



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:01 PM UTC

PDB ID : 2OVW / pdb_00002ovw
Title : ENDOGLUCANASE I COMPLEXED WITH CELLOBIOSE
Authors : Sulzenbacher, G.; Davies, G.J.; Schulein, M.
Deposited on : 1997-04-04
Resolution : 2.30 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

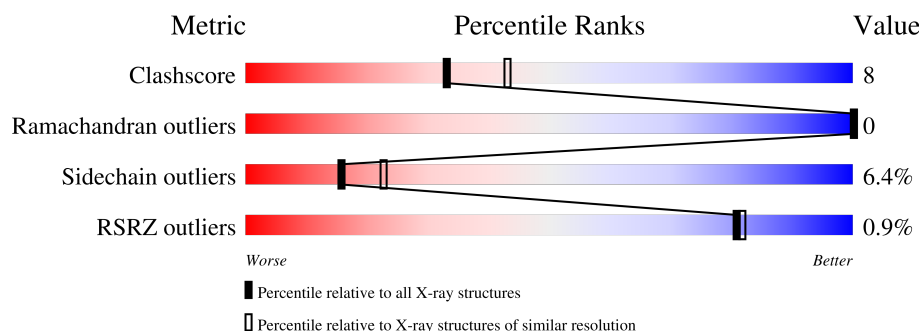
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	411	
1	B	411	
1	C	411	
1	D	411	
2	E	2	
2	F	2	

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13393 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 ENDOGLUCANASE I.

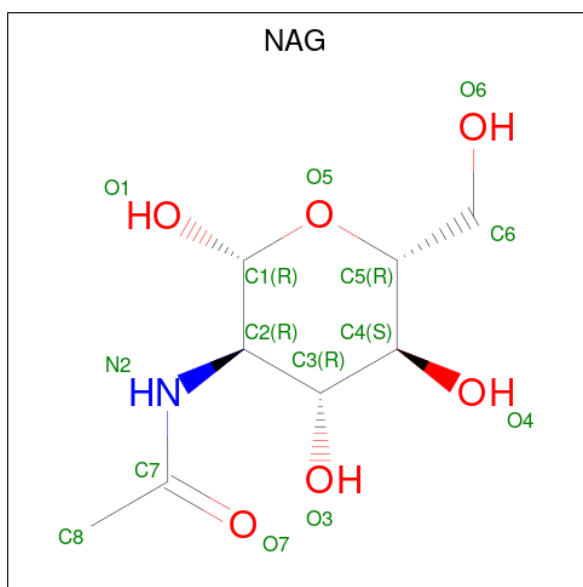
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			
1	B	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			
1	C	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			
1	D	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

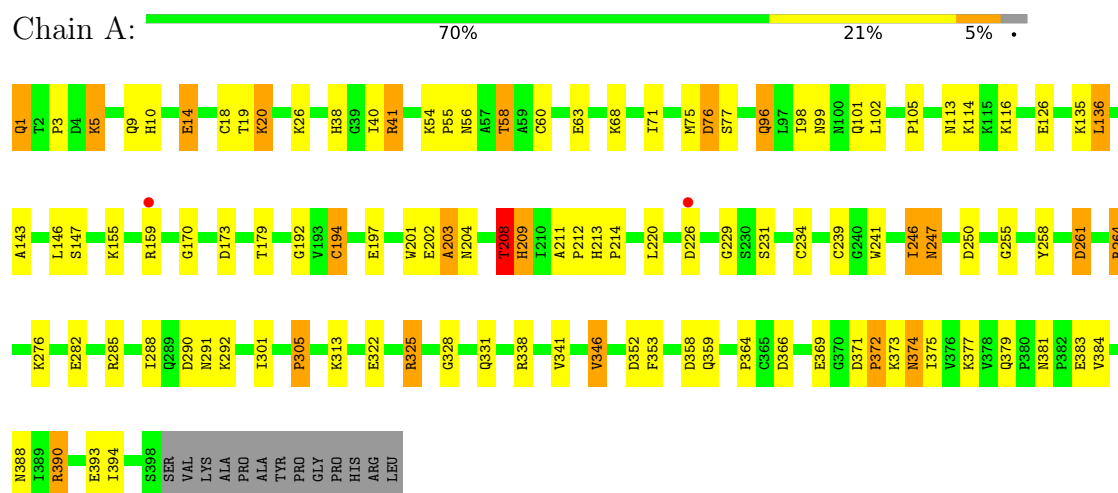
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O	0	0
			277	277		
4	B	268	Total	O	0	0
			268	268		
4	C	268	Total	O	0	0
			268	268		
4	D	288	Total	O	0	0
			288	288		

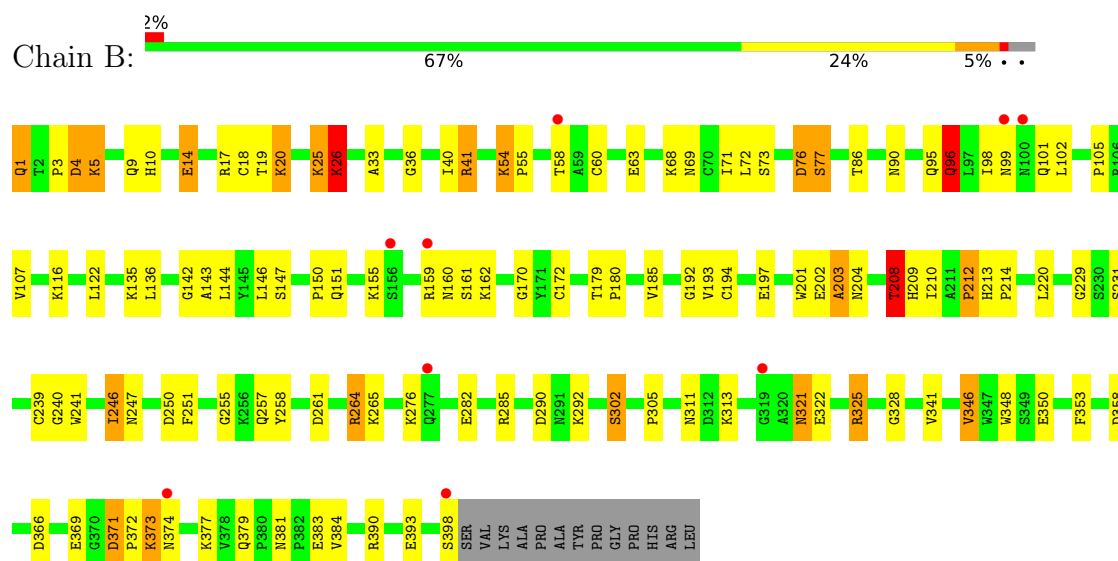
3 Residue-property plots

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: ENDOGLUCANASE I

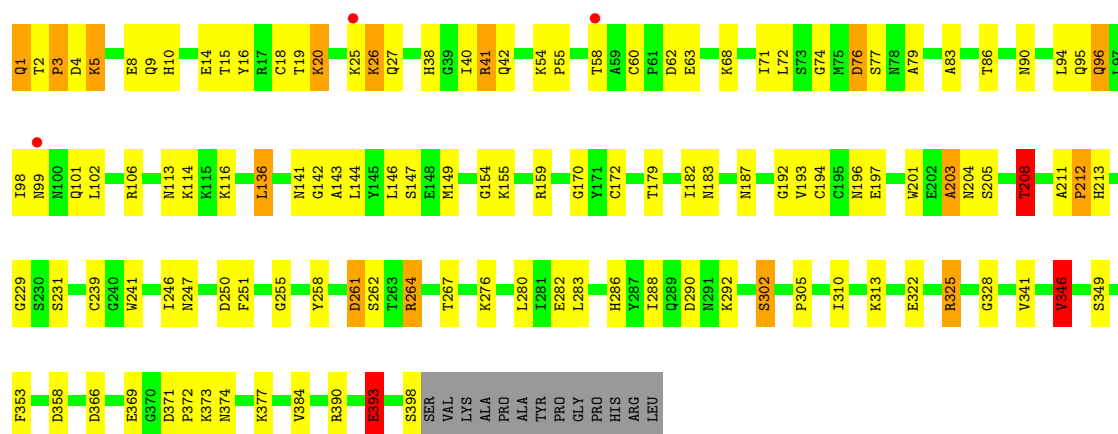


• Molecule 1: ENDOGLUCANASE I



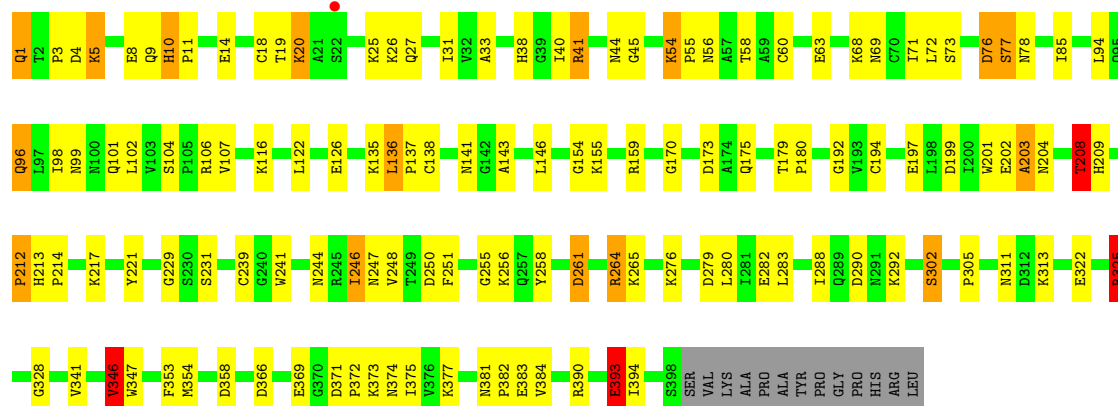
• Molecule 1: ENDOGLUCANASE I





• Molecule 1: ENDOGLUCANASE I

Chain D: 65% 27%



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E: 50% 50%



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F: 50% 50%



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G: 50% 50%



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

Chain H:  50% 50%

BG1
BG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.93Å 78.31Å 142.47Å 90.00° 96.98° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (15.00-2.30) 86.2 (15.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , (Not available) 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13393	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.25% 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: PCA, BGC, NAG

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	0.85	0/3076	1.87	78/4155 (1.9%)
1	B	0.85	0/3076	1.90	86/4155 (2.1%)
1	C	0.87	0/3076	1.89	77/4155 (1.9%)
1	D	0.88	1/3076 (0.0%)	1.88	86/4155 (2.1%)
All	All	0.86	1/12304 (0.0%)	1.88	327/16620 (2.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	60	CYS	CA-CB	6.16	1.60	1.53

