



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 07:45 am GMT

PDB ID : 6F7K
Title : Crystal structure of Dettilon tailspike protein (gp208)
Authors : Roske, Y.; Heinemann, U.
Deposited on : 2017-12-11
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

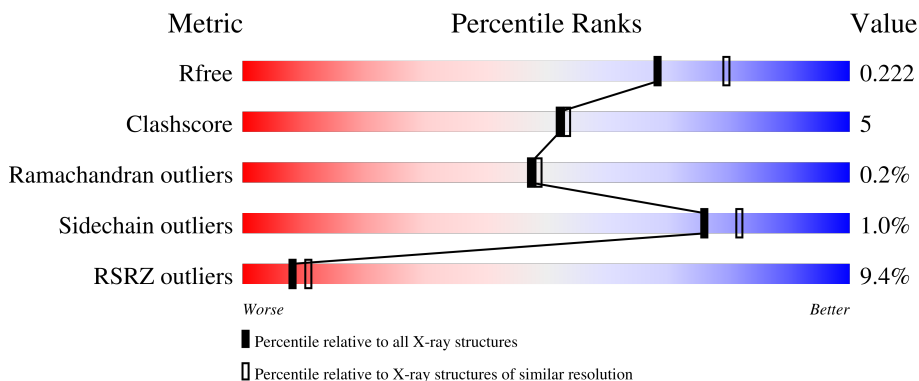
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



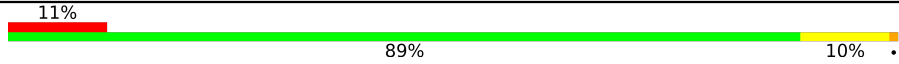

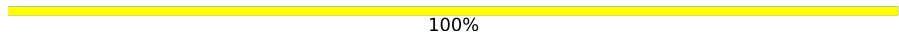
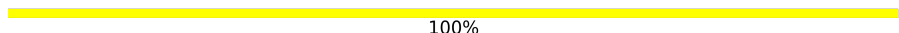
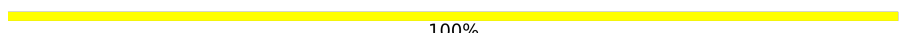
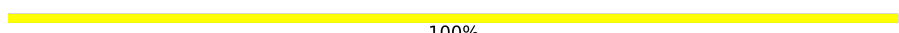
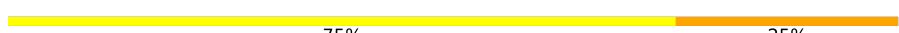

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	547	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">9% 87% 12%</p>
1	B	547	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">10% 88% 12%</p>
1	C	547	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">10% 89% 11%</p>
1	D	547	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">9% 86% 14%</p>
1	F	547	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">9% 85% 15%</p>

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Mol	Chain	Length	Quality of chain
1	G	547	 11% 89% 10%
2	E	6	 67% 33%
2	H	6	 100%
2	K	6	 100%
2	L	6	 100%
2	M	6	 100%
3	I	4	 75% 25%
4	J	2	 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26526 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.

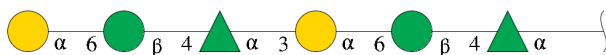
- Molecule 1 is a protein called Tailspike.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	546	4086	2563	687	820	16	0	2	0
1	B	547	4092	2565	688	822	17	0	2	0
1	C	547	4089	2563	688	821	17	0	1	0
1	D	547	4094	2568	688	821	17	0	2	0
1	F	547	4090	2565	688	821	16	0	2	0
1	G	547	4093	2567	688	821	17	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	MET	-	initiating methionine	UNP A0A0C5PVE3
B	252	MET	-	initiating methionine	UNP A0A0C5PVE3
C	252	MET	-	initiating methionine	UNP A0A0C5PVE3
D	252	MET	-	initiating methionine	UNP A0A0C5PVE3
F	252	MET	-	initiating methionine	UNP A0A0C5PVE3
G	252	MET	-	initiating methionine	UNP A0A0C5PVE3

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	6	65	36	29	0	0	0
2	H	6	65	36	29	0	0	0
2	K	6	65	36	29	0	0	0
2	L	6	65	36	29	0	0	0
2	M	6	65	36	29	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	I	4	43	24	19	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	J	2	22	12	10	0	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

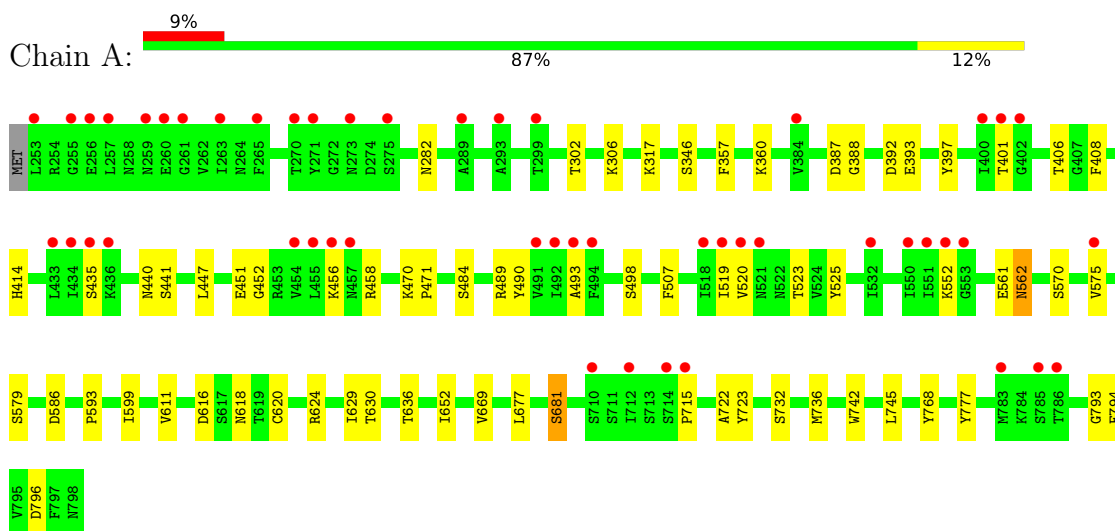
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	287	Total O 287 287	0	0
6	B	224	Total O 224 224	0	0
6	C	295	Total O 295 295	0	0
6	D	276	Total O 276 276	0	0
6	F	255	Total O 255 255	0	0
6	G	251	Total O 251 251	0	0

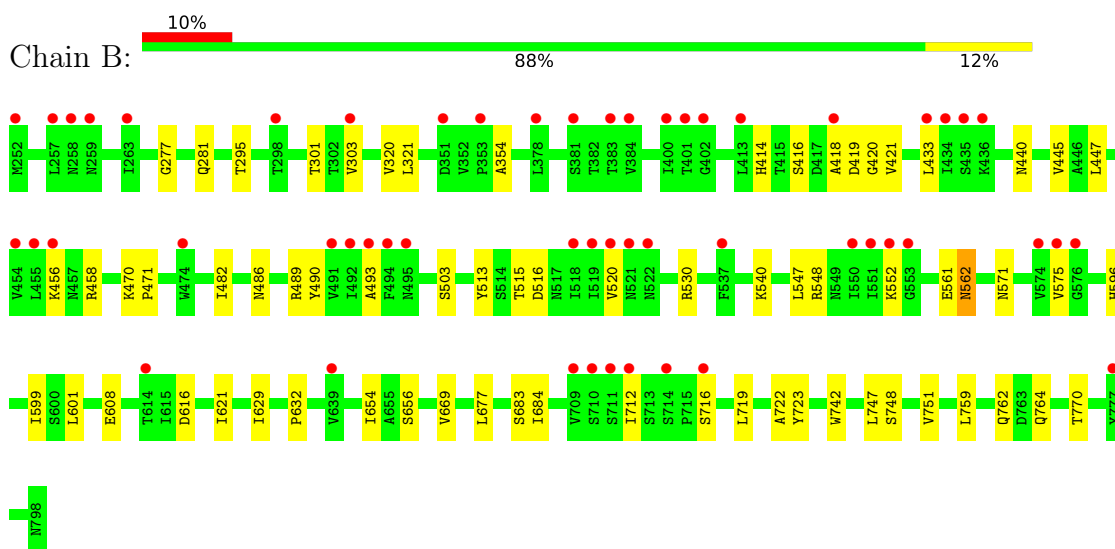
3 Residue-property plots [i](#)

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.

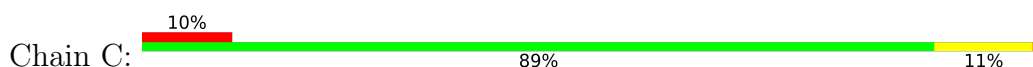
- Molecule 1: Tailspike

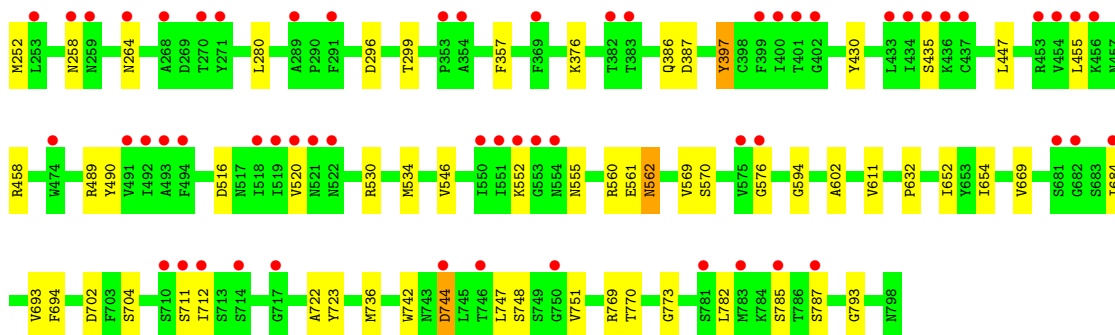


- Molecule 1: Tailspike



- Molecule 1: Tailspike





- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain E: 67% 33%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain H: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain K: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain L: 100%



- Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain M: 100%

RAM1
BMA2
GLA3
RAM4
BMA5
GLA6

- Molecule 3: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose

Chain I:  75% 25%

GLA1
RAM2
BMA3
GLA4

- Molecule 4: beta-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose

Chain J:  50% 50%

RAM1
BMA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.42Å 160.83Å 161.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.10 48.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.76-2.10) 99.5 (48.76-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.183 , 0.221 0.189 , 0.222	Depositor DCC
R_{free} test set	2432 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.452	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.015 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26526	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.93% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, RAM, GLA, EDO

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	0.66	0/4175	0.66	0/5680
1	B	0.63	0/4181	0.64	0/5687
1	C	0.64	0/4175	0.64	1/5679 (0.0%)
1	D	0.63	0/4183	0.65	0/5690
1	F	0.64	0/4179	0.64	0/5686
1	G	0.62	0/4182	0.64	2/5689 (0.0%)
All	All	0.64	0/25075	0.65	3/34111 (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	A	0	2
1	D	0	1
1	G	0	3
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	453	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	458	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	G	458	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	618	ASN	Mainchain
1	A	630	THR	Mainchain
1	D	648	GLN	Mainchain
1	G	397	TYR	Sidechain
1	G	555	ASN	Mainchain
1	G	652	ILE	Mainchain

