



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 PM UTC

PDB ID : 1L1Y / pdb_000011ly
Title : The Crystal Structure and Catalytic Mechanism of Cellobiohydrolase CelS, the Major Enzymatic Component of the Clostridium thermocellum cellulosome
Authors : Guimaraes, B.G.; Souchon, H.; Lytle, B.L.; Wu, J.H.D.; Alzari, P.M.
Deposited on : 2002-02-20
Resolution : 2.40 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

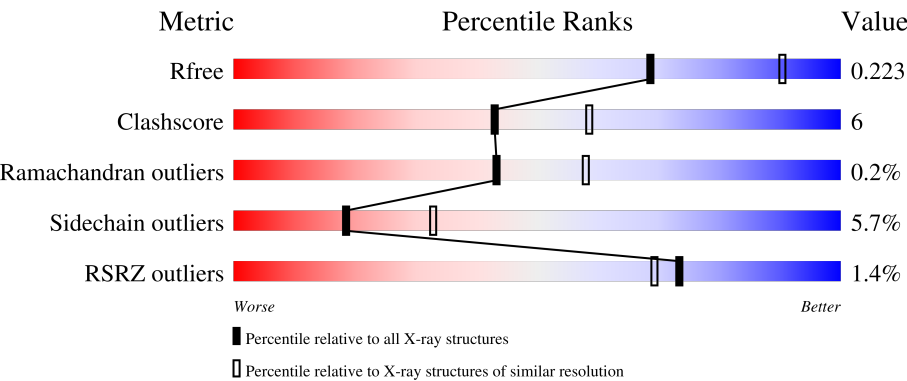
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	678	3% 78% 14% • 5%
1	B	678	% 81% 12% • 5%
1	C	678	% 78% 14% • 5%
1	D	678	% 82% 10% • 5%
1	E	678	% 83% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	678	% 81%12%5%
2	G	2	100%
2	H	2	50%50%
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	50%50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32457 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 cellobiohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5103	3285	825	973	20			
1	B	642	Total	C	N	O	S	0	0	0
			5128	3299	835	974	20			
1	C	642	Total	C	N	O	S	0	0	0
			5109	3287	832	970	20			
1	D	642	Total	C	N	O	S	0	0	0
			5136	3303	836	977	20			
1	E	642	Total	C	N	O	S	0	0	0
			5124	3298	832	974	20			
1	F	642	Total	C	N	O	S	0	0	0
			5130	3300	833	977	20			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			22	12	10			
2	H	2	Total	C	O	0	0	0
			22	12	10			
2	I	2	Total	C	O	0	0	0
			22	12	10			
2	J	2	Total	C	O	0	0	0
			22	12	10			
2	K	2	Total	C	O	0	0	0
			22	12	10			
2	L	2	Total	C	O	0	0	0
			22	12	10			

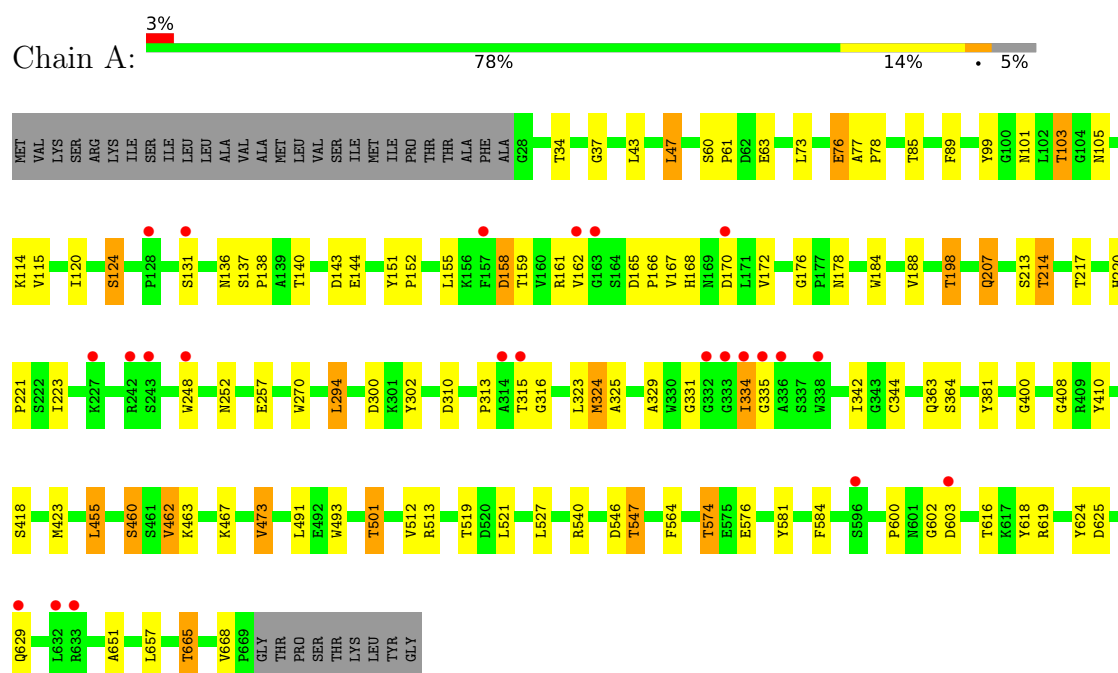
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total 169	O 169	0	0
3	B	204	Total 204	O 204	0	0
3	C	214	Total 214	O 214	0	0
3	D	326	Total 326	O 326	0	0
3	E	286	Total 286	O 286	0	0
3	F	396	Total 396	O 396	0	0

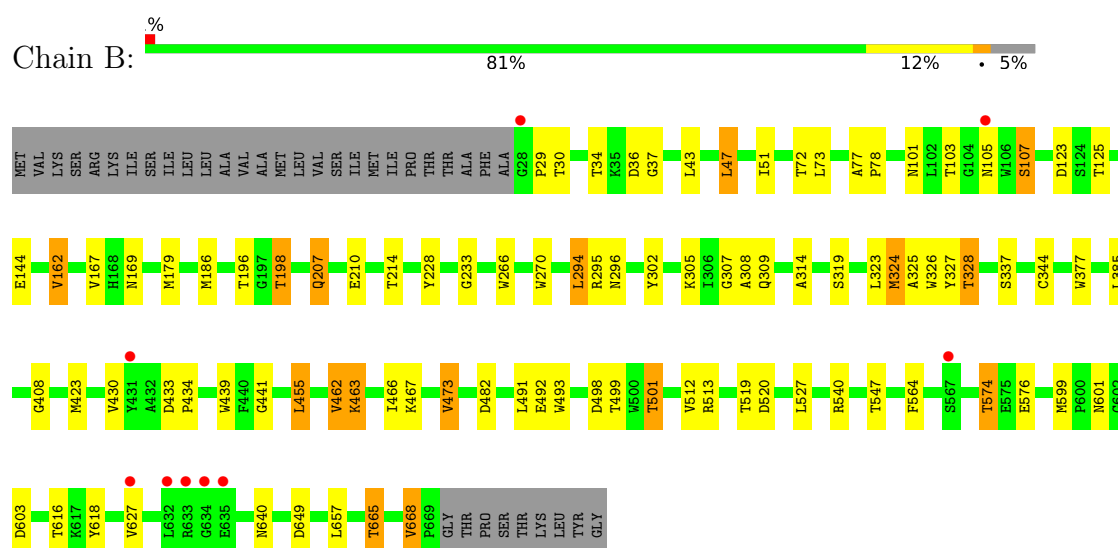
3 Residue-property plots [i](#)

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.

