



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 01:18 pm BST

PDB ID : 9S88 / pdb_00009s88
Title : Amuc0121_S1_15 in complex with O6 sulfated Lewis A antigen (6'S-LeA)
Authors : Dey, D.; Cartmell, A.
Deposited on : 2025-08-05
Resolution : 1.92 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

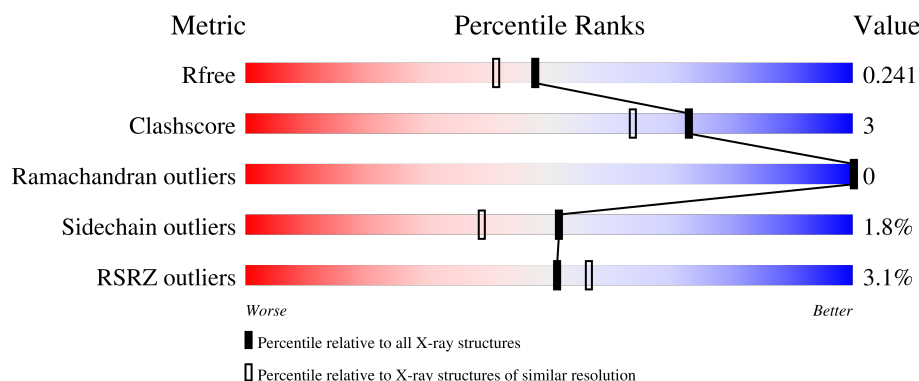
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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.



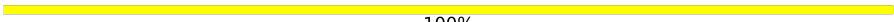



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	496	<div> <div>%</div> <div>93% 5% .</div> </div>
1	B	496	<div> <div>10%</div> <div>92% 6% .</div> </div>
1	C	496	<div> <div>3%</div> <div>91% 7% ..</div> </div>
1	D	496	<div> <div>%</div> <div>93% 7%</div> </div>
1	E	496	<div> <div>%</div> <div>92% 7% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	3	 100%
2	J	3	 100%
2	K	3	 67%  33%
2	L	3	 33%  67%
2	M	3	 33%  67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	E	602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19672 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 Sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	8	0
			3841	2428	684	712	17			
1	B	487	Total	C	N	O	S	0	0	0
			3758	2379	662	701	16			
1	C	488	Total	C	N	O	S	0	3	0
			3797	2400	672	709	16			
1	D	495	Total	C	N	O	S	0	4	0
			3863	2437	685	725	16			
1	E	489	Total	C	N	O	S	0	6	0
			3837	2424	685	712	16			

There are 20 discrepancies between the modelled and reference sequences:

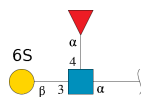
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	SER	CYS	conflict	UNP B2ULS2
A	237	LYS	ARG	conflict	UNP B2ULS2
A	249	VAL	ILE	conflict	UNP B2ULS2
A	512	SER	PRO	conflict	UNP B2ULS2
B	78	SER	CYS	conflict	UNP B2ULS2
B	237	LYS	ARG	conflict	UNP B2ULS2
B	249	VAL	ILE	conflict	UNP B2ULS2
B	512	SER	PRO	conflict	UNP B2ULS2
C	78	SER	CYS	conflict	UNP B2ULS2
C	237	LYS	ARG	conflict	UNP B2ULS2
C	249	VAL	ILE	conflict	UNP B2ULS2
C	512	SER	PRO	conflict	UNP B2ULS2
D	78	SER	CYS	conflict	UNP B2ULS2
D	237	LYS	ARG	conflict	UNP B2ULS2
D	249	VAL	ILE	conflict	UNP B2ULS2
D	512	SER	PRO	conflict	UNP B2ULS2
E	78	SER	CYS	conflict	UNP B2ULS2
E	237	LYS	ARG	conflict	UNP B2ULS2
E	249	VAL	ILE	conflict	UNP B2ULS2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	512	SER	PRO	conflict	UNP B2ULS2

- Molecule 2 is an oligosaccharide called 6-O-sulfo-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	S	0	0	0
			40	20	1	18	1			
2	J	3	Total	C	N	O	S	0	0	0
			40	20	1	18	1			
2	K	3	Total	C	N	O	S	0	0	0
			40	20	1	18	1			
2	L	3	Total	C	N	O	S	0	0	0
			40	20	1	18	1			
2	M	3	Total	C	N	O	S	0	0	0
			40	20	1	18	1			

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		
3	E	1	Total	I	0	0
			1	1		

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		
4	C	2	Total	Br	0	0
			2	2		
4	D	1	Total	Br	0	0
			1	1		
4	E	2	Total	Br	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0

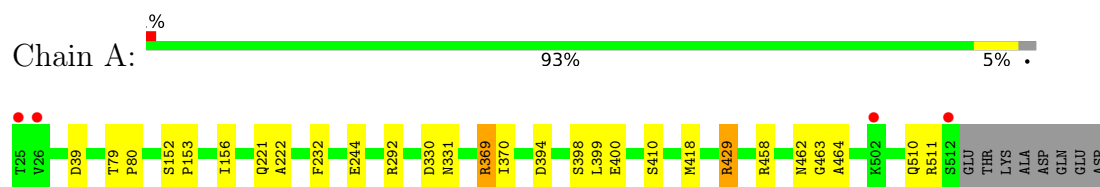
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	106	Total O 106 106	0	0
6	B	15	Total O 15 15	0	0
6	C	52	Total O 52 52	0	0
6	D	76	Total O 76 76	0	0
6	E	114	Total O 114 114	0	0

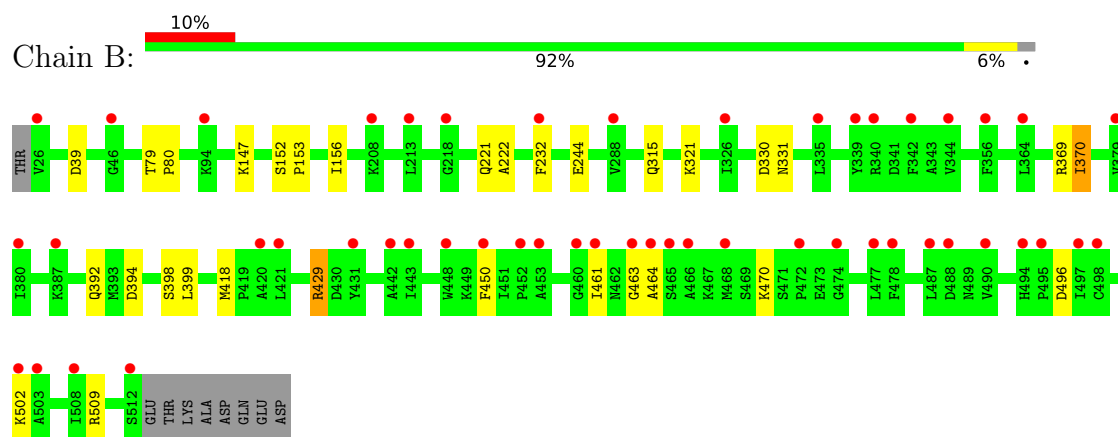
3 Residue-property plots [i](#)

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.

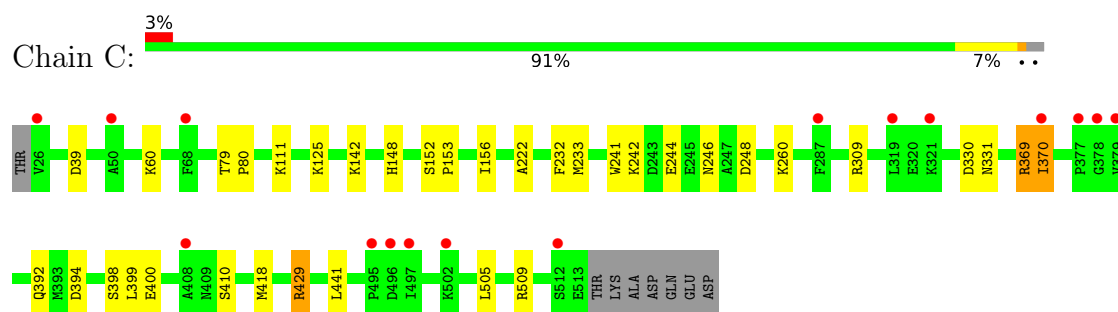
• Molecule 1: Sulfatase



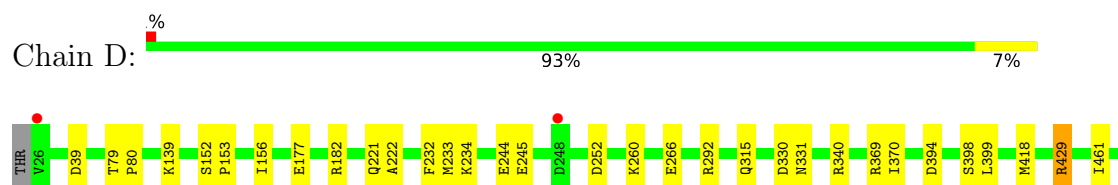
• Molecule 1: Sulfatase



• Molecule 1: Sulfatase

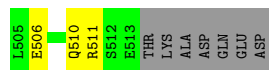


• Molecule 1: Sulfatase





- Molecule 1: Sulfatase



- Molecule 2: 6-O-sulfo-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 2: 6-O-sulfo-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 2: 6-O-sulfo-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 2: 6-O-sulfo-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 2: 6-O-sulfo-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.04Å 64.15Å 151.36Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	57.86 – 1.92 57.86 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.4 (57.86-1.92) 99.8 (57.86-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.208 , 0.236 0.215 , 0.241	Depositor DCC
R_{free} test set	9703 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19672	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: BR, FUC, G6S, CA, IOD, NDG