5.2 Too-close contacts [i](#)

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	4086	0	3937	52	0
1	B	4092	0	3940	48	0
1	C	4089	0	3935	41	0
1	D	4094	0	3946	46	0
1	F	4090	0	3937	65	0
1	G	4093	0	3944	41	0
2	E	65	0	57	2	0
2	H	65	0	57	0	0
2	K	65	0	56	0	0
2	L	65	0	55	0	0
2	M	65	0	56	0	0
3	I	43	0	37	1	0
4	J	22	0	19	1	0
5	A	4	0	6	2	0
6	A	287	0	0	9	0
6	B	224	0	0	10	0
6	C	295	0	0	4	0
6	D	276	0	0	4	0
6	F	255	0	0	1	0
6	G	251	0	0	1	0
All	All	26526	0	23982	268	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (268) 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)
6:A:909:HOH:O	1:F:523:THR:HB	1.67	0.94
1:G:397:TYR:HH	1:G:430:TYR:HE1	1.01	0.92
1:D:456:LYS:O	1:D:456:LYS:HD3	1.69	0.92
1:B:456:LYS:O	1:B:456:LYS:HD3	1.71	0.90
1:F:520[A]:VAL:HG12	1:F:552:LYS:HB3	1.63	0.80
1:F:586:ASP:OD2	1:F:624:ARG:NH1	2.14	0.80
1:A:489:ARG:HD2	1:F:523:THR:HG21	1.65	0.79
1:D:491:VAL:O	6:D:901:HOH:O	2.01	0.78
1:F:415:THR:HG22	1:F:419:ASP:OD2	1.83	0.78
1:A:523:THR:HG21	1:G:489:ARG:HD2	1.67	0.76
1:F:577:ASN:H	1:F:618:ASN:HD22	1.35	0.74
1:D:456:LYS:O	1:D:456:LYS:CD	2.38	0.71
1:C:264:ASN:O	6:C:901:HOH:O	2.07	0.70
1:A:736:MET:CE	1:F:793:GLY:HA2	2.21	0.70
1:C:457:ASN:HD22	1:C:495:ASN:HD21	1.38	0.70
1:B:458:ARG:HD3	1:D:397:TYR:OH	1.92	0.70
1:A:397:TYR:CE2	1:F:458:ARG:HD2	2.27	0.69
1:G:296:ASP:OD2	1:G:299:THR:HG23	1.93	0.69
1:G:376:LYS:H	1:G:386:GLN:HE22	1.40	0.69
1:F:518:ILE:HG22	1:F:520[B]:VAL:HG23	1.75	0.69
1:G:520:VAL:HG12	1:G:552:LYS:HB3	1.76	0.66
1:F:376:LYS:H	1:F:386:GLN:HE22	1.43	0.66
6:A:901:HOH:O	2:E:3:GLA:O6	2.14	0.65
1:D:527:CYS:H	1:D:559:ASN:HD22	1.44	0.64
1:B:420:GLY:HA3	6:B:902:HOH:O	1.98	0.63
1:D:586:ASP:OD1	1:D:624:ARG:NH1	2.32	0.63
6:B:1053:HOH:O	1:D:552:LYS:HE2	1.99	0.62
1:D:299:THR:O	1:D:301:THR:HG23	1.99	0.62
1:A:736:MET:HE1	1:F:793:GLY:HA2	1.82	0.62
1:B:301:THR:HG22	6:B:915:HOH:O	1.99	0.62
1:F:577:ASN:H	1:F:618:ASN:ND2	1.97	0.62
1:B:596:HIS:HE1	6:B:998:HOH:O	1.82	0.62
5:A:801:EDO:H11	6:A:1131:HOH:O	1.99	0.61
1:G:711:SER:HA	1:G:785:SER:HB2	1.83	0.61
1:A:561:GLU:O	1:A:562:ASN:HB2	2.01	0.60
1:F:681:SER:O	1:F:715:PRO:HA	2.02	0.60
1:A:458:ARG:HD2	1:G:397:TYR:CZ	2.36	0.60
1:G:748:SER:HB3	6:G:966:HOH:O	2.02	0.59
1:F:520[B]:VAL:HG12	1:F:521:ASN:CG	2.22	0.59
1:D:622:ASP:OD2	1:D:626:ASN:HB2	2.02	0.59
1:F:552:LYS:HE3	1:G:576:GLY:HA3	1.85	0.58
1:B:747:LEU:HB3	1:B:751:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ILE:HD13	1:B:669:VAL:HG11	1.86	0.58
1:F:737:PHE:CD1	1:F:793:GLY:HA3	2.39	0.58
1:D:470:LYS:HB3	1:D:471:PRO:HA	1.87	0.57
1:G:744:ASP:O	1:G:787:SER:OG	2.21	0.57
1:B:561:GLU:O	1:B:562:ASN:HB2	2.04	0.57
1:B:759:LEU:HA	1:B:762:GLN:HE21	1.68	0.57
1:A:393:GLU:CD	1:A:393:GLU:H	2.08	0.57
1:A:520:VAL:HG12	1:A:552:LYS:HB3	1.85	0.57
1:A:736:MET:HE2	1:F:793:GLY:HA2	1.86	0.57
1:C:520:VAL:HG12	1:C:552:LYS:HB3	1.86	0.56
1:F:722:ALA:HB1	1:F:723:TYR:CG	2.41	0.56
1:C:669:VAL:HG23	1:C:696:ALA:HB3	1.86	0.55
1:D:282:ASN:HA	1:D:317:LYS:HD2	1.88	0.55
1:A:561:GLU:O	1:A:562:ASN:CB	2.53	0.55
1:B:677:LEU:HB3	1:B:719:LEU:HD11	1.88	0.55
1:F:470:LYS:HB3	1:F:471:PRO:HA	1.89	0.55
1:A:777:TYR:O	6:A:902:HOH:O	2.18	0.54
1:B:303:VAL:O	6:B:901:HOH:O	2.18	0.54
1:A:736:MET:O	1:A:793:GLY:HA3	2.07	0.54
1:B:561:GLU:O	1:B:562:ASN:CB	2.55	0.54
1:B:433:LEU:HD13	1:C:456:LYS:HD2	1.89	0.54
1:D:503:SER:HB3	6:D:905:HOH:O	2.06	0.54
1:B:575:VAL:HA	1:B:616:ASP:O	2.08	0.54
1:C:470:LYS:HB3	1:C:471:PRO:HA	1.89	0.54
1:F:520[B]:VAL:HA	1:F:552:LYS:O	2.08	0.54
1:G:258:ASN:OD1	1:G:264:ASN:ND2	2.38	0.53
1:A:414:HIS:H	1:A:414:HIS:CD2	2.25	0.53
1:C:540:LYS:NZ	6:C:902:HOH:O	2.21	0.53
1:A:397:TYR:CZ	1:F:458:ARG:HD2	2.44	0.53
1:D:258:ASN:HB2	1:D:263:ILE:HD11	1.90	0.53
1:A:360:LYS:HE3	1:A:392:ASP:OD2	2.09	0.53
1:A:599:ILE:O	1:A:629:ILE:HA	2.09	0.53
1:D:408:PHE:O	1:D:441:SER:HB3	2.10	0.52
1:D:570:SER:HA	1:D:611:VAL:O	2.10	0.52
1:F:552:LYS:HZ1	1:G:552:LYS:HE2	1.73	0.52
1:A:282:ASN:HA	1:A:317:LYS:HD2	1.91	0.52
1:A:408:PHE:O	1:A:441:SER:HB3	2.09	0.52
1:A:470:LYS:HB3	1:A:471:PRO:HA	1.91	0.52
1:C:561:GLU:O	1:C:562:ASN:CB	2.57	0.52
1:F:518:ILE:HG22	1:F:520[B]:VAL:CG2	2.38	0.52
1:G:570:SER:HA	1:G:611:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:GLU:CD	1:D:393:GLU:H	2.12	0.51
1:F:421:VAL:HG11	1:F:423:TYR:CZ	2.45	0.51
1:A:401:THR:HA	1:A:435:SER:O	2.10	0.51
1:A:768:TYR:OH	1:F:740:ASP:O	2.22	0.51
5:A:801:EDO:H22	2:E:6:GLA:O3	2.10	0.51
1:G:357:PHE:CE2	1:G:387:ASP:HB3	2.46	0.51
1:F:303:VAL:O	6:F:901:HOH:O	2.19	0.51
1:F:520[A]:VAL:HA	1:F:552:LYS:O	2.11	0.51
1:F:746:THR:HG22	1:F:746:THR:O	2.11	0.51
1:A:575:VAL:HA	1:A:616:ASP:O	2.10	0.50
1:F:714:SER:N	1:F:715:PRO:CD	2.74	0.50
1:B:354:ALA:HB1	6:B:902:HOH:O	2.12	0.50
1:D:329:ASP:OD1	1:D:356:LYS:NZ	2.42	0.50
1:F:622:ASP:OD2	1:F:626:ASN:HB2	2.11	0.50
1:F:388:GLY:HA2	1:F:408:PHE:CE1	2.47	0.50
1:D:512:GLY:O	1:D:544:ASN:HA	2.12	0.50
1:G:654:ILE:HD13	1:G:669:VAL:HG11	1.93	0.50
1:C:406:THR:HG22	1:C:440:ASN:HB3	1.94	0.50
1:G:376:LYS:H	1:G:386:GLN:NE2	2.07	0.49
1:C:349:LYS:NZ	6:C:914:HOH:O	2.45	0.49
1:A:732:SER:HB2	1:A:796:ASP:O	2.12	0.49
1:F:279:HIS:CD2	1:G:280:LEU:HD22	2.47	0.49
1:B:503:SER:HA	1:B:530:ARG:O	2.13	0.49
1:D:454:VAL:N	6:D:901:HOH:O	2.46	0.49
1:D:769:ARG:NH2	1:D:776:LEU:HD12	2.28	0.49
1:F:734:THR:HG22	1:F:735:SER:N	2.27	0.49
1:G:447:LEU:HD22	1:G:490:TYR:CE2	2.48	0.49
1:B:520:VAL:HA	1:B:552:LYS:O	2.13	0.48
1:C:457:ASN:H	1:C:495:ASN:HD22	1.60	0.48
1:F:561:GLU:O	1:F:562:ASN:CB	2.60	0.48
1:A:519:ILE:HD12	1:A:519:ILE:N	2.29	0.48
1:C:575:VAL:HA	1:C:616:ASP:O	2.13	0.48
1:F:357:PHE:CE2	1:F:387:ASP:HB3	2.49	0.48
1:F:599:ILE:O	1:F:629:ILE:HA	2.13	0.48
1:B:489:ARG:HA	1:B:516:ASP:O	2.13	0.48
1:A:570:SER:HA	1:A:611:VAL:O	2.14	0.48
1:C:548:ARG:HA	1:C:571:ASN:O	2.14	0.48
1:F:452:GLY:HA3	1:F:490:TYR:CE2	2.48	0.48
1:B:277:GLY:O	1:B:281:GLN:HG3	2.14	0.48
1:C:520:VAL:HA	1:C:552:LYS:O	2.13	0.48
1:A:742:TRP:CH2	1:G:770:THR:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:ALA:HB1	1:B:723:TYR:CG	2.48	0.47
1:D:252:MET:HE1	1:D:255:GLY:HA3	1.96	0.47
1:G:546:VAL:HB	1:G:569:VAL:HG12	1.96	0.47
1:F:561:GLU:O	1:F:562:ASN:HB2	2.14	0.47
1:F:733:SER:O	1:G:693[B]:VAL:HG21	2.14	0.47
1:A:493:ALA:HA	1:A:520:VAL:O	2.13	0.47
1:B:493:ALA:HA	1:B:520:VAL:O	2.14	0.47
1:D:722:ALA:HB2	1:D:764:GLN:HG2	1.96	0.47
1:G:747:LEU:HD22	1:G:751:VAL:HG12	1.97	0.47
1:B:748:SER:O	1:B:751:VAL:HG12	2.14	0.47
1:F:552:LYS:NZ	1:G:552:LYS:HE2	2.29	0.47
1:G:684:ILE:HG23	1:G:712:ILE:HG22	1.96	0.47
1:B:470:LYS:HB3	1:B:471:PRO:HA	1.96	0.46
1:B:520:VAL:HG12	1:B:552:LYS:HB3	1.96	0.46
1:F:376:LYS:H	1:F:386:GLN:NE2	2.11	0.46
1:F:512:GLY:O	1:F:544:ASN:HA	2.15	0.46
1:F:722:ALA:HB1	1:F:723:TYR:CD2	2.50	0.46
1:D:302:THR:CG2	1:D:306:LYS:HE3	2.44	0.46
1:F:577:ASN:HD22	1:F:618:ASN:HD21	1.63	0.46
1:B:456:LYS:O	1:B:456:LYS:CD	2.56	0.46
1:A:652:ILE:HG23	1:A:669:VAL:HG12	1.98	0.46
1:B:548:ARG:HA	1:B:571:ASN:O	2.16	0.46
1:D:561:GLU:O	1:D:562:ASN:CB	2.63	0.46
1:D:575:VAL:HA	1:D:616:ASP:O	2.16	0.46
1:C:457:ASN:H	1:C:495:ASN:ND2	2.13	0.46
1:F:315:LYS:O	1:F:317:LYS:HD3	2.16	0.46
1:F:770:THR:HG22	1:G:742:TRP:CH2	2.51	0.45
1:A:611:VAL:HA	1:A:636:THR:O	2.16	0.45
1:C:301:THR:OG1	1:C:325:PHE:HB3	2.16	0.45
1:A:736:MET:HE3	1:A:794:PHE:CZ	2.52	0.45
1:C:561:GLU:O	1:C:562:ASN:CG	2.55	0.45
1:D:695:ARG:NH2	6:D:913:HOH:O	2.42	0.45
1:C:489:ARG:HA	1:C:516:ASP:O	2.17	0.45
1:A:742:TRP:CZ2	1:G:770:THR:HG22	2.52	0.45
6:A:909:HOH:O	1:F:523:THR:CB	2.45	0.45
1:G:489:ARG:HA	1:G:516:ASP:O	2.17	0.45
1:A:451:GLU:HA	1:A:489:ARG:O	2.16	0.44
1:A:456:LYS:NZ	6:A:916:HOH:O	2.49	0.44
1:B:596:HIS:CD2	1:B:596:HIS:O	2.70	0.44
1:C:635:ALA:HB1	1:C:638:ASN:ND2	2.32	0.44
1:B:303:VAL:HA	6:B:901:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ALA:HB1	1:A:723:TYR:CD2	2.53	0.44
1:F:280:LEU:HD21	1:G:280:LEU:HD21	1.99	0.44
1:A:388:GLY:HA2	1:A:408:PHE:CE1	2.53	0.44
1:A:677:LEU:HB3	6:A:1104:HOH:O	2.18	0.44
3:I:1:GLA:H5	4:J:2:BMA:H61	1.99	0.44
1:C:349:LYS:HD3	6:C:1169:HOH:O	2.18	0.44
1:D:524:VAL:O	1:D:556:THR:HA	2.18	0.44
1:A:616:ASP:HB2	6:A:1105:HOH:O	2.18	0.44
1:A:681:SER:O	1:A:715:PRO:HA	2.18	0.44
1:C:750:GLY:CA	1:D:750:GLY:HA2	2.47	0.44
1:G:435:SER:HA	1:G:455:LEU:O	2.18	0.44
1:B:486:ASN:HA	1:B:513:TYR:O	2.18	0.43
1:G:520:VAL:HA	1:G:552:LYS:O	2.18	0.43
1:C:457:ASN:HD22	1:C:495:ASN:ND2	2.09	0.43
1:C:556:THR:O	1:C:579:SER:HA	2.18	0.43
1:D:466:SER:HB2	1:D:478:TYR:CZ	2.54	0.43
1:A:452:GLY:HA3	1:A:490:TYR:CE2	2.54	0.43
1:D:519:ILE:N	1:D:519:ILE:HD12	2.34	0.43
1:F:699:ASN:HA	1:F:797:PHE:CZ	2.53	0.43
1:C:783:MET:HE2	1:C:787:SER:HB2	2.01	0.43
1:D:722:ALA:HB1	1:D:723:TYR:CG	2.53	0.43
1:A:302:THR:HG22	1:A:306:LYS:HE3	2.01	0.43
1:D:769:ARG:HD3	1:D:782:LEU:HD11	2.01	0.43
1:B:621:ILE:HD11	1:D:571:ASN:HB3	2.01	0.43
1:F:435:SER:HA	1:F:455:LEU:O	2.19	0.43
1:G:769:ARG:HD3	1:G:782:LEU:CD1	2.49	0.43
1:D:486:ASN:HA	1:D:513:TYR:O	2.18	0.42
1:D:665:PHE:HB3	1:D:667:LEU:O	2.20	0.42
1:B:742:TRP:CZ2	1:D:770:THR:HG22	2.54	0.42
1:C:722:ALA:HB1	1:C:723:TYR:CG	2.54	0.42
1:C:737:PHE:CD1	1:C:791:LEU:HD21	2.54	0.42
1:F:612:GLY:HA2	1:F:637:GLY:O	2.19	0.42
1:B:440:ASN:OD1	1:B:440:ASN:C	2.57	0.42
1:A:722:ALA:HB1	1:A:723:TYR:CG	2.54	0.42
1:C:773:GLY:HA3	1:D:745:LEU:O	2.19	0.42
1:D:526:ALA:HA	1:D:558:ASN:O	2.19	0.42
1:F:734:THR:CG2	1:F:735:SER:N	2.82	0.42
1:B:320:VAL:C	6:B:908:HOH:O	2.57	0.42
1:B:684:ILE:HG23	1:B:712:ILE:HG22	2.00	0.42
1:G:561:GLU:O	1:G:562:ASN:CB	2.66	0.42
1:C:534:MET:CE	1:C:551:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:736:MET:O	1:G:793:GLY:HA3	2.19	0.42
1:A:484:SER:HB2	1:A:507:PHE:CD2	2.55	0.42
1:B:515:THR:HA	1:B:547:LEU:O	2.20	0.42
1:D:376:LYS:HG3	1:D:386:GLN:OE1	2.20	0.42
1:F:602:ALA:HA	1:F:632:PRO:HG3	2.01	0.42
1:B:445:VAL:O	1:B:482:ILE:HA	2.19	0.42
1:F:451:GLU:HA	1:F:489:ARG:O	2.20	0.42
1:A:586:ASP:OD1	1:A:624:ARG:NH1	2.51	0.41
1:B:419:ASP:O	6:B:902:HOH:O	2.21	0.41
1:B:654:ILE:CD1	1:B:669:VAL:HG11	2.49	0.41
1:C:681:SER:O	1:C:715:PRO:HA	2.20	0.41
1:B:321:LEU:HD23	6:B:908:HOH:O	2.20	0.41
1:F:319:LEU:HD23	1:F:339:VAL:HG22	2.01	0.41
1:A:357:PHE:CE2	1:A:387:ASP:HB3	2.56	0.41
1:B:416:SER:OG	1:B:418:ALA:HB3	2.20	0.41
1:B:599:ILE:O	1:B:629:ILE:HA	2.20	0.41
1:G:654:ILE:CD1	1:G:669:VAL:HG11	2.50	0.41
1:G:722:ALA:HB1	1:G:723:TYR:CG	2.55	0.41
1:B:540:LYS:HB2	1:B:608:GLU:HG2	2.01	0.41
1:C:501:GLY:O	1:C:528:TRP:HB3	2.19	0.41
1:D:520:VAL:HG12	1:D:552:LYS:HB2	2.01	0.41
1:F:401:THR:HA	1:F:435:SER:O	2.20	0.41
1:A:745:LEU:O	1:G:773:GLY:HA3	2.20	0.41
1:C:746:THR:CG2	1:C:784:LYS:HD2	2.50	0.41
1:C:357:PHE:CE2	1:C:387:ASP:HB3	2.55	0.41
1:A:447:LEU:HD22	1:A:490:TYR:CE2	2.55	0.41
1:A:552:LYS:HG3	1:G:552:LYS:NZ	2.36	0.41
1:D:447:LEU:HD22	1:D:490:TYR:CE2	2.56	0.41
1:B:770:THR:HG22	1:C:742:TRP:CZ2	2.55	0.41
1:C:796:ASP:OD2	1:D:702:ASP:OD2	2.39	0.41
1:D:759:LEU:HD23	1:D:759:LEU:HA	1.94	0.41
1:F:584:ASN:O	1:F:588:ILE:HG12	2.21	0.41
1:F:677:LEU:HD11	1:F:707:VAL:HG11	2.03	0.41
1:B:601:LEU:O	1:B:632:PRO:HD3	2.21	0.41
1:C:506:TYR:HA	1:C:533:ASP:O	2.21	0.41
1:F:301:THR:OG1	1:F:305:ILE:HD12	2.21	0.41
1:F:773:GLY:HA2	1:G:747:LEU:HD12	2.01	0.41
1:G:560:ARG:O	1:G:594:GLY:HA3	2.21	0.41
1:B:759:LEU:HD22	1:B:762:GLN:HE22	1.85	0.41
1:C:326:MET:CE	1:C:349:LYS:HE3	2.51	0.41
1:A:593:PRO:HA	6:A:951:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:HD22	1:B:490:TYR:CE2	2.56	0.40
1:C:484:SER:HB2	1:C:507:PHE:CD2	2.56	0.40
1:C:561:GLU:O	1:C:562:ASN:HB2	2.21	0.40
1:A:406:THR:HA	1:A:440:ASN:O	2.21	0.40
1:A:498:SER:HA	1:A:525:TYR:O	2.22	0.40
1:C:415:THR:HG23	1:C:419:ASP:OD2	2.21	0.40
1:C:560:ARG:HD2	1:C:592:TYR:O	2.21	0.40
1:G:694:PHE:HA	1:G:702:ASP:O	2.21	0.40
1:F:706:THR:HG23	1:F:790:ILE:HG12	2.03	0.40
1:B:414:HIS:CE1	1:B:421:VAL:HG13	2.56	0.40
1:C:413:LEU:HD23	1:C:413:LEU:HA	1.82	0.40
1:D:444:CYS:HB2	1:D:481:GLY:O	2.22	0.40
1:F:311:HIS:CE1	1:F:315:LYS:HG3	2.55	0.40
1:F:320:VAL:HA	1:F:340:GLU:O	2.22	0.40
1:F:556:THR:O	1:F:579:SER:HA	2.21	0.40
1:G:602:ALA:HA	1:G:632:PRO:HG3	2.03	0.40
1:A:579:SER:O	1:A:620:CYS:HA	2.21	0.40
1:B:722:ALA:HB2	1:B:764:GLN:HG2	2.03	0.40
1:D:252:MET:CE	1:D:255:GLY:HA3	2.50	0.40
1:D:312:CYS:SG	1:D:319:LEU:HB2	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	546/547 (100%)	528 (97%)	17 (3%)	1 (0%)	47 49
1	B	547/547 (100%)	525 (96%)	21 (4%)	1 (0%)	47 49
1	C	546/547 (100%)	523 (96%)	22 (4%)	1 (0%)	47 49
1	D	547/547 (100%)	527 (96%)	19 (4%)	1 (0%)	47 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	547/547 (100%)	525 (96%)	21 (4%)	1 (0%)	47	49
1	G	547/547 (100%)	526 (96%)	20 (4%)	1 (0%)	47	49
All	All	3280/3282 (100%)	3154 (96%)	120 (4%)	6 (0%)	47	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	ASN
1	B	562	ASN
1	C	562	ASN
1	D	562	ASN
1	F	562	ASN
1	G	562	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/447 (100%)	446 (100%)	2 (0%)	91	94
1	B	449/447 (100%)	445 (99%)	4 (1%)	78	84
1	C	448/447 (100%)	441 (98%)	7 (2%)	62	69
1	D	449/447 (100%)	445 (99%)	4 (1%)	78	84
1	F	448/447 (100%)	443 (99%)	5 (1%)	73	79
1	G	449/447 (100%)	444 (99%)	5 (1%)	73	79
All	All	2691/2682 (100%)	2664 (99%)	27 (1%)	76	82