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	ARG	CD-NE-CZ	14.96	145.34	124.40
1	C	325	ARG	CD-NE-CZ	14.91	145.27	124.40
1	A	325	ARG	CD-NE-CZ	14.60	144.84	124.40
1	A	264	ARG	CD-NE-CZ	13.71	143.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	CD-NE-CZ	13.51	143.31	124.40
1	B	264	ARG	CD-NE-CZ	12.66	142.13	124.40
1	D	325	ARG	CD-NE-CZ	11.75	140.86	124.40
1	B	41	ARG	CD-NE-CZ	11.64	140.70	124.40
1	D	261	ASP	CA-CB-CG	11.31	123.91	112.60
1	A	41	ARG	CD-NE-CZ	11.15	140.02	124.40
1	D	41	ARG	CD-NE-CZ	10.82	139.55	124.40
1	C	41	ARG	CD-NE-CZ	10.44	139.01	124.40
1	D	264	ARG	CD-NE-CZ	9.68	137.95	124.40
1	B	346	VAL	N-CA-CB	9.60	125.53	111.52
1	A	261	ASP	CA-CB-CG	9.24	121.84	112.60
1	C	346	VAL	N-CA-CB	9.15	124.89	111.52
1	D	346	VAL	N-CA-CB	8.87	124.47	111.52
1	A	346	VAL	N-CA-CB	8.84	124.43	111.52
1	B	390	ARG	CD-NE-CZ	8.51	136.31	124.40
1	D	141	ASN	CA-CB-CG	8.40	121.00	112.60
1	D	247	ASN	OD1-CG-ND2	8.21	130.81	122.60
1	A	226	ASP	CA-CB-CG	-8.10	104.50	112.60
1	D	325	ARG	NE-CZ-NH1	8.04	129.54	121.50
1	C	346	VAL	CB-CA-C	-7.97	98.69	110.33
1	A	359	GLN	OE1-CD-NE2	-7.93	114.67	122.60
1	C	373	LYS	CA-CB-CG	7.85	129.81	114.10
1	B	398	SER	CA-C-O	-7.83	107.50	120.80
1	D	373	LYS	CB-CA-C	-7.79	97.85	110.79
1	C	63	GLU	N-CA-C	7.78	119.76	111.28
1	A	373	LYS	CB-CA-C	-7.71	97.99	110.79
1	B	76	ASP	CA-CB-CG	7.65	120.25	112.60
1	A	331	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	A	247	ASN	OD1-CG-ND2	7.58	130.18	122.60
1	B	151	GLN	OE1-CD-NE2	7.48	130.08	122.60
1	B	63	GLU	N-CA-C	7.43	119.38	111.28
1	A	63	GLU	N-CA-C	7.33	119.28	111.28
1	D	63	GLU	N-CA-C	7.31	119.25	111.28
1	A	170	GLY	N-CA-C	7.30	125.73	115.43
1	C	241	TRP	N-CA-CB	7.30	122.29	110.90
1	D	179	THR	CA-C-N	7.18	127.17	119.28
1	D	179	THR	C-N-CA	7.18	127.17	119.28
1	C	251	PHE	CA-CB-CG	-7.16	106.64	113.80
1	D	76	ASP	CA-CB-CG	7.16	119.76	112.60
1	B	255	GLY	N-CA-C	7.13	123.51	112.45
1	D	390	ARG	CD-NE-CZ	7.13	134.38	124.40
1	C	179	THR	CA-C-N	7.11	127.10	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	THR	C-N-CA	7.11	127.10	119.28
1	D	10	HIS	CA-CB-CG	7.10	120.90	113.80
1	A	373	LYS	CA-CB-CG	7.08	128.26	114.10
1	B	10	HIS	CA-CB-CG	7.06	120.86	113.80
1	A	325	ARG	NE-CZ-NH1	7.05	128.55	121.50
1	B	373	LYS	CB-CA-C	-7.03	99.12	110.79
1	B	398	SER	CA-CB-OG	7.02	125.14	111.10
1	A	346	VAL	CB-CA-C	-6.98	100.13	110.33
1	B	213	HIS	CA-CB-CG	6.93	120.73	113.80
1	A	374	ASN	CA-CB-CG	-6.90	105.70	112.60
1	D	251	PHE	CA-CB-CG	-6.89	106.91	113.80
1	C	187	ASN	OD1-CG-ND2	-6.89	115.71	122.60
1	A	353	PHE	CA-CB-CG	6.89	120.69	113.80
1	A	390	ARG	CD-NE-CZ	6.87	134.02	124.40
1	D	154	GLY	CA-C-N	6.83	129.76	120.54
1	D	154	GLY	C-N-CA	6.83	129.76	120.54
1	D	229	GLY	CA-C-N	6.81	129.71	120.38
1	D	229	GLY	C-N-CA	6.81	129.71	120.38
1	B	241	TRP	N-CA-CB	6.81	122.73	110.95
1	D	214	PRO	N-CA-CB	6.81	109.66	103.33
1	D	170	GLY	N-CA-C	6.80	125.01	115.43
1	D	69	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	B	150	PRO	N-CA-CB	6.76	109.36	103.27
1	A	76	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	179	THR	CA-C-N	6.75	126.70	119.28
1	A	179	THR	C-N-CA	6.75	126.70	119.28
1	B	203	ALA	N-CA-C	6.75	118.05	108.74
1	D	353	PHE	CA-CB-CG	6.74	120.53	113.80
1	D	3	PRO	N-CA-CB	6.73	109.21	103.35
1	B	346	VAL	CB-CA-C	-6.70	100.55	110.33
1	A	255	GLY	N-CA-C	6.67	122.79	112.45
1	D	246	ILE	CA-C-O	6.66	126.80	120.14
1	D	4	ASP	CA-CB-CG	6.63	119.23	112.60
1	C	213	HIS	CA-CB-CG	6.61	120.41	113.80
1	B	208	THR	N-CA-CB	6.56	123.32	111.37
1	D	213	HIS	CA-C-N	6.55	126.47	119.85
1	D	213	HIS	C-N-CA	6.55	126.47	119.85
1	B	251	PHE	CA-CB-CG	-6.52	107.28	113.80
1	B	247	ASN	OD1-CG-ND2	6.51	129.11	122.60
1	C	261	ASP	CA-CB-CG	6.47	119.07	112.60
1	C	373	LYS	CB-CA-C	-6.46	100.07	110.79
1	C	328	GLY	N-CA-C	6.45	122.89	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	CYS	N-CA-C	6.44	120.54	110.17
1	D	27	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	B	311	ASN	CA-CB-CG	6.43	119.03	112.60
1	D	203	ALA	N-CA-C	6.42	117.61	108.74
1	A	203	ALA	N-CA-C	6.41	117.59	108.74
1	C	325	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	358	ASP	N-CA-C	6.39	120.98	112.30
1	A	358	ASP	N-CA-C	6.38	120.97	112.30
1	C	4	ASP	CA-CB-CG	6.37	118.97	112.60
1	C	255	GLY	N-CA-C	6.37	122.32	112.45
1	D	44	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	D	213	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	192	GLY	N-CA-C	-6.34	101.68	111.64
1	B	264	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	C	3	PRO	N-CA-CB	6.30	108.83	103.35
1	C	208	THR	N-CA-CB	6.26	122.77	111.37
1	A	208	THR	N-CA-CB	6.26	122.76	111.37
1	A	285	ARG	CD-NE-CZ	6.26	133.16	124.40
1	D	45	GLY	CA-C-O	-6.26	112.76	118.95
1	D	78	ASN	N-CA-CB	-6.26	100.92	110.12
1	B	63	GLU	CB-CA-C	-6.24	100.43	110.79
1	D	373	LYS	CA-CB-CG	6.24	126.57	114.10
1	D	180	PRO	N-CA-CB	6.22	110.11	103.39
1	C	203	ALA	N-CA-C	6.22	117.32	108.74
1	B	179	THR	CA-C-N	6.21	126.11	119.28
1	B	179	THR	C-N-CA	6.21	126.11	119.28
1	A	136	LEU	CA-C-O	6.21	126.17	120.09
1	D	212	PRO	CB-CA-C	-6.21	103.95	111.46
1	C	358	ASP	N-CA-C	6.17	120.69	112.30
1	A	241	TRP	N-CA-CB	6.16	120.51	110.90
1	D	244	ASN	CA-CB-CG	-6.16	106.44	112.60
1	A	213	HIS	CA-CB-CG	6.15	119.95	113.80
1	B	77	SER	CA-C-O	6.14	127.06	120.55
1	C	76	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	286	HIS	N-CA-CB	6.12	121.88	111.66
1	C	136	LEU	CA-C-O	6.10	127.04	120.08
1	D	208	THR	N-CA-CB	6.09	122.45	111.37
1	C	194	CYS	N-CA-C	6.08	119.84	110.42
1	D	241	TRP	N-CA-CB	6.07	121.46	110.95
1	D	136	LEU	CA-C-O	6.07	127.00	120.08
1	A	328	GLY	N-CA-C	6.04	121.98	111.78
1	C	170	GLY	N-CA-C	6.04	123.94	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	GLY	N-CA-C	6.02	122.14	111.73
1	D	393	GLU	N-CA-CB	6.01	118.88	110.04
1	A	14	GLU	CA-C-O	-6.01	113.90	120.81
1	B	371	ASP	N-CA-C	-6.00	102.21	109.83
1	A	371	ASP	N-CA-C	-5.99	102.22	109.83
1	B	170	GLY	N-CA-C	5.99	123.87	115.43
1	A	204	ASN	CA-CB-CG	5.98	118.58	112.60
1	D	106	ARG	NE-CZ-NH2	-5.97	113.82	119.20
1	C	79	ALA	O-C-N	5.97	128.95	122.15
1	A	18	CYS	N-CA-C	5.96	118.92	109.50
1	D	255	GLY	N-CA-C	5.94	121.66	112.45
1	A	194	CYS	N-CA-C	5.94	119.62	110.42
1	A	372	PRO	CA-C-N	5.92	128.22	120.28
1	A	372	PRO	C-N-CA	5.92	128.22	120.28
1	B	353	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	285	ARG	CD-NE-CZ	5.92	132.68	124.40
1	B	204	ASN	CA-CB-CG	5.90	118.50	112.60
1	C	183	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	D	371	ASP	N-CA-C	-5.88	102.36	109.83
1	D	60	CYS	N-CA-C	5.86	119.17	109.79
1	B	4	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	10	HIS	CA-CB-CG	5.85	119.65	113.80
1	C	192	GLY	N-CA-C	-5.84	102.46	111.64
1	C	282	GLU	N-CA-C	5.84	119.03	108.69
1	C	371	ASP	CA-C-N	5.84	125.98	119.32
1	C	371	ASP	C-N-CA	5.84	125.98	119.32
1	C	371	ASP	N-CA-C	-5.80	102.46	109.83
1	D	346	VAL	CB-CA-C	-5.79	101.87	110.33
1	A	381	ASN	CA-CB-CG	-5.79	106.81	112.60
1	C	42	GLN	OE1-CD-NE2	5.78	128.38	122.60
1	D	18	CYS	N-CA-C	5.78	118.63	109.50
1	D	194	CYS	N-CA-C	5.77	119.47	110.17
1	C	212	PRO	CB-CA-C	-5.77	103.54	111.21
1	B	69	ASN	CA-CB-CG	-5.76	106.84	112.60