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	0.61	0/3929	0.97	4/5303 (0.1%)
1	B	0.56	0/3846	0.98	9/5194 (0.2%)
1	C	0.60	0/3885	0.97	4/5245 (0.1%)
1	D	0.59	0/3951	0.98	7/5333 (0.1%)
1	E	0.62	0/3925	0.98	3/5297 (0.1%)
All	All	0.60	0/19536	0.98	27/26372 (0.1%)

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	4
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	2
All	All	0	15

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LYS	CB-CG-CD	7.18	127.80	111.30
1	D	473	GLU	CG-CD-OE2	-6.74	102.89	118.40
1	B	244	GLU	CB-CG-CD	6.63	123.87	112.60
1	B	244	GLU	CG-CD-OE1	6.47	133.29	118.40
1	D	473	GLU	CG-CD-OE1	6.31	132.92	118.40
1	E	39	ASP	CA-CB-CG	6.25	118.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	233	MET	CG-SD-CE	5.74	113.52	100.90
1	E	330	ASP	CA-CB-CG	5.72	118.32	112.60
1	D	233	MET	CG-SD-CE	-5.68	88.41	100.90
1	D	39	ASP	CA-CB-CG	5.49	118.08	112.60
1	C	39	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	330	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	330	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	221	GLN	CB-CA-C	5.45	121.26	110.42
1	A	369	ARG	CG-CD-NE	-5.39	100.15	112.00
1	D	330	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	39	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	221	GLN	CB-CA-C	5.33	121.03	110.42
1	B	321	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	330	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	221	GLN	CB-CA-C	5.21	120.79	110.42
1	C	369	ARG	CG-CD-NE	-5.20	100.56	112.00
1	B	244	GLU	CG-CD-OE2	-5.20	106.44	118.40
1	B	496	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	461	ILE	N-CA-C	-5.10	108.31	113.20
1	E	221	GLN	CB-CA-C	5.07	120.51	110.42

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ARG	Sidechain
1	A	369	ARG	Sidechain
1	A	429[A]	ARG	Sidechain
1	A	511	ARG	Sidechain
1	B	369	ARG	Sidechain
1	B	429	ARG	Sidechain
1	B	509	ARG	Sidechain
1	C	369	ARG	Sidechain
1	C	429	ARG	Sidechain
1	D	292	ARG	Sidechain
1	D	369	ARG	Sidechain
1	D	429[A]	ARG	Sidechain
1	D	509	ARG	Sidechain
1	E	369	ARG	Sidechain
1	E	511	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3841	0	3843	20	0
1	B	3758	0	3751	23	0
1	C	3797	0	3784	28	0
1	D	3863	0	3843	19	2
1	E	3837	0	3834	32	1
2	I	40	0	29	0	0
2	J	40	0	29	0	0
2	K	40	0	29	1	0
2	L	40	0	29	1	0
2	M	40	0	29	0	0
3	A	1	0	0	0	0
3	E	1	0	0	1	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	3	1
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	106	0	0	1	0
6	B	15	0	0	0	0
6	C	52	0	0	1	0
6	D	76	0	0	1	0
6	E	114	0	0	2	0
All	All	19672	0	19200	122	2

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 3.