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	SER
1	A	681	SER
1	B	295	THR
1	B	656	SER

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Mol	Chain	Res	Type
1	B	683	SER
1	B	716	SER
1	C	415	THR
1	C	632	PRO
1	C	669	VAL
1	C	710	SER
1	C	733[A]	SER
1	C	733[B]	SER
1	C	784	LYS
1	D	315	LYS
1	D	417	ASP
1	D	656	SER
1	D	746	THR
1	F	356	LYS
1	F	383	THR
1	F	417	ASP
1	F	700	ARG
1	F	784	LYS
1	G	252	MET
1	G	530	ARG
1	G	534	MET
1	G	704	SER
1	G	744	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	HIS
1	A	462	ASN
1	A	720	ASN
1	A	764	GLN
1	B	596	HIS
1	C	495	ASN
1	D	559	ASN
1	F	386	GLN
1	F	618	ASN
1	G	386	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

36 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	RAM	E	1	2	11,11,11	1.76	2 (18%)	15,16,16	2.22	3 (20%)
2	BMA	E	2	2	11,11,12	1.66	1 (9%)	15,15,17	1.36	2 (13%)
2	GLA	E	3	2	11,11,12	1.89	3 (27%)	15,15,17	0.71	0
2	RAM	E	4	2	10,10,11	2.17	3 (30%)	14,14,16	1.89	4 (28%)
2	BMA	E	5	2	11,11,12	1.84	2 (18%)	15,15,17	1.21	3 (20%)
2	GLA	E	6	2	11,11,12	1.83	3 (27%)	15,15,17	0.63	0
2	RAM	H	1	2	11,11,11	1.74	2 (18%)	15,16,16	1.35	3 (20%)
2	BMA	H	2	2	11,11,12	1.79	3 (27%)	15,15,17	1.47	3 (20%)
2	GLA	H	3	2	11,11,12	1.68	1 (9%)	15,15,17	0.72	0
2	RAM	H	4	2	10,10,11	2.19	4 (40%)	14,14,16	1.04	0
2	BMA	H	5	2	11,11,12	1.58	2 (18%)	15,15,17	1.14	2 (13%)
2	GLA	H	6	2	11,11,12	1.73	2 (18%)	15,15,17	0.89	0
3	GLA	I	1	3	11,11,12	1.50	2 (18%)	15,15,17	1.25	2 (13%)
3	RAM	I	2	3	10,10,11	2.22	3 (30%)	14,14,16	1.14	1 (7%)
3	BMA	I	3	3	11,11,12	1.82	2 (18%)	15,15,17	1.05	2 (13%)
3	GLA	I	4	3	11,11,12	1.81	3 (27%)	15,15,17	0.72	0
4	RAM	J	1	4	11,11,11	1.53	2 (18%)	15,16,16	1.95	3 (20%)
4	BMA	J	2	4	11,11,12	1.73	2 (18%)	15,15,17	1.26	2 (13%)
2	RAM	K	1	2	11,11,11	1.72	2 (18%)	15,16,16	1.16	0
2	BMA	K	2	2	11,11,12	1.43	2 (18%)	15,15,17	1.39	2 (13%)
2	GLA	K	3	2	11,11,12	1.62	2 (18%)	15,15,17	0.79	0
2	RAM	K	4	2	10,10,11	2.25	3 (30%)	14,14,16	1.71	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	K	5	2	11,11,12	1.79	3 (27%)	15,15,17	1.14	2 (13%)
2	GLA	K	6	2	11,11,12	1.88	3 (27%)	15,15,17	0.73	0
2	RAM	L	1	2	11,11,11	1.69	2 (18%)	15,16,16	2.84	4 (26%)
2	BMA	L	2	2	11,11,12	1.83	2 (18%)	15,15,17	2.03	4 (26%)
2	GLA	L	3	2	11,11,12	1.75	3 (27%)	15,15,17	0.81	0
2	RAM	L	4	2	10,10,11	2.40	4 (40%)	14,14,16	1.03	1 (7%)
2	BMA	L	5	2	11,11,12	1.70	3 (27%)	15,15,17	0.70	1 (6%)
2	GLA	L	6	2	11,11,12	1.69	3 (27%)	15,15,17	0.42	0
2	RAM	M	1	2	11,11,11	1.78	2 (18%)	15,16,16	2.03	3 (20%)
2	BMA	M	2	2	11,11,12	1.45	2 (18%)	15,15,17	1.56	3 (20%)
2	GLA	M	3	2	11,11,12	1.70	2 (18%)	15,15,17	0.41	0
2	RAM	M	4	2	10,10,11	2.19	4 (40%)	14,14,16	1.50	3 (21%)
2	BMA	M	5	2	11,11,12	1.78	3 (27%)	15,15,17	1.12	2 (13%)
2	GLA	M	6	2	11,11,12	1.76	2 (18%)	15,15,17	0.41	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	RAM	E	1	2	-	-	0/1/1/1
2	BMA	E	2	2	-	0/2/19/22	0/1/1/1
2	GLA	E	3	2	-	0/2/19/22	0/1/1/1
2	RAM	E	4	2	-	-	0/1/1/1
2	BMA	E	5	2	-	0/2/19/22	0/1/1/1
2	GLA	E	6	2	-	0/2/19/22	0/1/1/1
2	RAM	H	1	2	-	-	0/1/1/1
2	BMA	H	2	2	-	1/2/19/22	0/1/1/1
2	GLA	H	3	2	-	1/2/19/22	0/1/1/1
2	RAM	H	4	2	-	-	0/1/1/1
2	BMA	H	5	2	-	0/2/19/22	0/1/1/1
2	GLA	H	6	2	-	0/2/19/22	0/1/1/1
3	GLA	I	1	3	-	0/2/19/22	0/1/1/1
3	RAM	I	2	3	-	-	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	GLA	I	4	3	-	0/2/19/22	0/1/1/1
4	RAM	J	1	4	-	-	0/1/1/1
4	BMA	J	2	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RAM	K	1	2	-	-	0/1/1/1
2	BMA	K	2	2	-	2/2/19/22	0/1/1/1
2	GLA	K	3	2	-	0/2/19/22	0/1/1/1
2	RAM	K	4	2	-	-	0/1/1/1
2	BMA	K	5	2	-	0/2/19/22	0/1/1/1
2	GLA	K	6	2	-	0/2/19/22	0/1/1/1
2	RAM	L	1	2	-	-	0/1/1/1
2	BMA	L	2	2	-	2/2/19/22	0/1/1/1
2	GLA	L	3	2	-	0/2/19/22	0/1/1/1
2	RAM	L	4	2	-	-	0/1/1/1
2	BMA	L	5	2	-	0/2/19/22	0/1/1/1
2	GLA	L	6	2	-	0/2/19/22	0/1/1/1
2	RAM	M	1	2	-	-	0/1/1/1
2	BMA	M	2	2	-	0/2/19/22	0/1/1/1
2	GLA	M	3	2	-	0/2/19/22	0/1/1/1
2	RAM	M	4	2	-	-	0/1/1/1
2	BMA	M	5	2	-	2/2/19/22	0/1/1/1
2	GLA	M	6	2	-	0/2/19/22	0/1/1/1