1	A	60	CYS	N-CA-C	5.76	119.01	109.79
1	A	192	GLY	N-CA-C	-5.76	102.60	111.64
1	B	373	LYS	CA-CB-CG	5.76	125.62	114.10
1	D	328	GLY	N-CA-C	5.75	121.68	111.73
1	A	58	THR	N-CA-CB	5.73	118.80	110.26
1	B	325	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	C	86	THR	CA-C-O	-5.72	115.15	121.33
1	B	54	LYS	N-CA-CB	5.71	118.27	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	212	PRO	N-CA-CB	5.71	108.39	103.36
1	B	26	LYS	O-C-N	-5.70	116.14	122.86
1	D	204	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	76	ASP	CA-C-O	-5.66	115.49	121.88
1	C	212	PRO	N-CA-CB	5.66	108.60	103.34
1	D	246	ILE	CB-CG1-CD1	5.66	125.68	113.80
1	A	352	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	209	HIS	CA-CB-CG	5.65	119.45	113.80
1	B	143	ALA	N-CA-C	5.63	118.58	109.40
1	A	214	PRO	N-CA-CB	5.63	108.57	103.33
1	C	27	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	C	196	ASN	OD1-CG-ND2	5.63	128.23	122.60
1	B	214	PRO	N-CA-CB	5.63	108.56	103.33
1	D	214	PRO	CB-CA-C	-5.62	103.62	110.98
1	B	350	GLU	CA-CB-CG	5.61	125.33	114.10
1	C	325	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	D	192	GLY	N-CA-C	-5.61	102.83	111.64
1	D	311	ASN	CA-CB-CG	5.60	118.20	112.60
1	A	371	ASP	CA-C-N	5.60	125.70	119.32
1	A	371	ASP	C-N-CA	5.60	125.70	119.32
1	B	86	THR	CA-C-O	-5.59	115.29	121.33
1	D	264	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	B	18	CYS	N-CA-C	5.59	118.33	109.50
1	C	90	ASN	CA-CB-CG	5.58	118.18	112.60
1	D	56	ASN	CA-C-N	5.58	129.53	120.60
1	D	56	ASN	C-N-CA	5.58	129.53	120.60
1	A	213	HIS	CA-C-N	5.58	125.48	119.85
1	A	213	HIS	C-N-CA	5.58	125.48	119.85
1	D	282	GLU	N-CA-C	5.58	118.56	108.69
1	B	371	ASP	CA-C-N	5.58	125.68	119.32
1	B	371	ASP	C-N-CA	5.58	125.68	119.32
1	C	116	LYS	CA-CB-CG	5.57	125.23	114.10
1	C	393	GLU	N-CA-CB	5.56	118.21	110.04
1	D	372	PRO	CA-C-N	5.55	127.72	120.28
1	D	372	PRO	C-N-CA	5.55	127.72	120.28
1	C	302	SER	CB-CA-C	5.54	118.66	109.53
1	B	60	CYS	N-CA-C	5.53	118.64	109.79
1	C	398	SER	CA-C-O	-5.51	111.43	120.80
1	B	96	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	56	ASN	CA-C-N	5.51	129.91	120.72
1	A	56	ASN	C-N-CA	5.51	129.91	120.72
1	A	3	PRO	N-CA-CB	5.49	108.13	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	HIS	CA-C-N	5.48	125.39	119.85
1	B	213	HIS	C-N-CA	5.48	125.39	119.85
1	D	54	LYS	N-CA-CB	5.47	117.93	110.05
1	B	229	GLY	CA-C-N	5.47	127.87	120.38
1	B	229	GLY	C-N-CA	5.47	127.87	120.38
1	C	204	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	246	ILE	CA-C-O	5.44	125.58	120.14
1	C	143	ALA	N-CA-C	5.44	118.27	109.40
1	C	349	SER	CA-C-O	5.44	127.11	120.25
1	B	36	GLY	O-C-N	-5.43	116.90	122.17
1	A	41	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	B	180	PRO	N-CA-CB	5.43	109.25	103.39
1	C	194	CYS	CB-CA-C	-5.42	100.86	109.80
1	B	302	SER	CB-CA-C	5.42	118.47	109.53
1	B	282	GLU	CA-C-N	-5.39	115.60	122.77
1	B	282	GLU	C-N-CA	-5.39	115.60	122.77
1	C	213	HIS	CA-C-N	5.38	125.28	119.85
1	C	213	HIS	C-N-CA	5.38	125.28	119.85
1	B	379	GLN	CA-C-N	5.37	125.01	119.05
1	B	379	GLN	C-N-CA	5.37	125.01	119.05
1	C	390	ARG	CD-NE-CZ	5.37	131.91	124.40
1	C	60	CYS	N-CA-C	5.37	118.37	109.79
1	B	105	PRO	CB-CA-C	-5.36	104.37	111.23
1	A	194	CYS	CB-CA-C	-5.36	100.96	109.80
1	D	106	ARG	N-CA-CB	5.36	119.18	110.77
1	C	106	ARG	N-CA-CB	5.35	119.17	110.77
1	D	382	PRO	N-CA-CB	5.34	108.07	103.31
1	A	338	ARG	CG-CD-NE	5.34	123.75	112.00
1	C	229	GLY	CA-C-N	5.34	127.69	120.38
1	C	229	GLY	C-N-CA	5.34	127.69	120.38
1	A	229	GLY	CA-C-N	5.34	127.69	120.38
1	A	229	GLY	C-N-CA	5.34	127.69	120.38
1	B	202	GLU	N-CA-CB	5.32	118.92	110.84
1	A	14	GLU	CA-C-N	5.30	130.84	122.36
1	A	14	GLU	C-N-CA	5.30	130.84	122.36
1	A	282	GLU	CA-C-N	-5.29	115.64	123.05
1	A	282	GLU	C-N-CA	-5.29	115.64	123.05
1	B	212	PRO	CB-CA-C	-5.28	105.07	111.46
1	B	247	ASN	N-CA-C	5.28	118.91	111.52
1	C	241	TRP	CA-C-O	5.28	126.90	120.25
1	B	321	ASN	CB-CG-ND2	-5.27	108.49	116.40
1	C	141	ASN	CA-CB-CG	5.27	117.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ASN	CA-CB-CG	-5.27	107.33	112.60
1	D	202	GLU	N-CA-CB	5.27	118.85	110.84
1	A	105	PRO	N-CA-C	5.27	119.76	111.38
1	D	371	ASP	CA-C-N	5.27	125.32	119.32
1	D	371	ASP	C-N-CA	5.27	125.32	119.32
1	D	288	ILE	N-CA-CB	5.26	119.77	111.99
1	C	18	CYS	N-CA-C	5.24	117.78	109.50
1	A	203	ALA	CB-CA-C	-5.24	99.48	111.95
1	A	209	HIS	CA-CB-CG	5.23	119.03	113.80
1	C	282	GLU	CA-C-N	-5.23	115.81	122.77
1	C	282	GLU	C-N-CA	-5.23	115.81	122.77
1	D	358	ASP	N-CA-C	5.23	120.44	112.54
1	A	305	PRO	N-CA-CB	5.22	108.30	103.39
1	D	282	GLU	CA-C-N	-5.21	115.85	122.77
1	D	282	GLU	C-N-CA	-5.21	115.85	122.77
1	B	160	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	116	LYS	CA-CB-CG	5.20	124.49	114.10
1	A	364	PRO	N-CA-C	5.19	121.10	114.92
1	B	194	CYS	CB-CA-C	-5.19	100.73	109.50
1	D	143	ALA	N-CA-C	5.19	117.86	109.40
1	A	173	ASP	N-CA-CB	5.18	119.43	111.24
1	D	199	ASP	CA-CB-CG	-5.18	107.42	112.60
1	D	116	LYS	CA-CB-CG	5.17	124.44	114.10
1	A	143	ALA	N-CA-C	5.17	117.82	109.40
1	D	302	SER	CB-CA-C	5.16	118.05	109.53
1	C	15	THR	N-CA-CB	5.16	119.98	111.62
1	B	76	ASP	CA-C-O	-5.16	115.58	121.82
1	B	17	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	211	ALA	CA-C-N	5.16	124.92	119.76
1	A	211	ALA	C-N-CA	5.16	124.92	119.76
1	A	282	GLU	N-CA-C	5.16	117.83	109.06
1	B	202	GLU	CB-CG-CD	-5.15	103.84	112.60
1	A	291	ASN	CA-CB-CG	-5.15	107.45	112.60
1	C	76	ASP	CA-C-O	-5.15	115.59	121.82
1	B	321	ASN	CA-CB-CG	-5.14	107.46	112.60
1	B	90	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	62	ASP	CA-CB-CG	-5.14	107.46	112.60
1	C	353	PHE	CA-CB-CG	5.13	118.93	113.80
1	D	381	ASN	CA-CB-CG	-5.13	107.47	112.60
1	D	85	ILE	N-CA-CB	-5.12	104.98	111.64
1	B	142	GLY	N-CA-C	-5.12	101.06	113.18
1	B	122	LEU	N-CA-C	5.11	119.57	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	PRO	N-CA-CB	5.11	107.80	103.35
1	B	77	SER	CA-C-N	5.11	127.13	120.28
1	B	77	SER	C-N-CA	5.11	127.13	120.28
1	D	104	SER	CA-C-N	5.10	125.00	119.85
1	D	104	SER	C-N-CA	5.10	125.00	119.85
1	B	240	GLY	CA-C-N	5.08	130.09	122.47
1	B	240	GLY	C-N-CA	5.08	130.09	122.47
1	C	142	GLY	N-CA-C	-5.08	101.14	113.18
1	B	105	PRO	N-CA-C	5.08	119.28	111.21
1	A	379	GLN	CA-C-N	5.07	124.68	119.05
1	A	379	GLN	C-N-CA	5.07	124.68	119.05
1	B	14	GLU	CA-C-O	-5.07	114.91	120.69
1	C	154	GLY	CA-C-N	5.06	127.38	120.54
1	C	154	GLY	C-N-CA	5.06	127.38	120.54
1	A	1	PCA	O-C-N	-5.05	114.91	123.00
1	D	248	VAL	CA-C-O	5.05	127.10	120.78
1	D	247	ASN	N-CA-C	5.05	118.59	111.52
1	C	149	MET	N-CA-CB	-5.05	103.88	109.74
1	C	63	GLU	CB-CA-C	-5.05	102.41	110.79
1	B	210	ILE	CA-C-O	-5.04	114.78	120.67
1	C	74	GLY	N-CA-C	-5.04	106.79	112.33
1	C	372	PRO	CA-C-N	5.02	127.00	120.28
1	C	372	PRO	C-N-CA	5.02	127.00	120.28
1	C	247	ASN	N-CA-C	5.01	118.54	111.52
1	A	288	ILE	N-CA-CB	5.01	118.64	111.82
1	B	381	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	202	GLU	N-CA-CB	5.01	118.45	110.84
1	C	83	ALA	N-CA-C	-5.00	107.18	113.28
1	D	122	LEU	N-CA-C	5.00	119.44	113.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Mainchain
1	B	1	PCA	Mainchain
1	C	1	PCA	Mainchain
1	D	1	PCA	Mainchain