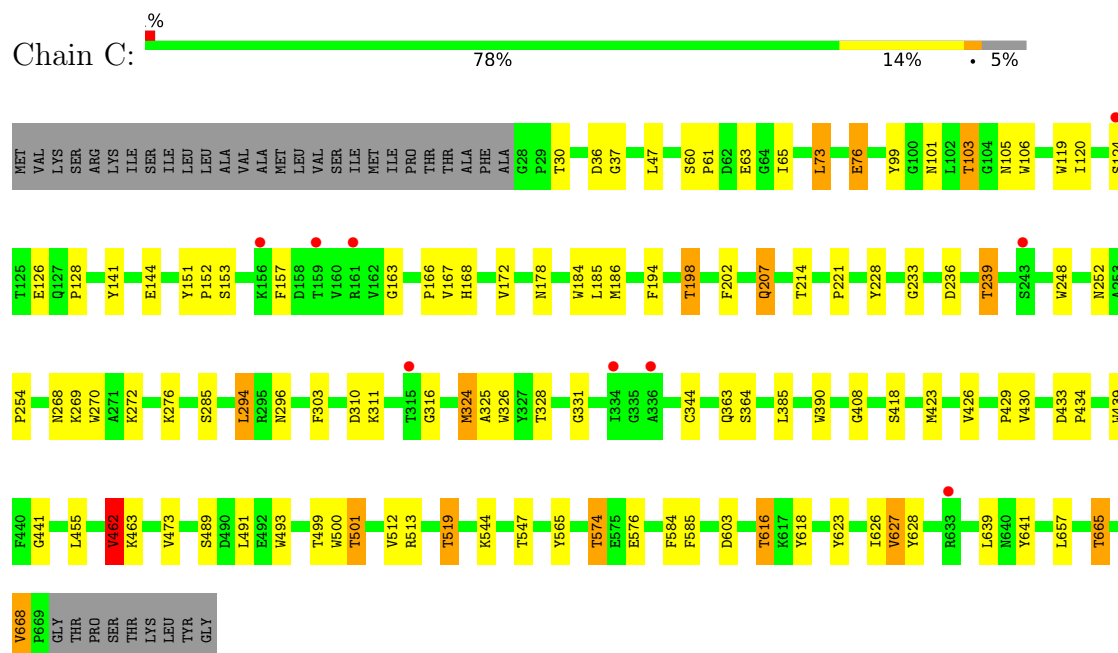
• Molecule 1: cellobiohydrolase



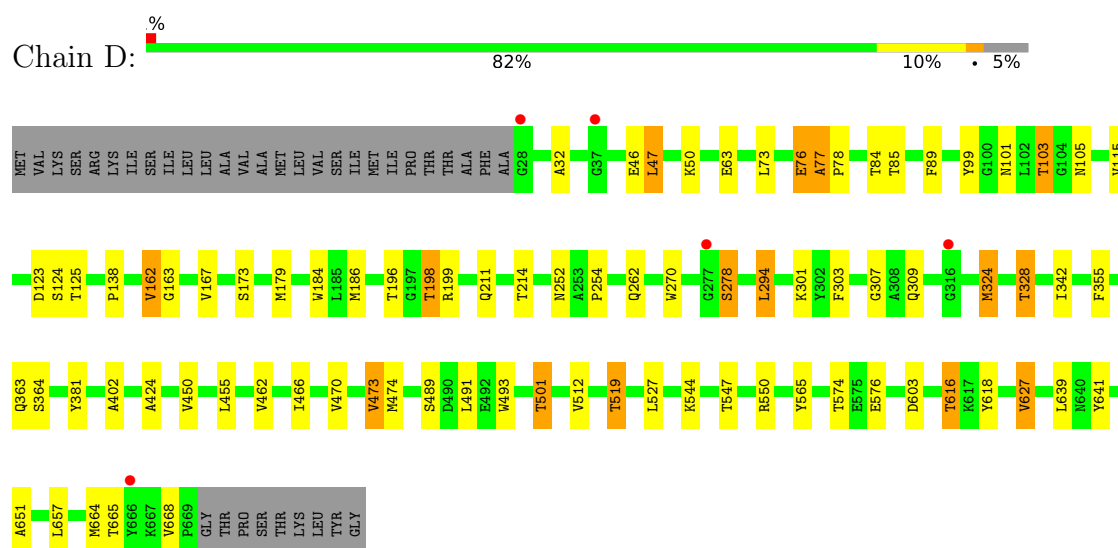
• Molecule 1: cellobiohydrolase



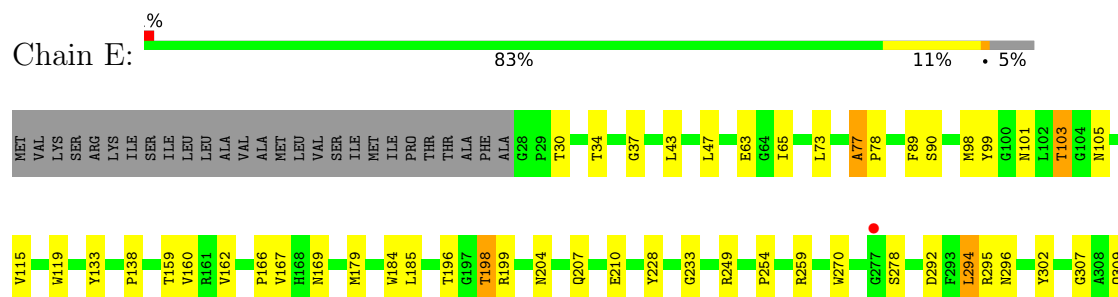
- Molecule 1: cellobiohydrolase

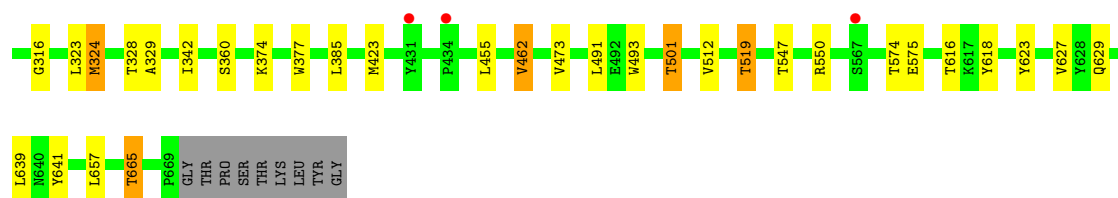


- Molecule 1: cellobiohydrolase

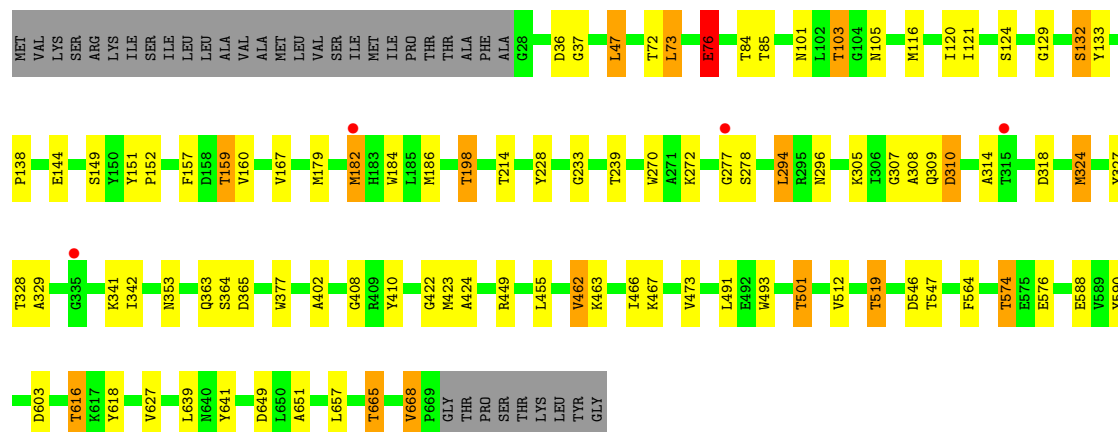
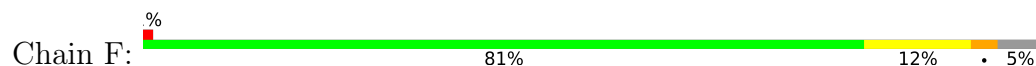


- Molecule 1: cellobiohydrolase





- Molecule 1: cellobiohydrolase



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



BGC1
BGC2

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



BGC1
BGC2

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



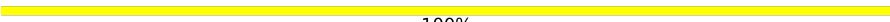
BGC1
BGC2

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



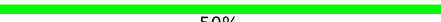
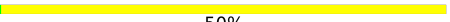
BGC1
BGC2

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

Chain K:  100%

BGC1
BGC2

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

Chain L:  50%  50%

BGC1
BGC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	147.24Å 207.20Å 213.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.40) 99.4 (15.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.189 , 0.224 0.188 , 0.223	Depositor DCC
R_{free} test set	12676 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32457	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: BGC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	1/5282 (0.0%)	0.96	9/7213 (0.1%)
1	B	0.65	2/5307 (0.0%)	0.89	0/7241
1	C	0.65	1/5288 (0.0%)	0.91	2/7218 (0.0%)
1	D	0.74	2/5315 (0.0%)	0.97	2/7251 (0.0%)
1	E	0.69	2/5303 (0.0%)	0.93	0/7236
1	F	0.74	2/5309 (0.0%)	0.95	5/7244 (0.1%)
All	All	0.69	10/31804 (0.0%)	0.94	18/43403 (0.0%)

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	B	0	1
1	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	324	MET	SD-CE	-12.24	1.49	1.79
1	B	324	MET	SD-CE	-11.23	1.51	1.79
1	C	324	MET	SD-CE	-10.34	1.53	1.79
1	F	324	MET	SD-CE	-9.86	1.54	1.79
1	E	324	MET	SD-CE	-9.48	1.55	1.79
1	A	324	MET	SD-CE	-7.01	1.62	1.79
1	D	627	VAL	CA-CB	6.14	1.62	1.54
1	F	182	MET	SD-CE	-5.40	1.66	1.79
1	B	186	MET	SD-CE	5.09	1.92	1.79
1	E	98	MET	SD-CE	5.00	1.92	1.79

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	GLU	N-CA-C	-6.52	100.99	108.49
1	A	400	GLY	N-CA-C	6.06	119.82	112.49
1	A	462	VAL	N-CA-CB	-5.67	105.97	112.21
1	A	188	VAL	N-CA-C	5.65	115.85	110.42
1	C	157	PHE	N-CA-C	5.64	118.37	111.82
1	F	310	ASP	N-CA-C	5.62	115.99	108.23
1	D	76	GLU	N-CA-C	-5.36	99.39	110.80
1	A	546	ASP	CA-C-N	5.36	127.45	120.28
1	A	546	ASP	C-N-CA	5.36	127.45	120.28
1	F	157	PHE	N-CA-C	5.31	117.15	111.36
1	D	328	THR	OG1-CB-CG2	-5.30	98.69	109.30
1	F	546	ASP	CA-C-N	5.22	127.53	120.38
1	F	546	ASP	C-N-CA	5.22	127.53	120.38
1	F	76	GLU	N-CA-C	-5.17	99.78	110.80
1	C	462	VAL	N-CA-CB	-5.14	106.56	112.21
1	A	120	ILE	CA-C-N	-5.13	118.89	122.59
1	A	120	ILE	C-N-CA	-5.13	118.89	122.59
1	A	170	ASP	N-CA-C	5.12	117.75	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	327	TYR	Peptide
1	F	327	TYR	Peptide