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	GLA	O5-C1	5.20	1.52	1.43
2	L	4	RAM	O5-C1	5.10	1.51	1.43
2	E	6	GLA	O5-C1	4.99	1.51	1.43
2	K	6	GLA	O5-C1	4.92	1.51	1.43
2	K	4	RAM	O5-C1	4.87	1.51	1.43
2	E	5	BMA	O5-C1	4.84	1.51	1.43
2	E	4	RAM	O5-C1	4.71	1.51	1.43
3	I	3	BMA	O5-C1	4.71	1.51	1.43
2	H	3	GLA	O5-C1	4.70	1.51	1.43
3	I	4	GLA	O5-C1	4.69	1.51	1.43
2	H	4	RAM	O5-C1	4.66	1.51	1.43
3	I	2	RAM	O5-C1	4.66	1.51	1.43
2	K	5	BMA	O5-C1	4.63	1.51	1.43
2	M	6	GLA	O5-C1	4.58	1.51	1.43
2	H	6	GLA	O5-C1	4.55	1.51	1.43
2	L	3	GLA	O5-C1	4.55	1.51	1.43
2	M	3	GLA	O5-C1	4.53	1.51	1.43
2	M	4	RAM	O5-C1	4.51	1.50	1.43
2	L	2	BMA	O5-C1	4.40	1.50	1.43
2	M	5	BMA	O5-C1	4.34	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BMA	O5-C1	4.34	1.50	1.43
2	K	3	GLA	O5-C1	4.28	1.50	1.43
2	L	6	GLA	O5-C1	4.24	1.50	1.43
2	M	1	RAM	O4-C4	-4.15	1.33	1.43
2	H	2	BMA	O5-C1	4.14	1.50	1.43
4	J	2	BMA	O5-C1	4.11	1.50	1.43
2	L	5	BMA	O5-C1	4.09	1.50	1.43
2	L	1	RAM	O4-C4	-4.03	1.33	1.43
2	M	4	RAM	O4-C4	-4.03	1.33	1.43
2	K	4	RAM	O4-C4	-4.01	1.33	1.43
2	E	1	RAM	O4-C4	-4.01	1.33	1.43
3	I	2	RAM	O4-C4	-3.99	1.33	1.43
3	I	1	GLA	O5-C1	3.98	1.50	1.43
2	L	4	RAM	O4-C4	-3.96	1.33	1.43
2	H	1	RAM	O4-C4	-3.92	1.33	1.43
2	H	5	BMA	O5-C1	3.75	1.49	1.43
2	E	4	RAM	O4-C4	-3.71	1.34	1.43
2	K	1	RAM	O5-C1	3.70	1.52	1.42
2	H	4	RAM	O4-C4	-3.68	1.34	1.43
2	K	1	RAM	O4-C4	-3.57	1.34	1.43
2	E	1	RAM	O5-C1	3.49	1.51	1.42
2	K	2	BMA	O5-C1	3.47	1.49	1.43
4	J	2	BMA	C2-C3	-3.39	1.47	1.52
2	M	1	RAM	O5-C1	3.18	1.50	1.42
2	L	2	BMA	C2-C3	-3.17	1.47	1.52
2	H	1	RAM	O5-C1	3.15	1.50	1.42
4	J	1	RAM	O4-C4	3.12	1.50	1.43
2	M	2	BMA	O5-C1	3.11	1.48	1.43
4	J	1	RAM	O5-C1	2.95	1.50	1.42
2	H	2	BMA	C2-C3	-2.95	1.48	1.52
2	L	1	RAM	O5-C1	2.86	1.50	1.42
3	I	3	BMA	C2-C3	-2.84	1.48	1.52
2	H	5	BMA	C2-C3	-2.63	1.48	1.52
2	L	4	RAM	O5-C5	2.62	1.49	1.43
2	M	6	GLA	C2-C3	-2.58	1.48	1.52
2	M	2	BMA	C2-C3	-2.57	1.48	1.52
2	M	5	BMA	C2-C3	-2.53	1.48	1.52
2	L	5	BMA	C2-C3	-2.47	1.48	1.52
3	I	4	GLA	O5-C5	2.47	1.48	1.43
2	K	6	GLA	C2-C3	-2.45	1.48	1.52
2	E	4	RAM	O5-C5	2.44	1.48	1.43
2	M	5	BMA	O5-C5	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	6	GLA	C2-C3	-2.41	1.49	1.52
3	I	1	GLA	C2-C3	-2.41	1.49	1.52
2	L	3	GLA	C2-C3	-2.40	1.49	1.52
2	L	4	RAM	C2-C3	-2.39	1.49	1.52
2	K	6	GLA	O5-C5	2.38	1.48	1.43
2	K	5	BMA	O5-C5	2.35	1.48	1.43
3	I	2	RAM	C2-C3	-2.32	1.49	1.52
2	M	3	GLA	C2-C3	-2.31	1.49	1.52
2	H	2	BMA	O5-C5	2.31	1.48	1.43
2	H	6	GLA	C2-C3	-2.29	1.49	1.52
2	H	4	RAM	O5-C5	2.26	1.48	1.43
2	E	3	GLA	C2-C3	-2.23	1.49	1.52
2	E	5	BMA	O5-C5	2.23	1.48	1.43
2	H	4	RAM	C2-C3	-2.22	1.49	1.52
2	E	6	GLA	C2-C3	-2.20	1.49	1.52
2	E	6	GLA	O5-C5	2.18	1.47	1.43
2	M	4	RAM	C2-C3	-2.18	1.49	1.52
3	I	4	GLA	C2-C3	-2.16	1.49	1.52
2	L	3	GLA	O5-C5	2.16	1.47	1.43
2	K	5	BMA	C2-C3	-2.16	1.49	1.52
2	L	6	GLA	O5-C5	2.15	1.47	1.43
2	K	4	RAM	O5-C5	2.15	1.48	1.43
2	M	4	RAM	O5-C5	2.14	1.48	1.43
2	L	5	BMA	O5-C5	2.06	1.47	1.43
2	K	3	GLA	C2-C3	-2.06	1.49	1.52
2	K	2	BMA	O5-C5	2.06	1.47	1.43
2	E	3	GLA	O5-C5	2.03	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	RAM	O4-C4-C5	9.49	130.69	109.67
2	E	1	RAM	O4-C4-C5	7.02	125.23	109.67
2	M	1	RAM	O4-C4-C5	6.31	123.65	109.67
2	L	2	BMA	C1-O5-C5	5.57	119.73	112.19
4	J	1	RAM	O4-C4-C5	4.78	120.26	109.67
2	E	4	RAM	O4-C4-C5	4.63	119.93	109.67
2	K	4	RAM	C1-C2-C3	3.50	113.96	109.67
2	M	2	BMA	C6-C5-C4	-3.35	105.15	113.00
4	J	1	RAM	O4-C4-C3	3.33	118.05	110.35
4	J	1	RAM	C3-C4-C5	3.32	114.94	109.77
2	L	1	RAM	C3-C4-C5	3.31	114.93	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	BMA	C1-O5-C5	-3.31	107.71	112.19
2	H	2	BMA	C6-C5-C4	-3.29	105.29	113.00
2	M	5	BMA	O5-C5-C6	3.22	112.25	107.20
2	L	2	BMA	O5-C5-C4	3.13	118.44	110.83
2	H	1	RAM	O4-C4-C5	3.03	116.39	109.67
2	E	2	BMA	C1-C2-C3	3.00	113.35	109.67
2	M	4	RAM	O4-C4-C5	2.93	116.15	109.67
2	E	4	RAM	C3-C4-C5	2.86	114.23	109.77
3	I	2	RAM	C1-C2-C3	2.84	113.16	109.67
2	M	4	RAM	C1-C2-C3	2.84	113.16	109.67
3	I	1	GLA	C1-C2-C3	2.84	113.16	109.67
2	K	2	BMA	C2-C3-C4	2.83	115.79	110.89
2	M	2	BMA	C1-O5-C5	2.77	115.94	112.19
2	E	5	BMA	O5-C5-C6	2.69	111.42	107.20
2	M	4	RAM	O4-C4-C3	-2.62	104.29	110.35
2	E	1	RAM	O4-C4-C3	2.58	116.32	110.35
2	K	4	RAM	O4-C4-C5	2.57	115.36	109.67
2	M	2	BMA	C3-C4-C5	2.56	114.80	110.24
2	H	5	BMA	C1-O5-C5	-2.54	108.75	112.19
2	K	4	RAM	C2-C3-C4	2.52	115.25	110.89
2	K	5	BMA	C1-C2-C3	2.50	112.74	109.67
2	H	2	BMA	C3-C4-C5	2.45	114.61	110.24
3	I	3	BMA	O5-C5-C6	2.41	110.98	107.20
2	E	5	BMA	C1-C2-C3	2.35	112.56	109.67
2	E	5	BMA	O5-C1-C2	2.34	114.39	110.77
2	M	5	BMA	C1-O5-C5	-2.31	109.06	112.19
2	H	5	BMA	O5-C5-C6	2.30	110.81	107.20
2	K	4	RAM	C3-C4-C5	2.30	113.35	109.77
2	L	4	RAM	O4-C4-C5	2.23	114.62	109.67
2	L	2	BMA	O5-C1-C2	2.22	114.19	110.77
2	K	5	BMA	O5-C5-C6	2.21	110.67	107.20
2	E	4	RAM	O5-C5-C4	2.21	113.48	109.52
2	E	2	BMA	O5-C5-C6	2.21	110.66	107.20
2	H	1	RAM	C6-C5-C4	-2.17	109.05	113.07
2	E	1	RAM	C4-C3-C2	2.17	114.61	110.82
3	I	3	BMA	C1-O5-C5	-2.16	109.27	112.19
2	H	1	RAM	O5-C5-C4	2.16	113.39	109.52
2	L	2	BMA	C3-C4-C5	2.15	114.07	110.24
2	L	1	RAM	O5-C5-C4	2.14	113.36	109.52
2	K	2	BMA	C3-C4-C5	2.14	114.05	110.24
3	I	1	GLA	O5-C1-C2	2.13	114.06	110.77
2	H	2	BMA	C1-O5-C5	2.07	115.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	RAM	O4-C4-C3	2.04	115.06	110.35
2	M	1	RAM	C3-C4-C5	2.03	112.93	109.77
2	L	1	RAM	C4-C3-C2	2.02	114.36	110.82
2	E	4	RAM	C2-C3-C4	2.02	114.38	110.89
2	L	5	BMA	O5-C5-C6	2.02	110.36	107.20
4	J	2	BMA	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