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	3022	0	2905	40	1
1	B	3022	0	2905	45	1
1	C	3022	0	2905	53	0
1	D	3022	0	2905	51	0
2	E	23	0	21	1	0
2	F	23	0	21	1	0
2	G	23	0	21	1	0
2	H	23	0	21	2	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	277	0	0	2	0
4	B	268	0	0	4	0
4	C	268	0	0	5	0
4	D	288	0	0	5	0
All	All	13393	0	11808	188	1

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 8.

All (188) 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:203:ALA:HB2	1:B:208:THR:HG23	1.42	1.00
1:C:203:ALA:HB2	1:C:208:THR:HG23	1.47	0.95
1:D:203:ALA:HB2	1:D:208:THR:HG23	1.48	0.94
1:C:5:LYS:H	1:C:5:LYS:HE2	1.34	0.93
1:B:5:LYS:H	1:B:5:LYS:HE2	1.35	0.91
1:D:5:LYS:H	1:D:5:LYS:HE2	1.35	0.91
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.52	0.89
1:A:5:LYS:H	1:A:5:LYS:HE2	1.38	0.85
1:D:197:GLU:OE2	2:H:1:BGC:H1	1.82	0.79
1:A:197:GLU:OE2	2:E:1:BGC:H1	1.86	0.74
1:C:201:TRP:CZ3	1:C:208:THR:HG21	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HB2	1:B:55:PRO:HD2	1.71	0.72
1:B:261:ASP:OD2	1:B:264:ARG:HD3	1.91	0.71
1:D:201:TRP:CZ3	1:D:208:THR:HG21	2.26	0.70
1:D:261:ASP:OD2	1:D:264:ARG:HD3	1.92	0.69
1:A:54:LYS:HB2	1:A:55:PRO:HD2	1.75	0.69
1:A:261:ASP:OD2	1:A:264:ARG:HD3	1.92	0.68
1:B:116:LYS:HD3	4:B:658:HOH:O	1.94	0.68
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.28	0.67
1:B:366:ASP:OD1	1:B:369:GLU:HG2	1.94	0.67
1:D:54:LYS:HB2	1:D:55:PRO:HD2	1.76	0.67
1:C:197:GLU:OE2	2:G:1:BGC:H1	1.96	0.65
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.31	0.65
1:D:14:GLU:OE1	1:D:26:LYS:HD2	1.98	0.64
1:D:305:PRO:HG3	1:D:313:LYS:HG2	1.80	0.64
1:A:19:THR:HA	1:A:393:GLU:HG2	1.80	0.63
1:C:54:LYS:HB2	1:C:55:PRO:HD2	1.81	0.62
1:B:197:GLU:OE2	2:F:1:BGC:H1	2.00	0.61
1:D:96:GLN:HE21	1:D:96:GLN:HA	1.66	0.60
1:D:256:LYS:HE2	4:D:1098:HOH:O	2.02	0.60
1:C:261:ASP:OD2	1:C:264:ARG:HD3	2.01	0.60
1:D:279:ASP:OD2	4:D:1023:HOH:O	2.16	0.59
1:C:366:ASP:CG	1:C:369:GLU:HG2	2.27	0.59
1:C:9:GLN:OE1	1:C:76:ASP:HB2	2.02	0.59
1:C:20:LYS:HG3	1:C:393:GLU:HG3	1.85	0.59
1:B:19:THR:HA	1:B:393:GLU:HG2	1.86	0.58
1:C:305:PRO:HG3	1:C:313:LYS:HG2	1.84	0.58
1:B:366:ASP:CG	1:B:369:GLU:HG2	2.29	0.58
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.68	0.58
1:A:20:LYS:HG3	1:A:393:GLU:HG3	1.86	0.57
1:B:305:PRO:HG3	1:B:313:LYS:HG2	1.86	0.57
1:B:20:LYS:HG3	1:B:393:GLU:HG3	1.87	0.56
1:B:54:LYS:HB2	1:B:55:PRO:CD	2.36	0.56
1:C:96:GLN:HE21	1:C:96:GLN:HA	1.70	0.56
1:D:9:GLN:OE1	1:D:76:ASP:HB2	2.05	0.56
1:D:54:LYS:HG2	4:D:793:HOH:O	2.05	0.55
1:A:366:ASP:OD1	1:A:369:GLU:HG2	2.06	0.55
1:B:136:LEU:HD11	1:B:384:VAL:HB	1.88	0.55
1:D:136:LEU:HD11	1:D:384:VAL:HB	1.89	0.55
1:C:366:ASP:OD1	1:C:369:GLU:HG2	2.06	0.54
1:D:20:LYS:HG3	1:D:393:GLU:HG3	1.89	0.54
1:C:322:GLU:OE1	1:C:325:ARG:NH1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ASP:OD1	1:D:369:GLU:HG2	2.08	0.54
1:C:54:LYS:HG2	4:C:565:HOH:O	2.08	0.53
1:C:94:LEU:HB3	1:C:346:VAL:HG22	1.90	0.53
1:A:136:LEU:HD11	1:A:384:VAL:HB	1.89	0.53
1:B:374:ASN:HA	1:B:377:LYS:HE2	1.89	0.53
1:C:136:LEU:HD11	1:C:384:VAL:HB	1.91	0.53
1:D:19:THR:HA	1:D:393:GLU:HG2	1.89	0.53
1:B:54:LYS:HG2	4:B:523:HOH:O	2.08	0.53
1:B:96:GLN:HE21	1:B:96:GLN:HA	1.74	0.52
1:D:366:ASP:CG	1:D:369:GLU:HG2	2.34	0.52
1:D:135:LYS:HD3	1:D:383:GLU:HG2	1.91	0.52
1:A:305:PRO:HG3	1:A:313:LYS:HG2	1.92	0.51
1:B:172:CYS:HB3	1:B:193:VAL:HG12	1.91	0.51
1:D:77:SER:HB2	4:D:1081:HOH:O	2.11	0.50
1:B:208:THR:HG22	1:B:209:HIS:H	1.76	0.50
1:A:322:GLU:OE1	1:A:325:ARG:NH1	2.42	0.50
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.52	0.50
1:B:33:ALA:HA	1:B:107:VAL:HG12	1.93	0.50
1:C:203:ALA:CB	1:C:208:THR:HG23	2.32	0.49
1:C:72:LEU:HD23	1:C:72:LEU:C	2.37	0.49
1:A:9:GLN:OE1	1:A:76:ASP:HB2	2.12	0.49
1:D:203:ALA:CB	1:D:208:THR:HG23	2.33	0.49
1:D:374:ASN:HA	1:D:377:LYS:HE2	1.94	0.49
1:B:116:LYS:HE2	4:B:647:HOH:O	2.13	0.49
1:C:19:THR:HA	1:C:393:GLU:HG2	1.94	0.49
1:A:372:PRO:HA	1:A:375:ILE:HD12	1.94	0.49
1:A:388:ASN:OD1	1:A:390:ARG:NE	2.46	0.49
1:D:5:LYS:HE2	1:D:5:LYS:N	2.18	0.49
1:B:135:LYS:HD3	1:B:383:GLU:HG2	1.95	0.49
1:C:16:TYR:CE2	1:C:26:LYS:HG3	2.47	0.48
1:A:374:ASN:HA	1:A:377:LYS:HE2	1.95	0.48
1:B:72:LEU:C	1:B:72:LEU:HD23	2.38	0.48
1:C:201:TRP:CH2	1:C:208:THR:HG21	2.49	0.48
1:A:247:ASN:HB2	1:A:301:ILE:HG23	1.96	0.48
1:C:40:ILE:HA	1:C:71:ILE:O	2.14	0.48
1:D:322:GLU:OE1	1:D:325:ARG:NH1	2.44	0.48
1:A:54:LYS:HB2	1:A:55:PRO:CD	2.44	0.48
1:A:212:PRO:HD2	1:A:239:CYS:O	2.14	0.47
1:D:72:LEU:C	1:D:72:LEU:HD23	2.39	0.47
1:C:172:CYS:HB3	1:C:193:VAL:HG12	1.96	0.47
1:C:264:ARG:HH22	1:C:290:ASP:CG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD21	1:C:283:LEU:HD11	1.96	0.47
1:C:313:LYS:NZ	4:C:947:HOH:O	2.47	0.47
1:D:54:LYS:HB2	1:D:55:PRO:CD	2.43	0.47
1:C:211:ALA:HA	1:C:212:PRO:HD2	1.84	0.47
1:B:257:GLN:HB3	1:C:377:LYS:O	2.15	0.47
1:D:40:ILE:HA	1:D:71:ILE:O	2.15	0.47
1:B:40:ILE:HA	1:B:71:ILE:O	2.15	0.47
1:C:8:GLU:HG2	1:C:10:HIS:CE1	2.50	0.47
1:A:126:GLU:HB2	1:A:394:ILE:HA	1.96	0.46
1:A:220:LEU:C	1:A:220:LEU:HD23	2.40	0.46
1:C:374:ASN:HA	1:C:377:LYS:HE2	1.97	0.46
1:B:14:GLU:OE2	1:B:26:LYS:HD3	2.15	0.46
1:D:137:PRO:HG2	1:D:375:ILE:HG23	1.96	0.46
1:A:40:ILE:HA	1:A:71:ILE:O	2.14	0.46
1:A:146:LEU:HA	1:A:341:VAL:O	2.16	0.46
1:B:257:GLN:HG2	1:B:258:TYR:CE2	2.50	0.46
1:C:26:LYS:HB3	1:C:26:LYS:HE2	1.56	0.46
1:D:25:LYS:HA	1:D:25:LYS:HD3	1.76	0.46
1:D:54:LYS:CB	1:D:55:PRO:HD2	2.46	0.46
1:C:212:PRO:HD2	1:C:239:CYS:O	2.15	0.46
1:C:14:GLU:HB3	1:C:26:LYS:HD2	1.98	0.46
1:B:208:THR:HG22	1:B:209:HIS:N	2.30	0.46
1:C:203:ALA:HB2	1:C:208:THR:CG2	2.33	0.45
1:D:33:ALA:HA	1:D:107:VAL:HG12	1.98	0.45
1:D:347:TRP:CE3	1:D:354:MET:HE1	2.52	0.45
1:D:98:ILE:O	1:D:99:ASN:C	2.60	0.45
1:D:201:TRP:CH2	1:D:208:THR:HG21	2.52	0.45
1:B:9:GLN:OE1	1:B:76:ASP:HB2	2.17	0.45
1:B:146:LEU:HA	1:B:341:VAL:O	2.16	0.45
1:C:25:LYS:HA	1:C:25:LYS:HD3	1.78	0.45
1:A:38:HIS:CD2	1:A:75:MET:HG3	2.52	0.45
1:D:280:LEU:HD21	1:D:283:LEU:HD11	1.99	0.44
1:A:264:ARG:HH22	1:A:290:ASP:CG	2.25	0.44
1:C:182:ILE:HD12	1:C:193:VAL:HG22	2.00	0.44
1:A:54:LYS:HG2	4:A:523:HOH:O	2.17	0.44
1:A:98:ILE:O	1:A:99:ASN:C	2.61	0.44
1:D:8:GLU:OE2	1:D:38:HIS:NE2	2.31	0.44
1:B:322:GLU:OE1	1:B:325:ARG:NH1	2.47	0.44
1:D:264:ARG:HH22	1:D:290:ASP:CG	2.25	0.44
1:B:95:GLN:NE2	4:B:608:HOH:O	2.43	0.44
1:B:193:VAL:HG13	1:B:220:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:O	1:A:258:TYR:HA	2.18	0.44
1:A:208:THR:HG22	1:A:209:HIS:H	1.82	0.43
1:B:250:ASP:O	1:B:258:TYR:HA	2.18	0.43
1:C:144:LEU:C	1:C:144:LEU:HD23	2.43	0.43
1:A:20:LYS:HE3	4:A:637:HOH:O	2.17	0.43
1:B:264:ARG:HH22	1:B:290:ASP:CG	2.27	0.43
1:C:14:GLU:HG2	4:C:1035:HOH:O	2.17	0.43
1:A:366:ASP:CG	1:A:369:GLU:HG2	2.44	0.43
1:A:366:ASP:OD1	1:A:366:ASP:C	2.62	0.43
1:A:113:ASN:O	1:A:114:LYS:HB2	2.18	0.43
1:A:14:GLU:OE1	1:A:26:LYS:HD2	2.19	0.43
1:A:246:ILE:H	1:A:246:ILE:HG13	1.73	0.43
1:B:212:PRO:HD2	1:B:239:CYS:O	2.18	0.43
1:D:212:PRO:HD2	1:D:239:CYS:O	2.19	0.43
1:C:5:LYS:HE2	1:C:5:LYS:N	2.16	0.42
1:C:283:LEU:HB2	1:C:310:ILE:HB	2.00	0.42
1:D:250:ASP:O	1:D:258:TYR:HA	2.18	0.42
1:B:98:ILE:O	1:B:99:ASN:C	2.62	0.42
1:D:137:PRO:O	1:D:138:CYS:C	2.62	0.42
1:D:146:LEU:HA	1:D:341:VAL:O	2.19	0.42
1:D:10:HIS:HA	1:D:11:PRO:HD3	1.88	0.42
1:D:73:SER:HB3	4:D:889:HOH:O	2.18	0.42
1:D:175:GLN:HG2	2:H:1:BGC:O2	2.19	0.42
1:B:54:LYS:CB	1:B:55:PRO:CD	2.95	0.42
1:C:98:ILE:O	1:C:99:ASN:C	2.62	0.42
1:A:135:LYS:HD3	1:A:383:GLU:HG2	2.01	0.42
1:C:267:THR:HB	1:C:288:ILE:HB	2.02	0.42
1:D:217:LYS:HE3	1:D:221:TYR:CE2	2.55	0.42
1:B:348:TRP:CE2	1:B:372:PRO:HB3	2.54	0.42
1:C:20:LYS:HE3	4:C:679:HOH:O	2.19	0.42
1:D:173:ASP:HB2	1:D:197:GLU:OE1	2.20	0.41
1:B:25:LYS:HA	1:B:25:LYS:HD3	1.88	0.41
1:D:8:GLU:CD	1:D:38:HIS:HE2	2.24	0.41
1:A:264:ARG:NH2	1:A:290:ASP:OD1	2.53	0.41
1:C:250:ASP:O	1:C:258:TYR:HA	2.20	0.41
1:C:264:ARG:NH2	1:C:290:ASP:OD1	2.53	0.41
1:B:371:ASP:OD1	1:B:373:LYS:HB2	2.19	0.41
1:C:95:GLN:NE2	4:C:650:HOH:O	2.45	0.41
1:D:94:LEU:HB3	1:D:346:VAL:HG22	2.03	0.41
1:B:144:LEU:C	1:B:144:LEU:HD23	2.45	0.41
1:C:54:LYS:HB2	1:C:55:PRO:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:SER:O	1:C:262:SER:OG	2.36	0.41
1:B:4:ASP:OD2	1:B:73:SER:HA	2.20	0.41
1:B:161:SER:HB2	1:B:185:VAL:HG13	2.03	0.41
1:C:8:GLU:OE2	1:C:38:HIS:NE2	2.37	0.41
1:C:146:LEU:HA	1:C:341:VAL:O	2.21	0.41
1:B:257:GLN:HG2	1:B:258:TYR:CD2	2.56	0.40
1:C:366:ASP:OD1	1:C:366:ASP:C	2.64	0.40
1:A:201:TRP:CH2	1:A:208:THR:HG21	2.55	0.40
1:D:126:GLU:HB2	1:D:394:ILE:HA	2.02	0.40
1:C:113:ASN:O	1:C:114:LYS:HB2	2.20	0.40
1:D:31:ILE:HG23	1:D:107:VAL:HB	2.03	0.40
1:D:54:LYS:CB	1:D:55:PRO:CD	2.98	0.40
1:C:2:THR:HA	1:C:3:PRO:HD3	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASP:O	1:B:321:ASN:ND2[2_656]	2.09	0.11