All (122) 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:E:494:HIS:NE2	4:E:602:BR:BR	2.45	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ASP:OD1	1:C:309[B]:ARG:NH2	1.92	1.01
1:E:494:HIS:CE1	4:E:602:BR:BR	2.72	0.97
1:D:398:SER:C	1:D:418:MET:HE2	1.97	0.88
1:B:398:SER:C	1:B:418:MET:HE2	1.99	0.87
1:E:398:SER:C	1:E:418:MET:HE2	2.00	0.87
1:C:398:SER:C	1:C:418:MET:HE2	1.99	0.87
1:A:398:SER:C	1:A:418[A]:MET:HE2	2.00	0.86
1:D:398:SER:C	1:D:418:MET:CE	2.53	0.82
1:E:398:SER:C	1:E:418:MET:CE	2.53	0.82
1:D:177:GLU:OE2	1:D:182[B]:ARG:HD2	1.79	0.82
1:C:370:ILE:CD1	1:C:392:GLN:NE2	2.43	0.81
1:B:370:ILE:CD1	1:B:392:GLN:NE2	2.43	0.81
1:C:398:SER:C	1:C:418:MET:CE	2.53	0.81
1:A:398:SER:C	1:A:418[A]:MET:CE	2.54	0.80
1:B:398:SER:C	1:B:418:MET:CE	2.54	0.79
1:E:357[A]:ARG:NH2	6:E:701:HOH:O	2.22	0.72
1:C:370:ILE:HD12	1:C:392:GLN:NE2	2.15	0.61
6:C:750:HOH:O	2:K:3:FUC:O4	2.14	0.61
1:B:370:ILE:HD12	1:B:392:GLN:NE2	2.16	0.60
1:E:398:SER:HB3	1:E:418:MET:HE2	1.83	0.60
1:B:398:SER:O	1:B:418:MET:CE	2.50	0.60
1:D:398:SER:O	1:D:418:MET:CE	2.50	0.60
1:C:111:LYS:HG2	1:D:266:GLU:HG2	1.84	0.60
1:A:398:SER:O	1:A:418[A]:MET:CE	2.50	0.60
1:E:504:LYS:HE3	3:E:601:IOD:I	2.72	0.60
1:C:398:SER:O	1:C:418:MET:CE	2.49	0.59
1:E:398:SER:O	1:E:418:MET:CE	2.51	0.59
1:E:156[A]:ILE:HD11	1:E:158:PHE:CD2	2.38	0.58
1:B:398:SER:HB3	1:B:418:MET:HE2	1.86	0.58
1:C:398:SER:HB3	1:C:418:MET:HE2	1.86	0.57
1:D:394:ASP:OD2	1:D:429[A]:ARG:HD2	2.05	0.57
1:A:398:SER:HB3	1:A:418[A]:MET:HE2	1.86	0.57
1:D:398:SER:HB3	1:D:418:MET:HE2	1.87	0.57
1:E:506:GLU:O	1:E:510:GLN:HG2	2.05	0.57
1:B:394:ASP:OD2	1:B:429:ARG:HD2	2.05	0.57
1:C:394:ASP:OD2	1:C:429:ARG:HD2	2.05	0.56
1:E:399:LEU:HA	1:E:418:MET:HE3	1.89	0.55
1:E:177:GLU:OE2	1:E:182[B]:ARG:NH2	2.40	0.53
1:E:398:SER:O	1:E:418:MET:HE3	2.08	0.53
1:A:394:ASP:OD2	1:A:429[A]:ARG:HD2	2.07	0.53
1:C:398:SER:O	1:C:418:MET:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:SER:O	1:B:418:MET:HE3	2.08	0.52
1:A:399:LEU:HA	1:A:418[A]:MET:HE3	1.91	0.52
1:C:399:LEU:HA	1:C:418:MET:HE3	1.92	0.52
1:E:494:HIS:HE1	4:E:602:BR:BR	2.44	0.52
1:D:398:SER:O	1:D:418:MET:HE3	2.10	0.52
1:B:370:ILE:HD11	1:B:392:GLN:NE2	2.24	0.51
1:D:398:SER:O	1:D:418:MET:HE2	2.10	0.51
1:A:398:SER:O	1:A:418[A]:MET:HE3	2.10	0.51
1:E:463:GLY:O	1:E:464:ALA:HB3	2.10	0.51
1:B:463:GLY:O	1:B:464:ALA:HB3	2.10	0.51
1:B:399:LEU:HA	1:B:418:MET:HE3	1.91	0.51
1:C:370:ILE:HD11	1:C:392:GLN:NE2	2.24	0.51
2:L:1:NDG:HA	2:L:3:FUC:H5	1.76	0.50
1:D:399:LEU:HA	1:D:418:MET:HE3	1.92	0.50
1:A:463:GLY:O	1:A:464:ALA:HB3	2.11	0.50
1:A:458[B]:ARG:NH1	1:A:462:ASN:O	2.32	0.50
1:E:399:LEU:N	1:E:418:MET:CE	2.74	0.50
1:C:398:SER:O	1:C:418:MET:HE2	2.11	0.49
1:B:450:PHE:CE2	1:B:502:LYS:HG3	2.48	0.49
1:D:399:LEU:N	1:D:418:MET:CE	2.76	0.49
1:E:153:PRO:O	1:E:156[A]:ILE:HD12	2.13	0.49
1:C:370:ILE:HD12	1:C:392:GLN:HE21	1.76	0.48
1:E:398:SER:O	1:E:418:MET:HE2	2.13	0.48
1:D:399:LEU:HA	1:D:418:MET:CE	2.44	0.48
1:E:153:PRO:O	1:E:156[A]:ILE:CD1	2.62	0.48
1:B:222:ALA:HB2	1:B:232:PHE:HA	1.96	0.47
1:B:399:LEU:N	1:B:418:MET:CE	2.77	0.47
1:E:399:LEU:HA	1:E:418:MET:CE	2.43	0.47
1:A:399:LEU:N	1:A:418[A]:MET:CE	2.77	0.47
1:C:399:LEU:N	1:C:418:MET:CE	2.77	0.47
1:C:399:LEU:HA	1:C:418:MET:CE	2.44	0.47
1:C:441:LEU:HD12	1:C:509:ARG:HD2	1.95	0.47
1:B:398:SER:O	1:B:418:MET:HE2	2.12	0.47
1:C:399:LEU:HD23	1:C:418:MET:HE1	1.96	0.47
1:E:398:SER:CB	1:E:418:MET:HE2	2.43	0.47
1:A:399:LEU:HA	1:A:418[A]:MET:CE	2.45	0.47
1:A:398:SER:O	1:A:418[A]:MET:HE2	2.10	0.47
1:A:399:LEU:HD23	1:A:418[A]:MET:HE1	1.97	0.47
1:E:236:GLY:HA2	6:E:798:HOH:O	2.14	0.47
1:B:398:SER:CB	1:B:418:MET:HE2	2.45	0.47
1:B:370:ILE:HD12	1:B:392:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429[A]:ARG:NH2	6:D:703:HOH:O	2.47	0.46
1:D:398:SER:CB	1:D:418:MET:HE2	2.46	0.46
1:B:399:LEU:HD23	1:B:418:MET:HE1	1.98	0.45
1:C:79:THR:N	1:C:80:PRO:HD2	2.32	0.45
1:C:398:SER:CB	1:C:418:MET:HE2	2.46	0.45
1:A:79:THR:N	1:A:80:PRO:HD2	2.31	0.45
1:E:156[A]:ILE:HD11	1:E:158:PHE:CE2	2.52	0.45
1:E:399:LEU:HD23	1:E:418:MET:HE1	1.98	0.45
1:B:370:ILE:CD1	1:B:392:GLN:HE21	2.28	0.45
1:B:399:LEU:HA	1:B:418:MET:CE	2.46	0.45
1:D:79:THR:N	1:D:80:PRO:HD2	2.31	0.45
1:C:400:GLU:OE1	1:C:410:SER:OG	2.32	0.45
1:E:156[A]:ILE:CD1	1:E:158:PHE:CD2	3.01	0.44
1:C:152:SER:CB	1:C:153:PRO:CD	2.96	0.44
1:D:222:ALA:HB2	1:D:232:PHE:HA	1.99	0.44
1:A:398:SER:CB	1:A:418[A]:MET:HE2	2.47	0.43
1:E:79:THR:N	1:E:80:PRO:HD2	2.33	0.43
1:A:429[A]:ARG:NH2	6:A:702:HOH:O	2.51	0.43
1:C:222:ALA:HB2	1:C:232:PHE:HA	2.00	0.43
1:B:79:THR:N	1:B:80:PRO:HD2	2.33	0.43
1:D:152:SER:CB	1:D:153:PRO:CD	2.97	0.43
1:B:450:PHE:CE2	1:B:502:LYS:CG	3.02	0.43
1:C:148:HIS:HB3	1:E:51:LYS:HB2	2.01	0.43
1:A:400:GLU:OE1	1:A:410:SER:OG	2.32	0.42
1:E:156[A]:ILE:CD1	1:E:158:PHE:HD2	2.32	0.42
1:A:152:SER:CB	1:A:153:PRO:CD	2.97	0.42
1:C:152:SER:HB2	1:C:153:PRO:CD	2.49	0.42
1:A:222:ALA:HB2	1:A:232:PHE:HA	2.01	0.42
1:E:276:ASP:HA	1:E:277:ILE:HA	1.90	0.41
1:D:399:LEU:HD23	1:D:418:MET:HE1	2.01	0.41
1:B:152:SER:CB	1:B:153:PRO:CD	2.98	0.41
1:E:222:ALA:HB2	1:E:232:PHE:HA	2.00	0.41
1:C:441:LEU:HD12	1:C:509:ARG:CD	2.51	0.41
1:E:153:PRO:HA	1:E:156[A]:ILE:HD12	2.02	0.41
1:A:152:SER:HB2	1:A:153:PRO:CD	2.51	0.41
1:D:152:SER:HB2	1:D:153:PRO:CD	2.51	0.40
1:C:505:LEU:O	1:C:509:ARG:HG3	2.22	0.40
1:E:72:TYR:OH	1:E:365:GLU:OE2	2.37	0.40
1:C:241:TRP:CG	1:C:246:ASN:HD21	2.39	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLU:OE2	1:E:482:LYS:NZ[1_545]	2.18	0.02
1:D:252:ASP:OD2	4:E:602:BR:BR[1_545]	2.19	0.01

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	494/496 (100%)	476 (96%)	18 (4%)	0	100	100
1	B	485/496 (98%)	467 (96%)	18 (4%)	0	100	100
1	C	489/496 (99%)	472 (96%)	17 (4%)	0	100	100
1	D	497/496 (100%)	480 (97%)	17 (3%)	0	100	100
1	E	493/496 (99%)	473 (96%)	20 (4%)	0	100	100
All	All	2458/2480 (99%)	2368 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	408/407 (100%)	403 (99%)	5 (1%)	63	57
1	B	399/407 (98%)	393 (98%)	6 (2%)	57	47
1	C	403/407 (99%)	394 (98%)	9 (2%)	45	32
1	D	410/407 (101%)	399 (97%)	11 (3%)	39	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	407/407 (100%)	400 (98%)	7 (2%)	53	41
All	All	2027/2035 (100%)	1989 (98%)	38 (2%)	51	37

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ILE
1	A	244	GLU
1	A	331	ASN
1	A	370	ILE
1	A	510	GLN
1	B	156	ILE
1	B	315	GLN
1	B	331	ASN
1	B	370	ILE
1	B	461	ILE
1	B	470	LYS
1	C	60	LYS
1	C	125	LYS
1	C	142	LYS
1	C	156	ILE
1	C	242	LYS
1	C	244	GLU
1	C	260	LYS
1	C	331	ASN
1	C	370	ILE
1	D	139	LYS
1	D	156	ILE
1	D	234	LYS
1	D	244	GLU
1	D	260	LYS
1	D	315	GLN
1	D	331	ASN
1	D	340	ARG
1	D	370	ILE
1	D	517[A]	ASP
1	D	517[B]	ASP
1	E	51	LYS
1	E	125	LYS
1	E	156[A]	ILE
1	E	156[B]	ILE
1	E	244	GLU

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Mol	Chain	Res	Type
1	E	331	ASN
1	E	370	ILE

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

Mol	Chain	Res	Type
1	A	347	ASN
1	A	510	GLN
1	B	122	HIS
1	B	347	ASN
1	B	392	GLN
1	C	122	HIS
1	C	347	ASN
1	D	122	HIS
1	D	347	ASN
1	E	122	HIS
1	E	347	ASN
1	E	493	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