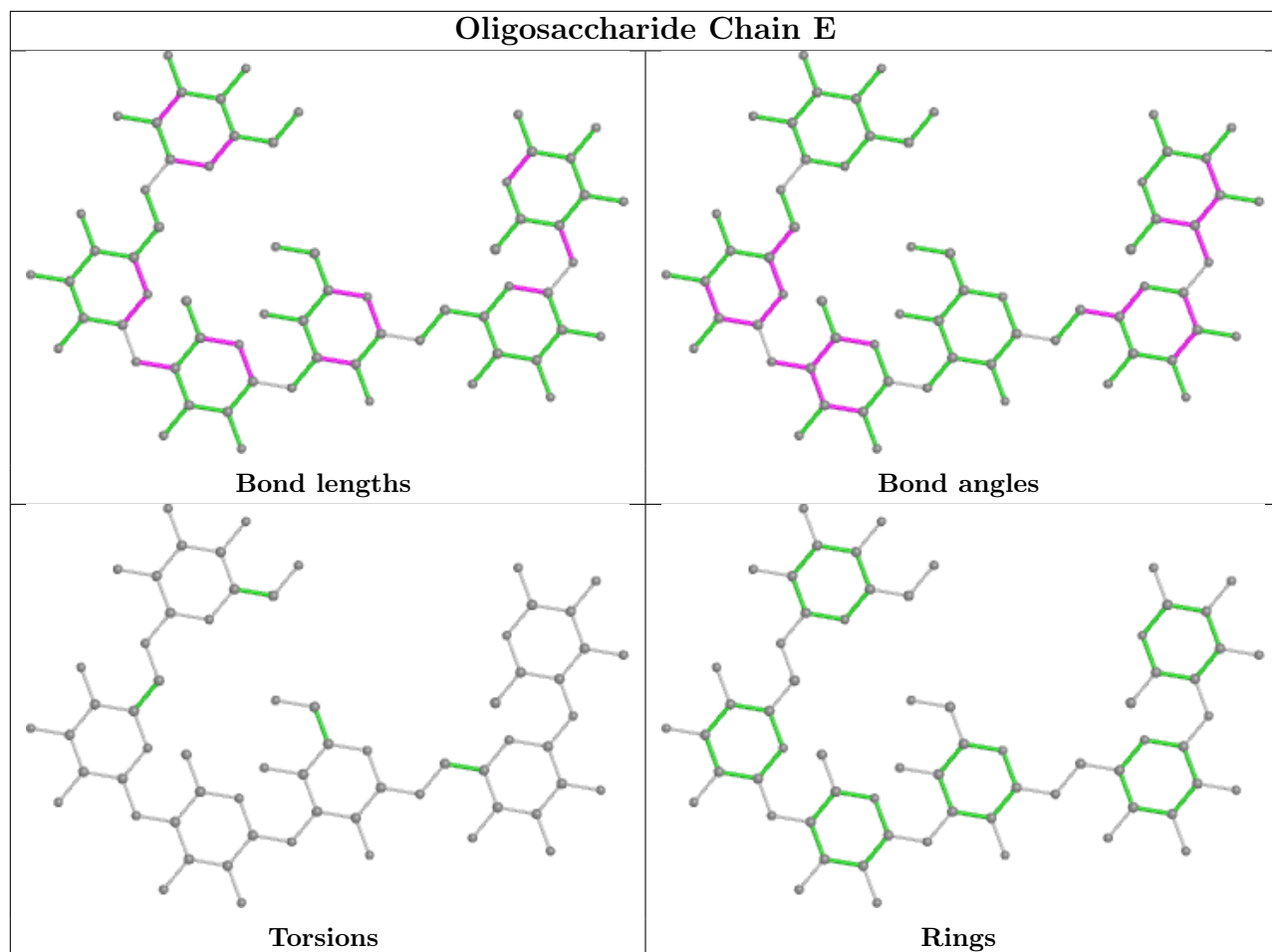
Mol	Chain	Res	Type	Atoms
2	L	2	BMA	O5-C5-C6-O6
2	L	2	BMA	C4-C5-C6-O6
2	K	2	BMA	C4-C5-C6-O6
2	K	2	BMA	O5-C5-C6-O6
4	J	2	BMA	C4-C5-C6-O6
2	H	2	BMA	C4-C5-C6-O6
4	J	2	BMA	O5-C5-C6-O6
2	M	5	BMA	O5-C5-C6-O6
2	H	3	GLA	O5-C5-C6-O6
2	M	5	BMA	C4-C5-C6-O6

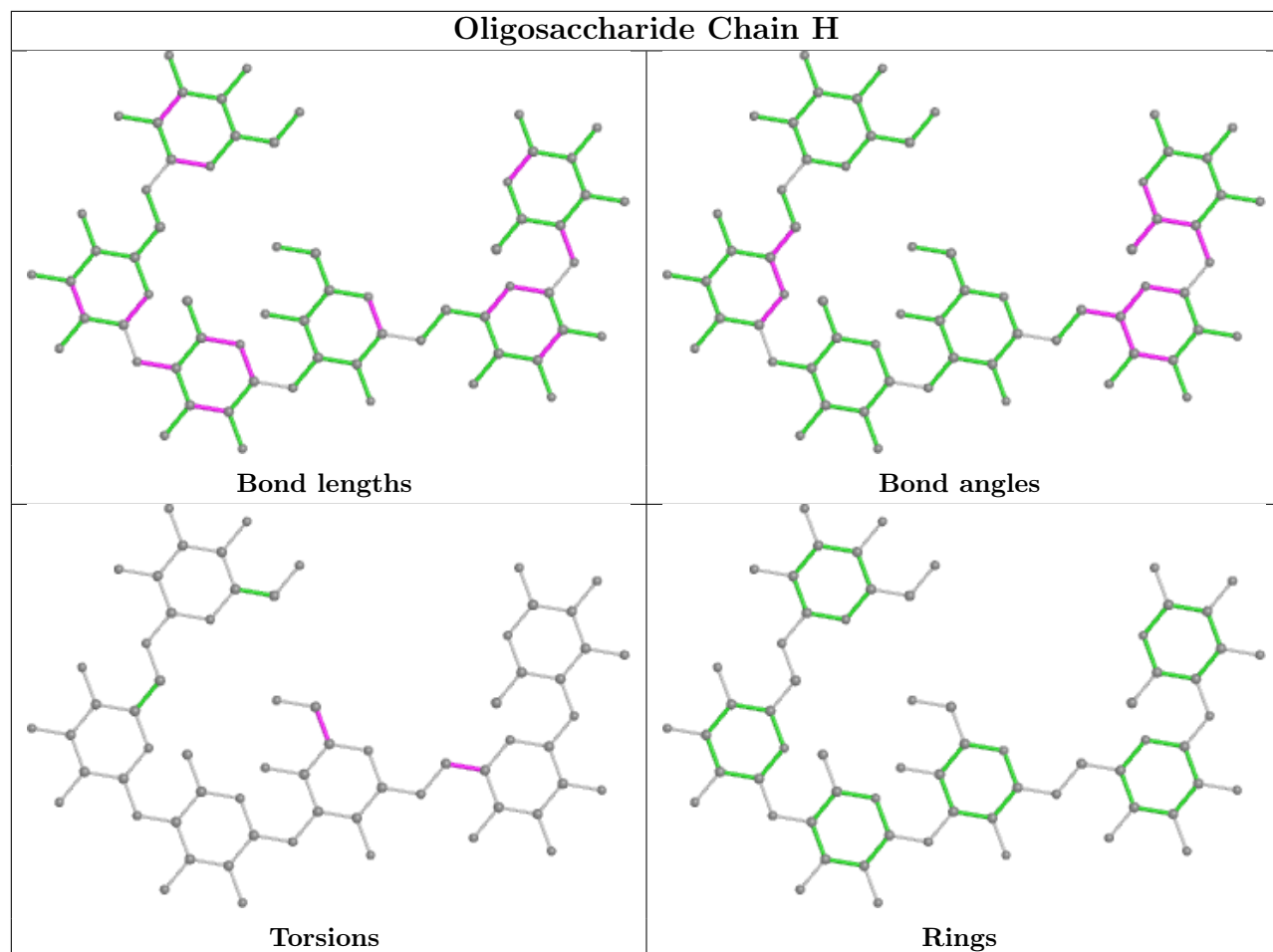
There are no ring outliers.

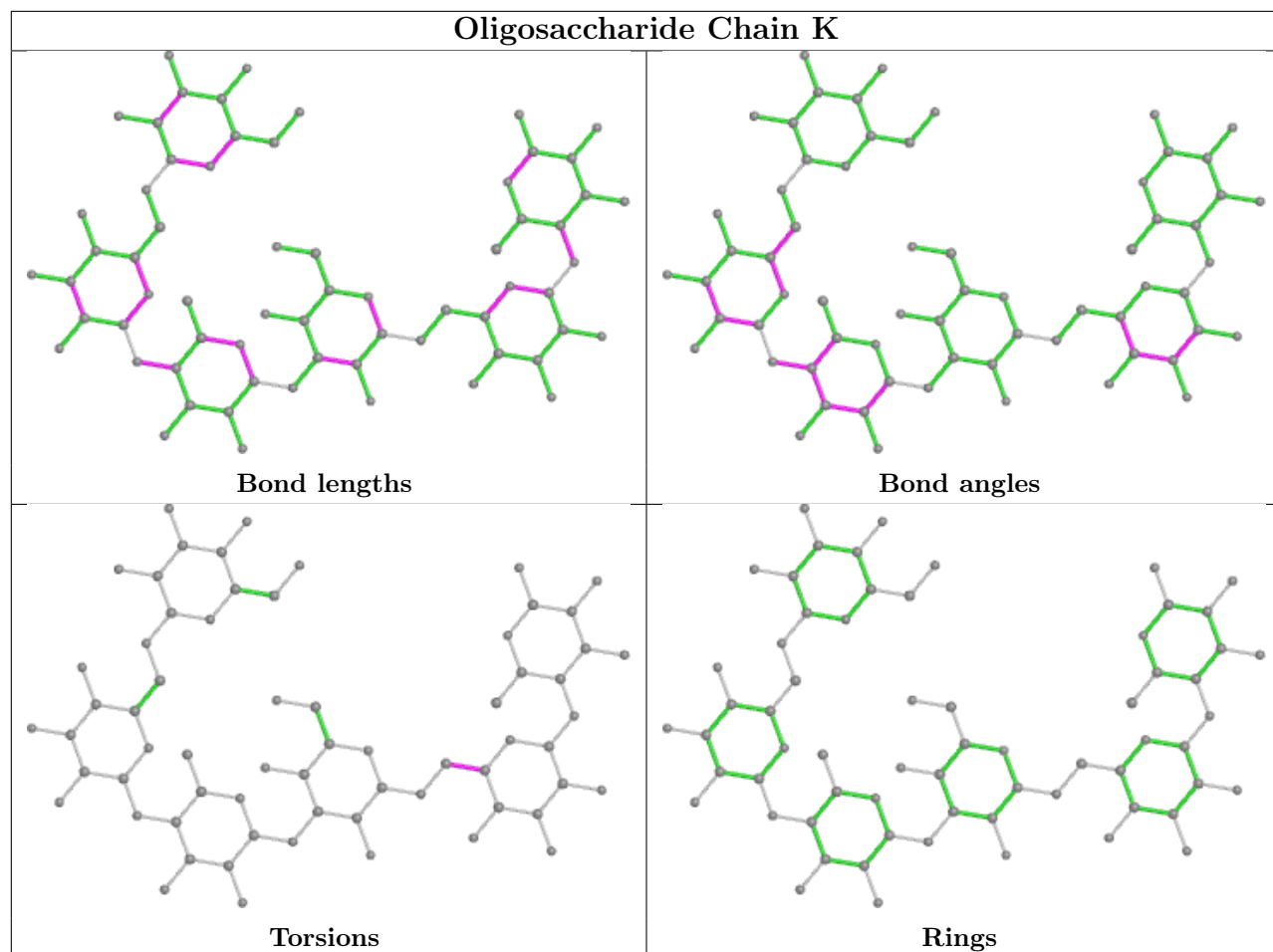
4 monomers are involved in 3 short contacts:

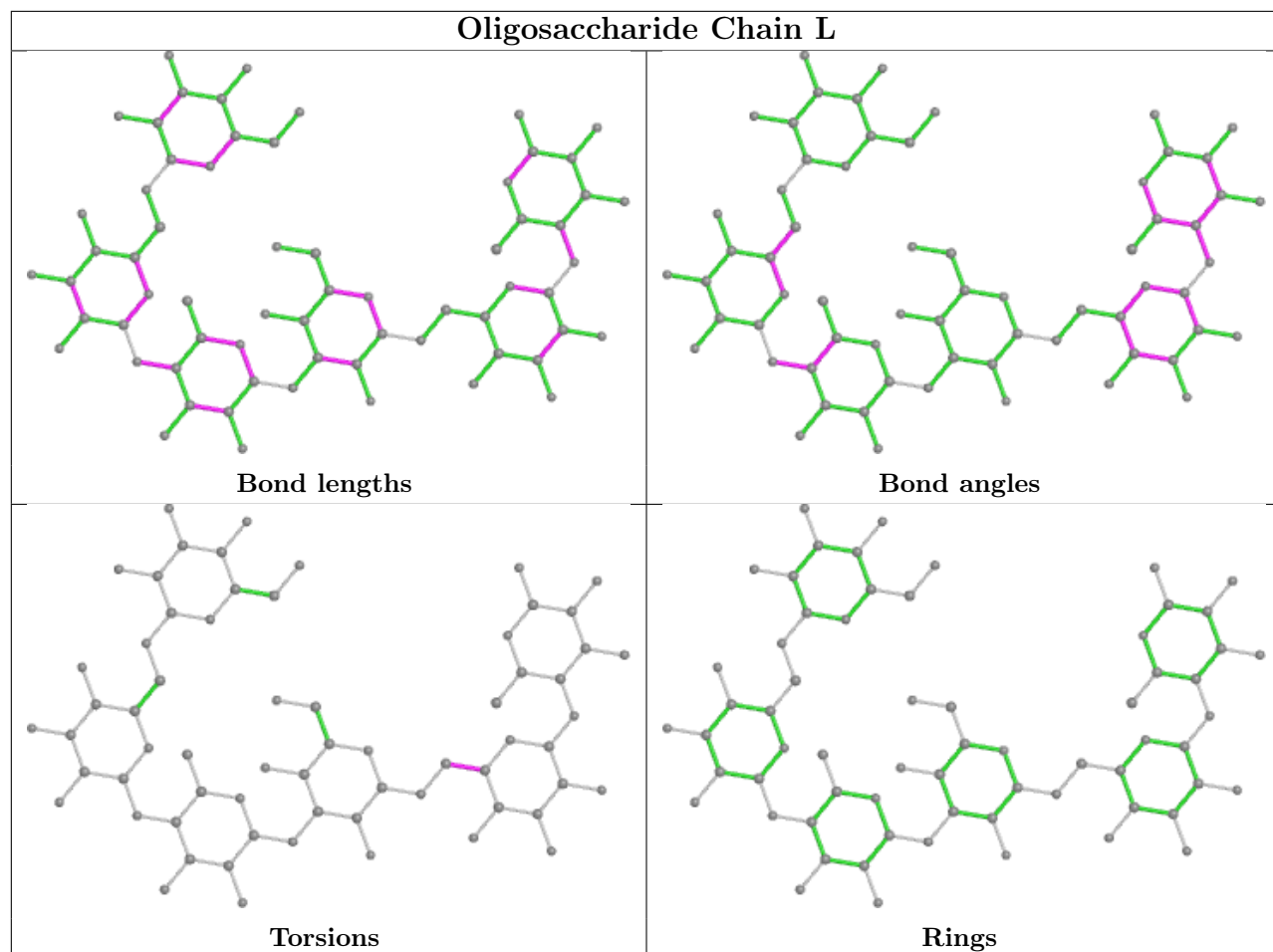
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	GLA	1	0
4	J	2	BMA	1	0
2	E	3	GLA	1	0
2	E	6	GLA	1	0