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	396/411 (96%)	381 (96%)	15 (4%)	0	100	100
1	B	396/411 (96%)	381 (96%)	15 (4%)	0	100	100
1	C	396/411 (96%)	382 (96%)	14 (4%)	0	100	100
1	D	396/411 (96%)	382 (96%)	14 (4%)	0	100	100
All	All	1584/1644 (96%)	1526 (96%)	58 (4%)	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	323/333 (97%)	305 (94%)	18 (6%)	19	28
1	B	323/333 (97%)	300 (93%)	23 (7%)	13	19
1	C	323/333 (97%)	302 (94%)	21 (6%)	15	22
1	D	323/333 (97%)	302 (94%)	21 (6%)	15	22
All	All	1292/1332 (97%)	1209 (94%)	83 (6%)	16	23

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	20	LYS
1	A	41	ARG
1	A	58	THR
1	A	68	LYS
1	A	77	SER
1	A	96	GLN
1	A	101	GLN
1	A	102	LEU
1	A	147	SER
1	A	155	LYS
1	A	159	ARG
1	A	208	THR
1	A	231	SER
1	A	246	ILE
1	A	276	LYS
1	A	292	LYS
1	A	346	VAL
1	B	5	LYS
1	B	20	LYS
1	B	25	LYS
1	B	26	LYS
1	B	41	ARG
1	B	58	THR

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Mol	Chain	Res	Type
1	B	68	LYS
1	B	77	SER
1	B	96	GLN
1	B	101	GLN
1	B	102	LEU
1	B	147	SER
1	B	155	LYS
1	B	159	ARG
1	B	162	LYS
1	B	208	THR
1	B	231	SER
1	B	246	ILE
1	B	265	LYS
1	B	276	LYS
1	B	292	LYS
1	B	302	SER
1	B	346	VAL
1	C	5	LYS
1	C	20	LYS
1	C	26	LYS
1	C	41	ARG
1	C	58	THR
1	C	68	LYS
1	C	77	SER
1	C	96	GLN
1	C	101	GLN
1	C	102	LEU
1	C	147	SER
1	C	155	LYS
1	C	159	ARG
1	C	208	THR
1	C	231	SER
1	C	246	ILE
1	C	276	LYS
1	C	292	LYS
1	C	302	SER
1	C	346	VAL
1	C	393	GLU
1	D	5	LYS
1	D	20	LYS
1	D	41	ARG
1	D	58	THR

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Mol	Chain	Res	Type
1	D	68	LYS
1	D	77	SER
1	D	96	GLN
1	D	101	GLN
1	D	102	LEU
1	D	155	LYS
1	D	159	ARG
1	D	208	THR
1	D	231	SER
1	D	246	ILE
1	D	265	LYS
1	D	276	LYS
1	D	292	LYS
1	D	302	SER
1	D	325	ARG
1	D	346	VAL
1	D	393	GLU

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

Mol	Chain	Res	Type
1	A	96	GLN
1	A	321	ASN
1	B	95	GLN
1	B	96	GLN
1	B	99	ASN
1	B	321	ASN
1	C	95	GLN
1	C	96	GLN
1	C	277	GLN
1	C	321	ASN
1	D	96	GLN
1	D	99	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	PCA	D	1	1	7,8,9	1.65	1 (14%)	9,10,12	2.24	4 (44%)
1	PCA	A	1	1	7,8,9	1.29	1 (14%)	9,10,12	1.88	4 (44%)
1	PCA	B	1	1	7,8,9	1.26	0	9,10,12	1.73	3 (33%)
1	PCA	C	1	1	7,8,9	1.57	1 (14%)	9,10,12	2.63	5 (55%)

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
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	PCA	CG-CD	2.60	1.57	1.50
1	C	1	PCA	O-C	2.19	1.28	1.20
1	A	1	PCA	O-C	2.19	1.28	1.20

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	OE-CD-CG	-5.56	116.81	126.72
1	D	1	PCA	OE-CD-CG	-3.92	119.73	126.72
1	C	1	PCA	O-C-CA	-3.54	115.66	124.77
1	D	1	PCA	CB-CA-C	-3.32	108.10	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-N	-3.23	117.96	124.96
1	A	1	PCA	OE-CD-CG	-3.10	121.18	126.72
1	C	1	PCA	CA-N-CD	-2.70	104.33	113.58
1	D	1	PCA	O-C-CA	-2.63	118.01	124.77
1	B	1	PCA	OE-CD-CG	-2.59	122.09	126.72
1	B	1	PCA	O-C-CA	-2.58	118.13	124.77
1	B	1	PCA	OE-CD-N	-2.38	119.81	124.96
1	D	1	PCA	CA-N-CD	-2.36	105.50	113.58
1	C	1	PCA	OE-CD-N	-2.28	120.02	124.96
1	A	1	PCA	CA-N-CD	-2.18	106.10	113.58
1	A	1	PCA	O-C-CA	-2.14	119.26	124.77
1	C	1	PCA	CB-CA-C	-2.12	109.75	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	BGC	E	1	2	12,12,12	1.00	0	17,17,17	1.79	4 (23%)
2	BGC	E	2	2	11,11,12	1.42	1 (9%)	15,15,17	1.07	1 (6%)
2	BGC	F	1	2	12,12,12	1.25	0	17,17,17	1.69	4 (23%)
2	BGC	F	2	2	11,11,12	1.23	1 (9%)	15,15,17	1.27	2 (13%)
2	BGC	G	1	2	12,12,12	1.20	0	17,17,17	1.71	2 (11%)
2	BGC	G	2	2	11,11,12	1.36	1 (9%)	15,15,17	1.18	1 (6%)
2	BGC	H	1	2	12,12,12	1.15	0	17,17,17	1.48	3 (17%)
2	BGC	H	2	2	11,11,12	1.40	2 (18%)	15,15,17	1.44	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	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	BGC	G	2	2	-	1/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	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	E	2	BGC	O5-C5	3.57	1.50	1.43
2	G	2	BGC	O5-C5	3.14	1.49	1.43
2	F	2	BGC	O5-C5	2.71	1.48	1.43
2	H	2	BGC	O5-C5	2.59	1.48	1.43
2	H	2	BGC	C2-C3	2.54	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BGC	O3-C3-C2	-4.17	100.55	110.38
2	G	1	BGC	O3-C3-C2	-4.12	100.66	110.38
2	F	1	BGC	O3-C3-C2	-4.08	100.76	110.38
2	H	2	BGC	O2-C2-C1	-3.61	100.96	109.22
2	H	1	BGC	O3-C3-C2	-3.27	102.67	110.38
2	E	1	BGC	C4-C3-C2	-3.06	105.46	110.83
2	F	2	BGC	O2-C2-C1	-3.04	102.26	109.22
2	E	1	BGC	O5-C1-C2	2.91	115.42	110.30
2	G	2	BGC	O2-C2-C1	-2.81	102.79	109.22
2	G	1	BGC	C4-C3-C2	-2.63	106.21	110.83
2	F	2	BGC	O3-C3-C2	2.50	115.15	110.05
2	E	2	BGC	O2-C2-C1	-2.45	103.61	109.22
2	H	1	BGC	C4-C3-C2	-2.33	106.74	110.83
2	F	1	BGC	C4-C3-C2	-2.32	106.76	110.83
2	E	1	BGC	O1-C1-O5	2.30	117.25	110.41
2	F	1	BGC	O5-C5-C6	2.25	112.01	106.44
2	F	1	BGC	O5-C5-C4	-2.18	105.77	109.70
2	H	1	BGC	O5-C5-C6	2.07	111.57	106.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