15 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	NDG	I	1	2	15,15,15	0.33	0	21,21,21	1.18	2 (9%)
2	G6S	I	2	5,2	15,15,16	0.66	0	20,22,24	1.38	3 (15%)
2	FUC	I	3	2	10,10,11	0.37	0	14,14,16	0.96	1 (7%)
2	NDG	J	1	2	15,15,15	0.53	0	21,21,21	1.37	3 (14%)
2	G6S	J	2	5,2	15,15,16	0.54	0	20,22,24	1.43	3 (15%)
2	FUC	J	3	2	10,10,11	0.44	0	14,14,16	2.00	2 (14%)
2	NDG	K	1	2	15,15,15	0.70	1 (6%)	21,21,21	2.95	9 (42%)
2	G6S	K	2	5,2	15,15,16	0.61	0	20,22,24	1.30	3 (15%)
2	FUC	K	3	2	10,10,11	0.41	0	14,14,16	1.60	3 (21%)
2	NDG	L	1	2	15,15,15	0.78	0	21,21,21	1.79	4 (19%)
2	G6S	L	2	5,2	15,15,16	0.63	0	20,22,24	1.26	2 (10%)
2	FUC	L	3	2	10,10,11	0.41	0	14,14,16	1.23	3 (21%)
2	NDG	M	1	2	15,15,15	0.42	0	21,21,21	1.51	3 (14%)
2	G6S	M	2	5,2	15,15,16	0.56	0	20,22,24	1.02	2 (10%)
2	FUC	M	3	2	10,10,11	0.41	0	14,14,16	0.84	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	NDG	I	1	2	-	1/6/26/26	0/1/1/1
2	G6S	I	2	5,2	-	0/6/23/26	0/1/1/1
2	FUC	I	3	2	-	-	0/1/1/1
2	NDG	J	1	2	-	1/6/26/26	0/1/1/1
2	G6S	J	2	5,2	-	0/6/23/26	0/1/1/1
2	FUC	J	3	2	-	-	0/1/1/1
2	NDG	K	1	2	-	1/6/26/26	0/1/1/1
2	G6S	K	2	5,2	-	0/6/23/26	0/1/1/1
2	FUC	K	3	2	-	-	0/1/1/1
2	NDG	L	1	2	-	2/6/26/26	0/1/1/1
2	G6S	L	2	5,2	-	0/6/23/26	0/1/1/1
2	FUC	L	3	2	-	-	0/1/1/1
2	NDG	M	1	2	-	2/6/26/26	0/1/1/1
2	G6S	M	2	5,2	-	0/6/23/26	0/1/1/1
2	FUC	M	3	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NDG	C1-C2	2.15	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NDG	O5-C1-C2	7.60	117.15	109.52
2	J	3	FUC	C1-C2-C3	6.25	117.35	109.67
2	K	1	NDG	C1-C2-N2	5.49	117.09	110.73
2	M	1	NDG	C3-C4-C5	4.76	118.74	110.24
2	K	1	NDG	C1-O5-C5	4.60	122.34	113.66
2	L	1	NDG	C3-C2-N2	4.52	119.15	110.62
2	L	1	NDG	C4-C3-C2	4.34	116.70	110.34
2	J	2	G6S	O6-S-O7	-4.32	93.79	106.88
2	K	3	FUC	C1-C2-C3	4.06	114.65	109.67
2	L	2	G6S	C1-O5-C5	-3.65	107.24	112.19
2	K	1	NDG	C4-C3-C2	3.46	115.41	110.34
2	J	1	NDG	C3-C4-C5	3.43	116.35	110.24
2	K	1	NDG	C3-C4-C5	3.27	116.06	110.24
2	K	1	NDG	O3-C3-C2	-3.25	103.09	109.66
2	I	1	NDG	C3-C4-C5	3.01	115.61	110.24
2	K	1	NDG	O1-C1-O5	-2.95	101.52	110.38
2	K	2	G6S	O9-S-O7	2.83	118.31	108.49
2	J	2	G6S	O6-S-O8	2.79	115.32	106.88
2	K	1	NDG	C1-C2-C3	2.76	114.31	110.54
2	I	2	G6S	O2-C2-C1	2.73	114.74	109.15
2	L	1	NDG	O3-C3-C4	-2.65	104.21	110.35
2	I	2	G6S	O2-C2-C3	-2.63	104.86	110.14
2	K	3	FUC	O3-C3-C2	-2.63	104.96	109.99
2	K	1	NDG	O1-C1-C2	2.61	114.63	109.22
2	I	1	NDG	C3-C2-N2	2.50	115.34	110.62
2	L	2	G6S	O9-S-O8	2.43	116.95	108.49
2	J	1	NDG	C3-C2-N2	2.40	115.15	110.62
2	M	2	G6S	O6-S-O7	-2.39	99.64	106.88
2	J	3	FUC	C3-C4-C5	-2.38	106.07	109.77
2	L	3	FUC	C3-C4-C5	-2.37	106.08	109.77
2	I	3	FUC	O3-C3-C2	-2.31	105.56	109.99
2	L	3	FUC	O3-C3-C2	2.31	114.42	109.99
2	I	2	G6S	O4-C4-C5	2.24	114.85	109.30
2	M	1	NDG	C1-O5-C5	2.24	117.88	113.66
2	L	1	NDG	C1-C2-N2	2.23	113.31	110.73
2	K	2	G6S	O2-C2-C3	2.17	114.49	110.14
2	L	3	FUC	C2-C3-C4	-2.15	107.17	110.89
2	J	2	G6S	O8-S-O7	2.14	120.81	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	NDG	O4-C4-C5	-2.13	104.01	109.30
2	J	1	NDG	C1-O5-C5	2.11	117.64	113.66
2	K	2	G6S	O4-C4-C3	-2.07	105.56	110.35
2	K	3	FUC	C3-C4-C5	-2.05	106.58	109.77
2	M	2	G6S	O9-S-O8	2.00	115.45	108.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

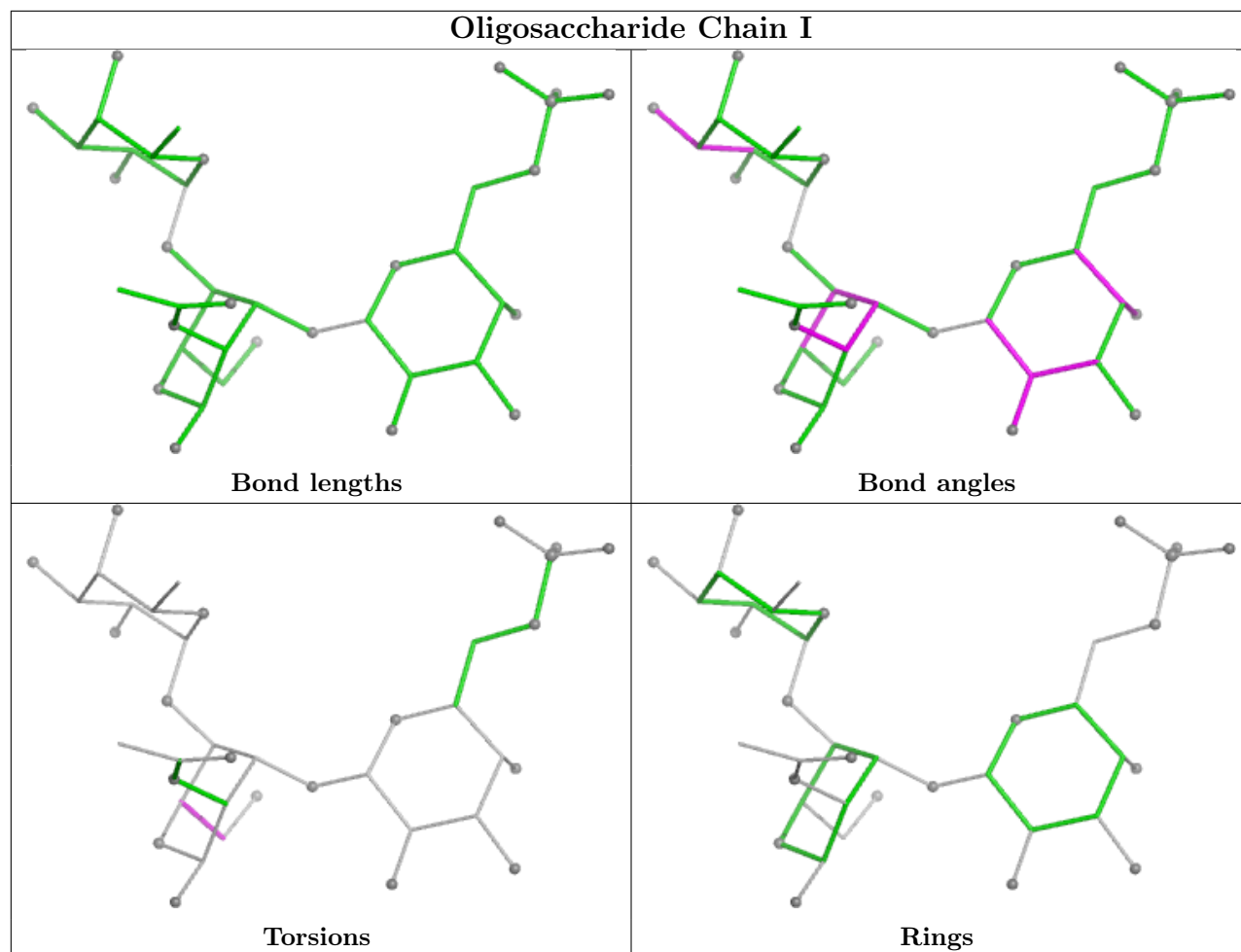
Mol	Chain	Res	Type	Atoms
2	M	1	NDG	O5-C5-C6-O6
2	L	1	NDG	O5-C5-C6-O6
2	I	1	NDG	O5-C5-C6-O6
2	J	1	NDG	O5-C5-C6-O6
2	K	1	NDG	O5-C5-C6-O6
2	M	1	NDG	C4-C5-C6-O6
2	L	1	NDG	C4-C5-C6-O6

