120.38
1	C	343	TYR	C-N-CA	7.01	127.60	120.38
1	C	181	ARG	N-CA-C	6.92	119.86	108.99
1	B	65	HIS	CA-C-N	6.91	127.49	119.47
1	B	65	HIS	C-N-CA	6.91	127.49	119.47
1	C	344	PRO	N-CA-C	6.89	119.11	110.70
1	A	344	PRO	N-CA-C	6.87	119.08	110.70
1	B	344	PRO	N-CA-C	6.87	119.08	110.70
1	A	65	HIS	CA-C-N	6.87	127.44	119.47
1	A	65	HIS	C-N-CA	6.87	127.44	119.47
1	A	174	ARG	N-CA-C	-6.80	101.55	110.53
1	B	181	ARG	N-CA-C	6.67	119.21	109.07
1	A	139	ASN	CA-C-N	6.67	126.35	119.82
1	A	139	ASN	C-N-CA	6.67	126.35	119.82
1	B	161	ALA	CA-C-N	6.67	126.17	119.24
1	B	161	ALA	C-N-CA	6.67	126.17	119.24
1	A	181	ARG	N-CA-C	6.64	119.42	108.99
1	C	139	ASN	CA-C-N	6.63	126.32	119.82
1	C	139	ASN	C-N-CA	6.63	126.32	119.82
1	B	316	TYR	CA-C-N	6.63	126.61	119.78
1	B	316	TYR	C-N-CA	6.63	126.61	119.78
1	C	161	ALA	CA-C-N	6.62	126.13	119.24
1	C	161	ALA	C-N-CA	6.62	126.13	119.24
1	C	191	THR	CA-C-N	6.62	142.89	127.00
1	C	191	THR	C-N-CA	6.62	142.89	127.00
1	B	139	ASN	CA-C-N	6.54	126.23	119.82
1	B	139	ASN	C-N-CA	6.54	126.23	119.82
1	C	316	TYR	CA-C-N	6.46	126.43	119.78
1	C	316	TYR	C-N-CA	6.46	126.43	119.78
1	A	88	ARG	N-CA-C	6.36	118.29	111.36
1	B	191	THR	CA-C-N	6.32	142.16	127.00
1	B	191	THR	C-N-CA	6.32	142.16	127.00
1	A	316	TYR	CA-C-N	6.27	126.24	119.78
1	A	316	TYR	C-N-CA	6.27	126.24	119.78
1	C	184	CYS	N-CA-C	6.26	119.10	108.90
1	A	184	CYS	N-CA-C	6.21	119.02	108.90
1	B	273	THR	N-CA-C	-6.16	102.14	111.56
1	B	182	ASP	N-CA-C	6.13	119.88	111.54
1	C	174	ARG	N-CA-C	-6.01	101.58	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ALA	N-CA-C	-6.01	104.81	111.36
1	B	184	CYS	N-CA-C	5.97	118.63	108.90
1	A	147	GLN	CA-C-N	5.92	125.88	119.78
1	A	147	GLN	C-N-CA	5.92	125.88	119.78
1	C	147	GLN	CA-C-N	5.89	125.84	119.78
1	C	147	GLN	C-N-CA	5.89	125.84	119.78
1	B	147	GLN	CA-C-N	5.86	125.82	119.78
1	B	147	GLN	C-N-CA	5.86	125.82	119.78
1	B	174	ARG	N-CA-C	-5.85	101.82	110.48
1	C	164	ALA	N-CA-C	-5.84	105.00	111.36
1	C	366	ASN	N-CA-C	5.84	119.60	111.90
1	B	366	ASN	N-CA-C	5.80	119.56	111.90
1	A	164	ALA	N-CA-C	-5.80	104.88	111.14
1	B	218	MSE	N-CA-C	5.80	118.01	110.53
1	A	366	ASN	N-CA-C	5.77	119.52	111.90
1	A	182	ASP	N-CA-C	5.68	119.27	111.54
1	C	268	GLY	CA-C-N	5.68	125.79	119.32
1	C	268	GLY	C-N-CA	5.68	125.79	119.32
1	B	268	GLY	CA-C-N	5.65	125.76	119.32
1	B	268	GLY	C-N-CA	5.65	125.76	119.32
1	A	56	ASP	N-CA-C	-5.64	99.21	108.41
1	A	328	GLU	N-CA-C	5.64	119.18	111.39
1	A	268	GLY	CA-C-N	5.64	126.01	119.47
1	A	268	GLY	C-N-CA	5.64	126.01	119.47
1	B	102	ILE	CA-C-N	5.59	126.14	120.38
1	B	102	ILE	C-N-CA	5.59	126.14	120.38
1	B	60	TRP	N-CA-C	5.59	117.41	108.41
1	C	102	ILE	CA-C-N	5.55	126.10	120.38
1	C	102	ILE	C-N-CA	5.55	126.10	120.38
1	C	182	ASP	N-CA-C	5.55	119.09	111.54
1	C	60	TRP	N-CA-C	5.55	117.34	108.41
1	C	328	GLU	N-CA-C	5.52	119.05	111.54
1	C	56	ASP	N-CA-C	-5.50	99.44	108.41
1	B	328	GLU	N-CA-C	5.49	119.01	111.54
1	A	60	TRP	N-CA-C	5.46	117.20	108.41
1	C	357	TYR	N-CA-C	-5.44	105.51	111.82
1	C	88	ARG	N-CA-C	5.42	118.35	111.69
1	C	152	HIS	N-CA-C	5.41	117.05	108.67
1	C	419	LEU	CD1-CG-CD2	5.40	122.69	110.80
1	A	102	ILE	CA-C-N	5.40	125.94	120.38
1	A	102	ILE	C-N-CA	5.40	125.94	120.38
1	B	56	ASP	N-CA-C	-5.39	99.62	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	MSE	N-CA-C	5.39	117.49	110.53
1	C	216	THR	N-CA-C	5.37	117.34	109.24
1	A	357	TYR	N-CA-C	-5.36	105.60	111.82
1	C	163	GLN	N-CA-C	5.36	118.00	109.96
1	A	218	MSE	N-CA-C	5.34	117.42	110.53
1	B	152	HIS	N-CA-C	5.33	116.93	108.67
1	B	216	THR	N-CA-C	5.32	117.28	109.24
1	C	400	ALA	N-CA-C	5.29	119.68	113.23
1	A	152	HIS	N-CA-C	5.25	116.80	108.67
1	B	321	ARG	N-CA-C	5.20	117.38	108.90
1	C	388	ALA	N-CA-C	5.19	118.16	110.48
1	B	357	TYR	N-CA-C	-5.18	105.82	111.82
1	B	88	ARG	N-CA-C	5.17	118.05	111.69
1	A	321	ARG	N-CA-C	5.15	117.30	108.90
1	A	216	THR	N-CA-C	5.14	117.01	109.24
1	C	173	PRO	CA-N-CD	-5.14	104.81	112.00
1	B	400	ALA	N-CA-C	5.13	119.49	113.23
1	B	436	GLN	N-CA-C	-5.11	106.28	112.88
1	B	163	GLN	N-CA-C	5.10	117.61	109.96
1	C	321	ARG	N-CA-C	5.10	117.21	108.90
1	C	105	GLY	N-CA-C	5.07	117.84	111.09
1	A	163	GLN	N-CA-C	5.07	117.56	109.96
1	A	161	ALA	CA-C-N	5.05	126.15	119.84
1	A	161	ALA	C-N-CA	5.05	126.15	119.84
1	A	400	ALA	N-CA-C	5.04	119.37	113.23
1	A	105	GLY	N-CA-C	5.02	117.91	110.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2982	0	2905	109	0
1	B	2982	0	2905	106	0
1	C	2982	0	2905	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23	0	21	3	0
2	E	23	0	21	3	0
2	F	23	0	21	3	0
3	A	4	0	1	0	0
3	B	4	0	1	0	0
4	A	203	0	0	1	0
4	B	210	0	0	0	0
4	C	212	0	0	2	0
All	All	9648	0	8780	272	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 15.