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	5103	0	4667	72	0
1	B	5128	0	4727	60	0
1	C	5109	0	4686	67	0
1	D	5136	0	4737	54	0
1	E	5124	0	4720	57	0
1	F	5130	0	4726	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	22	0	19	0	0
2	H	22	0	19	1	0
2	I	22	0	19	0	0
2	J	22	0	19	0	0
2	K	22	0	19	0	0
2	L	22	0	19	0	0
3	A	169	0	0	8	0
3	B	204	0	0	4	0
3	C	214	0	0	10	0
3	D	326	0	0	5	0
3	E	286	0	0	7	0
3	F	396	0	0	15	0
All	All	32457	0	28377	367	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 6.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:HG21	1:A:576:GLU:OE1	1.58	1.03
1:C:294:LEU:HG	1:C:324:MET:HE1	1.40	1.03
1:A:105:ASN:HB2	3:A:840:HOH:O	1.62	0.97
3:C:703:HOH:O	1:E:169:ASN:HB3	1.66	0.95
1:C:103:THR:HG22	1:C:105:ASN:H	1.35	0.91
1:F:278:SER:HB3	3:F:1064:HOH:O	1.76	0.86
1:C:294:LEU:HG	1:C:324:MET:CE	2.05	0.85
1:C:574:THR:HG21	1:C:576:GLU:OE1	1.76	0.85
1:F:574:THR:HG21	1:F:576:GLU:OE1	1.74	0.85
1:F:116:MET:HG3	1:F:182:MET:SD	2.16	0.85
1:A:76:GLU:O	1:A:214:THR:HG21	1.77	0.84
1:E:103:THR:HG22	1:E:105:ASN:H	1.42	0.84
1:F:120:ILE:CG2	1:F:182:MET:SD	2.68	0.82
1:F:76:GLU:O	1:F:214:THR:HG21	1.78	0.82
1:B:37:GLY:HA2	1:B:665:THR:HG21	1.63	0.81
1:B:599:MET:HB2	1:B:603:ASP:HB2	1.63	0.80
1:D:294:LEU:HG	1:D:324:MET:HE1	1.65	0.77
1:B:501:THR:HG21	1:D:309:GLN:HE21	1.49	0.77
1:F:294:LEU:HG	1:F:324:MET:HE1	1.66	0.76
1:F:310:ASP:HB2	3:F:842:HOH:O	1.85	0.76
1:E:501:THR:HG23	1:F:307:GLY:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:SER:HB2	3:A:829:HOH:O	1.85	0.76
1:B:294:LEU:HG	1:B:324:MET:HE1	1.69	0.75
1:E:99:TYR:O	1:E:103:THR:HB	1.86	0.75
1:F:519:THR:HG22	3:F:715:HOH:O	1.87	0.75
1:B:37:GLY:HA2	1:B:665:THR:CG2	2.17	0.75
1:C:363:GLN:HE22	1:F:364:SER:H	1.31	0.74
1:E:574:THR:HG23	3:E:814:HOH:O	1.87	0.74
1:F:120:ILE:HG23	1:F:182:MET:SD	2.28	0.73
1:D:574:THR:HG22	1:D:641:TYR:H	1.53	0.72
1:E:501:THR:HG21	1:F:309:GLN:HE21	1.54	0.72
1:C:268:ASN:HD21	1:C:272:LYS:HZ2	1.38	0.72
1:D:198:THR:HB	3:D:834:HOH:O	1.89	0.72
1:E:629:GLN:HB3	3:E:859:HOH:O	1.90	0.72
1:A:162:VAL:HG23	1:A:302:TYR:HB3	1.72	0.71
1:A:103:THR:HG22	1:A:105:ASN:H	1.56	0.70
1:F:37:GLY:HA2	1:F:665:THR:CG2	2.20	0.70
1:B:307:GLY:O	1:D:501:THR:CG2	2.40	0.70
1:A:47:LEU:HD13	1:A:651:ALA:HB2	1.74	0.69
1:E:254:PRO:HB2	1:E:324:MET:CE	2.22	0.69
1:B:574:THR:HG21	1:B:576:GLU:OE1	1.93	0.69
1:A:103:THR:CG2	1:A:105:ASN:H	2.06	0.69
1:B:501:THR:CG2	1:D:307:GLY:O	2.41	0.69
1:D:76:GLU:O	1:D:214:THR:HG21	1.93	0.69
1:E:101:ASN:HB2	1:E:270:TRP:CE3	2.28	0.69
1:C:364:SER:H	1:F:363:GLN:HE22	1.41	0.68
1:F:121:ILE:HG13	1:F:182:MET:HG2	1.76	0.68
1:A:294:LEU:HG	1:A:324:MET:HE1	1.76	0.68
1:E:37:GLY:HA2	1:E:665:THR:CG2	2.24	0.68
1:B:47:LEU:O	1:B:51:ILE:HG13	1.94	0.67
1:A:37:GLY:HA2	1:A:665:THR:CG2	2.24	0.67
1:E:254:PRO:HB2	1:E:324:MET:HE2	1.75	0.67
1:E:323:LEU:HD12	1:E:423:MET:HE1	1.76	0.67
1:C:623:TYR:O	1:C:627:VAL:HG12	1.93	0.67
1:C:513:ARG:HD3	3:C:878:HOH:O	1.94	0.66
1:C:99:TYR:O	1:C:103:THR:HB	1.94	0.66
1:D:254:PRO:HB2	1:D:324:MET:HE3	1.77	0.66
1:D:473:VAL:HG11	1:D:527:LEU:HD11	1.78	0.66
1:C:513:ARG:CD	3:C:878:HOH:O	2.44	0.66
1:E:307:GLY:O	1:F:501:THR:CG2	2.43	0.66
1:E:199:ARG:HD2	3:E:961:HOH:O	1.96	0.65
1:C:152:PRO:HG3	1:C:236:ASP:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:TRP:O	1:C:186:MET:HE1	1.95	0.65
1:A:364:SER:H	1:D:363:GLN:HE22	1.45	0.65
1:B:307:GLY:O	1:D:501:THR:HG23	1.96	0.65
1:B:323:LEU:HD12	1:B:423:MET:HE1	1.79	0.65
1:F:198:THR:CG2	3:F:924:HOH:O	2.44	0.64
1:C:269:LYS:HE3	3:C:889:HOH:O	1.97	0.64
1:A:363:GLN:HE22	1:D:364:SER:H	1.44	0.64
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.62	0.64
1:A:101:ASN:HB2	1:A:270:TRP:CE3	2.33	0.63
1:C:144:GLU:HB2	1:C:408:GLY:HA3	1.79	0.63
1:C:254:PRO:HB2	1:C:324:MET:HE3	1.80	0.63
1:E:37:GLY:HA2	1:E:665:THR:HG21	1.81	0.63
1:A:257:GLU:HB3	1:A:294:LEU:HD21	1.81	0.63
1:A:625:ASP:O	1:A:629:GLN:HG2	1.99	0.63
1:B:309:GLN:HE21	1:D:501:THR:HG21	1.64	0.63
1:F:305:LYS:HD2	3:F:1066:HOH:O	1.98	0.63
1:C:76:GLU:O	1:C:214:THR:HG21	1.99	0.63
1:D:254:PRO:HB2	1:D:324:MET:CE	2.29	0.63
1:F:101:ASN:HB2	1:F:270:TRP:CE3	2.34	0.62
1:E:309:GLN:HE21	1:F:501:THR:HG21	1.63	0.62
1:E:501:THR:CG2	1:F:307:GLY:O	2.47	0.61
1:D:103:THR:HG22	1:D:105:ASN:H	1.65	0.61
1:C:603:ASP:OD2	1:C:616:THR:HB	2.01	0.61
1:F:37:GLY:HA2	1:F:665:THR:HG21	1.81	0.61
1:E:196:THR:O	1:E:199:ARG:HG3	2.01	0.60
1:D:101:ASN:HB2	1:D:270:TRP:CE3	2.36	0.60
1:C:101:ASN:HB2	1:C:270:TRP:CE3	2.36	0.60
1:F:294:LEU:HG	1:F:324:MET:CE	2.31	0.60
1:B:101:ASN:HB2	1:B:270:TRP:CE3	2.37	0.60
1:F:121:ILE:CG1	1:F:182:MET:HG2	2.32	0.60
1:F:37:GLY:HA2	1:F:665:THR:HG23	1.84	0.59
1:D:550:ARG:HD2	1:D:664:MET:SD	2.42	0.59
1:A:248:TRP:CZ3	1:A:331:GLY:HA2	2.38	0.59
1:F:324:MET:HE3	3:F:747:HOH:O	2.02	0.59
1:B:169:ASN:HB2	3:B:873:HOH:O	2.02	0.58
1:A:124:SER:HB3	1:A:178:ASN:HD21	1.68	0.58
1:B:294:LEU:HG	1:B:324:MET:CE	2.33	0.58
1:A:37:GLY:HA2	1:A:665:THR:HG23	1.84	0.58
1:B:296:ASN:HB3	1:B:328:THR:HG21	1.86	0.58
1:D:76:GLU:O	1:D:77:ALA:C	2.47	0.58
1:D:294:LEU:HG	1:D:324:MET:CE	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HG23	1:A:334:ILE:HD11	1.86	0.57
1:B:77:ALA:H	1:B:78:PRO:HD2	1.70	0.57
1:C:124:SER:HB3	1:C:178:ASN:ND2	2.19	0.57
1:A:124:SER:HB3	1:A:178:ASN:ND2	2.20	0.57
1:F:103:THR:CG2	1:F:105:ASN:H	2.17	0.57
1:F:588:GLU:HG3	3:F:942:HOH:O	2.03	0.56
1:C:207:GLN:HA	1:C:207:GLN:HE21	1.69	0.56
1:C:385:LEU:HD22	1:C:462:VAL:HG21	1.86	0.56
1:D:99:TYR:O	1:D:103:THR:HB	2.06	0.56
1:A:114:LYS:HE3	3:A:838:HOH:O	2.05	0.56
1:C:36:ASP:OD1	1:C:668:VAL:HG12	2.06	0.56
1:A:547:THR:CG2	3:A:831:HOH:O	2.54	0.55
1:B:198:THR:HG22	3:B:806:HOH:O	2.06	0.55
1:A:519:THR:HG23	3:A:731:HOH:O	2.07	0.55
1:B:105:ASN:ND2	1:B:107:SER:OG	2.37	0.55
1:B:162:VAL:HG22	1:B:302:TYR:HB3	1.87	0.55
1:B:493:TRP:CZ3	1:B:512:VAL:HB	2.41	0.55
1:D:574:THR:HG21	1:D:576:GLU:OE1	2.07	0.55
1:F:493:TRP:CZ3	1:F:512:VAL:HB	2.42	0.55
1:B:601:ASN:HD21	1:B:616:THR:HB	1.71	0.54
1:E:294:LEU:HG	1:E:324:MET:HE1	1.88	0.54
1:A:37:GLY:HA2	1:A:665:THR:HG21	1.89	0.54
1:A:294:LEU:HG	1:A:324:MET:CE	2.36	0.54
1:A:581:TYR:O	1:A:584:PHE:HB2	2.08	0.54
1:A:463:LYS:O	1:A:467:LYS:HG2	2.09	0.53
1:B:439:TRP:CE2	1:B:441:GLY:HA3	2.43	0.53
1:B:325:ALA:HB1	1:B:344:CYS:HB3	1.90	0.53
1:B:324:MET:HE2	1:B:377:TRP:HH2	1.73	0.53
1:E:323:LEU:CD1	1:E:423:MET:HE1	2.37	0.53
1:E:77:ALA:H	1:E:78:PRO:HD2	1.74	0.53
1:E:574:THR:HG22	1:E:575:GLU:N	2.24	0.53
1:A:89:PHE:HE2	1:A:115:VAL:HG12	1.74	0.53
1:B:574:THR:O	1:B:640:ASN:HA	2.09	0.53
1:C:272:LYS:HE2	3:F:863:HOH:O	2.09	0.53
1:F:463:LYS:O	1:F:467:LYS:HG2	2.08	0.53
1:D:519:THR:CG2	3:D:999:HOH:O	2.56	0.52
1:A:213:SER:O	1:A:217:THR:HG23	2.09	0.52
1:F:84:THR:HG22	1:F:186:MET:HB3	1.89	0.52
1:E:37:GLY:HA2	1:E:665:THR:HG23	1.91	0.52
1:A:473:VAL:HG11	1:A:527:LEU:HD11	1.92	0.52
1:F:574:THR:CG2	1:F:576:GLU:OE1	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:O	1:A:77:ALA:C	2.51	0.52
1:C:198:THR:HG22	3:C:876:HOH:O	2.09	0.52
1:E:296:ASN:HB3	1:E:328:THR:HG21	1.90	0.52
1:E:360:SER:HG	1:E:377:TRP:CD1	2.28	0.51
1:F:151:TYR:HA	1:F:152:PRO:C	2.36	0.51
1:D:47:LEU:HD13	1:D:651:ALA:HB2	1.93	0.51
1:F:47:LEU:HD13	1:F:651:ALA:HB2	1.91	0.51
1:D:574:THR:HG22	1:D:641:TYR:N	2.25	0.51
1:F:310:ASP:HB3	3:F:717:HOH:O	2.11	0.51
1:B:324:MET:CE	1:B:377:TRP:HH2	2.24	0.51
1:A:166:PRO:HG3	1:A:316:GLY:O	2.11	0.50
1:E:103:THR:CG2	1:E:105:ASN:H	2.19	0.50
1:F:198:THR:HG23	3:F:924:HOH:O	2.09	0.50
1:F:103:THR:HG23	1:F:105:ASN:H	1.76	0.50
1:B:501:THR:HG23	1:D:307:GLY:O	2.10	0.50
1:D:262:GLN:HG3	1:D:355:PHE:CD2	2.45	0.50
1:B:519:THR:HG23	3:B:783:HOH:O	2.11	0.50
1:F:272:LYS:HD2	1:F:277:GLY:HA3	1.93	0.50
1:B:492:GLU:OE1	1:B:513:ARG:NH1	2.45	0.50
1:C:120:ILE:HA	1:C:186:MET:HE1	1.94	0.50
1:E:360:SER:HG	1:E:377:TRP:CG	2.30	0.50
1:A:619:ARG:HG2	1:A:624:TYR:CZ	2.45	0.50
1:A:140:THR:HB	1:A:155:LEU:HD22	1.93	0.50
1:B:36:ASP:OD1	1:B:668:VAL:HG12	2.12	0.50
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.94	0.50
1:F:272:LYS:HD2	1:F:277:GLY:CA	2.41	0.50
1:C:296:ASN:HB3	1:C:328:THR:HG21	1.94	0.49
1:E:34:THR:HG21	1:E:43:LEU:HD21	1.94	0.49
1:A:602:GLY:O	1:A:603:ASP:C	2.55	0.49
1:C:639:LEU:HD22	1:C:641:TYR:OH	2.13	0.49
1:E:249:ARG:HD3	3:E:883:HOH:O	2.11	0.49
1:F:294:LEU:CG	1:F:324:MET:HE1	2.39	0.49
1:A:144:GLU:HB2	1:A:408:GLY:HA3	1.93	0.49
1:B:34:THR:HG21	1:B:43:LEU:HD21	1.95	0.49
1:B:228:TYR:O	1:B:233:GLY:HA2	2.12	0.49
1:F:73:LEU:HD12	1:F:73:LEU:C	2.37	0.49
1:A:161:ARG:O	1:A:313:PRO:HG3	2.12	0.49
1:C:493:TRP:CZ3	1:C:512:VAL:HB	2.47	0.49
1:F:116:MET:CG	1:F:182:MET:SD	2.97	0.49