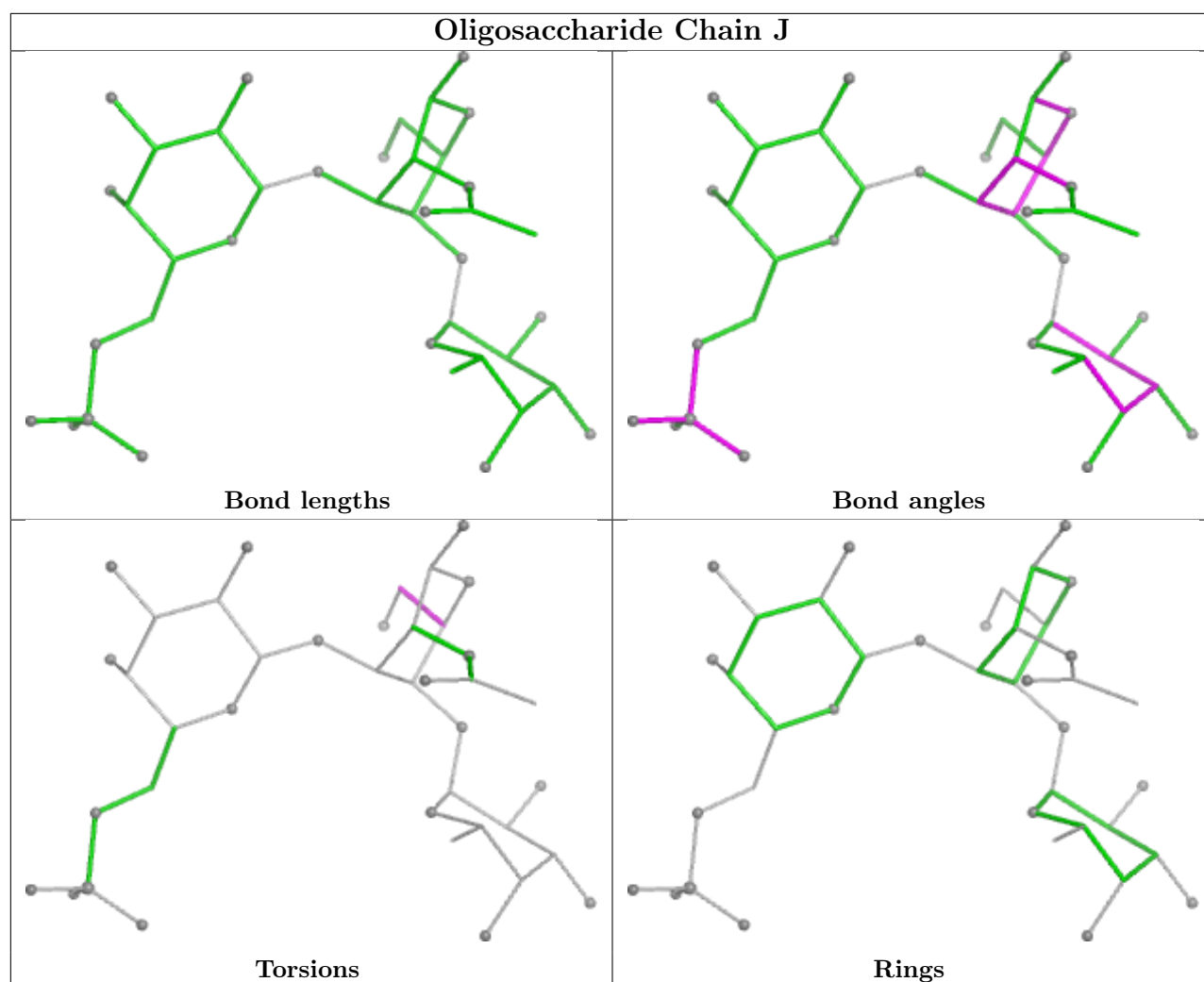
There are no ring outliers.

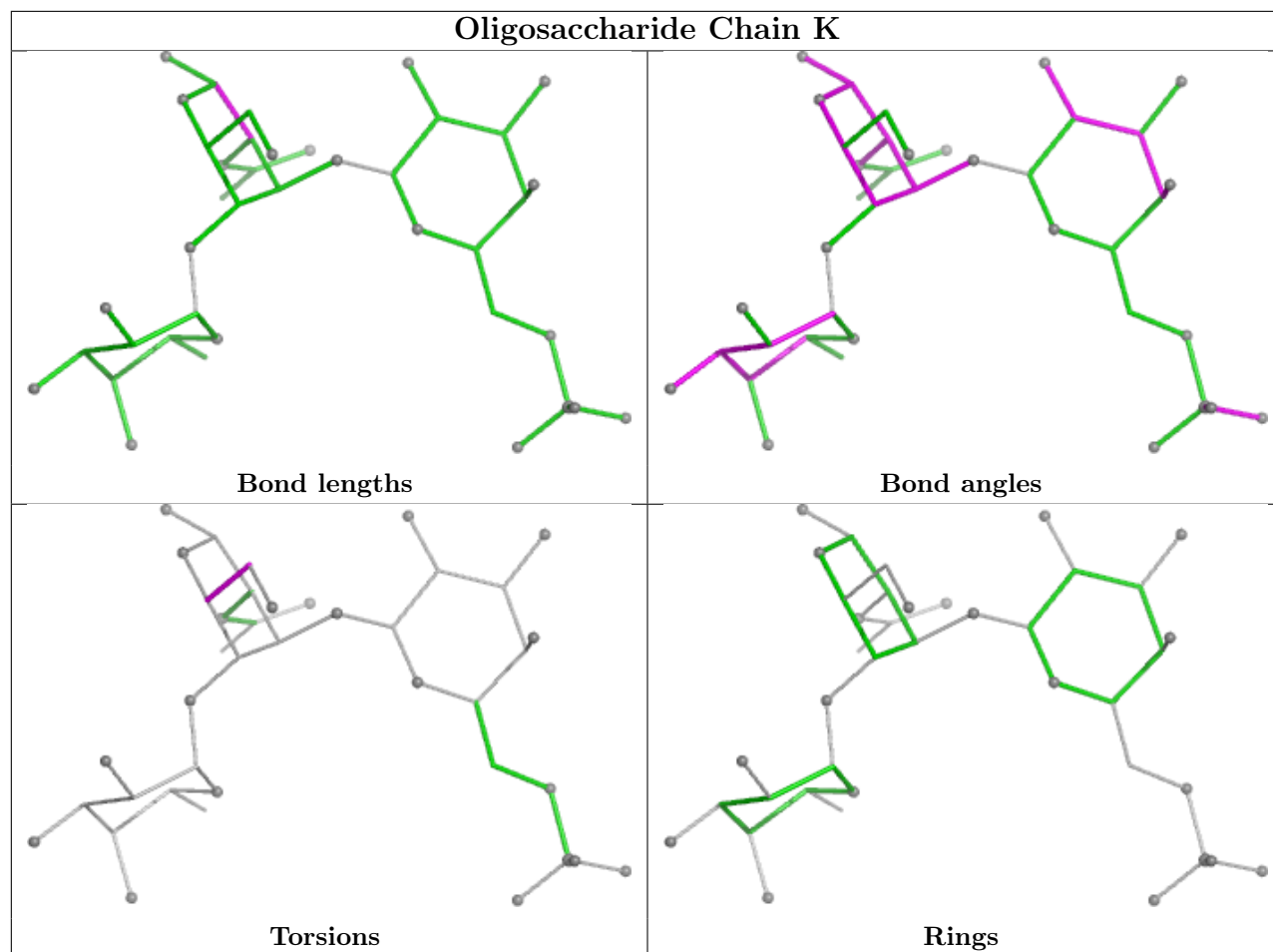
3 monomers are involved in 2 short contacts:

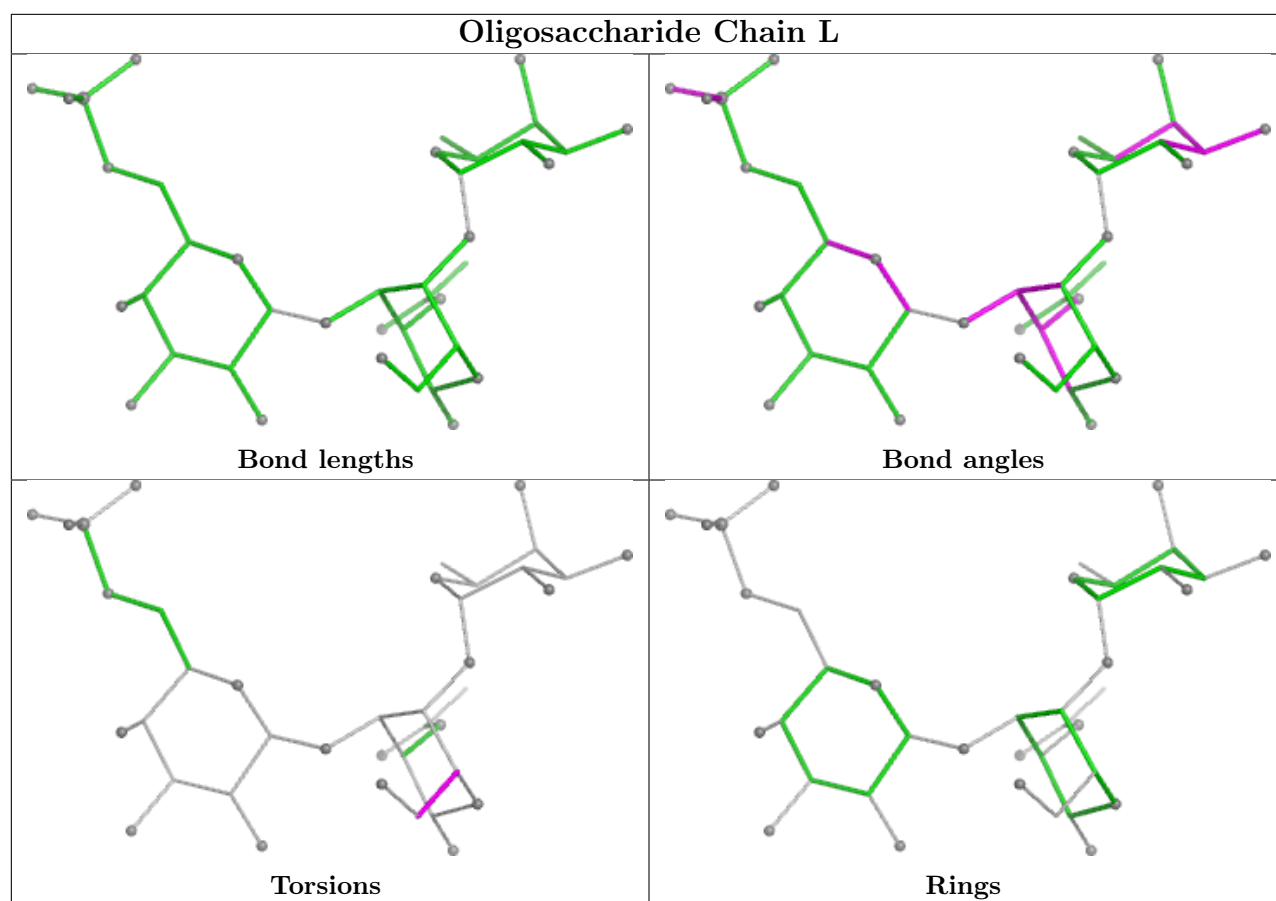
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NDG	1	0
2	L	3	FUC	1	0
2	K	3	FUC	1	0

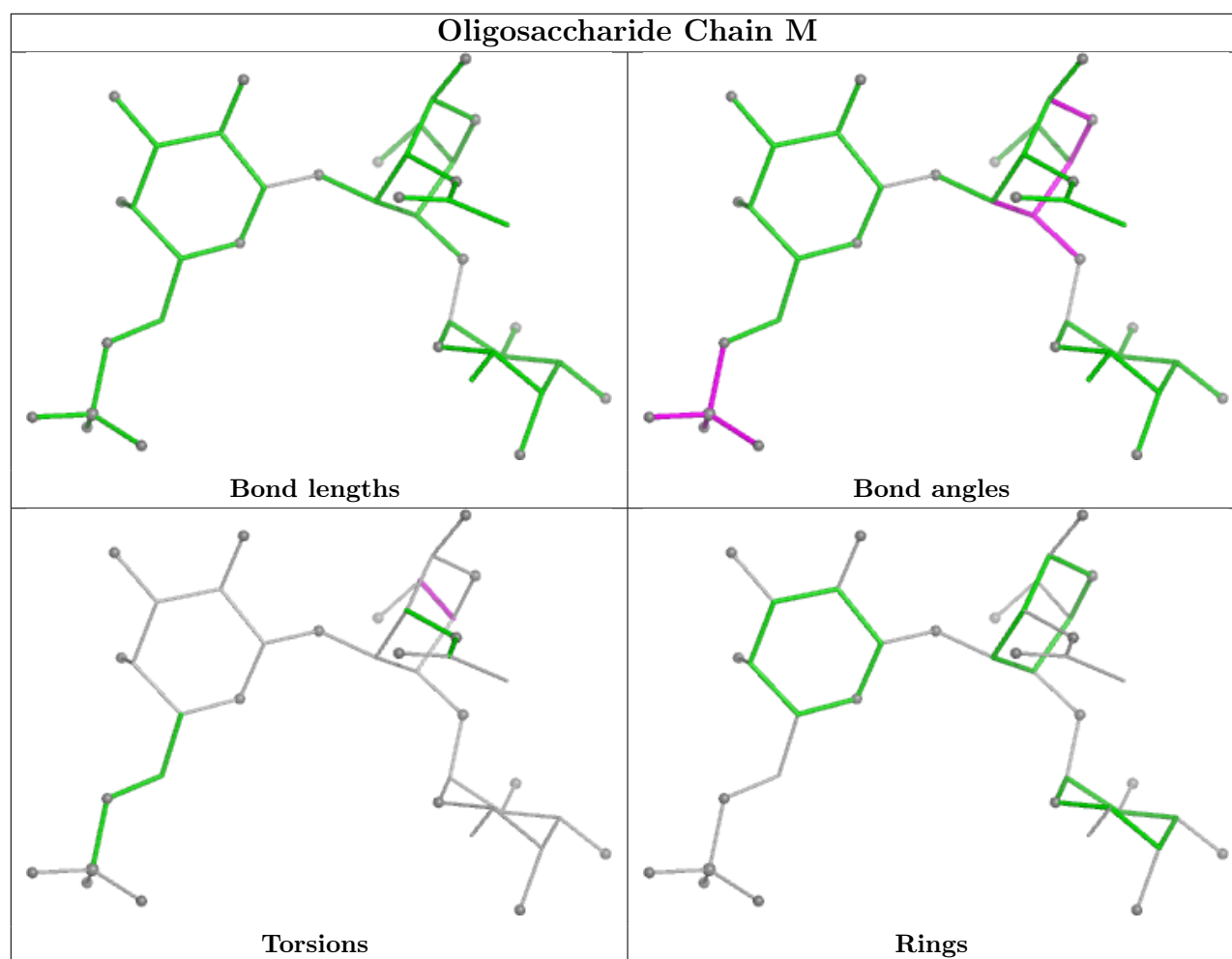
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	488/496 (98%)	-0.00	4 (0%) 82 88	14, 32, 50, 76	8 (1%)
1	B	487/496 (98%)	0.91	50 (10%) 12 16	34, 48, 74, 92	0
1	C	488/496 (98%)	0.49	16 (3%) 49 54	18, 39, 62, 79	3 (0%)
1	D	495/496 (99%)	0.17	3 (0%) 85 89	16, 35, 52, 71	4 (0%)
1	E	489/496 (98%)	-0.04	3 (0%) 85 89	14, 30, 49, 72	6 (1%)
All	All	2447/2480 (98%)	0.30	76 (3%) 51 56	14, 36, 62, 92	21 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	ALA	5.1
1	B	461	ILE	4.2
1	B	26	VAL	4.0
1	B	453	ALA	3.6
1	B	502	LYS	3.6
1	E	25	THR	3.4
1	B	497	ILE	3.2
1	B	495	PRO	3.2
1	D	26	VAL	3.2
1	B	468	MET	3.1
1	B	465	SER	3.1
1	B	448	TRP	3.1
1	C	26	VAL	3.0
1	C	378	GLY	2.9
1	B	94	LYS	2.9
1	E	465	SER	2.9
1	B	288	VAL	2.8
1	B	443	ILE	2.8
1	C	496[A]	ASP	2.8
1	B	498	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	321	LYS	2.7
1	B	450	PHE	2.6
1	C	502	LYS	2.6
1	B	487	LEU	2.6
1	B	474	GLY	2.6
1	B	490	VAL	2.6
1	C	379	VAL	2.6
1	A	25	THR	2.5
1	B	431	TYR	2.5
1	B	213	LEU	2.5
1	B	463	GLY	2.5
1	B	503	ALA	2.5
1	B	46	GLY	2.4
1	B	472	PRO	2.4
1	C	377	PRO	2.4
1	B	364	LEU	2.4
1	B	512	SER	2.4
1	B	508	ILE	2.3
1	D	248	ASP	2.3
1	C	408	ALA	2.3
1	B	342	PHE	2.3
1	B	478	PHE	2.3
1	B	340	ARG	2.3
1	B	379	VAL	2.3
1	B	460	GLY	2.2
1	C	512	SER	2.2
1	B	387	LYS	2.2
1	B	477	LEU	2.2
1	C	497	ILE	2.2
1	B	344	VAL	2.2
1	C	319	LEU	2.2
1	B	420	ALA	2.2
1	C	50	ALA	2.2
1	B	232	PHE	2.2
1	B	356	PHE	2.2
1	C	287	PHE	2.2
1	C	370	ILE	2.2
1	B	442	ALA	2.2
1	A	502	LYS	2.2
1	C	68	PHE	2.1
1	B	339	TYR	2.1
1	D	509	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	466	ALA	2.1
1	A	26	VAL	2.1
1	B	208	LYS	2.1
1	B	421	LEU	2.1
1	B	380	ILE	2.1
1	B	218	GLY	2.1
1	B	452	PRO	2.1
1	C	495	PRO	2.1
1	B	335	LEU	2.1
1	B	488	ASP	2.1
1	B	494	HIS	2.0
1	E	26	VAL	2.0
1	A	512	SER	2.0
1	B	326	ILE	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.