All (272) 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:265:MSE:HE3	1:B:273:THR:HG22	1.32	1.10
1:A:319:MSE:HE1	1:A:338:ARG:HB2	1.39	1.01
1:C:291:PRO:HB2	2:F:2:FRU:O6	1.67	0.93
1:A:291:PRO:HB2	2:D:2:FRU:O6	1.70	0.90
1:B:291:PRO:HB2	2:E:2:FRU:O6	1.73	0.89
1:A:283:LEU:HD22	1:A:285:THR:HG23	1.55	0.89
1:B:265:MSE:CE	1:B:273:THR:HG22	2.03	0.88
1:B:265:MSE:HE2	1:B:289:LEU:HD22	1.56	0.87
1:C:283:LEU:HD22	1:C:285:THR:HG23	1.57	0.85
1:A:359:VAL:HG22	1:A:392:GLN:O	1.77	0.84
1:B:269:PRO:HD3	1:B:292:ARG:HG3	1.60	0.83
1:A:269:PRO:HD3	1:A:292:ARG:HG3	1.62	0.81
1:A:283:LEU:HD22	1:A:285:THR:CG2	2.16	0.75
1:A:95:ARG:N	1:A:96:PRO:HD3	2.00	0.75
1:A:145:ASN:HD21	1:C:169:ARG:HH12	1.35	0.75
1:C:95:ARG:N	1:C:96:PRO:HD3	2.02	0.75
1:B:283:LEU:HD22	1:B:285:THR:HG23	1.69	0.74
1:C:269:PRO:HD3	1:C:292:ARG:HG3	1.69	0.74
1:B:169:ARG:HH12	1:C:145:ASN:HD21	1.34	0.73
1:B:265:MSE:HE1	1:B:274:LEU:HB2	1.71	0.73
1:C:138:SER:O	1:C:140:PRO:HD3	1.88	0.73
1:A:169:ARG:HH12	1:B:145:ASN:HD21	1.35	0.72
1:A:234:ALA:HB1	1:B:241:MSE:HE1	1.71	0.72
1:A:138:SER:O	1:A:140:PRO:HD3	1.91	0.71
1:C:283:LEU:HD22	1:C:285:THR:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ARG:N	1:B:96:PRO:HD3	2.03	0.71
1:A:241:MSE:HE1	1:C:234:ALA:HB1	1.71	0.71
1:A:319:MSE:HE3	1:A:359:VAL:HB	1.72	0.70
1:A:359:VAL:HG23	1:A:360:VAL:HG23	1.73	0.69
1:B:138:SER:O	1:B:140:PRO:HD3	1.91	0.69
1:C:89:GLN:HE22	1:C:97:GLY:H	1.40	0.68
1:C:53:ASN:HD22	1:C:88:ARG:HH22	1.39	0.68
1:B:265:MSE:HE3	1:B:273:THR:CG2	2.20	0.67
1:A:89:GLN:HE22	1:A:97:GLY:H	1.44	0.66
1:A:53:ASN:HD22	1:A:88:ARG:HH22	1.43	0.65
1:C:247:ASN:HD22	1:C:272:VAL:HG22	1.63	0.64
1:C:291:PRO:HB2	2:F:2:FRU:C6	2.28	0.64
1:A:247:ASN:HD22	1:A:272:VAL:HG22	1.64	0.63
1:B:89:GLN:HE22	1:B:97:GLY:H	1.47	0.63
1:A:173:PRO:HG3	1:B:143:TRP:CE3	2.34	0.62
1:B:53:ASN:HD22	1:B:88:ARG:HH22	1.46	0.62
1:C:53:ASN:ND2	1:C:88:ARG:HH22	1.98	0.62
1:B:173:PRO:HG3	1:C:143:TRP:CE3	2.34	0.62
1:C:344:PRO:HB2	1:C:345:PRO:HD3	1.80	0.62
1:A:344:PRO:HB2	1:A:345:PRO:HD3	1.82	0.62
1:B:344:PRO:HB2	1:B:345:PRO:HD3	1.81	0.61
1:C:91:SER:HB2	1:C:94:ALA:HB3	1.83	0.61
1:A:143:TRP:CE3	1:C:173:PRO:HG3	2.35	0.61
1:C:290:PHE:HB2	1:C:291:PRO:HD2	1.82	0.60
1:A:89:GLN:O	1:A:95:ARG:HD3	2.02	0.60
1:C:91:SER:O	1:C:95:ARG:HG3	2.02	0.60
1:C:89:GLN:O	1:C:95:ARG:HD3	2.02	0.59
1:C:242:ILE:HB	1:C:265:MSE:HG2	1.82	0.59
1:B:84:ASP:O	1:B:87:GLN:HB3	2.03	0.59
1:B:89:GLN:O	1:B:95:ARG:HD3	2.03	0.58
1:A:89:GLN:HB3	1:A:95:ARG:HG2	1.86	0.58
1:B:265:MSE:HB3	1:B:273:THR:CG2	2.33	0.58
1:A:106:ASP:CG	1:C:96:PRO:HG3	2.29	0.57
1:A:91:SER:O	1:A:95:ARG:HG3	2.05	0.57
1:A:94:ALA:C	1:A:96:PRO:HD3	2.30	0.57
1:B:91:SER:O	1:B:95:ARG:HG3	2.05	0.56
1:B:89:GLN:HB3	1:B:95:ARG:HG2	1.88	0.56
1:A:144:GLN:H	1:C:173:PRO:HD2	1.70	0.56
1:C:291:PRO:CB	2:F:2:FRU:O6	2.48	0.56
1:C:89:GLN:HB3	1:C:95:ARG:HG2	1.88	0.56