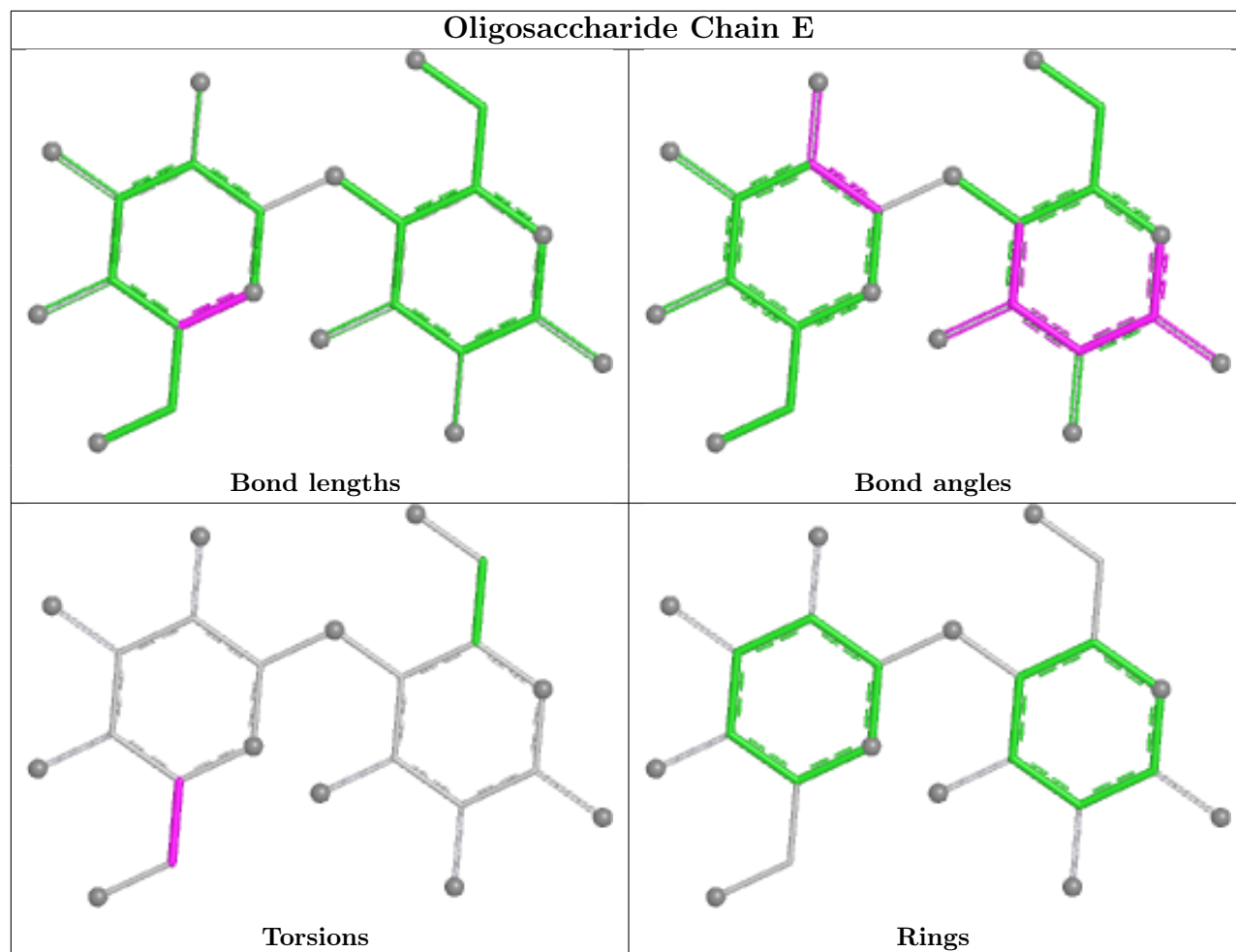
Mol	Chain	Res	Type	Atoms
2	H	2	BGC	C4-C5-C6-O6
2	F	2	BGC	C4-C5-C6-O6
2	E	2	BGC	C4-C5-C6-O6
2	G	2	BGC	C4-C5-C6-O6

There are no ring outliers.

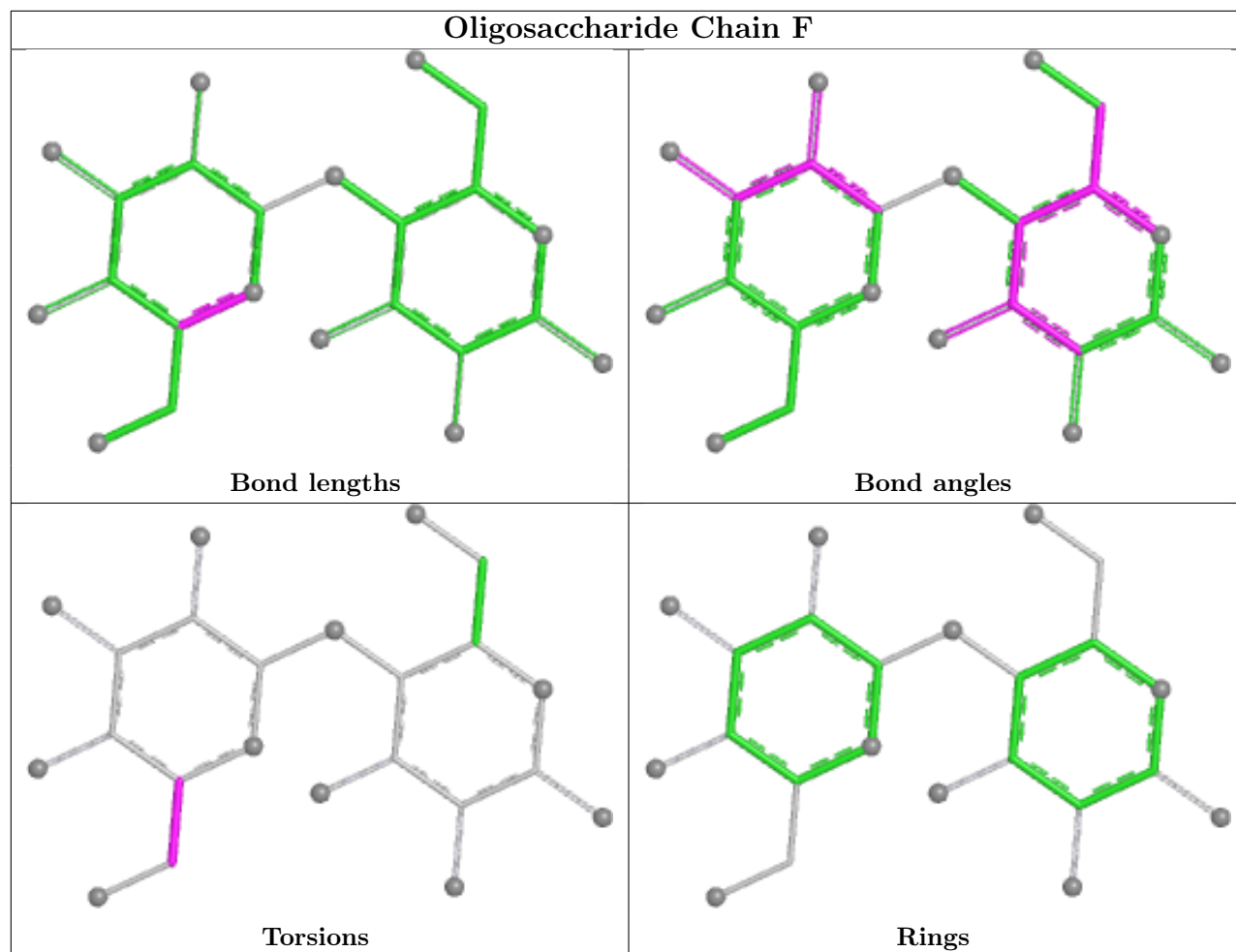
4 monomers are involved in 5 short contacts:

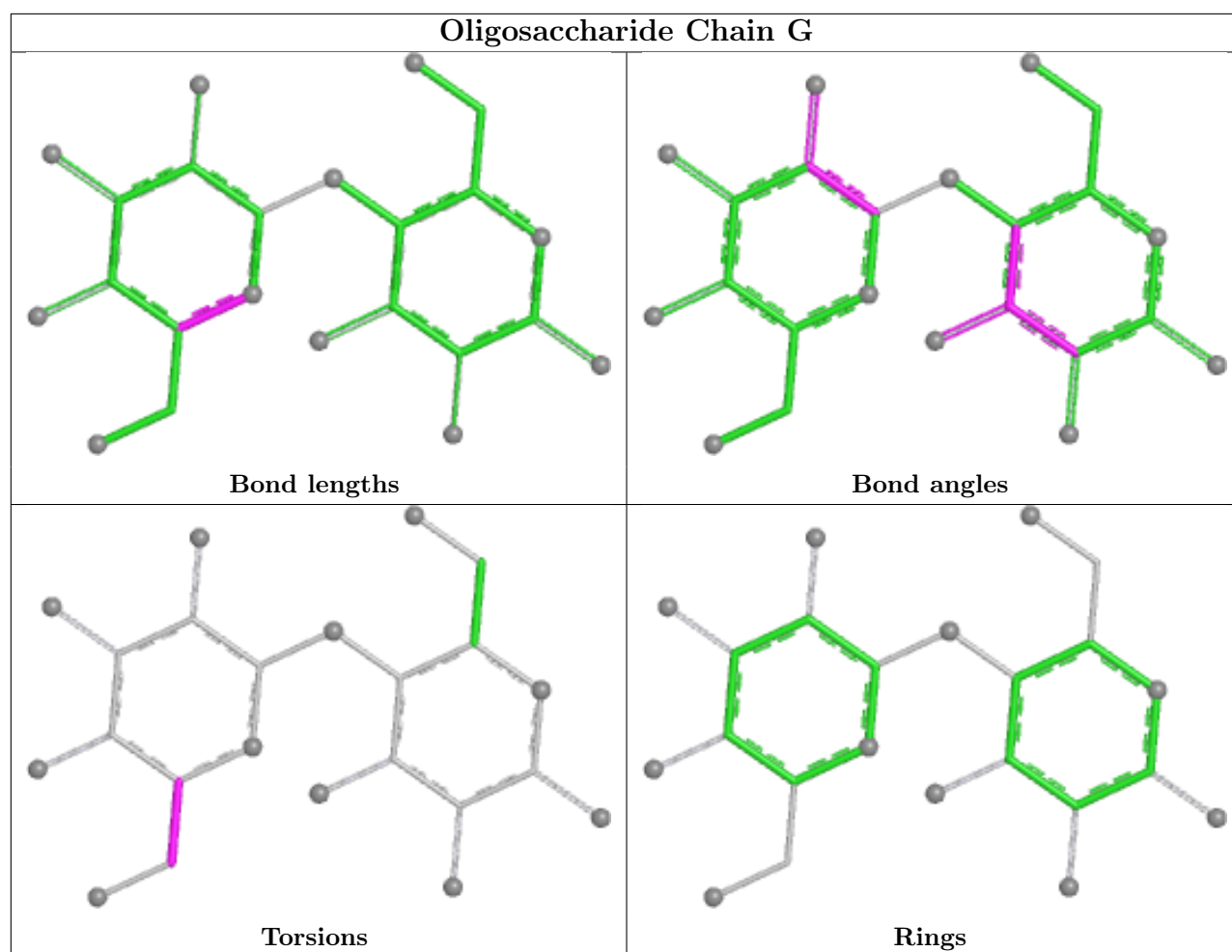
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	BGC	2	0
2	F	1	BGC	1	0
2	G	1	BGC	1	0
2	E	1	BGC	1	0