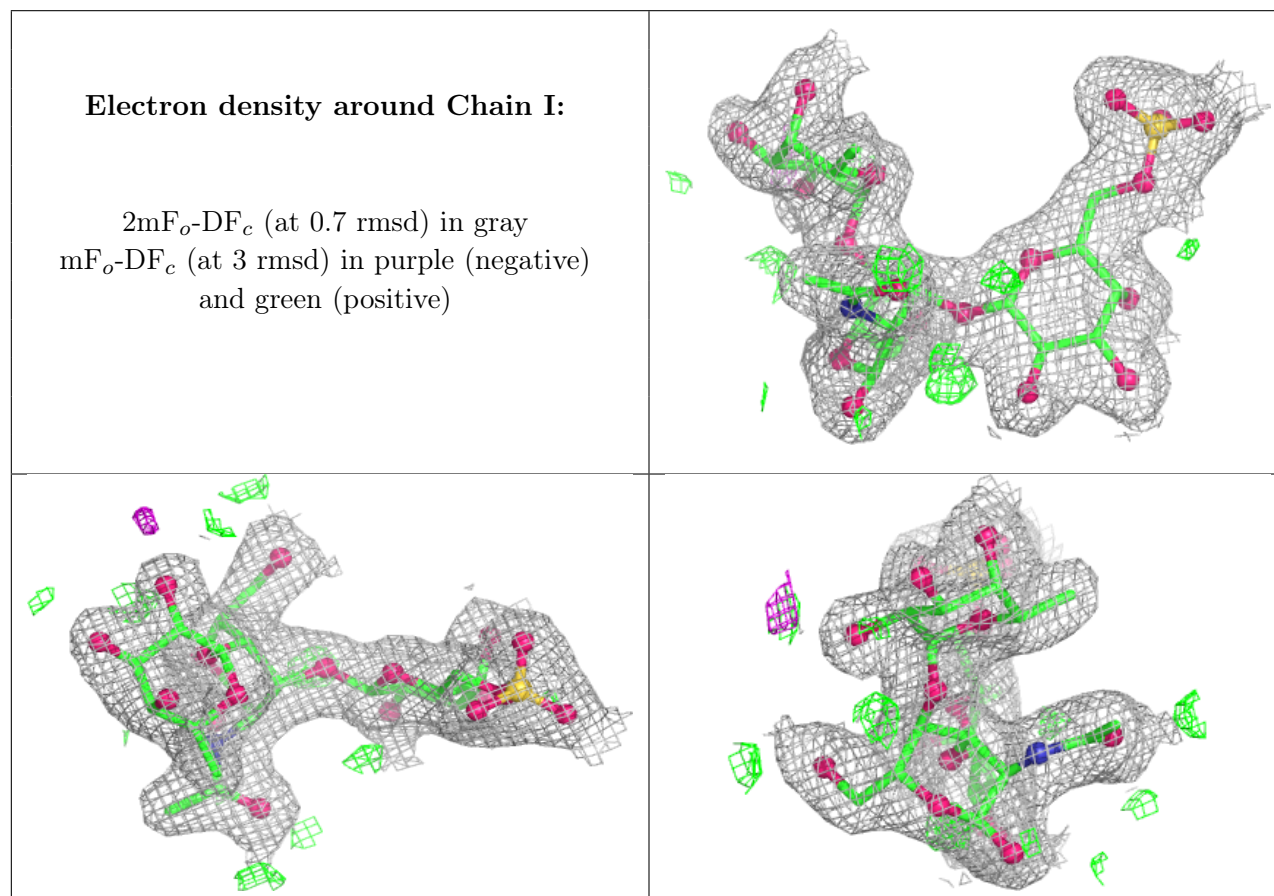
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	I	3	10/11	0.79	0.15	29,31,33,34	0
2	NDG	I	1	15/15	0.82	0.14	28,30,34,34	0
2	FUC	J	3	10/11	0.90	0.10	55,74,82,83	0
2	NDG	J	1	15/15	0.94	0.07	58,65,78,84	0
2	G6S	J	2	15/16	0.99	0.04	36,45,52,54	0
2	G6S	I	2	15/16	0.99	0.04	23,24,27,27	0
2	NDG	K	1	15/15	-	-	31,43,47,47	0
2	G6S	K	2	15/16	-	-	26,27,30,31	0
2	FUC	K	3	10/11	-	-	45,49,56,61	0
2	NDG	L	1	15/15	-	-	34,61,70,70	0
2	G6S	L	2	15/16	-	-	25,27,33,34	0
2	FUC	L	3	10/11	-	-	68,76,85,89	0
2	NDG	M	1	15/15	-	-	28,37,42,42	0
2	G6S	M	2	15/16	-	-	22,24,27,27	0

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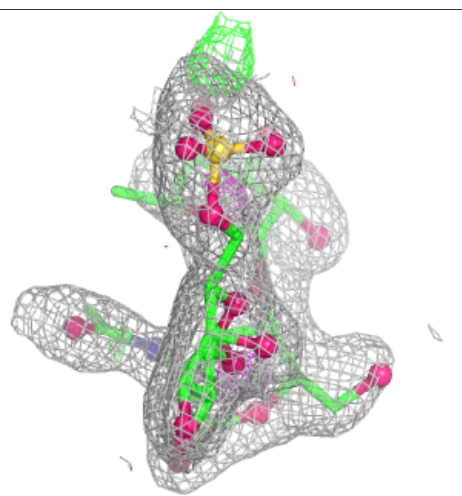
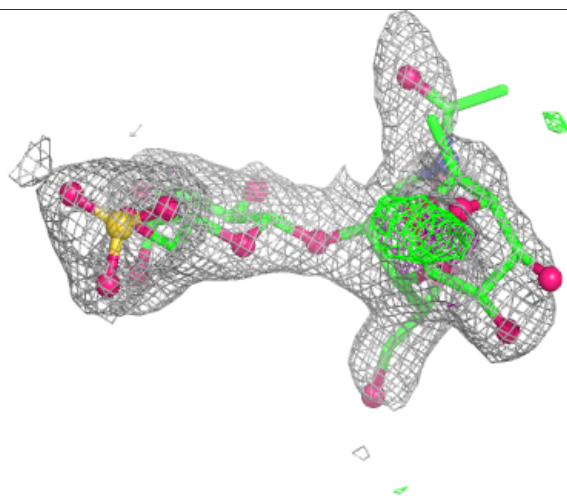
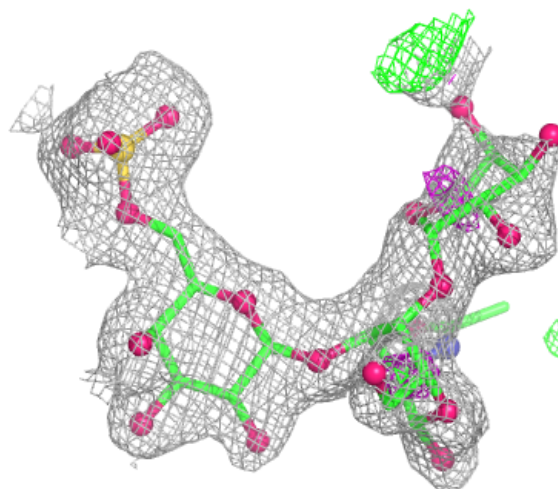
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FUC	M	3	10/11	-	-	35,41,42,42	0

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.