1:B:53:ASN:CB	1:C:104:PRO:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PRO:HG3	1:C:106:ASP:CG	2.31	0.55
1:A:96:PRO:HG3	1:B:106:ASP:CG	2.31	0.55
1:A:173:PRO:HD2	1:B:144:GLN:H	1.71	0.55
1:C:94:ALA:C	1:C:96:PRO:HD3	2.31	0.55
1:A:123:ALA:HA	1:A:181:ARG:O	2.07	0.55
1:A:53:ASN:ND2	1:A:88:ARG:HH22	2.05	0.54
1:B:404:ALA:HA	1:B:429:LEU:O	2.06	0.54
1:C:84:ASP:O	1:C:87:GLN:HB3	2.07	0.54
1:A:319:MSE:CE	1:A:338:ARG:HB2	2.25	0.54
1:A:112:GLN:HG3	1:A:163:GLN:O	2.08	0.54
1:B:291:PRO:HB2	2:E:2:FRU:C6	2.38	0.54
1:A:283:LEU:HG	1:B:311:ARG:HB2	1.90	0.54
1:B:328:GLU:O	1:C:335:HIS:HE1	1.91	0.54
1:C:364:GLY:O	1:C:398:GLY:HA3	2.08	0.53
1:B:119:TYR:CD2	1:C:149:GLY:HA3	2.43	0.53
1:C:326:CYS:O	1:C:364:GLY:HA3	2.09	0.53
1:A:291:PRO:HB2	2:D:2:FRU:C6	2.37	0.53
1:A:290:PHE:HB2	1:A:291:PRO:HD2	1.90	0.53
1:B:291:PRO:HD3	1:B:313:GLN:HB3	1.91	0.53
1:A:104:PRO:HB2	1:C:53:ASN:CB	2.39	0.53
1:A:311:ARG:HB2	1:C:283:LEU:HG	1.90	0.53
1:A:319:MSE:CE	1:A:359:VAL:HB	2.38	0.53
1:B:283:LEU:HD22	1:B:285:THR:CG2	2.38	0.53
1:A:169:ARG:HH22	1:B:145:ASN:HD22	1.57	0.53
1:B:283:LEU:HG	1:C:311:ARG:HB2	1.91	0.53
1:B:358:GLY:HA2	1:B:391:THR:O	2.08	0.53
1:A:91:SER:HB2	1:A:94:ALA:HB3	1.90	0.52
1:B:290:PHE:HB2	1:B:291:PRO:HD2	1.89	0.52
1:A:326:CYS:O	1:A:364:GLY:HA3	2.09	0.52
1:A:62:ILE:HD11	1:A:77:VAL:HA	1.91	0.52
1:B:53:ASN:ND2	1:B:88:ARG:HH22	2.08	0.52
1:C:234:ALA:HA	1:C:257:ALA:O	2.10	0.52
1:B:364:GLY:O	1:B:398:GLY:HA3	2.11	0.51
1:C:404:ALA:HA	1:C:429:LEU:O	2.10	0.51
1:B:94:ALA:C	1:B:96:PRO:HD3	2.34	0.51
1:B:178:ILE:HD12	1:B:213:PHE:CZ	2.45	0.51
1:C:112:GLN:HG3	1:C:163:GLN:O	2.11	0.51
1:B:247:ASN:HD22	1:B:272:VAL:HG22	1.75	0.51
1:B:123:ALA:HA	1:B:181:ARG:O	2.10	0.51
1:B:169:ARG:HH22	1:C:145:ASN:HD22	1.57	0.51
1:C:71:GLN:HG3	4:C:541:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:N	1:A:96:PRO:CD	2.71	0.51
1:A:379:PRO:HB2	1:A:382:ASN:ND2	2.25	0.51
1:A:148:PRO:HB2	1:A:152:HIS:CE1	2.46	0.51
1:C:358:GLY:HA2	1:C:391:THR:O	2.11	0.51
1:B:65:HIS:N	1:B:66:PRO:HD3	2.26	0.50
1:A:358:GLY:HA2	1:A:391:THR:O	2.12	0.50
1:B:112:GLN:HG3	1:B:163:GLN:O	2.11	0.50
1:A:53:ASN:CB	1:B:104:PRO:HB2	2.42	0.50
1:A:433:THR:HG22	1:A:434:ALA:N	2.26	0.50
1:A:328:GLU:O	1:B:335:HIS:HE1	1.95	0.50
1:C:148:PRO:HB2	1:C:152:HIS:CE1	2.47	0.50
1:A:149:GLY:HA3	1:C:119:TYR:CD2	2.47	0.50
1:B:291:PRO:HD3	1:B:313:GLN:O	2.12	0.50
1:A:408:VAL:HB	1:A:416:HIS:CE1	2.47	0.49
1:C:123:ALA:HA	1:C:181:ARG:O	2.12	0.49
1:C:92:PRO:HG3	1:C:95:ARG:NH2	2.27	0.49
1:B:53:ASN:HB3	1:C:104:PRO:HB2	1.94	0.49
1:B:62:ILE:HD11	1:B:77:VAL:HA	1.94	0.49
1:A:159:PRO:O	1:A:162:PRO:HD3	2.13	0.49
1:A:246:GLY:O	1:A:271:GLY:HA3	2.12	0.49
1:A:404:ALA:HA	1:A:429:LEU:O	2.12	0.49
1:A:71:GLN:HG3	4:A:1082:HOH:O	2.13	0.49
1:C:379:PRO:HB2	1:C:382:ASN:ND2	2.28	0.49
1:A:187:GLY:HA3	1:A:222:TYR:O	2.12	0.49
1:C:246:GLY:O	1:C:271:GLY:HA3	2.13	0.49
1:A:169:ARG:HH12	1:B:145:ASN:ND2	2.08	0.49
1:A:84:ASP:O	1:A:87:GLN:HB3	2.13	0.48