1:A:151:TYR:HA	1:A:152:PRO:C	2.38	0.49
1:B:210:GLU:HG2	3:B:879:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ALA:HB3	1:E:78:PRO:CD	2.43	0.49
1:E:159:THR:HG23	1:E:160:VAL:HG23	1.94	0.49
1:A:99:TYR:O	1:A:103:THR:HB	2.12	0.49
1:D:574:THR:CG2	1:D:641:TYR:H	2.25	0.49
1:F:310:ASP:HA	1:F:410:TYR:HB3	1.95	0.49
1:A:172:VAL:HA	1:A:176:GLY:O	2.13	0.48
1:D:493:TRP:CZ3	1:D:512:VAL:HB	2.48	0.48
1:F:133:TYR:OH	1:F:138:PRO:HB3	2.13	0.48
1:A:493:TRP:CZ3	1:A:512:VAL:HB	2.49	0.48
1:B:144:GLU:HB2	1:B:408:GLY:HA3	1.95	0.48
1:E:307:GLY:O	1:F:501:THR:HG22	2.13	0.48
1:A:665:THR:HG22	3:A:811:HOH:O	2.13	0.48
1:C:426:VAL:HG23	1:C:429:PRO:HG3	1.95	0.48
1:F:36:ASP:OD1	1:F:668:VAL:HG13	2.14	0.48
1:E:89:PHE:HE2	1:E:115:VAL:HG12	1.77	0.48
1:A:165:ASP:OD2	1:A:168:HIS:HB2	2.14	0.48
1:C:30:THR:O	1:C:565:TYR:HB3	2.13	0.48
1:B:105:ASN:ND2	1:B:107:SER:H	2.12	0.48
1:B:294:LEU:HB3	1:B:377:TRP:HZ2	1.79	0.48
1:B:482:ASP:C	1:B:482:ASP:OD1	2.57	0.48
1:D:77:ALA:HB3	1:D:78:PRO:HD3	1.94	0.48
1:F:519:THR:HG21	1:F:564:PHE:CZ	2.48	0.48
1:F:314:ALA:HB1	1:F:318:ASP:HB2	1.96	0.47
1:A:329:ALA:HB3	1:A:342:ILE:HD11	1.96	0.47
1:E:519:THR:HG22	3:E:814:HOH:O	2.15	0.47
1:B:463:LYS:O	1:B:467:LYS:HG2	2.14	0.47
1:D:103:THR:HG22	1:D:105:ASN:N	2.29	0.47
1:C:63:GLU:HG3	1:C:65:ILE:CD1	2.44	0.47
1:B:266:TRP:HB3	1:B:270:TRP:CZ3	2.49	0.47
1:B:473:VAL:HG11	1:B:527:LEU:HD11	1.96	0.47
1:D:76:GLU:O	1:D:78:PRO:O	2.33	0.47
1:E:133:TYR:OH	1:E:138:PRO:HB3	2.14	0.47
1:F:296:ASN:HB3	1:F:328:THR:HG21	1.97	0.47
1:A:136:ASN:HB3	3:A:844:HOH:O	2.14	0.47
1:F:519:THR:CG2	1:F:519:THR:O	2.62	0.47
1:E:162:VAL:HG13	1:E:302:TYR:O	2.14	0.46
1:E:254:PRO:CB	1:E:324:MET:CE	2.92	0.46
1:B:37:GLY:HA2	1:B:665:THR:HG23	1.97	0.46
1:E:166:PRO:HG3	1:E:316:GLY:O	2.16	0.46
1:A:547:THR:HG23	3:A:831:HOH:O	2.16	0.46
1:D:574:THR:CG2	1:D:641:TYR:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LYS:HD2	1:F:365:ASP:OD1	2.16	0.46
1:F:120:ILE:HG21	1:F:182:MET:SD	2.55	0.46
1:A:294:LEU:CG	1:A:324:MET:HE1	2.43	0.46
1:A:323:LEU:HD12	1:A:423:MET:HE1	1.98	0.46
1:B:123:ASP:OD2	1:B:125:THR:HB	2.16	0.46
1:C:37:GLY:HA2	1:C:665:THR:CG2	2.45	0.46
1:A:37:GLY:CA	1:A:665:THR:HG23	2.46	0.46
3:C:769:HOH:O	1:F:272:LYS:HE2	2.15	0.46
1:D:211:GLN:HG3	3:D:815:HOH:O	2.14	0.46
1:E:196:THR:HG22	1:E:199:ARG:HE	1.81	0.46
1:B:305:LYS:HB2	1:B:308:ALA:HB2	1.98	0.46
1:A:76:GLU:C	1:A:214:THR:HG21	2.40	0.46
1:B:439:TRP:CZ2	1:B:441:GLY:HA3	2.51	0.46
1:E:329:ALA:HB3	1:E:342:ILE:CG1	2.46	0.46
1:E:385:LEU:HD22	1:E:462:VAL:HG21	1.98	0.46
1:D:138:PRO:HD2	1:D:162:VAL:HG12	1.97	0.45
1:E:184:TRP:CZ2	1:E:185:LEU:HD22	2.50	0.45
1:A:501:THR:HG22	1:A:501:THR:O	2.16	0.45
1:B:455:LEU:HD22	1:B:540:ARG:NH1	2.31	0.45
1:E:204:ASN:HB2	3:E:740:HOH:O	2.16	0.45
1:A:455:LEU:HD22	1:A:540:ARG:NH1	2.31	0.45
1:D:603:ASP:OD2	1:D:616:THR:HB	2.16	0.45
1:A:207:GLN:HG3	1:A:220:HIS:CE1	2.51	0.45
1:C:151:TYR:HA	1:C:152:PRO:C	2.41	0.45
1:A:294:LEU:HB3	1:A:324:MET:HE1	1.99	0.45
1:F:228:TYR:O	1:F:233:GLY:HA2	2.16	0.45
1:B:385:LEU:HD22	1:B:462:VAL:HG21	1.98	0.45
1:C:166:PRO:HG3	1:C:316:GLY:O	2.16	0.45
1:C:268:ASN:HD21	1:C:272:LYS:NZ	2.11	0.45
1:D:123:ASP:OD2	1:D:125:THR:HB	2.17	0.45
1:D:519:THR:HG23	1:D:519:THR:O	2.17	0.45
1:E:493:TRP:CZ3	1:E:512:VAL:HB	2.52	0.45
1:B:167:VAL:HG23	1:B:295:ARG:NH1	2.31	0.45
1:E:65:ILE:HD11	1:E:119:TRP:CG	2.52	0.45
1:E:307:GLY:CA	1:F:501:THR:HG23	2.47	0.45
1:D:84:THR:HG22	1:D:186:MET:HB3	1.99	0.45
1:D:450:VAL:HG12	1:D:466:ILE:HD11	1.99	0.45
1:E:294:LEU:HB3	1:E:377:TRP:HZ2	1.81	0.45
1:F:519:THR:CG2	1:F:564:PHE:CZ	3.00	0.45
1:A:85:THR:HA	1:A:184:TRP:O	2.16	0.44
1:C:228:TYR:O	1:C:233:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:PHE:CZ	1:C:628:TYR:HD1	2.34	0.44
1:B:37:GLY:CA	1:B:665:THR:HG23	2.47	0.44
1:C:153:SER:O	1:C:239:THR:HA	2.17	0.44
1:F:329:ALA:HB3	1:F:342:ILE:HG12	1.99	0.44
1:C:198:THR:O	1:C:198:THR:CG2	2.66	0.44
1:F:639:LEU:HD22	1:F:641:TYR:OH	2.17	0.44
1:A:198:THR:HG23	1:A:198:THR:O	2.18	0.44
1:B:326:TRP:CG	1:B:430:VAL:HG21	2.53	0.44
1:A:89:PHE:CE2	1:A:115:VAL:HG12	2.52	0.44
1:A:138:PRO:HD2	1:A:162:VAL:HG11	1.99	0.44
1:C:73:LEU:HD13	1:C:584:PHE:CZ	2.52	0.44
1:B:433:ASP:HA	1:B:434:PRO:HA	1.87	0.44
1:C:198:THR:CG2	3:C:876:HOH:O	2.65	0.44
1:C:326:TRP:CD2	1:C:430:VAL:HG21	2.53	0.44
1:C:60:SER:HA	1:C:61:PRO:HD3	1.88	0.44
1:B:37:GLY:CA	1:B:665:THR:CG2	2.94	0.44
1:F:37:GLY:CA	1:F:665:THR:HG23	2.46	0.44
1:C:128:PRO:HD2	1:C:248:TRP:NE1	2.33	0.43
1:D:519:THR:HG22	3:D:999:HOH:O	2.16	0.43
1:E:501:THR:OG1	1:F:422:GLY:HA2	2.18	0.43
1:A:77:ALA:HB3	1:A:78:PRO:CD	2.48	0.43
1:C:105:ASN:HD22	1:C:106:TRP:N	2.16	0.43
1:C:141:TYR:CZ	1:C:311:LYS:HE3	2.53	0.43
1:C:186:MET:HE2	1:C:202:PHE:CE2	2.52	0.43
1:F:179:MET:HE2	1:F:341:LYS:HE2	1.99	0.43
1:C:126:GLU:C	1:C:128:PRO:HD3	2.43	0.43
1:E:37:GLY:CA	1:E:665:THR:HG23	2.49	0.43
1:C:163:GLY:HA3	1:C:303:PHE:O	2.19	0.43
1:F:308:ALA:C	1:F:310:ASP:H	2.26	0.43
1:A:363:GLN:NE2	1:D:364:SER:H	2.15	0.43
1:A:521:LEU:HD21	1:A:564:PHE:CD1	2.54	0.43
1:D:519:THR:CG2	1:D:519:THR:O	2.66	0.43
1:D:328:THR:HG23	1:D:342:ILE:O	2.19	0.43
1:A:325:ALA:HB1	1:A:344:CYS:HB3	2.01	0.43
1:F:353:ASN:CG	1:F:449:ARG:HD3	2.44	0.43
1:D:32:ALA:HB2	1:D:565:TYR:HB2	2.00	0.42
1:E:639:LEU:HD22	1:E:641:TYR:OH	2.20	0.42
1:F:149:SER:HA	1:F:590:TYR:CE2	2.54	0.42
1:C:124:SER:CB	1:C:178:ASN:ND2	2.82	0.42
1:D:89:PHE:HE2	1:D:115:VAL:HG12	1.85	0.42
1:F:462:VAL:HG12	1:F:466:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:TYR:CE2	1:A:103:THR:HG21	2.54	0.42
1:C:194:PHE:CD1	1:C:221:PRO:HD3	2.54	0.42
1:E:90:SER:HB2	1:E:259:ARG:HB3	2.02	0.42
1:B:501:THR:HG22	1:D:307:GLY:O	2.18	0.42
1:C:439:TRP:CE2	1:C:441:GLY:HA3	2.55	0.42
1:F:129:GLY:O	1:F:132:SER:HB2	2.20	0.42
1:F:519:THR:CG2	3:F:715:HOH:O	2.55	0.42
1:C:276:LYS:HA	3:C:720:HOH:O	2.20	0.42
1:F:278:SER:CA	3:F:1061:HOH:O	2.67	0.42
1:F:501:THR:HB	3:F:708:HOH:O	2.20	0.42
1:D:163:GLY:HA3	1:D:303:PHE:O	2.18	0.42
1:C:519:THR:HG23	3:C:877:HOH:O	2.20	0.42
1:F:324:MET:HE2	1:F:377:TRP:HH2	1.85	0.42
1:A:60:SER:HA	1:A:61:PRO:HD3	1.96	0.41
1:A:574:THR:CG2	1:A:576:GLU:OE1	2.48	0.41
1:E:294:LEU:HG	1:E:324:MET:CE	2.49	0.41
1:D:470:VAL:O	1:D:474:MET:HG2	2.20	0.41
1:E:198:THR:CG2	1:E:198:THR:O	2.69	0.41
1:B:314:ALA:HB3	1:B:319:SER:HB3	2.01	0.41
1:A:220:HIS:HB2	1:A:221:PRO:HD2	2.01	0.41
1:C:390:TRP:CD1	1:C:500:TRP:HB2	2.56	0.41
1:F:85:THR:HA	1:F:184:TRP:O	2.20	0.41
1:A:473:VAL:CG1	1:A:527:LEU:HD11	2.51	0.41
1:C:626:ILE:HG13	3:C:890:HOH:O	2.21	0.41
1:D:639:LEU:HD22	1:D:641:TYR:OH	2.21	0.41
1:E:292:ASP:O	1:E:295:ARG:HD3	2.20	0.41
1:F:665:THR:HG21	3:F:948:HOH:O	2.21	0.41
1:A:138:PRO:HD2	1:A:162:VAL:CG1	2.51	0.41
1:A:501:THR:O	1:A:501:THR:CG2	2.68	0.41
1:B:29:PRO:HB3	1:B:564:PHE:HA	2.02	0.41
1:C:248:TRP:CZ3	1:C:331:GLY:HA2	2.56	0.41
1:D:301:LYS:HE3	1:D:342:ILE:HD12	2.02	0.41
1:D:402:ALA:HA	1:D:424:ALA:O	2.21	0.41
1:E:228:TYR:O	1:E:233:GLY:HA2	2.21	0.41
1:E:547:THR:HG23	1:E:550:ARG:NH2	2.36	0.41
1:F:103:THR:HG22	1:F:105:ASN:H	1.85	0.41
1:B:498:ASP:O	1:B:499:THR:C	2.64	0.41
1:D:198:THR:CB	3:D:834:HOH:O	2.60	0.41
1:F:159:THR:HG22	1:F:160:VAL:HG23	2.03	0.41
1:F:402:ALA:HA	1:F:424:ALA:O	2.21	0.41
1:F:423:MET:HE2	3:F:953:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HG21	1:A:43:LEU:HD21	2.03	0.40
1:A:300:ASP:OD2	1:A:410:TYR:OH	2.28	0.40
1:F:603:ASP:OD2	1:F:616:THR:HB	2.22	0.40
1:C:168:HIS:O	1:C:172:VAL:HG23	2.21	0.40
1:C:194:PHE:CE1	1:C:221:PRO:HD3	2.56	0.40
1:D:46:GLU:OE2	1:D:50:LYS:NZ	2.52	0.40
1:B:520:ASP:OD2	2:H:1:BGC:O6	2.37	0.40
1:C:184:TRP:CE2	1:C:185:LEU:HB2	2.56	0.40
1:C:325:ALA:HB1	1:C:344:CYS:HB3	2.03	0.40
1:C:423:MET:HE3	1:C:423:MET:HB2	1.77	0.40
1:D:85:THR:HA	1:D:184:TRP:O	2.21	0.40
1:F:144:GLU:HB2	1:F:408:GLY:HA3	2.04	0.40
1:B:36:ASP:OD1	1:B:668:VAL:CG1	2.70	0.40
1:B:462:VAL:HG12	1:B:466:ILE:HD12	2.03	0.40
1:C:268:ASN:ND2	1:C:272:LYS:HZ2	2.14	0.40
1:C:433:ASP:HA	1:C:434:PRO:HA	1.91	0.40
1:C:501:THR:O	1:C:501:THR:CG2	2.69	0.40
1:E:278:SER:HB3	3:E:957:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/678 (94%)	607 (95%)	30 (5%)	3 (0%)	24	37
1	B	640/678 (94%)	623 (97%)	17 (3%)	0	100	100
1	C	640/678 (94%)	618 (97%)	22 (3%)	0	100	100
1	D	640/678 (94%)	622 (97%)	16 (2%)	2 (0%)	36	50
1	E	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	43	58
1	F	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	43	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3840/4068 (94%)	3716 (97%)	117 (3%)	7 (0%)	43	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	335	GLY
1	E	77	ALA
1	A	600	PRO
1	D	278	SER
1	F	76	GLU
1	D	77	ALA