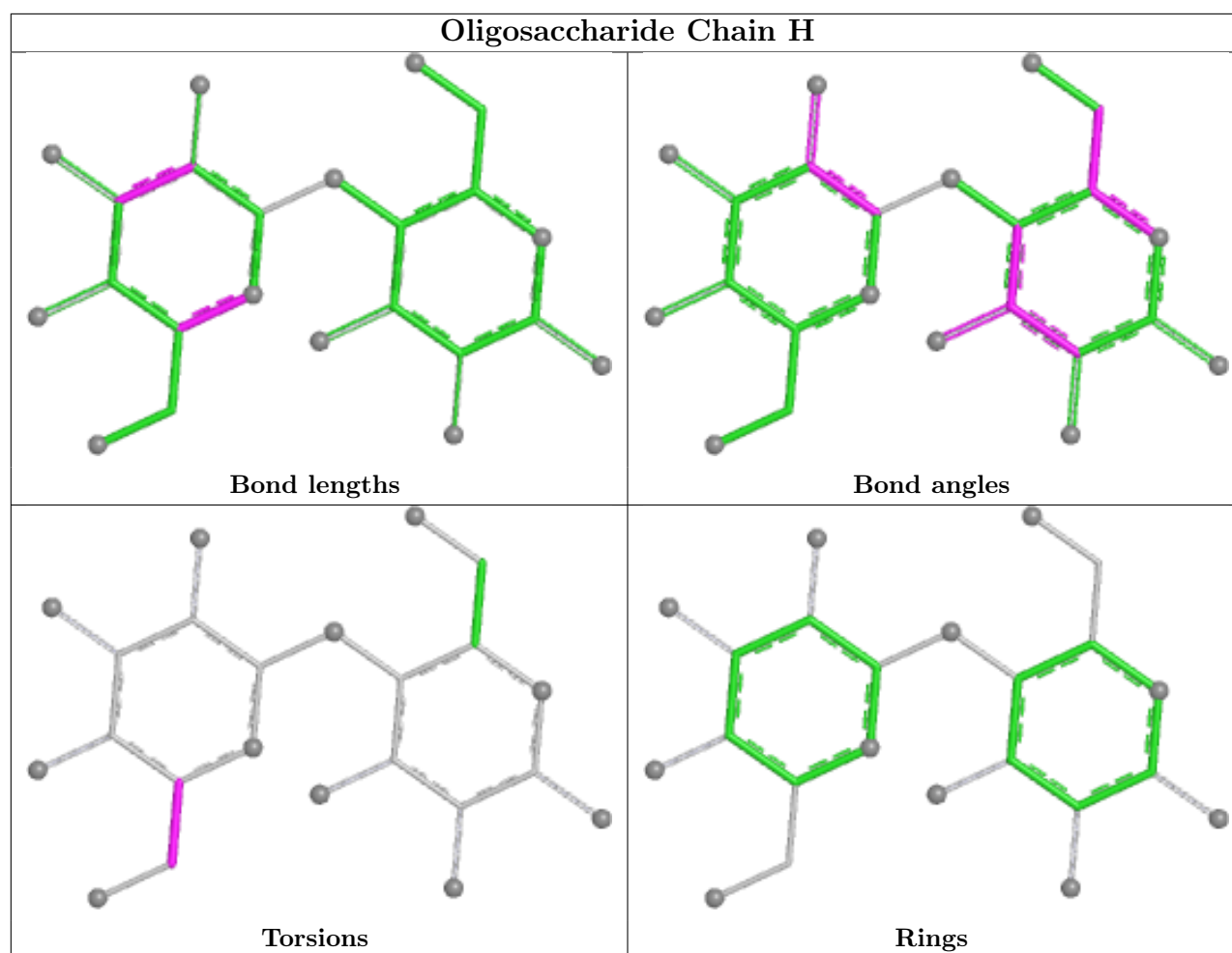
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain F







5.6 Ligand geometry [i](#)

8 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	NAG	A	413	1	14,14,15	1.16	1 (7%)	17,19,21	1.55	3 (17%)
3	NAG	D	413	1	14,14,15	1.23	1 (7%)	17,19,21	1.88	4 (23%)
3	NAG	C	412	1	14,14,15	1.25	1 (7%)	17,19,21	2.18	4 (23%)
3	NAG	C	413	1	14,14,15	1.20	1 (7%)	17,19,21	1.57	2 (11%)
3	NAG	B	412	1	14,14,15	1.29	1 (7%)	17,19,21	1.65	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	412	1	14,14,15	1.31	1 (7%)	17,19,21	1.57	4 (23%)
3	NAG	D	412	1	14,14,15	1.38	1 (7%)	17,19,21	1.81	5 (29%)
3	NAG	B	413	1	14,14,15	1.27	1 (7%)	17,19,21	2.01	8 (47%)

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
3	NAG	A	413	1	-	2/6/23/26	0/1/1/1
3	NAG	D	413	1	-	2/6/23/26	0/1/1/1
3	NAG	C	412	1	-	2/6/23/26	0/1/1/1
3	NAG	C	413	1	-	2/6/23/26	0/1/1/1
3	NAG	B	412	1	-	0/6/23/26	0/1/1/1
3	NAG	A	412	1	-	0/6/23/26	0/1/1/1
3	NAG	D	412	1	-	2/6/23/26	0/1/1/1
3	NAG	B	413	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	413	NAG	O7-C7	-3.96	1.14	1.23
3	D	412	NAG	O7-C7	-3.77	1.14	1.23
3	A	412	NAG	O7-C7	-3.70	1.15	1.23
3	B	413	NAG	O7-C7	-3.56	1.15	1.23
3	B	412	NAG	O7-C7	-3.55	1.15	1.23
3	C	412	NAG	O7-C7	-3.49	1.15	1.23
3	D	413	NAG	O7-C7	-3.27	1.15	1.23
3	C	413	NAG	O7-C7	-3.23	1.16	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	412	NAG	C1-O5-C5	-7.18	102.56	112.19
3	B	412	NAG	C1-O5-C5	-4.79	105.76	112.19
3	C	413	NAG	C1-O5-C5	4.51	118.24	112.19
3	D	413	NAG	C2-N2-C7	-4.50	116.86	122.90
3	D	412	NAG	O5-C1-C2	-4.28	104.67	111.29
3	B	413	NAG	O5-C1-C2	-4.25	104.72	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	413	NAG	C4-C3-C2	-3.90	105.30	111.02
3	A	413	NAG	O5-C1-C2	-3.45	105.96	111.29
3	D	412	NAG	C2-N2-C7	-3.38	118.37	122.90
3	A	412	NAG	O4-C4-C5	-3.27	101.26	109.32
3	C	412	NAG	O5-C1-C2	-3.21	106.32	111.29
3	A	412	NAG	C8-C7-N2	-2.95	111.23	116.12
3	B	413	NAG	C3-C4-C5	2.75	115.21	110.23
3	A	413	NAG	O3-C3-C2	-2.63	103.94	109.40
3	B	412	NAG	C8-C7-N2	-2.62	111.77	116.12
3	B	413	NAG	C8-C7-N2	-2.55	111.89	116.12
3	D	413	NAG	O6-C6-C5	2.55	120.00	111.33
3	D	412	NAG	C1-O5-C5	-2.52	108.81	112.19
3	B	413	NAG	C1-C2-N2	-2.42	106.61	110.43
3	A	412	NAG	C3-C4-C5	2.39	114.57	110.23
3	D	412	NAG	C6-C5-C4	-2.35	107.25	113.02
3	B	413	NAG	C1-O5-C5	2.32	115.29	112.19
3	B	413	NAG	C2-N2-C7	-2.31	119.80	122.90
3	A	413	NAG	O3-C3-C4	2.26	115.71	110.38
3	C	412	NAG	O5-C5-C4	-2.22	105.42	110.83
3	D	413	NAG	O5-C1-C2	-2.19	107.90	111.29
3	C	412	NAG	C4-C3-C2	-2.13	107.89	111.02
3	A	412	NAG	O5-C1-C2	-2.07	108.08	111.29
3	B	412	NAG	O7-C7-C8	2.07	125.73	122.05
3	D	412	NAG	C3-C4-C5	2.05	113.95	110.23
3	B	413	NAG	C6-C5-C4	-2.05	107.98	113.02
3	C	413	NAG	O3-C3-C4	-2.04	105.56	110.38
3	B	413	NAG	O7-C7-C8	2.00	125.62	122.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	413	NAG	O5-C5-C6-O6
3	A	413	NAG	C8-C7-N2-C2
3	A	413	NAG	O7-C7-N2-C2
3	D	413	NAG	C4-C5-C6-O6
3	C	412	NAG	C4-C5-C6-O6
3	D	412	NAG	C4-C5-C6-O6
3	D	412	NAG	O5-C5-C6-O6
3	C	412	NAG	O5-C5-C6-O6
3	C	413	NAG	O5-C5-C6-O6
3	C	413	NAG	C4-C5-C6-O6

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	397/411 (96%)	-0.24	2 (0%) 87 87	13, 26, 43, 52	0
1	B	397/411 (96%)	-0.02	9 (2%) 61 63	14, 27, 44, 51	0
1	C	397/411 (96%)	-0.13	3 (0%) 82 83	12, 27, 44, 53	0
1	D	397/411 (96%)	-0.31	1 (0%) 90 90	14, 25, 42, 51	0
All	All	1588/1644 (96%)	-0.18	15 (0%) 81 82	12, 26, 43, 53	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ARG	3.4
1	B	398	SER	3.3
1	B	99	ASN	3.1
1	B	156	SER	3.0
1	C	25	LYS	2.8
1	A	226	ASP	2.6
1	C	99	ASN	2.6
1	B	319	GLY	2.5
1	B	277	GLN	2.3
1	B	100	ASN	2.2
1	B	159	ARG	2.2
1	D	22	SER	2.1
1	B	374	ASN	2.1
1	B	58	THR	2.0
1	C	58	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	C	1	8/9	0.92	0.07	27,29,31,33	0
1	PCA	A	1	8/9	0.95	0.06	23,26,29,31	0
1	PCA	D	1	8/9	0.95	0.06	23,26,27,28	0
1	PCA	B	1	8/9	0.96	0.06	24,27,29,31	0