1:A:291:PRO:HD3	1:A:313:GLN:O	2.13	0.48
1:B:135:LEU:HD12	1:B:140:PRO:HG3	1.94	0.48
1:A:119:TYR:CD2	1:B:149:GLY:HA3	2.47	0.48
1:A:115:VAL:HG13	1:A:120:LEU:HD12	1.95	0.48
1:C:65:HIS:N	1:C:66:PRO:HD3	2.28	0.48
1:C:159:PRO:O	1:C:162:PRO:HD3	2.13	0.48
1:B:135:LEU:CD1	1:B:140:PRO:HG3	2.43	0.48
1:A:92:PRO:HG3	1:A:95:ARG:NH2	2.28	0.48
1:B:169:ARG:HH12	1:C:145:ASN:ND2	2.08	0.48
1:B:169:ARG:HH22	1:C:145:ASN:ND2	2.12	0.48
1:C:214:HIS:HE1	1:C:238:ASN:OD1	1.95	0.48
1:A:288:ASN:HB2	1:C:259:ILE:HD11	1.96	0.48
1:B:238:ASN:HA	1:B:261:SER:O	2.14	0.48
1:A:178:ILE:HD12	1:A:213:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:HA	1:A:261:SER:O	2.13	0.48
1:B:255:GLY:HA3	1:B:279:HIS:CE1	2.48	0.48
1:C:115:VAL:HG13	1:C:120:LEU:HD12	1.95	0.48
1:C:95:ARG:N	1:C:96:PRO:CD	2.72	0.48
1:A:145:ASN:ND2	1:C:169:ARG:HH12	2.08	0.47
1:B:173:PRO:HD2	1:C:144:GLN:H	1.78	0.47
1:C:196:SER:O	1:C:197:TYR:HB2	2.14	0.47
1:A:104:PRO:HB2	1:C:53:ASN:HB3	1.95	0.47
1:C:187:GLY:HA3	1:C:222:TYR:O	2.14	0.47
1:C:337:ARG:HG3	1:C:337:ARG:HH11	1.79	0.47
1:A:291:PRO:HD3	1:A:313:GLN:HB3	1.97	0.47
1:B:326:CYS:O	1:B:364:GLY:HA3	2.14	0.47
1:C:178:ILE:HD12	1:C:213:PHE:CZ	2.50	0.47
1:C:448:PRO:O	1:C:450:PRO:HD3	2.14	0.47
1:A:364:GLY:O	1:A:398:GLY:HA3	2.14	0.47
1:B:53:ASN:HB2	1:C:104:PRO:HB2	1.96	0.47
1:B:196:SER:O	1:B:197:TYR:HB2	2.14	0.47
1:C:135:LEU:HD12	1:C:140:PRO:HG3	1.97	0.47
1:C:315:PHE:HA	1:C:339:THR:O	2.15	0.47
1:B:159:PRO:O	1:B:162:PRO:HD3	2.14	0.47
1:A:106:ASP:OD1	1:A:152:HIS:HD2	1.98	0.47
1:B:248:CYS:CB	1:B:265:MSE:HG2	2.45	0.46
1:A:65:HIS:N	1:A:66:PRO:HD3	2.30	0.46
1:B:91:SER:HB3	1:B:94:ALA:HB3	1.96	0.46
1:C:62:ILE:HD11	1:C:77:VAL:HA	1.97	0.46
1:C:419:LEU:N	1:C:419:LEU:HD22	2.30	0.46
1:A:255:GLY:HA3	1:A:279:HIS:CE1	2.50	0.46
1:B:106:ASP:OD1	1:B:152:HIS:HD2	1.98	0.46
1:B:376:TYR:O	1:B:410:SER:HA	2.16	0.46
1:A:380:PRO:HA	1:A:383:ILE:HD12	1.96	0.46
1:C:290:PHE:HB2	1:C:291:PRO:CD	2.46	0.46
1:B:320:LEU:C	1:B:320:LEU:HD23	2.41	0.46
1:A:161:ALA:N	1:A:162:PRO:HD3	2.30	0.46
1:A:169:ARG:HH22	1:B:145:ASN:ND2	2.13	0.46
1:B:265:MSE:HB3	1:B:273:THR:HG22	1.98	0.46
1:C:106:ASP:OD1	1:C:152:HIS:HD2	1.98	0.46
1:A:214:HIS:HE1	1:A:238:ASN:OD1	1.99	0.45
1:A:196:SER:O	1:A:197:TYR:HB2	2.15	0.45
1:B:268:GLY:C	1:B:292:ARG:O	2.60	0.45
1:C:337:ARG:HD3	4:C:534:HOH:O	2.15	0.45
1:A:53:ASN:HB2	1:B:104:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PRO:HB2	1:B:152:HIS:CE1	2.51	0.45
1:C:161:ALA:N	1:C:162:PRO:HD3	2.32	0.45
1:B:161:ALA:N	1:B:162:PRO:HD3	2.31	0.45
1:C:218:MSE:HE3	1:C:218:MSE:HB3	1.80	0.45
1:A:53:ASN:HD21	1:A:88:ARG:HH12	1.65	0.45
1:A:379:PRO:HB2	1:A:382:ASN:HD22	1.82	0.45
1:B:214:HIS:HE1	1:B:238:ASN:OD1	2.00	0.45
1:B:187:GLY:HA3	1:B:222:TYR:O	2.17	0.45
1:A:145:ASN:HD22	1:C:169:ARG:HH22	1.65	0.44
1:C:268:GLY:C	1:C:292:ARG:O	2.60	0.44
1:C:311:ARG:HD3	1:C:311:ARG:C	2.42	0.44
1:A:315:PHE:HA	1:A:339:THR:O	2.17	0.44