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	512/556 (92%)	477 (93%)	35 (7%)	14	25
1	B	519/556 (93%)	490 (94%)	29 (6%)	19	33
1	C	513/556 (92%)	482 (94%)	31 (6%)	17	31
1	D	521/556 (94%)	490 (94%)	31 (6%)	17	31
1	E	518/556 (93%)	494 (95%)	24 (5%)	24	41
1	F	520/556 (94%)	493 (95%)	27 (5%)	21	36
All	All	3103/3336 (93%)	2926 (94%)	177 (6%)	18	33

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	63	GLU
1	A	73	LEU
1	A	103	THR
1	A	124	SER

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Mol	Chain	Res	Type
1	A	131	SER
1	A	137	SER
1	A	143	ASP
1	A	158	ASP
1	A	159	THR
1	A	167	VAL
1	A	198	THR
1	A	207	GLN
1	A	214	THR
1	A	252	ASN
1	A	294	LEU
1	A	310	ASP
1	A	315	THR
1	A	334	ILE
1	A	381	TYR
1	A	418	SER
1	A	455	LEU
1	A	460	SER
1	A	462	VAL
1	A	473	VAL
1	A	491	LEU
1	A	501	THR
1	A	513	ARG
1	A	547	THR
1	A	574	THR
1	A	616	THR
1	A	618	TYR
1	A	657	LEU
1	A	665	THR
1	A	668	VAL
1	B	30	THR
1	B	47	LEU
1	B	72	THR
1	B	73	LEU
1	B	103	THR
1	B	107	SER
1	B	162	VAL
1	B	179	MET
1	B	196	THR
1	B	198	THR
1	B	207	GLN
1	B	214	THR

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Mol	Chain	Res	Type
1	B	294	LEU
1	B	328	THR
1	B	337	SER
1	B	455	LEU
1	B	462	VAL
1	B	463	LYS
1	B	473	VAL
1	B	491	LEU
1	B	501	THR
1	B	547	THR
1	B	574	THR
1	B	618	TYR
1	B	627	VAL
1	B	649	ASP
1	B	657	LEU
1	B	665	THR
1	B	668	VAL
1	C	47	LEU
1	C	73	LEU
1	C	76	GLU
1	C	103	THR
1	C	167	VAL
1	C	198	THR
1	C	207	GLN
1	C	239	THR
1	C	252	ASN
1	C	285	SER
1	C	294	LEU
1	C	310	ASP
1	C	418	SER
1	C	455	LEU
1	C	462	VAL
1	C	463	LYS
1	C	473	VAL
1	C	489	SER
1	C	491	LEU
1	C	499	THR
1	C	501	THR
1	C	519	THR
1	C	544	LYS
1	C	547	THR
1	C	574	THR

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Mol	Chain	Res	Type
1	C	616	THR
1	C	618	TYR
1	C	627	VAL
1	C	657	LEU
1	C	665	THR
1	C	668	VAL
1	D	47	LEU
1	D	63	GLU
1	D	73	LEU
1	D	103	THR
1	D	124	SER
1	D	162	VAL
1	D	167	VAL
1	D	173	SER
1	D	179	MET
1	D	196	THR
1	D	198	THR
1	D	199	ARG
1	D	252	ASN
1	D	278	SER
1	D	294	LEU
1	D	381	TYR
1	D	455	LEU
1	D	462	VAL
1	D	473	VAL
1	D	489	SER
1	D	491	LEU
1	D	501	THR
1	D	519	THR
1	D	544	LYS
1	D	547	THR
1	D	616	THR
1	D	618	TYR
1	D	627	VAL
1	D	657	LEU
1	D	665	THR
1	D	668	VAL
1	E	30	THR
1	E	47	LEU
1	E	63	GLU
1	E	73	LEU
1	E	103	THR

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Mol	Chain	Res	Type
1	E	167	VAL
1	E	179	MET
1	E	198	THR
1	E	207	GLN
1	E	210	GLU
1	E	294	LEU
1	E	374	LYS
1	E	455	LEU
1	E	462	VAL
1	E	473	VAL
1	E	491	LEU
1	E	501	THR
1	E	519	THR
1	E	616	THR
1	E	618	TYR
1	E	623	TYR
1	E	627	VAL
1	E	657	LEU
1	E	665	THR
1	F	47	LEU
1	F	72	THR
1	F	73	LEU
1	F	76	GLU
1	F	103	THR
1	F	124	SER
1	F	132	SER
1	F	159	THR
1	F	167	VAL
1	F	198	THR
1	F	239	THR
1	F	294	LEU
1	F	455	LEU
1	F	462	VAL
1	F	473	VAL
1	F	491	LEU
1	F	501	THR
1	F	519	THR
1	F	547	THR
1	F	574	THR
1	F	616	THR
1	F	618	TYR
1	F	627	VAL

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Mol	Chain	Res	Type
1	F	649	ASP
1	F	657	LEU
1	F	665	THR
1	F	668	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	105	ASN
1	A	178	ASN
1	A	207	GLN
1	A	268	ASN
1	A	363	GLN
1	A	587	GLN
1	A	620	GLN
1	A	640	ASN
1	B	105	ASN
1	B	178	ASN
1	B	207	GLN
1	C	105	ASN
1	C	178	ASN
1	C	207	GLN
1	C	268	ASN
1	C	363	GLN
1	C	563	ASN
1	C	640	ASN
1	D	105	ASN
1	D	207	GLN
1	D	232	ASN
1	D	309	GLN
1	D	363	GLN
1	D	509	ASN
1	D	640	ASN
1	E	136	ASN
1	E	232	ASN
1	E	309	GLN
1	E	363	GLN
1	E	438	GLN
1	E	640	ASN
1	F	232	ASN
1	F	268	ASN

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Mol	Chain	Res	Type
1	F	309	GLN
1	F	363	GLN
1	F	407	ASN
1	F	640	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	G	1	2	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
2	BGC	G	2	2	11,11,12	0.49	0	15,15,17	0.81	1 (6%)
2	BGC	H	1	2	11,11,12	0.46	0	15,15,17	1.06	2 (13%)
2	BGC	H	2	2	11,11,12	0.60	0	15,15,17	0.79	0
2	BGC	I	1	2	11,11,12	0.80	0	15,15,17	1.06	1 (6%)
2	BGC	I	2	2	11,11,12	0.67	0	15,15,17	0.89	1 (6%)
2	BGC	J	1	2	11,11,12	0.73	0	15,15,17	1.47	1 (6%)
2	BGC	J	2	2	11,11,12	0.74	0	15,15,17	1.09	1 (6%)
2	BGC	K	1	2	11,11,12	0.74	0	15,15,17	0.90	1 (6%)
2	BGC	K	2	2	11,11,12	0.74	0	15,15,17	1.06	1 (6%)
2	BGC	L	1	2	11,11,12	0.70	0	15,15,17	1.16	1 (6%)
2	BGC	L	2	2	11,11,12	0.69	0	15,15,17	0.63	0

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	G	1	2	-	0/2/19/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/19/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/19/22	0/1/1/1
2	BGC	I	2	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/19/22	0/1/1/1
2	BGC	J	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	1	2	-	0/2/19/22	0/1/1/1
2	BGC	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	L	1	2	-	0/2/19/22	0/1/1/1
2	BGC	L	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	BGC	O5-C1-C2	-3.95	101.37	110.79
2	J	2	BGC	C1-O5-C5	3.64	117.06	112.19
2	L	1	BGC	O5-C1-C2	-3.32	102.87	110.79
2	K	2	BGC	C1-O5-C5	3.04	116.25	112.19
2	K	1	BGC	O5-C1-C2	-2.54	104.72	110.79
2	H	1	BGC	C1-O5-C5	2.53	115.58	112.19
2	G	2	BGC	C1-O5-C5	2.50	115.54	112.19
2	G	1	BGC	O5-C1-C2	-2.48	104.87	110.79
2	I	1	BGC	O5-C1-C2	-2.30	105.29	110.79
2	G	1	BGC	C1-O5-C5	2.17	115.09	112.19
2	I	2	BGC	C1-O5-C5	2.15	115.07	112.19
2	H	1	BGC	O5-C1-C2	-2.02	105.96	110.79

There are no chirality outliers.

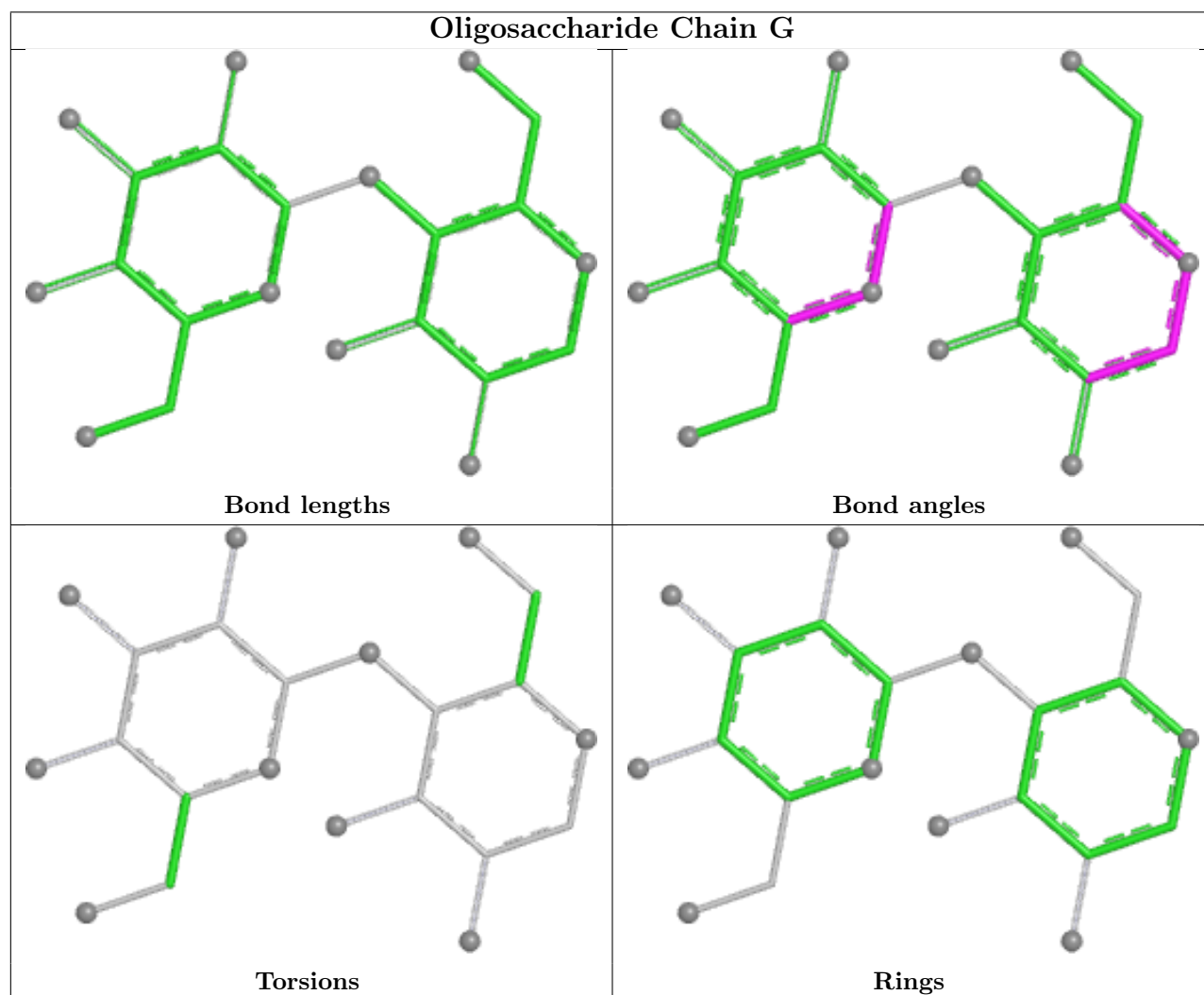
There are no torsion outliers.