6.3 Carbohydrates [i](#)

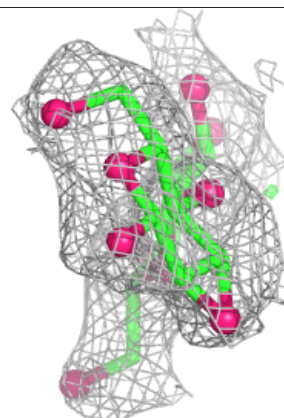
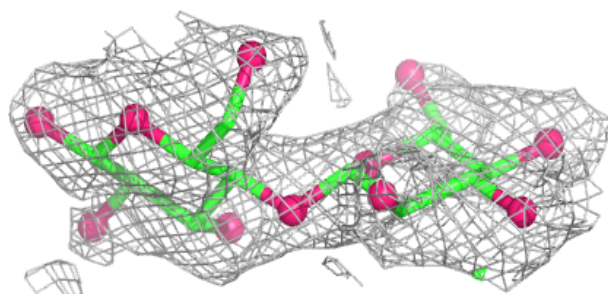
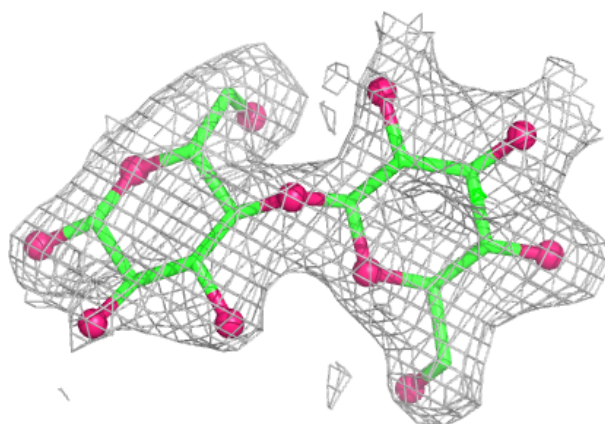
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	F	2	11/12	0.85	0.10	28,32,39,43	0
2	BGC	E	2	11/12	0.87	0.10	28,33,39,43	0
2	BGC	G	2	11/12	0.89	0.09	28,33,40,43	0
2	BGC	H	1	12/12	0.89	0.10	33,35,38,39	0
2	BGC	H	2	11/12	0.89	0.08	26,33,39,43	0
2	BGC	E	1	12/12	0.90	0.10	33,35,37,39	0
2	BGC	F	1	12/12	0.90	0.10	34,35,38,38	0
2	BGC	G	1	12/12	0.91	0.10	32,35,38,39	0

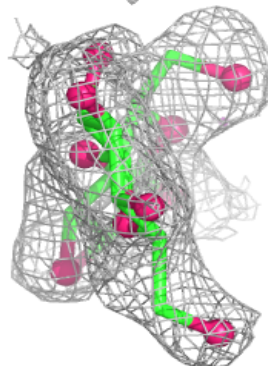
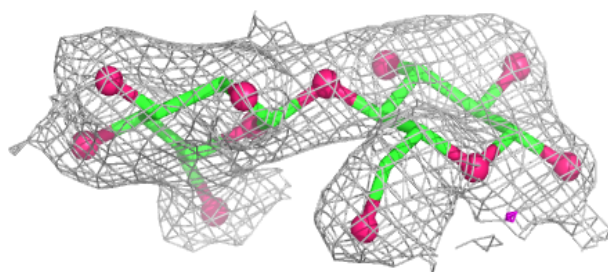
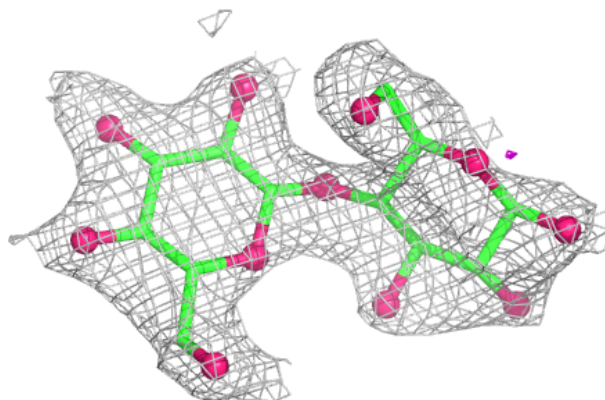
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

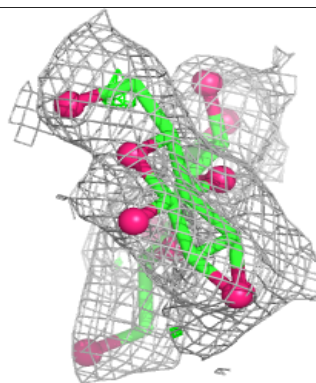
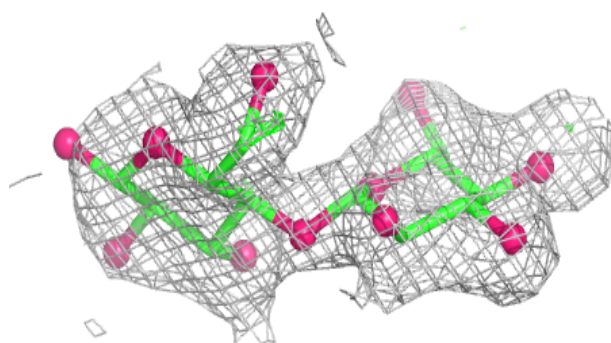
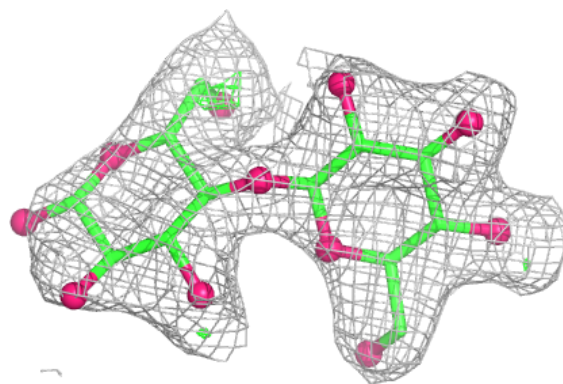
**Electron density around Chain F:**

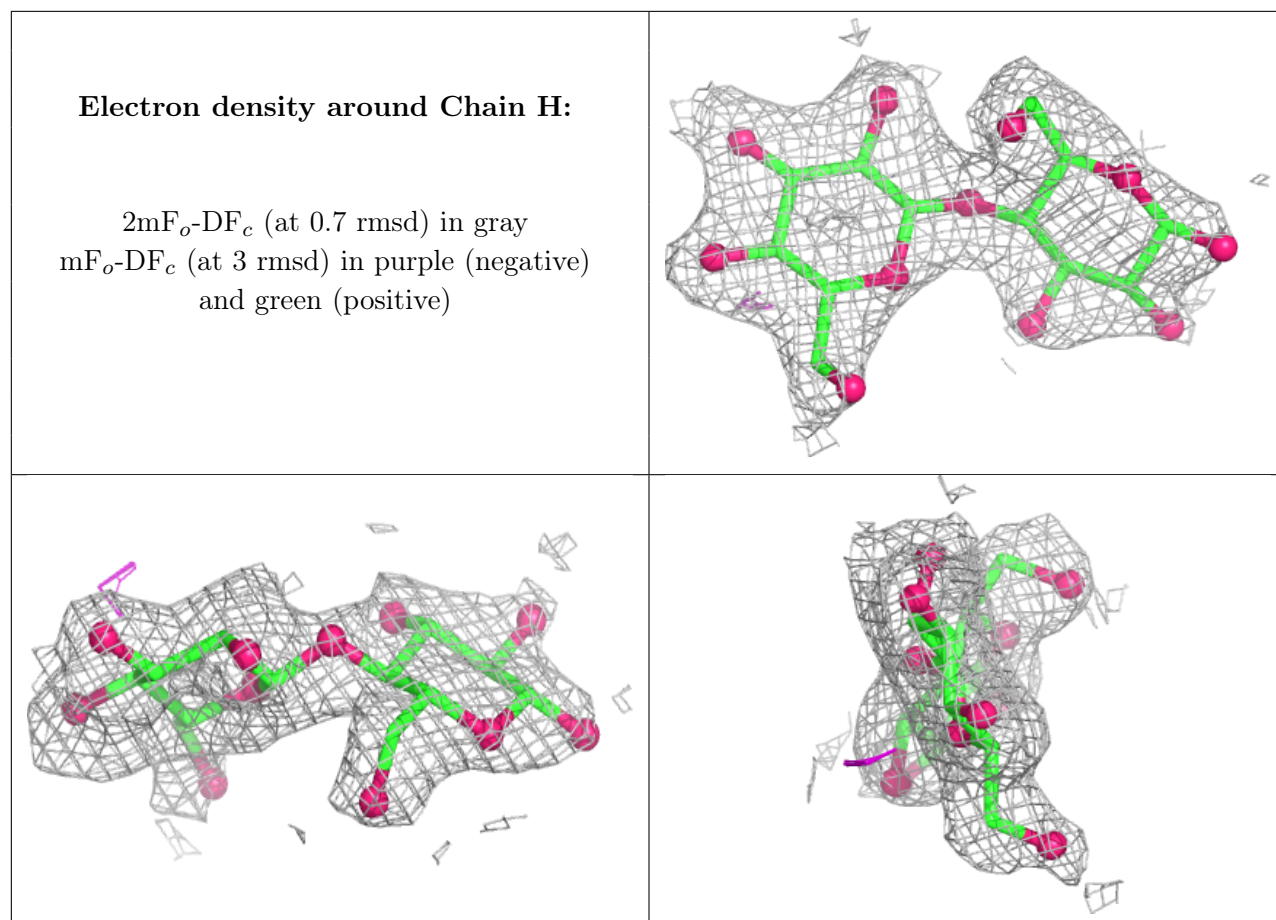
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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](#)

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	NAG	B	413	14/15	0.68	0.12	59,61,63,63	0
3	NAG	A	413	14/15	0.76	0.11	56,59,62,62	0
3	NAG	D	413	14/15	0.77	0.12	57,59,62,62	0
3	NAG	B	412	14/15	0.79	0.10	52,54,55,56	0
3	NAG	A	412	14/15	0.80	0.11	53,55,56,56	0
3	NAG	C	413	14/15	0.81	0.12	56,58,59,61	0
3	NAG	C	412	14/15	0.84	0.10	52,54,55,55	0
3	NAG	D	412	14/15	0.87	0.09	52,54,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.