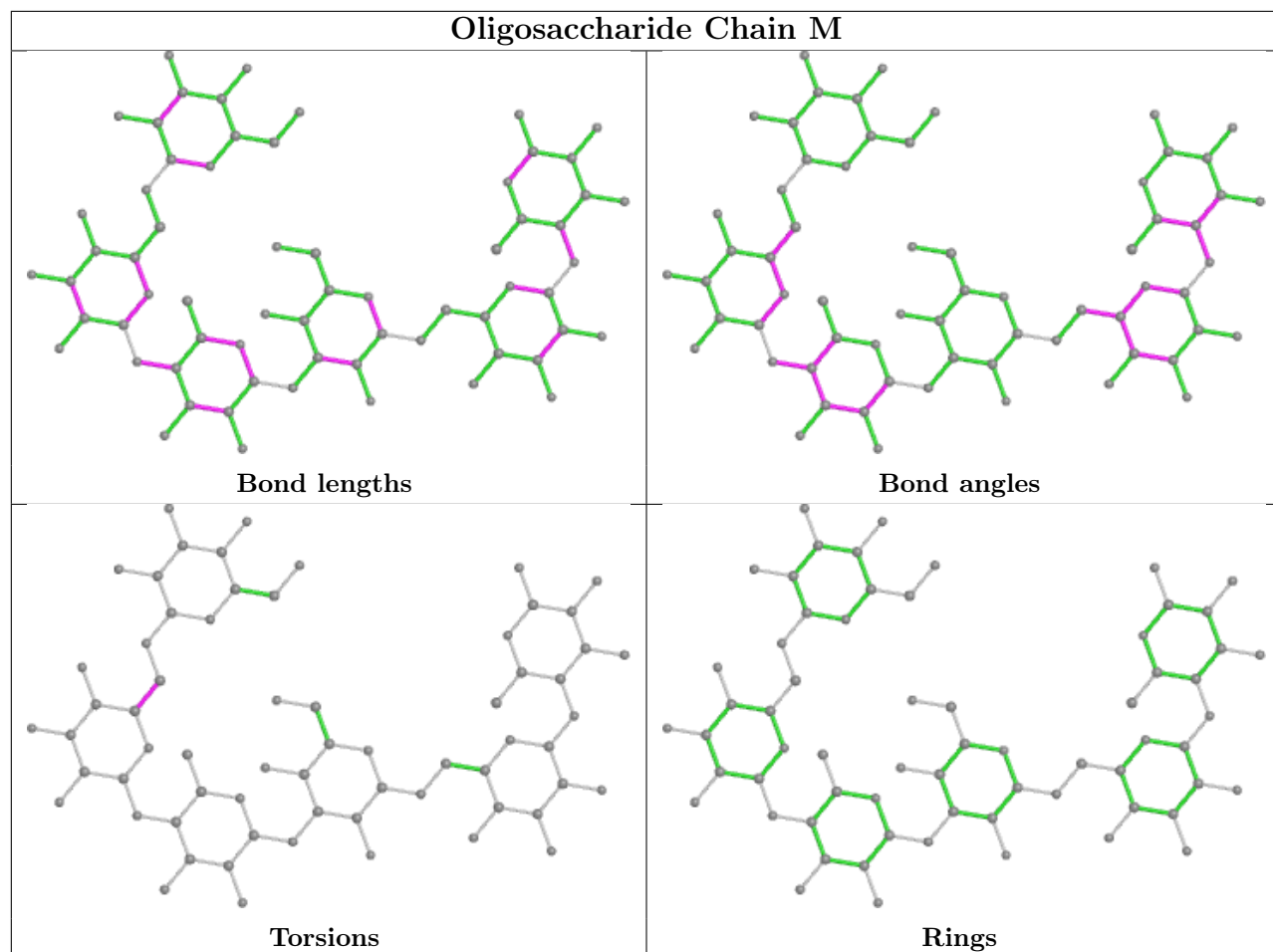
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

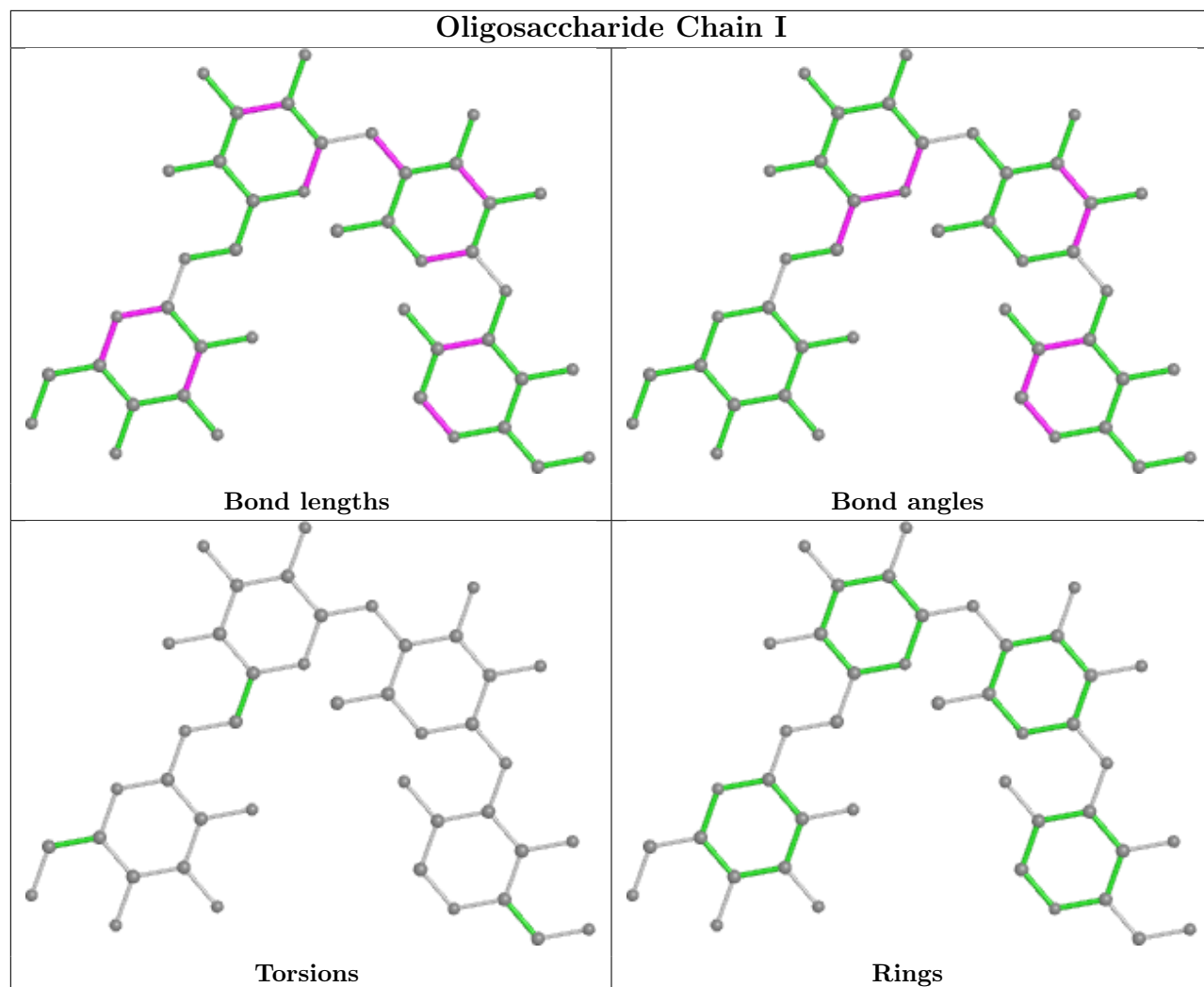


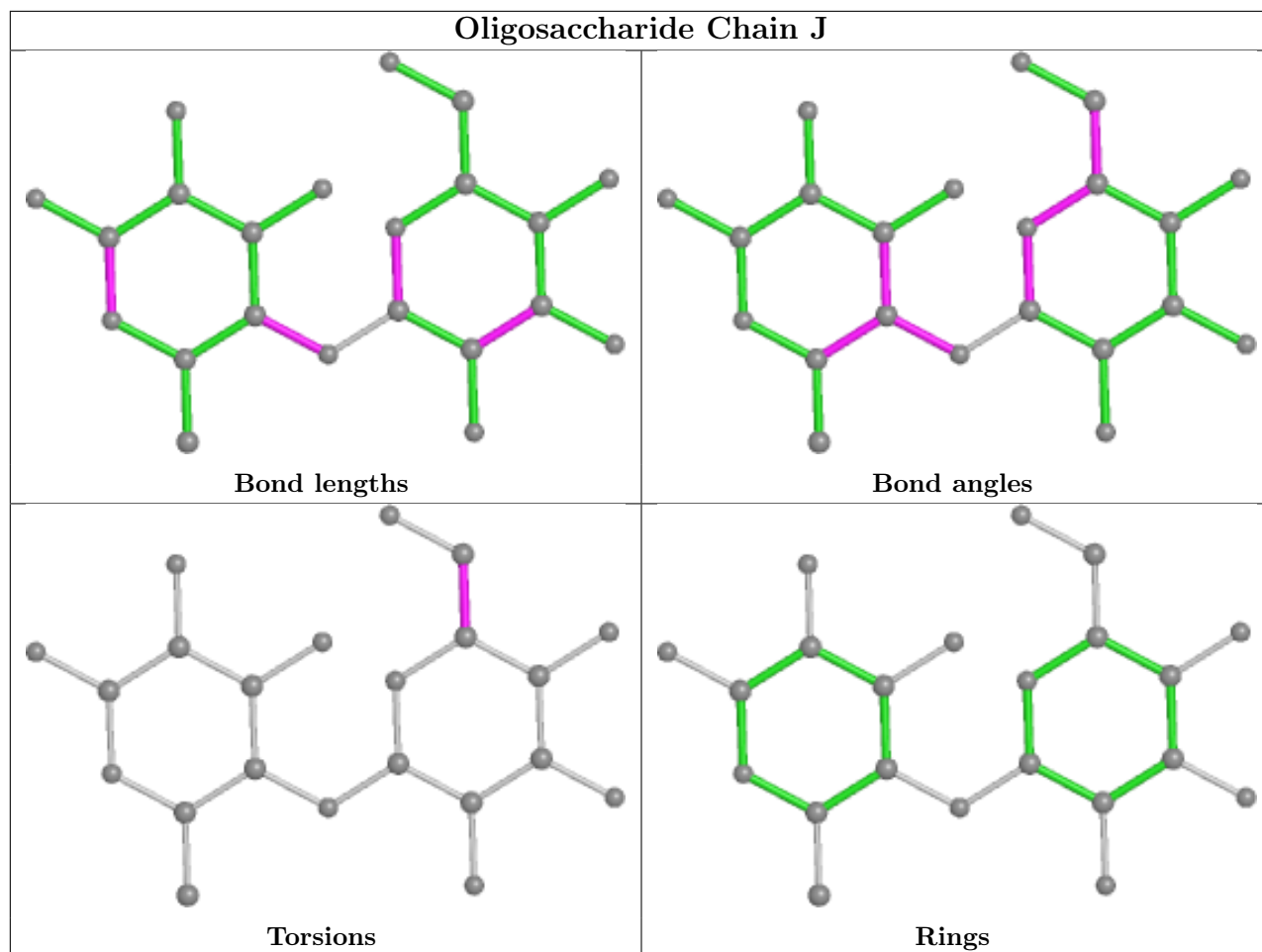












5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	EDO	A	801	-	3,3,3	0.54	0	2,2,2	0.09	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
5	EDO	A	801	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	EDO	2	0