1:B:243:ALA:HA	1:B:266:GLY:O	2.18	0.44
1:A:268:GLY:C	1:A:292:ARG:O	2.61	0.44
1:C:135:LEU:CD1	1:C:140:PRO:HG3	2.47	0.44
1:B:254:ALA:HA	1:B:277:GLU:O	2.17	0.44
1:B:234:ALA:HA	1:B:257:ALA:O	2.18	0.44
1:C:254:ALA:HA	1:C:277:GLU:O	2.18	0.44
1:A:55:TYR:CE2	1:A:81:ILE:HG23	2.53	0.44
1:A:291:PRO:CB	2:D:2:FRU:O6	2.55	0.43
1:C:55:TYR:CE2	1:C:81:ILE:HG23	2.53	0.43
1:C:202:THR:HA	1:C:225:HIS:O	2.17	0.43
1:C:238:ASN:HA	1:C:261:SER:O	2.18	0.43
1:B:55:TYR:CE2	1:B:81:ILE:HG23	2.53	0.43
1:B:332:THR:HA	1:B:370:SER:O	2.19	0.43
1:B:369:ILE:HD12	1:B:369:ILE:N	2.33	0.43
1:B:311:ARG:C	1:B:311:ARG:HD3	2.44	0.43
1:A:354:ASP:HB2	1:A:385:PRO:HD3	2.00	0.43
1:C:369:ILE:N	1:C:369:ILE:HD12	2.34	0.43
1:B:315:PHE:HA	1:B:339:THR:O	2.19	0.43
1:A:376:TYR:O	1:A:410:SER:HA	2.19	0.43
1:A:229:VAL:HG12	1:A:232:ALA:HB2	2.01	0.42
1:C:376:TYR:O	1:C:410:SER:HA	2.19	0.42
1:B:373:LEU:C	1:B:373:LEU:HD23	2.45	0.42
1:C:315:PHE:CD2	1:C:341:GLU:HA	2.54	0.42
1:A:344:PRO:HA	1:A:347:ILE:HG13	2.01	0.42
1:A:373:LEU:C	1:A:373:LEU:HD23	2.44	0.42
1:C:247:ASN:ND2	1:C:272:VAL:H	2.17	0.42
1:A:202:THR:HA	1:A:225:HIS:O	2.19	0.42
1:B:152:HIS:HE1	1:B:186:ASP:OD2	2.01	0.42
1:A:145:ASN:H	1:C:173:PRO:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:THR:HB	1:A:296:LEU:O	2.20	0.42
1:B:235:LEU:HG	1:B:236:ARG:N	2.34	0.42
1:B:256:GLN:O	1:B:257:ALA:C	2.63	0.42
1:C:337:ARG:HG3	1:C:337:ARG:NH1	2.34	0.42
1:A:173:PRO:HG2	1:B:145:ASN:H	1.83	0.42
1:A:332:THR:HA	1:A:370:SER:O	2.20	0.42
1:A:433:THR:HG22	1:A:434:ALA:H	1.84	0.42
1:A:291:PRO:HB3	1:A:315:PHE:CE2	2.55	0.42
1:A:104:PRO:HB2	1:C:53:ASN:HB2	2.01	0.42
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.94	0.42
1:B:269:PRO:N	1:B:292:ARG:O	2.53	0.42
1:A:138:SER:C	1:A:140:PRO:HD3	2.45	0.42
1:A:291:PRO:HD2	1:A:313:GLN:NE2	2.35	0.42
1:B:379:PRO:HB2	1:B:382:ASN:ND2	2.35	0.42
1:A:173:PRO:HD3	1:B:143:TRP:CG	2.55	0.41
1:B:132:ARG:NH2	1:B:147:GLN:HG2	2.35	0.41
1:A:288:ASN:OD1	1:A:311:ARG:HD2	2.20	0.41
1:B:173:PRO:HG2	1:C:145:ASN:H	1.84	0.41
1:B:176:SER:HA	1:B:211:ASP:O	2.20	0.41
1:A:218:MSE:HE3	1:A:218:MSE:HB3	1.88	0.41
1:C:92:PRO:HG3	1:C:95:ARG:HH21	1.85	0.41
1:C:332:THR:HA	1:C:370:SER:O	2.20	0.41
1:A:53:ASN:HB3	1:B:104:PRO:HB2	2.02	0.41
1:C:283:LEU:CD2	1:C:285:THR:HG23	2.41	0.41
1:A:143:TRP:CG	1:C:173:PRO:HD3	2.56	0.41
1:A:176:SER:HA	1:A:211:ASP:O	2.21	0.41
1:B:138:SER:C	1:B:140:PRO:HD3	2.44	0.41
1:C:176:SER:HA	1:C:211:ASP:O	2.20	0.41
1:A:234:ALA:HA	1:A:257:ALA:O	2.21	0.41
1:A:269:PRO:N	1:A:292:ARG:O	2.54	0.41
1:B:202:THR:HA	1:B:225:HIS:O	2.21	0.41
1:B:246:GLY:O	1:B:271:GLY:HA3	2.21	0.41
2:E:1:FRU:H12	2:E:2:FRU:H12	1.80	0.41
1:B:147:GLN:OE1	1:B:154:ARG:NH1	2.54	0.41
1:C:138:SER:C	1:C:140:PRO:HD3	2.45	0.41
1:C:291:PRO:HD3	1:C:313:GLN:HB3	2.03	0.41
1:B:408:VAL:HB	1:B:416:HIS:CE1	2.56	0.40
1:A:311:ARG:C	1:A:311:ARG:HD3	2.47	0.40
1:B:379:PRO:O	1:B:380:PRO:C	2.64	0.40
1:C:408:VAL:HB	1:C:416:HIS:CE1	2.56	0.40