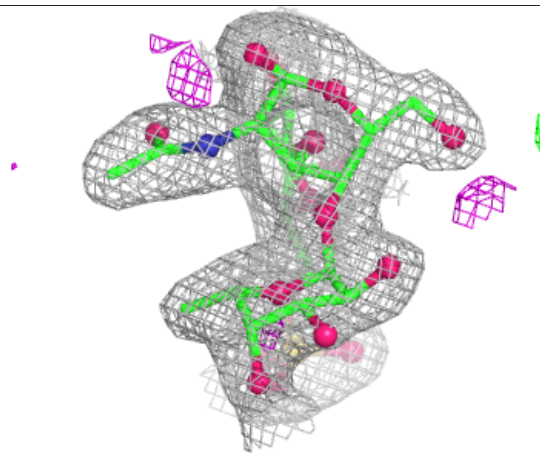
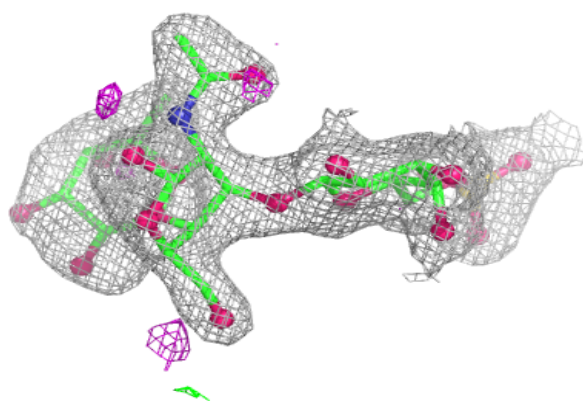
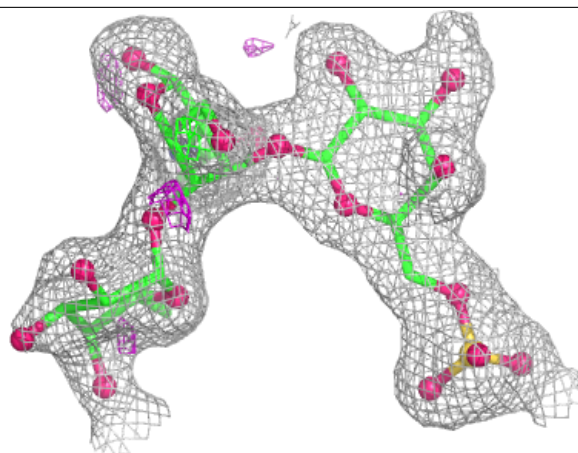
Electron density around Chain J:

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



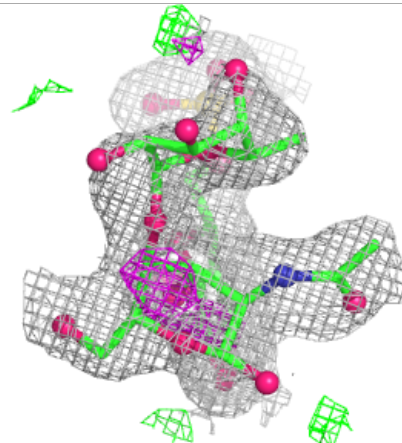
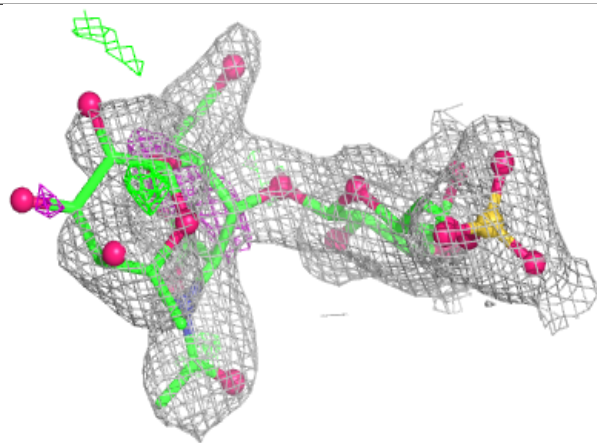
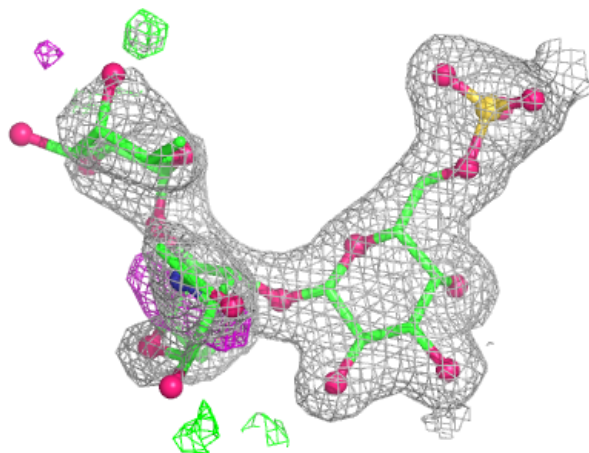
Electron density around Chain K:

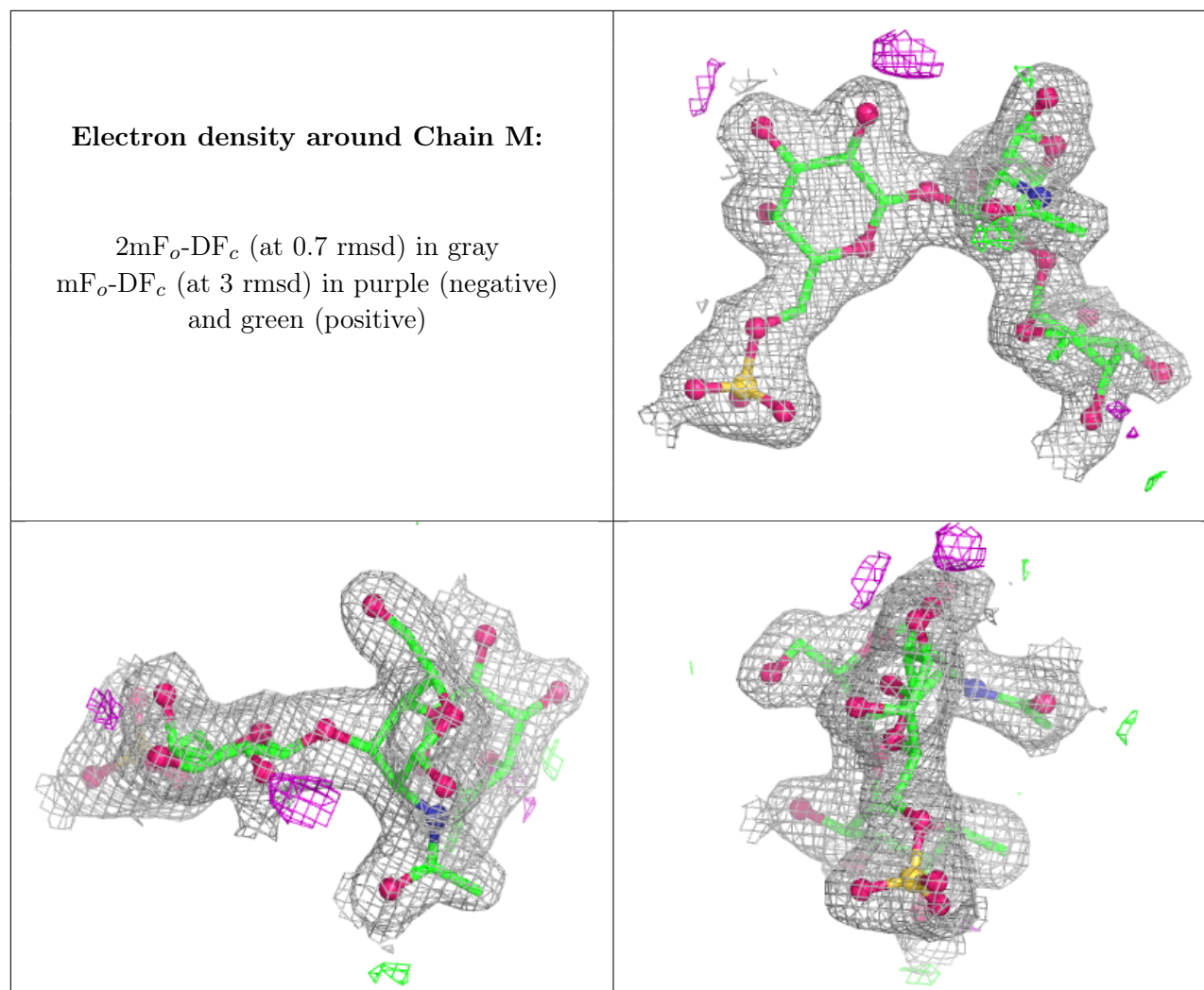
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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
3	IOD	A	601	1/1	0.89	0.35	148,148,148,148	0
3	IOD	E	601	1/1	0.96	0.19	113,113,113,113	0
4	BR	C	603	1/1	0.96	0.17	63,63,63,63	0
4	BR	E	602	1/1	0.97	0.11	63,63,63,63	0
5	CA	B	601	1/1	0.98	0.12	44,44,44,44	1
5	CA	E	604	1/1	0.98	0.03	23,23,23,23	1
4	BR	E	603	1/1	0.99	0.07	51,51,51,51	0
5	CA	A	603	1/1	0.99	0.02	22,22,22,22	1
4	BR	D	601	1/1	0.99	0.03	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	C	602	1/1	0.99	0.02	24,24,24,24	1
5	CA	D	602	1/1	0.99	0.03	22,22,22,22	1
4	BR	C	601	1/1	0.99	0.03	44,44,44,44	0
4	BR	A	602	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.