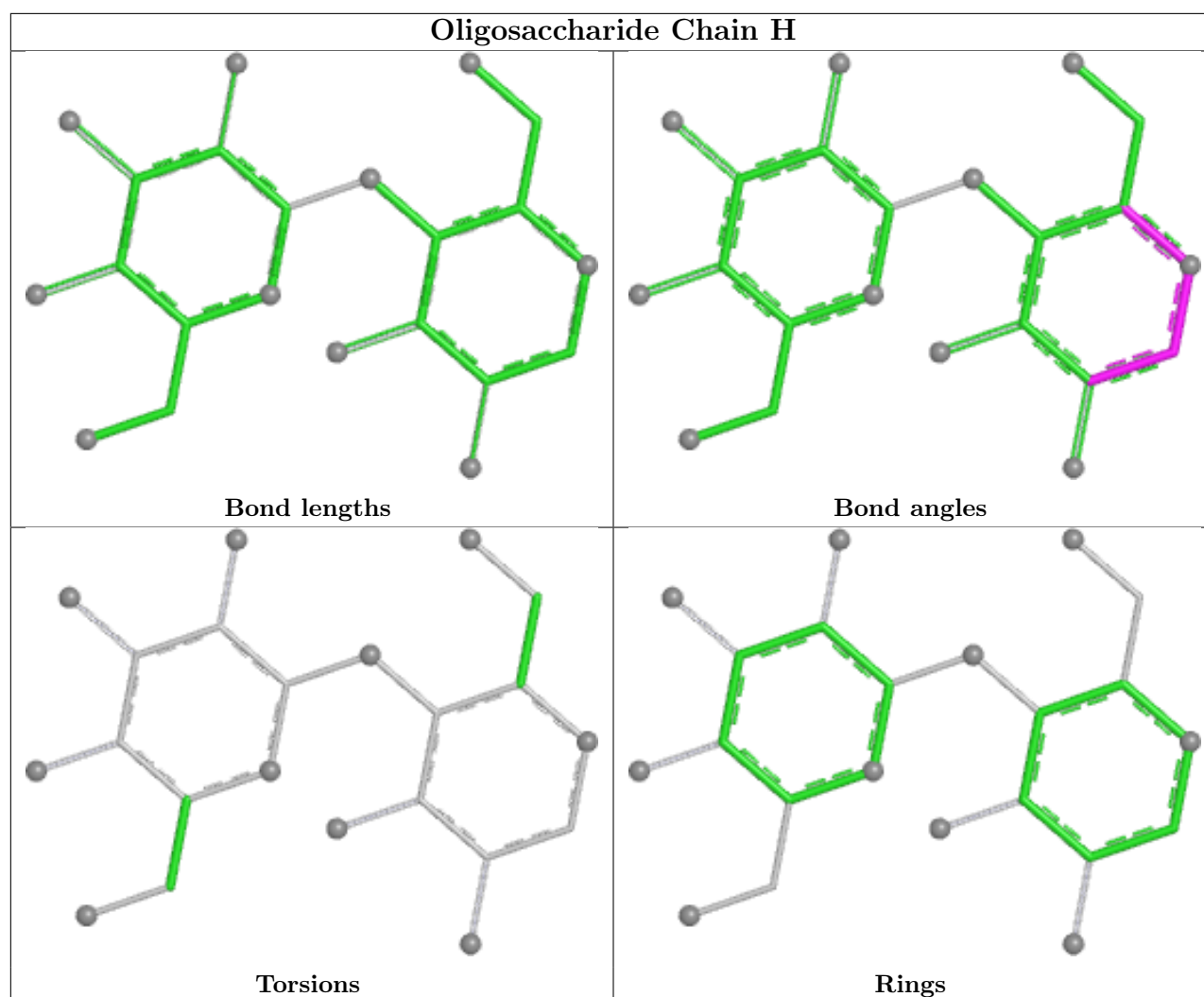
There are no ring outliers.

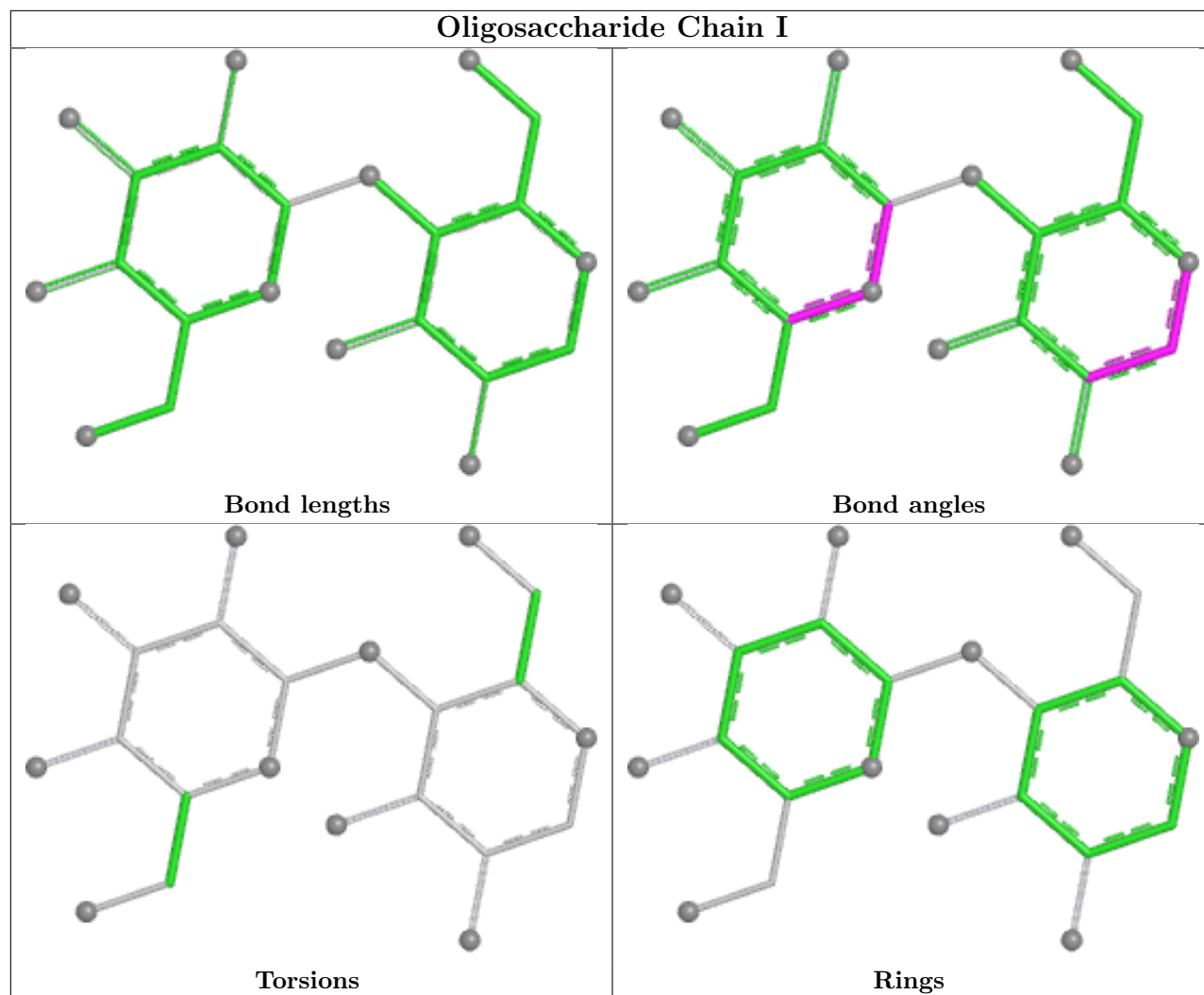
1 monomer is involved in 1 short contact:

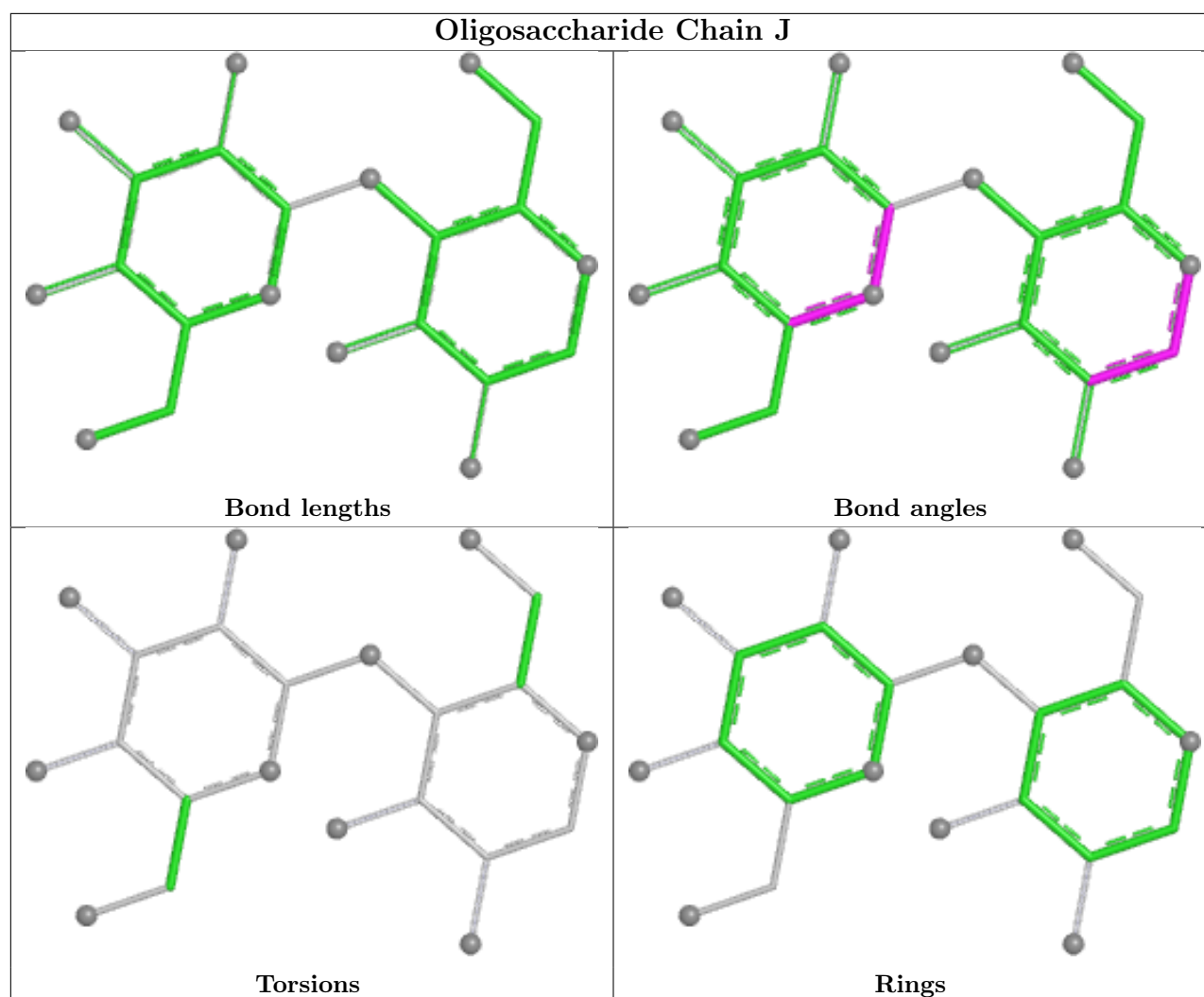
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	BGC	1	0