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	546/547 (99%)	0.38	49 (8%) 9 12	25, 47, 70, 88	0
1	B	547/547 (100%)	0.43	53 (9%) 7 10	27, 52, 75, 93	0
1	C	547/547 (100%)	0.41	52 (9%) 8 10	26, 46, 73, 93	0
1	D	547/547 (100%)	0.29	48 (8%) 10 12	25, 47, 68, 110	0
1	F	547/547 (100%)	0.32	48 (8%) 10 12	25, 47, 72, 97	0
1	G	547/547 (100%)	0.45	59 (10%) 5 7	28, 47, 72, 97	0
All	All	3281/3282 (99%)	0.38	309 (9%) 8 11	25, 48, 72, 110	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	252	MET	6.5
1	G	455	LEU	5.8
1	D	252	MET	5.8
1	A	455	LEU	5.2
1	D	455	LEU	5.2
1	B	455	LEU	5.0
1	A	520	VAL	4.9
1	C	455	LEU	4.8
1	A	494	PHE	4.8
1	B	520	VAL	4.7
1	F	255	GLY	4.7
1	G	433	LEU	4.7
1	D	493	ALA	4.7
1	D	494	PHE	4.7
1	F	520[A]	VAL	4.6
1	A	491	VAL	4.5
1	D	433	LEU	4.5
1	B	494	PHE	4.5
1	C	519	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	382	THR	4.3
1	F	455	LEU	4.3
1	B	252	MET	4.2
1	C	520	VAL	4.2
1	G	494	PHE	4.2
1	C	491	VAL	4.2
1	F	492	ILE	4.2
1	F	494	PHE	4.1
1	G	493	ALA	4.1
1	G	491	VAL	4.1
1	A	454	VAL	4.0
1	A	456	LYS	4.0
1	A	493	ALA	4.0
1	A	519	ILE	4.0
1	C	401	THR	4.0
1	C	712	ILE	4.0
1	C	434	ILE	3.9
1	A	434	ILE	3.9
1	A	492	ILE	3.9
1	D	518	ILE	3.9
1	A	435	SER	3.8
1	C	494	PHE	3.8
1	D	520	VAL	3.8
1	C	518	ILE	3.8
1	F	263	ILE	3.8
1	B	518	ILE	3.8
1	F	550	ILE	3.8
1	G	492	ILE	3.8
1	C	575	VAL	3.8
1	F	518	ILE	3.7
1	C	493	ALA	3.7
1	C	714	SER	3.7
1	F	717	GLY	3.7
1	B	519	ILE	3.7
1	C	492	ILE	3.7
1	B	384	VAL	3.7
1	F	454	VAL	3.7
1	A	263	ILE	3.6
1	D	492	ILE	3.6
1	F	493	ALA	3.6
1	F	436	LYS	3.6
1	A	253	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	454	VAL	3.6
1	G	436	LYS	3.5
1	A	550	ILE	3.5
1	C	681	SER	3.5
1	C	436	LYS	3.5
1	A	433	LEU	3.5
1	B	433	LEU	3.5
1	G	383	THR	3.5
1	A	257	LEU	3.5
1	D	491	VAL	3.5
1	F	271	TYR	3.5
1	B	492	ILE	3.5
1	B	710	SER	3.5
1	A	436	LYS	3.4
1	B	712	ILE	3.4
1	G	401	THR	3.4
1	C	253	LEU	3.4
1	A	401	THR	3.4
1	C	551	ILE	3.4
1	D	550	ILE	3.3
1	C	433	LEU	3.3
1	B	401	THR	3.3
1	G	259	ASN	3.3
1	A	518	ILE	3.3
1	C	400	ILE	3.3
1	D	434	ILE	3.3
1	F	551	ILE	3.3
1	B	491	VAL	3.2
1	C	553	GLY	3.2
1	D	454	VAL	3.2
1	F	261	GLY	3.2
1	F	433	LEU	3.2
1	D	519	ILE	3.2
1	B	575	VAL	3.2
1	B	413	LEU	3.2
1	F	435	SER	3.1
1	B	400	ILE	3.1
1	C	435	SER	3.1
1	C	437	CYS	3.1
1	G	710	SER	3.1
1	C	784	LYS	3.1
1	C	550	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	454	VAL	3.1
1	D	258	ASN	3.1
1	G	264	ASN	3.1
1	F	256	GLU	3.1
1	F	519	ILE	3.1
1	C	552	LYS	3.1
1	G	354	ALA	3.1
1	G	519	ILE	3.0
1	G	435	SER	3.0
1	D	259	ASN	3.0
1	D	553	GLY	3.0
1	A	551	ILE	3.0
1	G	270	THR	3.0
1	A	712	ILE	3.0
1	G	550	ILE	3.0
1	G	553	GLY	3.0
1	G	520	VAL	2.9
1	C	576	GLY	2.9
1	G	258	ASN	2.9
1	D	270	THR	2.9
1	G	518	ILE	2.9
1	G	576	GLY	2.9
1	D	551	ILE	2.9
1	C	710	SER	2.9
1	B	436	LYS	2.9
1	D	575	VAL	2.9
1	B	493	ALA	2.9
1	F	521	ASN	2.9
1	F	552	LYS	2.9
1	G	717	GLY	2.9
1	B	434	ILE	2.8
1	B	551	ILE	2.8
1	F	553	GLY	2.8
1	B	258	ASN	2.8
1	A	256	GLU	2.8
1	F	401	THR	2.8
1	G	453	ARG	2.8
1	A	255	GLY	2.8
1	B	576	GLY	2.8
1	G	399	PHE	2.8
1	B	552	LYS	2.8
1	A	575	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	435	SER	2.8
1	G	575	VAL	2.8
1	G	746	THR	2.8
1	C	717	GLY	2.8
1	B	257	LEU	2.8
1	F	270	THR	2.8
1	F	259	ASN	2.8
1	D	521	ASN	2.7
1	A	553	GLY	2.7
1	F	272	GLY	2.7
1	G	684	ILE	2.7
1	A	275	SER	2.7
1	C	785	SER	2.7
1	B	521	ASN	2.7
1	B	402	GLY	2.7
1	A	265	PHE	2.7
1	C	522	ASN	2.7
1	G	434	ILE	2.7
1	G	714	SER	2.7
1	G	785	SER	2.7
1	B	353	PRO	2.7
1	D	268	ALA	2.7
1	C	456	LYS	2.7
1	D	456	LYS	2.7
1	D	552	LYS	2.7
1	A	270	THR	2.7
1	D	271	TYR	2.7
1	C	521	ASN	2.7
1	F	491	VAL	2.7
1	F	712	ILE	2.7
1	F	265	PHE	2.6
1	B	298	THR	2.6
1	G	456	LYS	2.6
1	C	258	ASN	2.6
1	C	495	ASN	2.6
1	G	253	LEU	2.6
1	D	436	LYS	2.6
1	G	521	ASN	2.6
1	B	454	VAL	2.6
1	G	271	TYR	2.6
1	G	289	ALA	2.6
1	B	716	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	401	THR	2.6
1	B	553	GLY	2.6
1	D	253	LEU	2.6
1	B	456	LYS	2.5
1	F	576	GLY	2.5
1	G	400	ILE	2.5
1	B	714	SER	2.5
1	C	402	GLY	2.5
1	F	264	ASN	2.5
1	D	399	PHE	2.5
1	G	402	GLY	2.5
1	D	384	VAL	2.5
1	B	383	THR	2.5
1	F	434	ILE	2.5
1	A	714	SER	2.5
1	F	716	SER	2.5
1	G	750	GLY	2.5
1	D	274	ASP	2.5
1	A	384	VAL	2.5
1	F	575	VAL	2.5
1	B	435	SER	2.5
1	G	712	ILE	2.5
1	B	537	PHE	2.5
1	C	353	PRO	2.5
1	A	271	TYR	2.5
1	B	550	ILE	2.5
1	C	383	THR	2.4
1	G	783	MET	2.4
1	A	457	ASN	2.4
1	G	551	ILE	2.4
1	A	293	ALA	2.4
1	D	293	ALA	2.4
1	D	296	ASP	2.4
1	A	289	ALA	2.4
1	C	677	LEU	2.4
1	G	787	SER	2.4
1	D	576	GLY	2.4
1	G	268	ALA	2.4
1	G	353	PRO	2.4
1	A	710	SER	2.4
1	B	378	LEU	2.4
1	A	521	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	263	ILE	2.4
1	A	261	GLY	2.4
1	B	495	ASN	2.4
1	B	381	SER	2.4
1	B	474	TRP	2.4
1	C	711	SER	2.3
1	F	710	SER	2.3
1	C	264	ASN	2.3
1	D	265	PHE	2.3
1	B	574	VAL	2.3
1	F	303	VAL	2.3
1	F	274	ASP	2.3
1	F	402	GLY	2.3
1	A	786	THR	2.3
1	C	716	SER	2.3
1	D	356	LYS	2.3
1	C	684	ILE	2.3
1	C	686	LEU	2.3
1	D	292	ASN	2.3
1	D	261	GLY	2.3
1	G	474	TRP	2.3
1	D	353	PRO	2.3
1	G	437	CYS	2.3
1	B	418	ALA	2.2
1	G	369	PHE	2.2
1	B	709	VAL	2.2
1	F	400	ILE	2.2
1	G	554	ASN	2.2
1	A	785	SER	2.2
1	G	682	GLY	2.2
1	C	554	ASN	2.2
1	C	261	GLY	2.2
1	D	574	VAL	2.2
1	A	259	ASN	2.2
1	B	639	VAL	2.2
1	A	273	ASN	2.2
1	B	259	ASN	2.2
1	B	522	ASN	2.2
1	F	554	ASN	2.2
1	D	383	THR	2.2
1	C	532	ILE	2.1
1	F	532	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	574	VAL	2.1
1	G	291	PHE	2.1
1	G	552	LYS	2.1
1	D	400	ILE	2.1
1	C	780	SER	2.1
1	G	781	SER	2.1
1	D	295	THR	2.1
1	D	269	ASP	2.1
1	D	257	LEU	2.1
1	C	787	SER	2.1
1	B	777	TYR	2.1
1	B	614	THR	2.1
1	D	298	THR	2.1
1	F	456	LYS	2.1
1	G	522	ASN	2.1
1	A	400	ILE	2.1
1	F	688	SER	2.1
1	A	299	THR	2.1
1	F	495	ASN	2.1
1	D	495	ASN	2.1
1	B	711	SER	2.0
1	C	398	CYS	2.1
1	G	711	SER	2.0
1	A	532	ILE	2.0
1	C	505	ILE	2.0
1	F	718	ASN	2.0
1	G	744	ASP	2.0
1	B	303	VAL	2.0
1	A	715	PRO	2.0
1	A	402	GLY	2.0
1	B	351	ASP	2.0
1	F	522	ASN	2.0
1	G	681	SER	2.0
1	A	783	MET	2.0
1	A	260	GLU	2.0
1	D	437	CYS	2.0
1	F	453	ARG	2.0
1	A	552	LYS	2.0

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

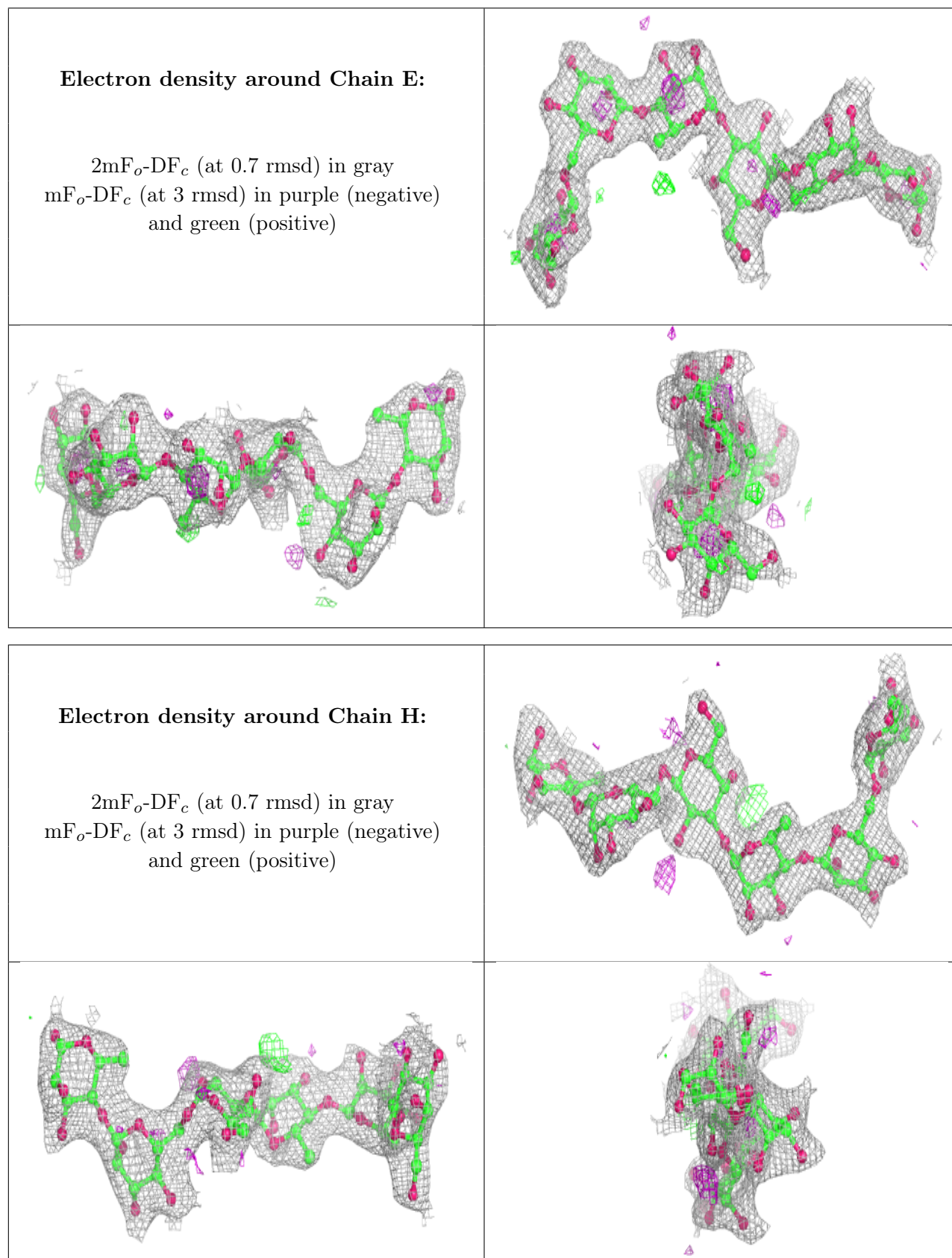
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