1:B:236:ARG:HG3	1:C:264:HIS:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PHE:CG	1:C:341:GLU:HA	2.57	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	397/410 (97%)	369 (93%)	25 (6%)	3 (1%)	16	6
1	B	397/410 (97%)	369 (93%)	25 (6%)	3 (1%)	16	6
1	C	397/410 (97%)	368 (93%)	26 (6%)	3 (1%)	16	6
All	All	1191/1230 (97%)	1106 (93%)	76 (6%)	9 (1%)	16	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	PRO
1	A	199	ASN
1	B	199	ASN
1	C	199	ASN
1	B	257	ALA
1	A	257	ALA
1	B	291	PRO
1	C	291	PRO
1	A	291	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/325 (99%)	299 (93%)	23 (7%)	13	4
1	B	322/325 (99%)	298 (92%)	24 (8%)	12	4
1	C	322/325 (99%)	297 (92%)	25 (8%)	11	3
All	All	966/975 (99%)	894 (92%)	72 (8%)	12	4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	92	PRO
1	A	103	PRO
1	A	120	LEU
1	A	140	PRO
1	A	148	PRO
1	A	159	PRO
1	A	173	PRO
1	A	192	PRO
1	A	283	LEU
1	A	291	PRO
1	A	304	ARG
1	A	317	PRO
1	A	322	LEU
1	A	337	ARG
1	A	344	PRO
1	A	349	ARG
1	A	379	PRO
1	A	385	PRO
1	A	390	PRO
1	A	419	LEU
1	A	443	ASP
1	A	450	PRO
1	B	66	PRO
1	B	67	GLU
1	B	92	PRO
1	B	103	PRO
1	B	120	LEU
1	B	140	PRO
1	B	148	PRO
1	B	159	PRO

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Mol	Chain	Res	Type
1	B	173	PRO
1	B	192	PRO
1	B	265	MSE
1	B	283	LEU
1	B	291	PRO
1	B	304	ARG
1	B	317	PRO
1	B	337	ARG
1	B	344	PRO
1	B	349	ARG
1	B	379	PRO
1	B	385	PRO
1	B	390	PRO
1	B	419	LEU
1	B	443	ASP
1	B	450	PRO
1	C	66	PRO
1	C	67	GLU
1	C	92	PRO
1	C	103	PRO
1	C	120	LEU
1	C	140	PRO
1	C	148	PRO
1	C	159	PRO
1	C	173	PRO
1	C	192	PRO
1	C	256	GLN
1	C	283	LEU
1	C	291	PRO
1	C	304	ARG
1	C	311	ARG
1	C	317	PRO
1	C	344	PRO
1	C	345	PRO
1	C	349	ARG
1	C	379	PRO
1	C	385	PRO
1	C	390	PRO
1	C	419	LEU
1	C	443	ASP
1	C	450	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	89	GLN
1	A	112	GLN
1	A	137	ASN
1	A	145	ASN
1	A	152	HIS
1	A	195	ASN
1	A	214	HIS
1	A	247	ASN
1	A	256	GLN
1	A	264	HIS
1	A	313	GLN
1	A	324	ASN
1	A	377	ASN
1	A	382	ASN
1	A	392	GLN
1	A	415	GLN
1	A	425	HIS
1	B	53	ASN
1	B	89	GLN
1	B	112	GLN
1	B	137	ASN
1	B	145	ASN
1	B	152	HIS
1	B	195	ASN
1	B	214	HIS
1	B	247	ASN
1	B	313	GLN
1	B	324	ASN
1	B	335	HIS
1	B	382	ASN
1	B	389	GLN
1	B	416	HIS
1	C	53	ASN
1	C	71	GLN
1	C	89	GLN
1	C	112	GLN
1	C	137	ASN
1	C	145	ASN
1	C	152	HIS
1	C	195	ASN
1	C	214	HIS

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Mol	Chain	Res	Type
1	C	238	ASN
1	C	247	ASN
1	C	264	HIS
1	C	313	GLN
1	C	324	ASN
1	C	335	HIS
1	C	377	ASN
1	C	382	ASN
1	C	392	GLN
1	C	425	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 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	FRU	D	1	2	11,12,12	3.93	3 (27%)	10,18,18	2.44	2 (20%)
2	FRU	D	2	2	11,11,12	1.13	1 (9%)	15,15,18	2.51	4 (26%)
2	FRU	E	1	2	11,12,12	3.32	3 (27%)	10,18,18	2.90	3 (30%)
2	FRU	E	2	2	11,11,12	1.13	1 (9%)	15,15,18	2.51	4 (26%)
2	FRU	F	1	2	11,12,12	3.12	3 (27%)	10,18,18	1.98	2 (20%)