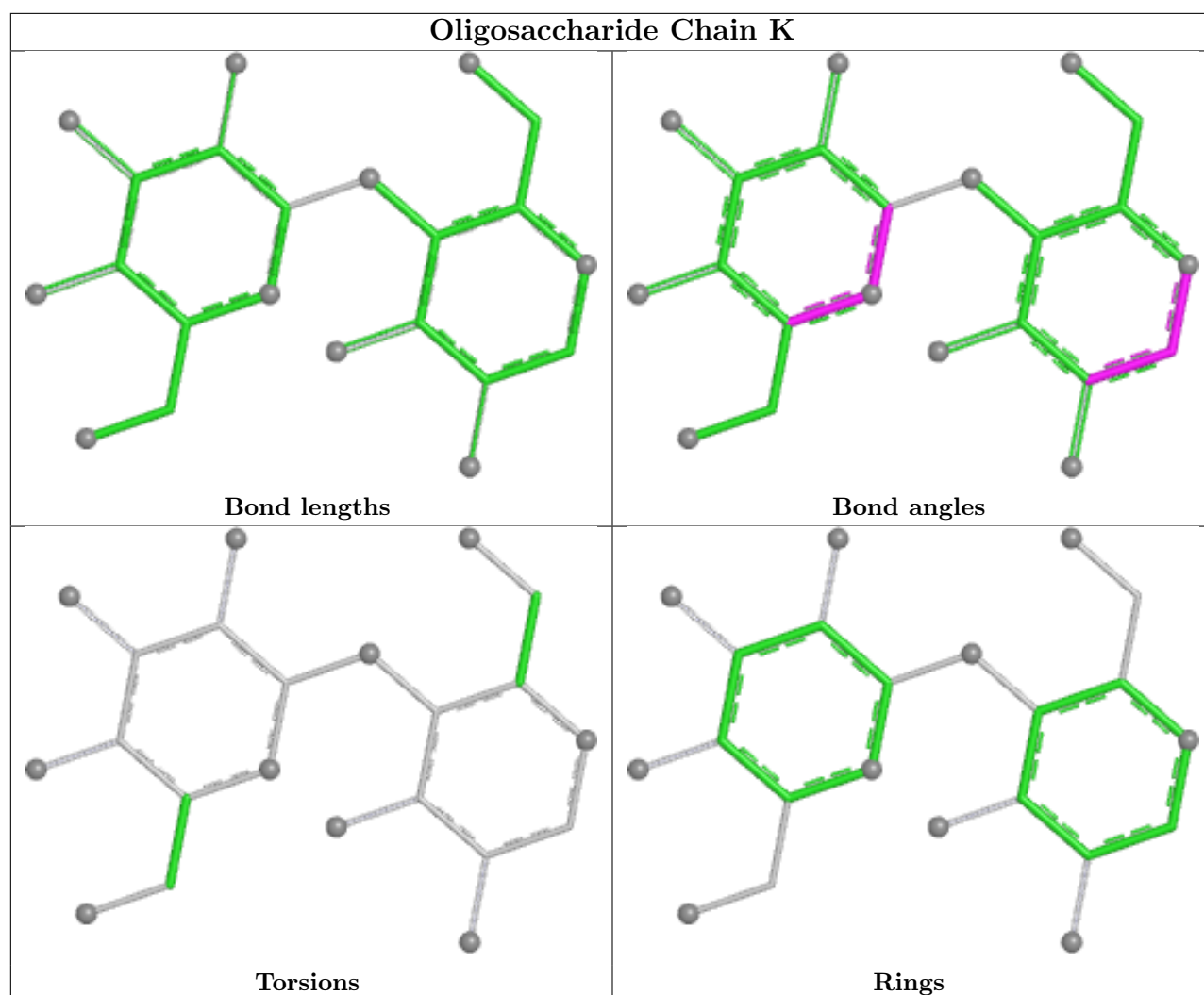
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

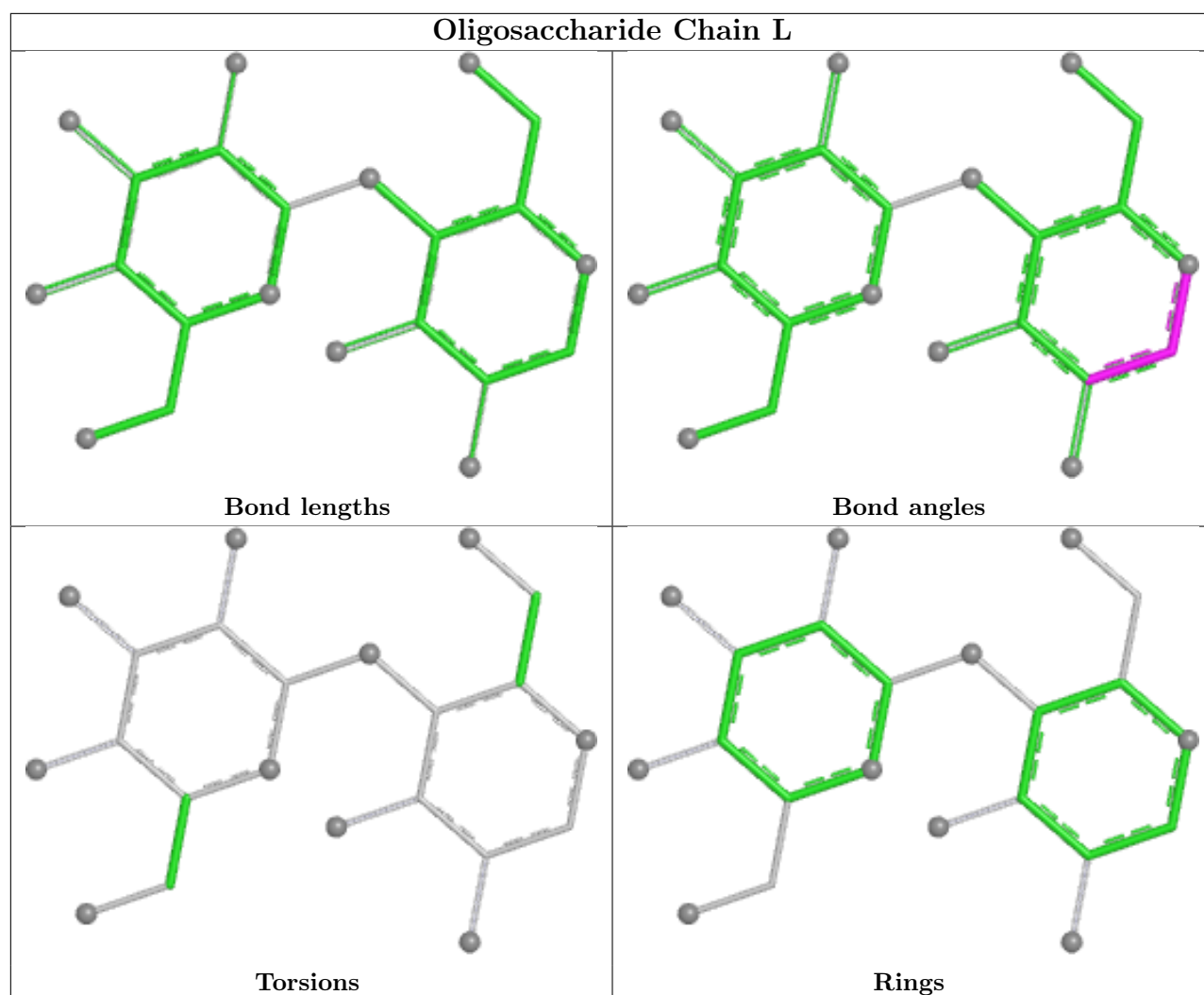












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	642/678 (94%)	0.14	23 (3%)	46 42	23, 40, 65, 73	0
1	B	642/678 (94%)	-0.25	9 (1%)	73 69	23, 37, 55, 69	0
1	C	642/678 (94%)	-0.16	9 (1%)	73 69	20, 37, 63, 73	0
1	D	642/678 (94%)	-0.32	5 (0%)	82 80	20, 31, 47, 55	0
1	E	642/678 (94%)	-0.58	4 (0%)	85 83	18, 29, 43, 56	0
1	F	642/678 (94%)	-0.68	4 (0%)	85 83	17, 26, 38, 53	0
All	All	3852/4068 (94%)	-0.31	54 (1%)	73 69	17, 32, 58, 73	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	567	SER	3.5
1	F	182	MET	3.5
1	F	277	GLY	3.2
1	A	335	GLY	3.1
1	C	334	ILE	3.1
1	D	28	GLY	3.0
1	E	277	GLY	3.0
1	C	336	ALA	3.0
1	A	603	ASP	3.0
1	B	28	GLY	2.9
1	A	334	ILE	2.9
1	A	315	THR	2.9
1	A	248	TRP	2.8
1	A	596	SER	2.7
1	C	315	THR	2.7
1	A	157	PHE	2.7
1	A	336	ALA	2.7
1	A	314	ALA	2.6
1	A	227	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	332	GLY	2.5
1	B	634	GLY	2.5
1	B	105	ASN	2.5
1	A	170	ASP	2.5
1	C	159	THR	2.5
1	B	633	ARG	2.4
1	A	163	GLY	2.4
1	A	333	GLY	2.4
1	B	567	SER	2.4
1	F	335	GLY	2.3
1	E	434	PRO	2.3
1	A	131	SER	2.3
1	C	243	SER	2.3
1	B	431	TYR	2.3
1	A	632	LEU	2.3
1	C	633	ARG	2.3
1	D	277	GLY	2.2
1	C	161	ARG	2.2
1	F	315	THR	2.2
1	D	316	GLY	2.2
1	A	162	VAL	2.2
1	A	629	GLN	2.2
1	C	156	LYS	2.2
1	B	635	GLU	2.1
1	A	242	ARG	2.1
1	A	633	ARG	2.1
1	A	243	SER	2.1
1	C	124	SER	2.1
1	D	37	GLY	2.1
1	B	627	VAL	2.0
1	A	338	TRP	2.0
1	A	128	PRO	2.0
1	E	431	TYR	2.0
1	B	632	LEU	2.0
1	D	666	TYR	2.0

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

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

6.3 Carbohydrates

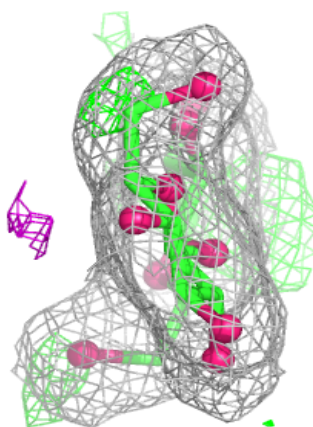
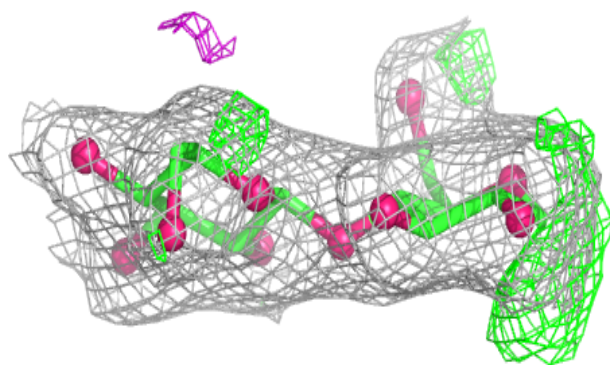
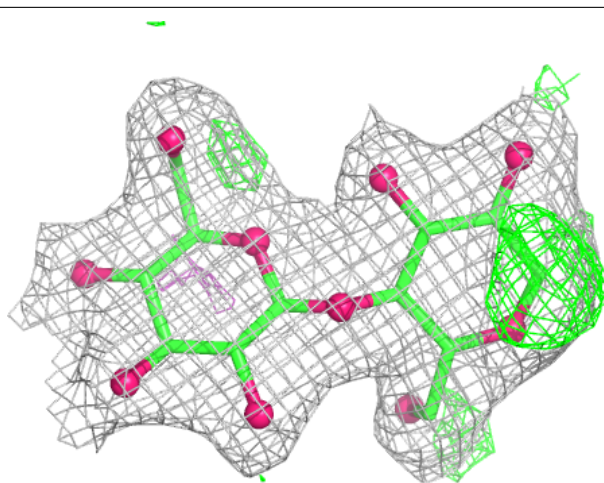
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G	1	11/12	0.87	0.09	34,35,37,37	0
2	BGC	I	1	11/12	0.88	0.08	30,36,39,40	0
2	BGC	J	1	11/12	0.89	0.09	35,37,43,44	0
2	BGC	H	1	11/12	0.90	0.08	38,38,41,41	0
2	BGC	K	1	11/12	0.90	0.08	26,29,34,34	0
2	BGC	L	1	11/12	0.91	0.07	28,31,36,37	0
2	BGC	G	2	11/12	0.92	0.08	33,34,35,35	0
2	BGC	H	2	11/12	0.95	0.05	31,33,34,35	0
2	BGC	J	2	11/12	0.95	0.05	30,31,32,33	0
2	BGC	K	2	11/12	0.96	0.05	24,25,26,27	0
2	BGC	I	2	11/12	0.97	0.05	31,32,33,35	0
2	BGC	L	2	11/12	0.98	0.04	24,27,29,30	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.