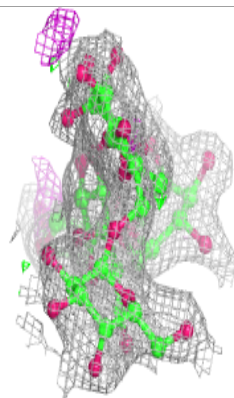
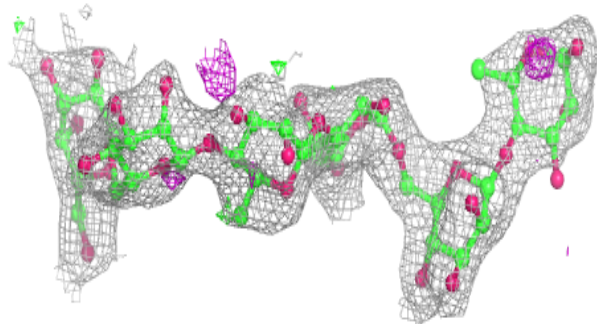
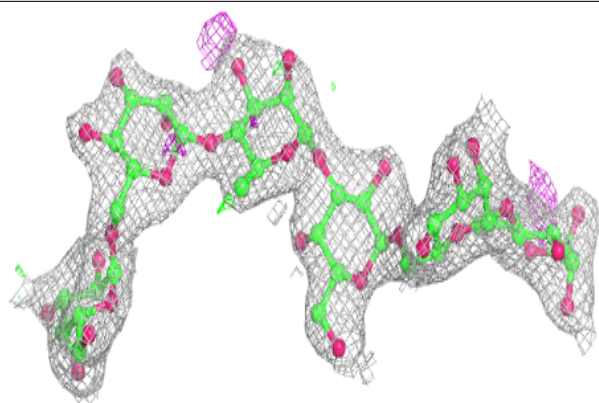
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLA	E	6	11/12	0.82	0.15	55,72,80,82	0
2	RAM	E	4	10/11	0.83	0.15	68,76,81,81	0
2	BMA	E	5	11/12	0.86	0.14	55,69,74,75	0
2	BMA	K	5	11/12	0.86	0.18	72,76,81,84	0
2	GLA	E	3	11/12	0.88	0.13	61,70,78,83	0
2	RAM	K	4	10/11	0.89	0.12	71,79,85,88	0
2	GLA	K	6	11/12	0.89	0.16	58,75,76,77	0
2	RAM	K	1	11/11	0.91	0.18	50,59,69,74	0
2	RAM	L	4	10/11	0.91	0.15	44,58,61,66	0
2	BMA	E	2	11/12	0.92	0.10	56,62,70,73	0
2	BMA	K	2	11/12	0.92	0.09	51,58,63,65	0
2	GLA	M	6	11/12	0.92	0.12	46,60,63,67	0
3	RAM	I	2	10/11	0.92	0.08	47,58,66,78	0
2	GLA	H	6	11/12	0.93	0.16	54,59,67,73	0
2	BMA	H	2	11/12	0.93	0.09	50,56,60,63	0
2	BMA	L	2	11/12	0.93	0.11	51,58,62,68	0
2	GLA	H	3	11/12	0.94	0.10	52,57,62,64	0
2	BMA	M	2	11/12	0.94	0.11	38,43,50,54	0
2	RAM	M	4	10/11	0.94	0.08	53,56,60,65	0
2	RAM	E	1	11/11	0.94	0.13	48,55,60,65	0
2	GLA	L	3	11/12	0.94	0.11	52,56,66,74	0
3	BMA	I	3	11/12	0.94	0.09	52,54,60,62	0
2	RAM	H	4	10/11	0.95	0.12	49,56,62,63	0
2	RAM	H	1	11/11	0.95	0.09	47,55,58,62	0
2	BMA	M	5	11/12	0.95	0.13	54,64,70,77	0
2	GLA	K	3	11/12	0.95	0.11	57,64,69,69	0
2	BMA	L	5	11/12	0.95	0.20	55,59,67,72	0
2	GLA	L	6	11/12	0.95	0.14	51,56,60,62	0
3	GLA	I	4	11/12	0.95	0.10	51,56,64,65	0
3	GLA	I	1	11/12	0.96	0.09	40,49,53,53	0
2	BMA	H	5	11/12	0.96	0.14	61,64,69,71	0
4	RAM	J	1	11/11	0.96	0.08	34,37,40,41	0
2	RAM	L	1	11/11	0.97	0.12	44,47,56,58	0
2	GLA	M	3	11/12	0.97	0.08	47,49,55,55	0
4	BMA	J	2	11/12	0.97	0.07	33,35,37,38	0
2	RAM	M	1	11/11	0.98	0.10	39,43,50,50	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.

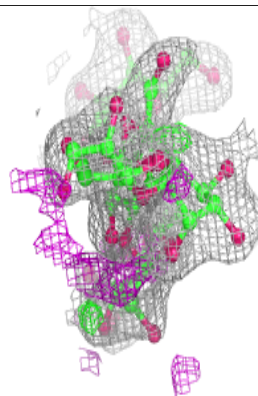
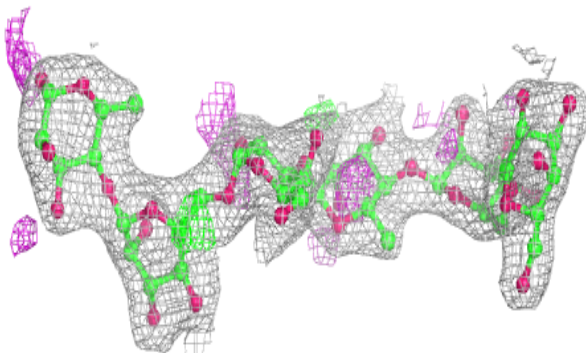
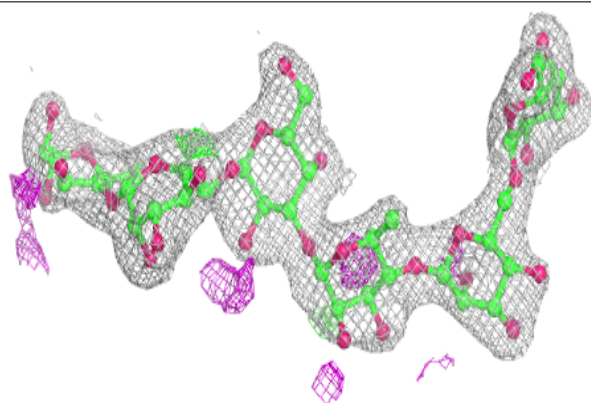


Electron density around Chain K:

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

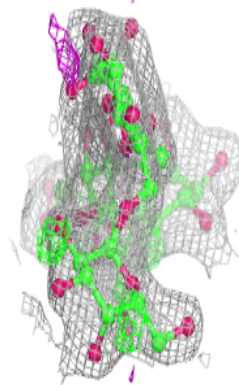
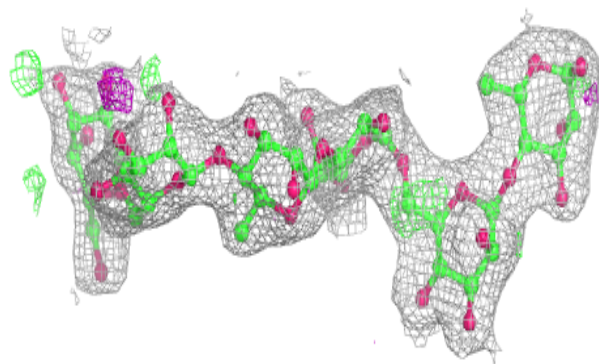
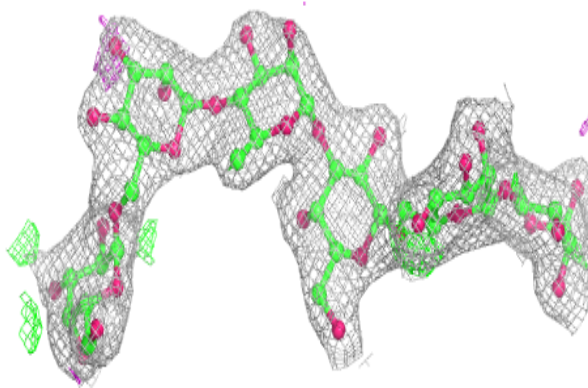
**Electron density around Chain L:**

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

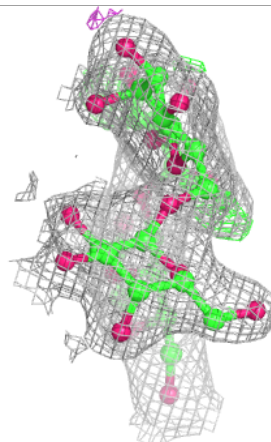
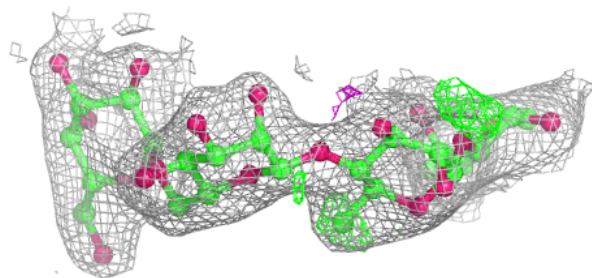
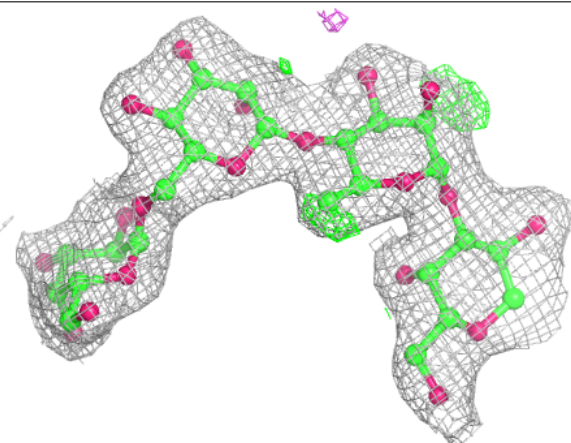


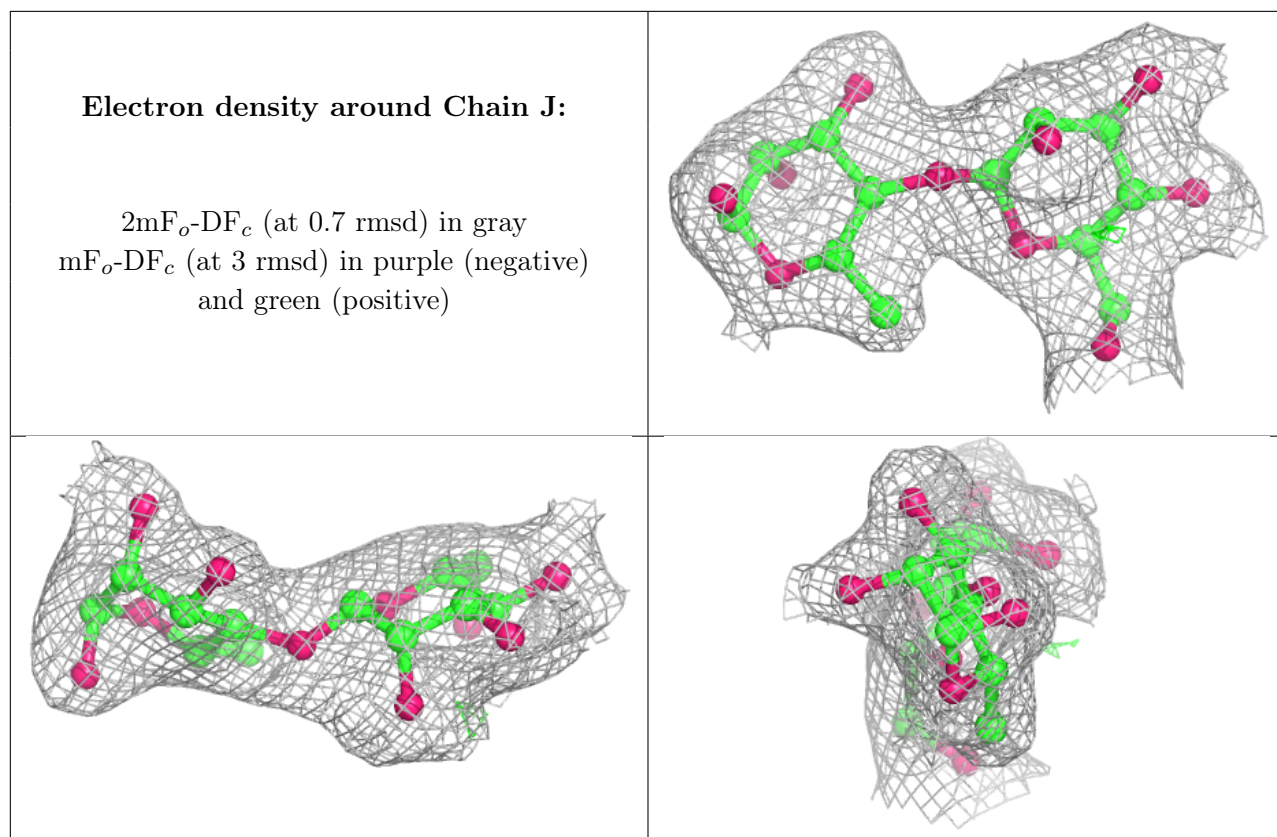
Electron density around Chain M:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	801	4/4	0.94	0.13	51,62,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.