2	FRU	F	2	2	11,11,12	1.14	1 (9%)	15,15,18	2.52	4 (26%)

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	FRU	D	1	2	-	0/5/24/24	0/1/1/1
2	FRU	D	2	2	-	1/4/20/24	0/1/1/1
2	FRU	E	1	2	-	2/5/24/24	0/1/1/1
2	FRU	E	2	2	-	1/4/20/24	0/1/1/1
2	FRU	F	1	2	-	0/5/24/24	0/1/1/1
2	FRU	F	2	2	-	1/4/20/24	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	FRU	O1-C1	-9.18	1.13	1.42
2	D	1	FRU	O1-C1	-9.18	1.13	1.42
2	E	1	FRU	O1-C1	-9.18	1.13	1.42
2	D	1	FRU	O6-C6	-8.34	1.07	1.42
2	E	1	FRU	O6-C6	-4.32	1.24	1.42
2	D	1	FRU	C1-C2	3.05	1.59	1.52
2	F	1	FRU	C1-C2	3.05	1.59	1.52
2	E	1	FRU	C1-C2	3.04	1.59	1.52
2	F	1	FRU	O6-C6	-2.66	1.31	1.42
2	F	2	FRU	C1-C2	2.23	1.59	1.51
2	D	2	FRU	C1-C2	2.22	1.59	1.51
2	E	2	FRU	C1-C2	2.22	1.59	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	FRU	O6-C6-C5	7.82	137.96	111.33
2	E	2	FRU	O3-C3-C2	7.54	132.75	111.08
2	D	2	FRU	O3-C3-C2	7.54	132.75	111.08
2	F	2	FRU	O3-C3-C2	7.54	132.73	111.08
2	D	1	FRU	O6-C6-C5	6.21	132.49	111.33
2	F	1	FRU	O6-C6-C5	4.57	126.91	111.33
2	F	2	FRU	O5-C2-C1	-3.34	102.16	109.22
2	E	2	FRU	O5-C2-C1	-3.32	102.19	109.22
2	D	2	FRU	O5-C2-C1	-3.32	102.20	109.22
2	D	1	FRU	O2-C2-O5	2.81	114.73	109.33
2	F	1	FRU	O2-C2-O5	2.81	114.72	109.33
2	E	1	FRU	O2-C2-O5	2.81	114.72	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	FRU	C6-C5-C4	-2.79	108.52	115.10
2	F	2	FRU	C6-C5-C4	-2.78	108.54	115.10
2	E	2	FRU	C6-C5-C4	-2.77	108.56	115.10
2	E	1	FRU	O5-C5-C6	-2.73	101.43	108.89
2	E	2	FRU	O5-C2-C3	-2.40	100.39	105.15
2	D	2	FRU	O5-C2-C3	-2.39	100.42	105.15
2	F	2	FRU	O5-C2-C3	-2.39	100.42	105.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

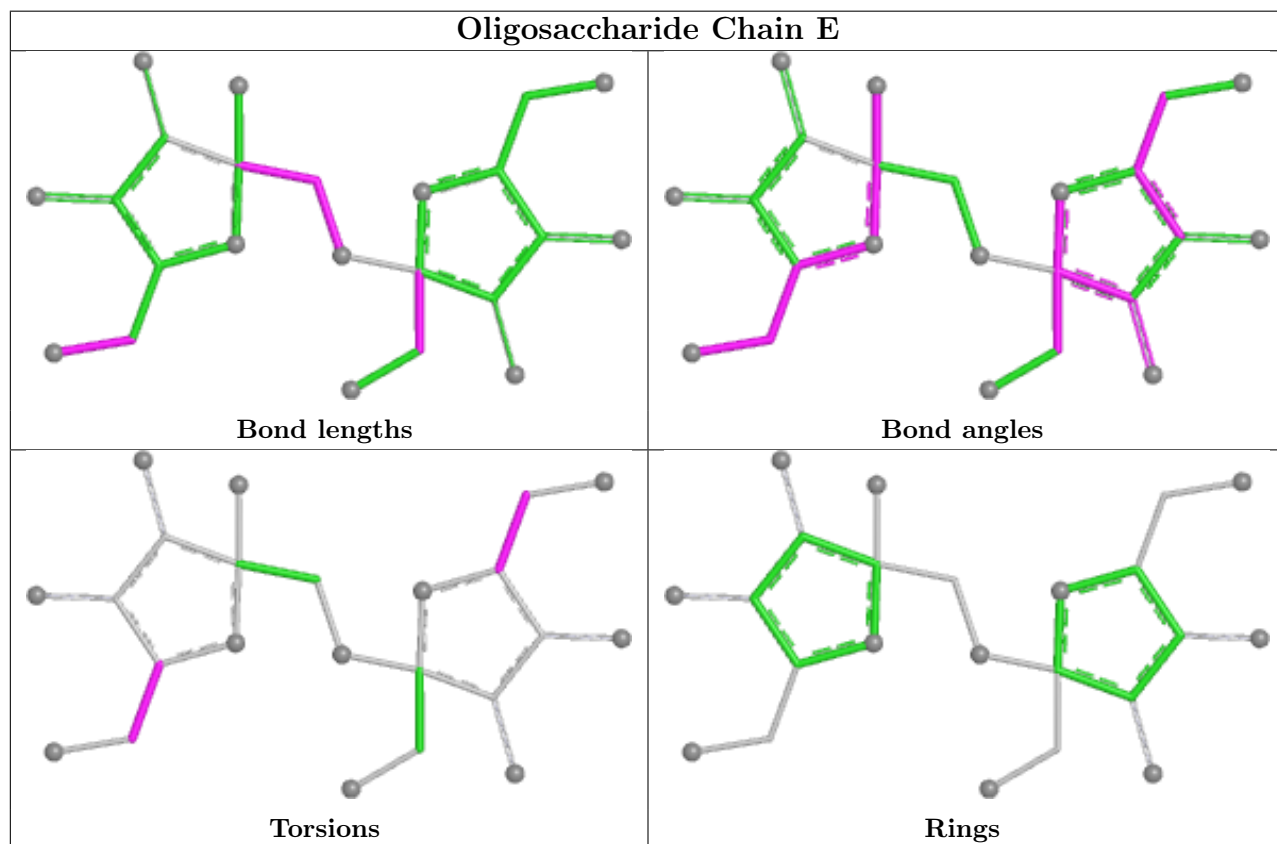
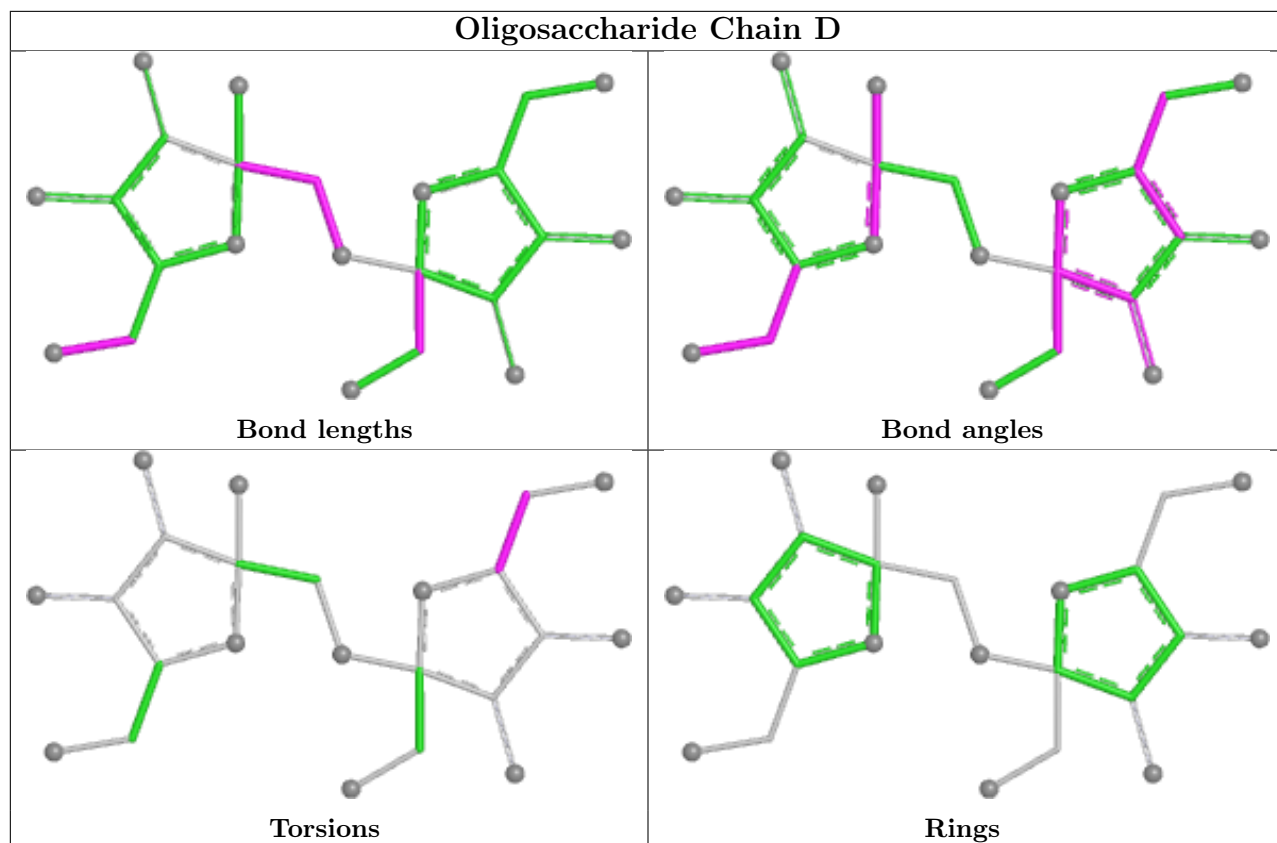
Mol	Chain	Res	Type	Atoms
2	E	1	FRU	C4-C5-C6-O6
2	E	1	FRU	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6
2	E	2	FRU	C4-C5-C6-O6
2	F	2	FRU	C4-C5-C6-O6

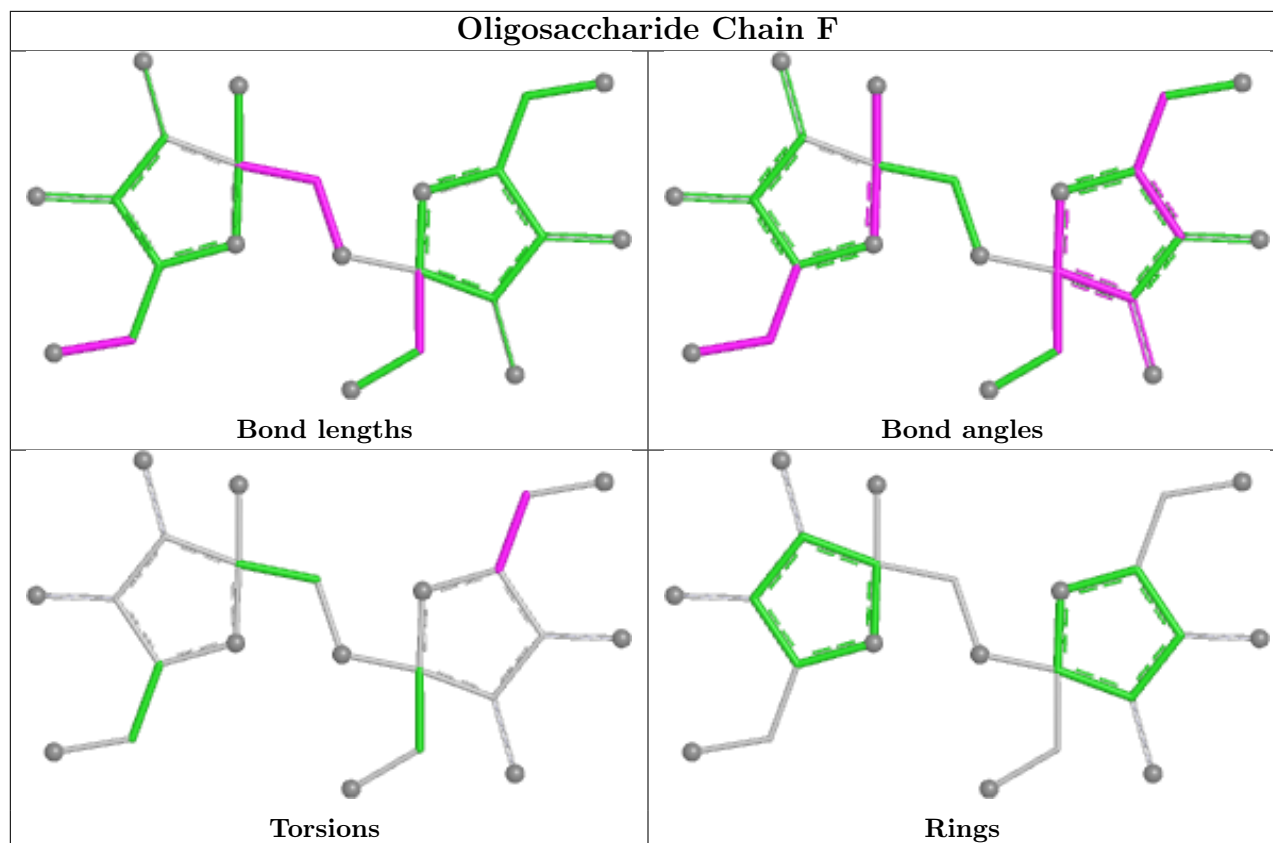
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	FRU	3	0
2	D	2	FRU	3	0
2	E	2	FRU	3	0
2	E	1	FRU	1	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](#)

2 ligands 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	$\# Z > 2$
3	2PO	A	1002	-	0,3,3	-	-	0,3,3	-	-
3	2PO	B	1001	-	0,3,3	-	-	0,3,3	-	-

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

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	395/410 (96%)	-1.34	0 100 100	10, 14, 25, 30	0
1	B	395/410 (96%)	-1.34	0 100 100	10, 14, 25, 30	0
1	C	395/410 (96%)	-1.34	0 100 100	10, 14, 25, 30	0
All	All	1185/1230 (96%)	-1.34	0 100 100	10, 14, 25, 30	0

There are no RSRZ outliers to report.

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](#)

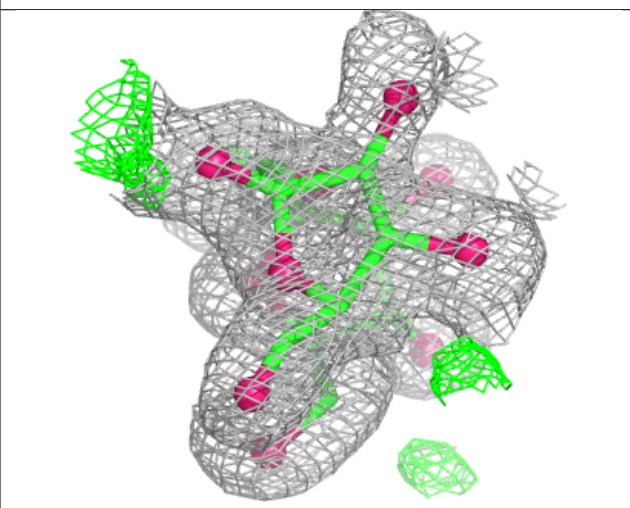
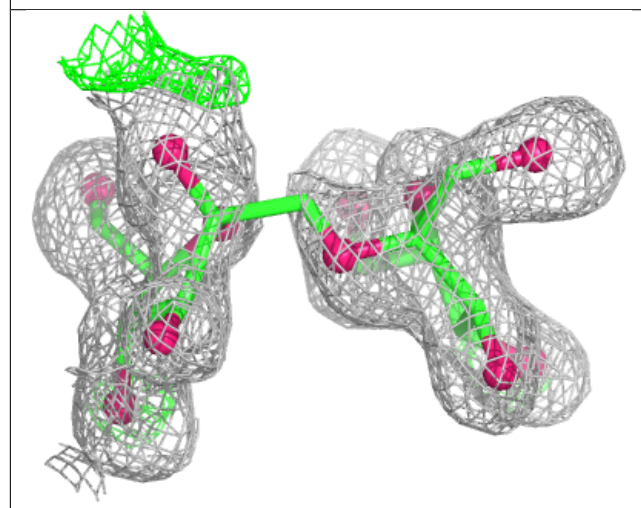
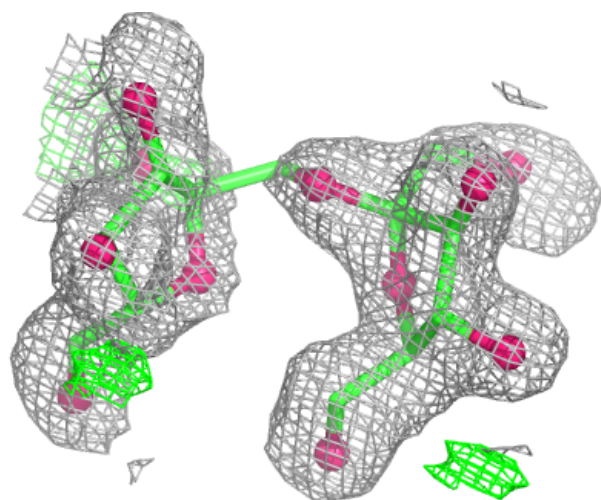
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	FRU	D	1	12/12	0.98	0.04	27,29,30,32	0