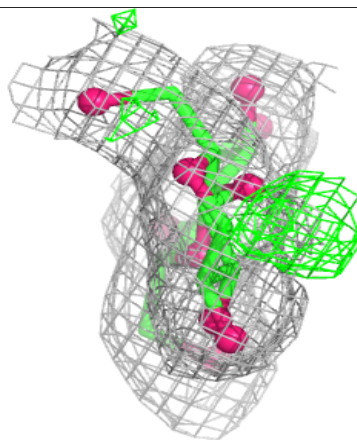
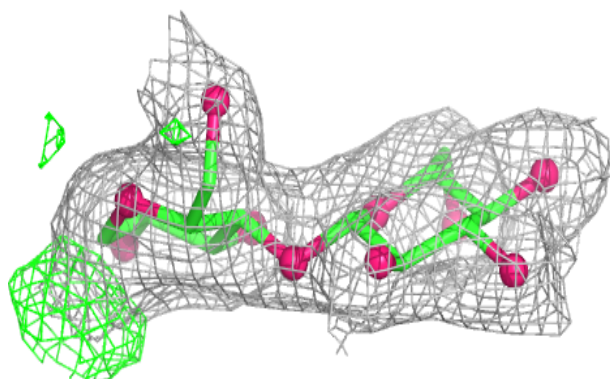
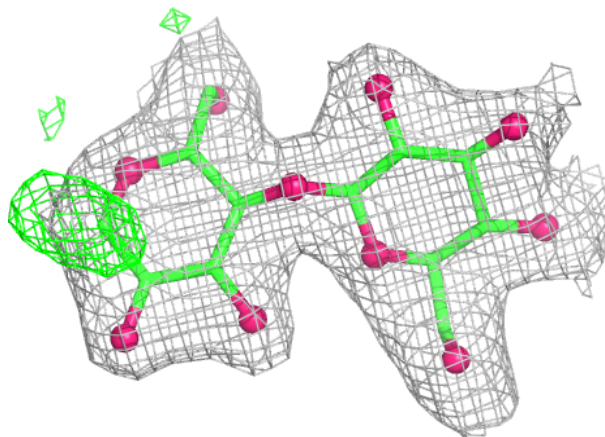
Electron density around Chain G:

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

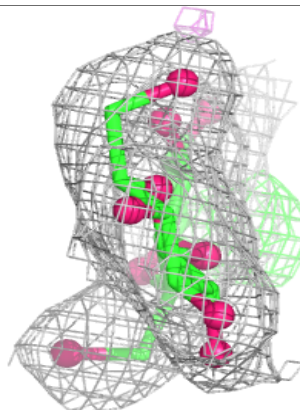
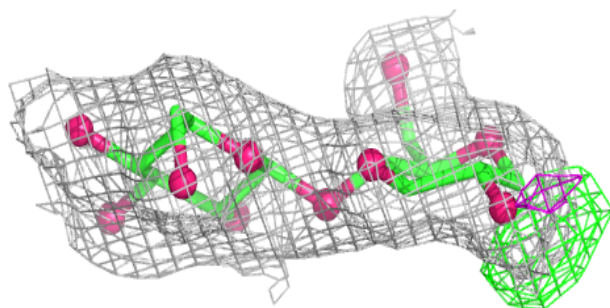
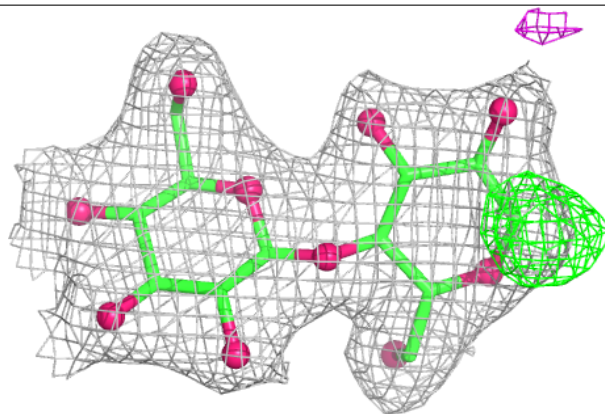


Electron density around Chain H:

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

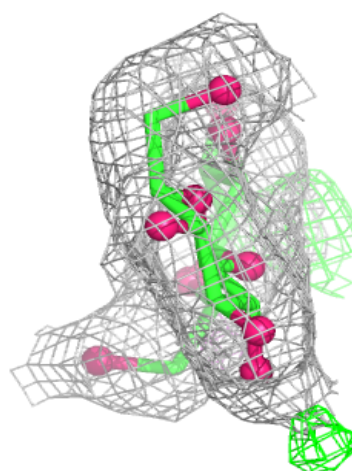
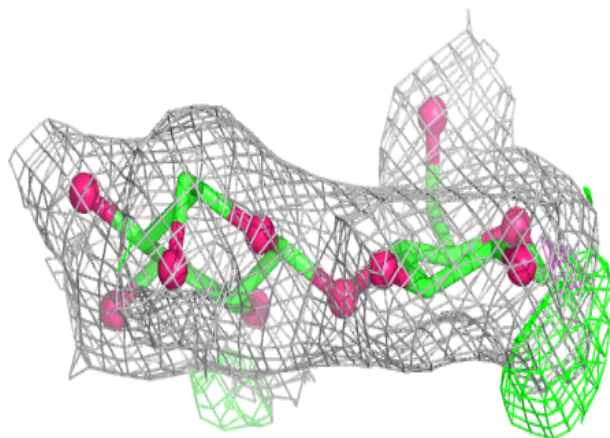
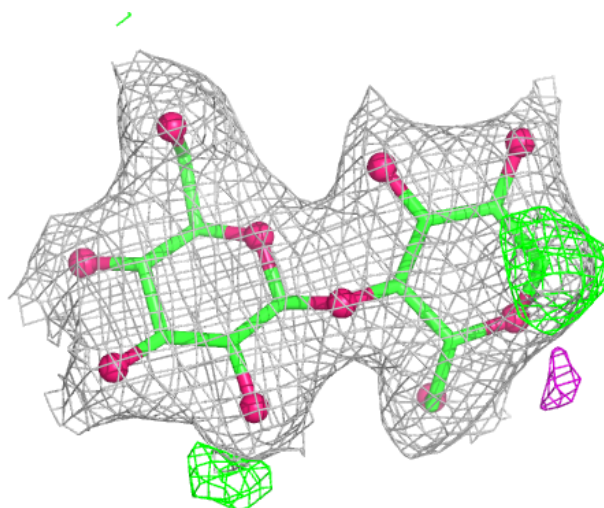
**Electron density around Chain I:**

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



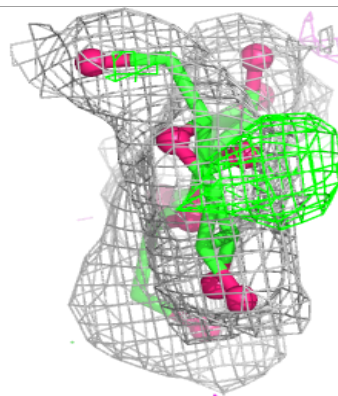
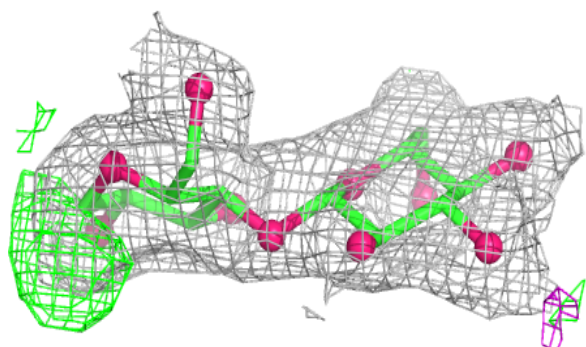
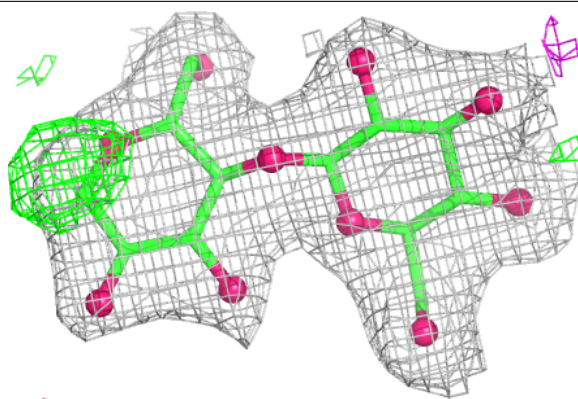
Electron density around Chain J:

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

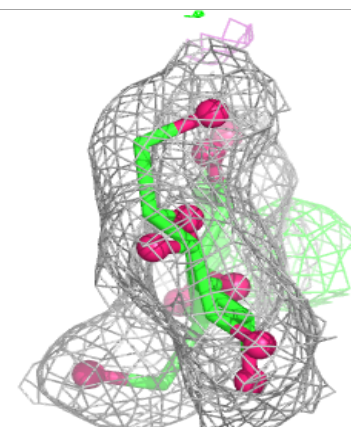
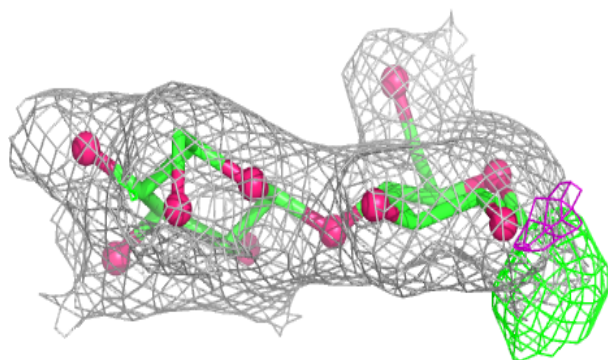
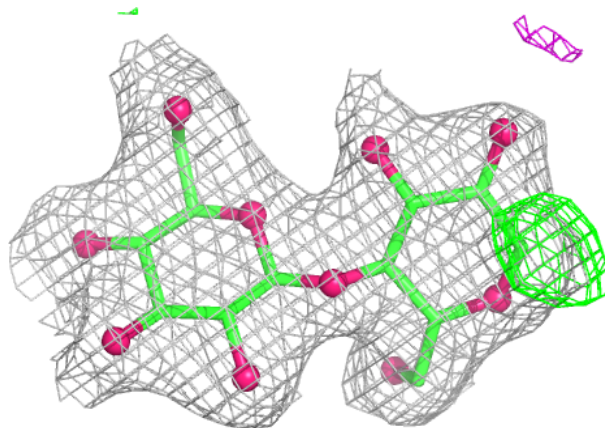


Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.