2	FRU	F	1	12/12	0.98	0.04	26,29,30,31	0
2	FRU	E	1	12/12	0.99	0.04	28,29,30,32	0
2	FRU	E	2	11/12	0.99	0.04	24,25,26,26	0
2	FRU	D	2	11/12	0.99	0.03	22,23,25,25	0
2	FRU	F	2	11/12	0.99	0.04	22,24,25,25	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.

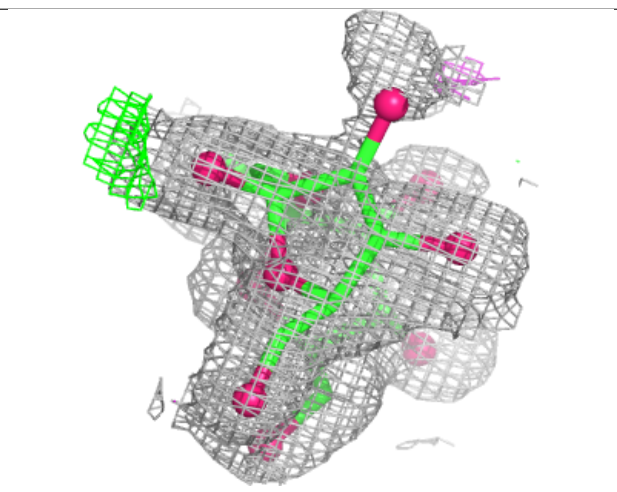
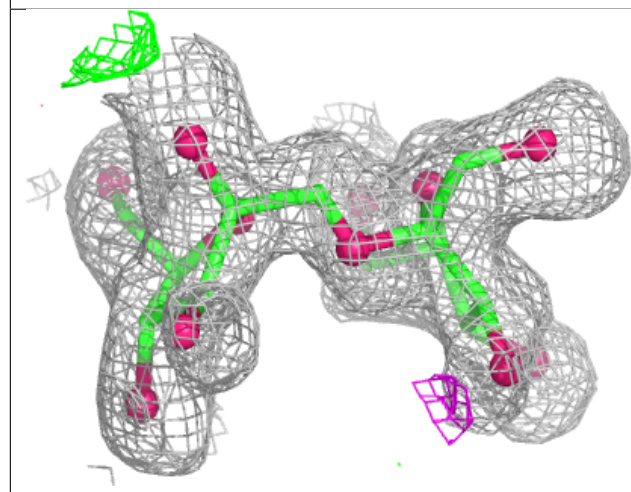
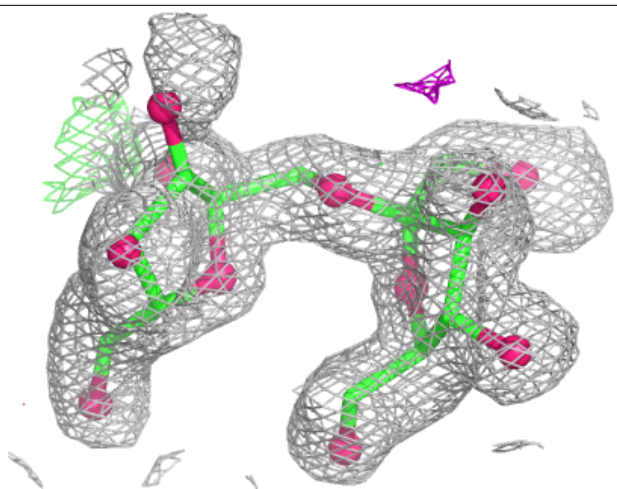
Electron density around Chain D:

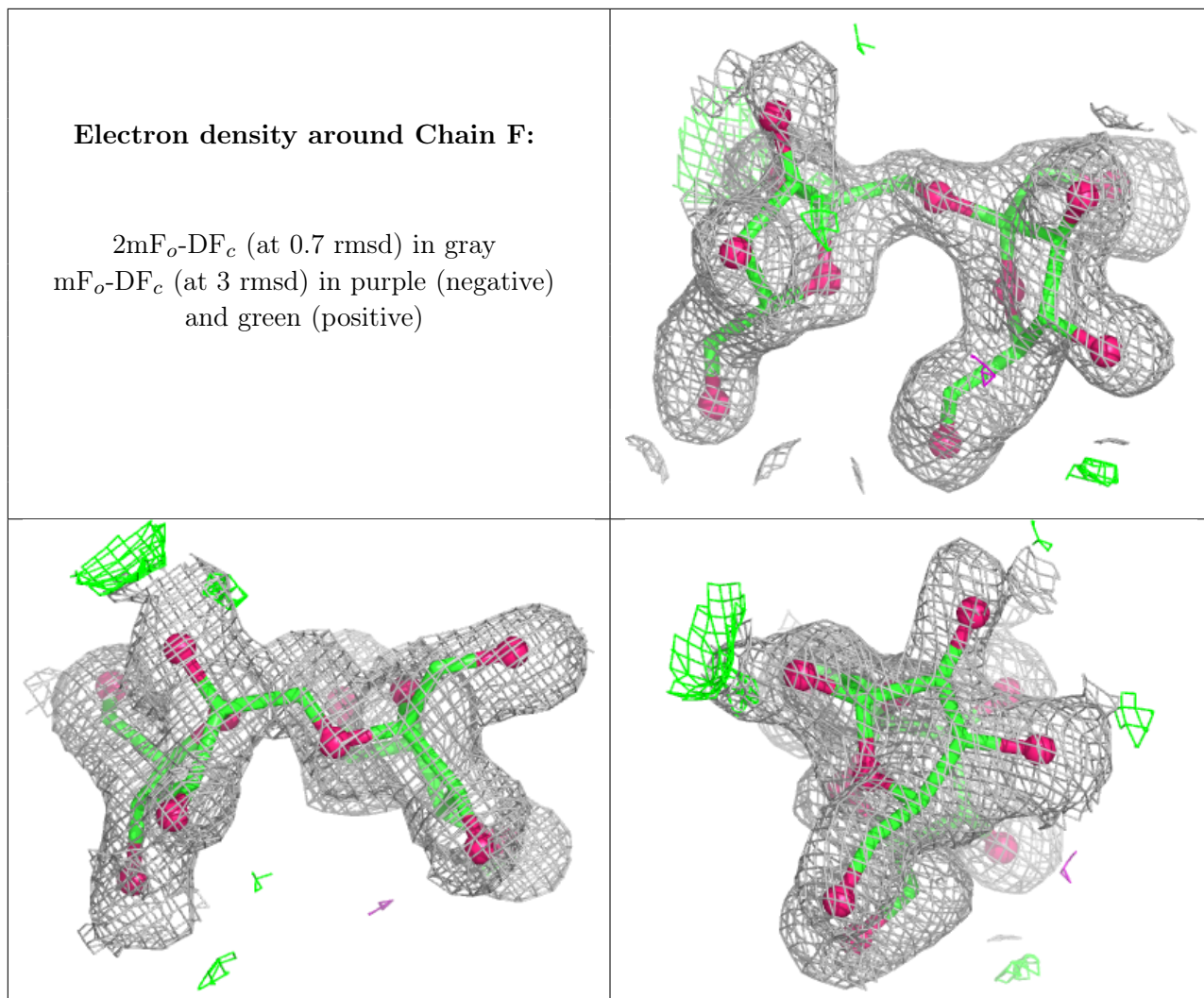
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\AA^2)	Q<0.9
3	2PO	A	1002	4/4	0.99	0.04	45,45,46,47	0
3	2PO	B	1001	4/4	0.99	0.05	33,33,33,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.