Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 10:07 PM EDT

PDB ID	:	7JTR
Title	:	Complex of maltose-binding protein (MBP) with single-chain Fv (scFv)
Authors	:	Loll, P.J.
Deposited on	:	2020-08-18
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

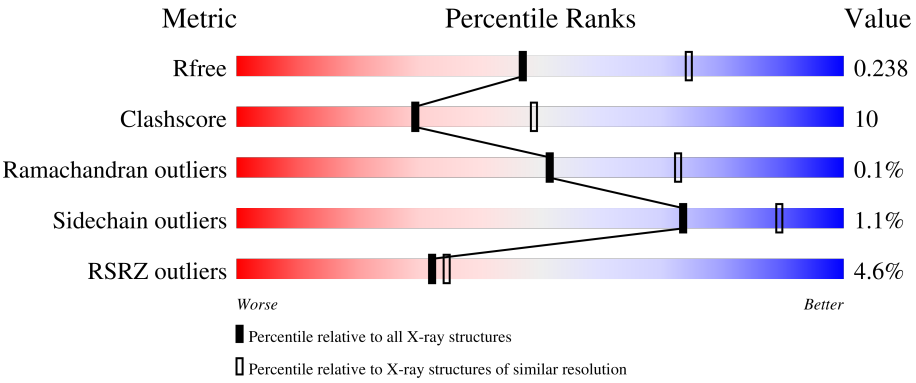
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	369	3% 80% 18% ·
1	C	369	5% 76% 22% ·
1	E	369	4% 84% 15% ·
1	G	369	6% 78% 20% ·
2	B	251	4% 69% 20% · 10%

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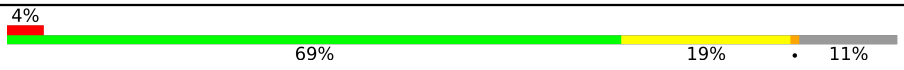
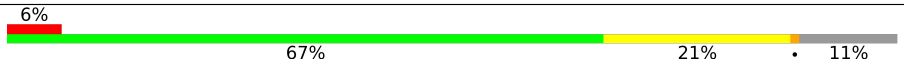
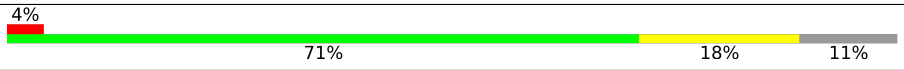
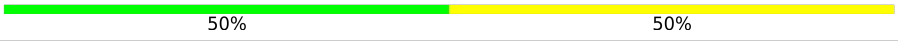
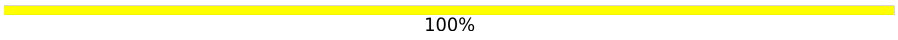
Mol	Chain	Length	Quality of chain
2	D	251	
2	F	251	
2	H	251	
3	J	2	
3	K	2	
3	L	2	
3	M	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18514 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 Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2871	1849	467	549	6			
1	C	369	Total	C	N	O	S	0	0	0
			2871	1849	467	549	6			
1	E	369	Total	C	N	O	S	0	0	0
			2871	1849	467	549	6			
1	G	369	Total	C	N	O	S	0	0	0
			2871	1849	467	549	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	VAL	ALA	variant	UNP P0AEX9
C	312	VAL	ALA	variant	UNP P0AEX9
E	312	VAL	ALA	variant	UNP P0AEX9
G	312	VAL	ALA	variant	UNP P0AEX9

- Molecule 2 is a protein called single-chain Fv antibody fragment (scFv).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1734	1096	288	341	9			
2	D	223	Total	C	N	O	S	0	0	0
			1721	1089	285	338	9			
2	F	224	Total	C	N	O	S	0	0	0
			1731	1094	289	339	9			
2	H	224	Total	C	N	O	S	0	0	0
			1731	1094	289	339	9			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	2	Total C O 23 12 11	0	0	0
3	K	2	Total C O 23 12 11	0	0	0
3	L	2	Total C O 23 12 11	0	0	0
3	M	2	Total C O 23 12 11	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is water.

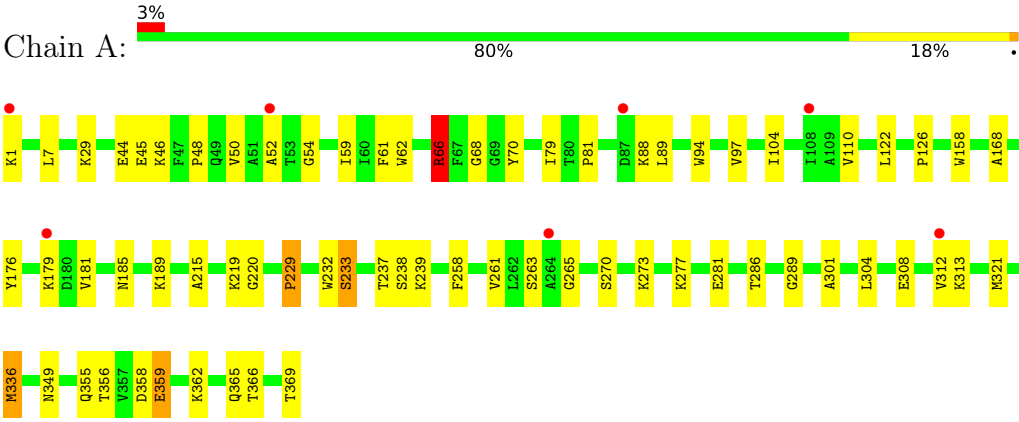
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	C	2	Total O 2 2	0	0
5	D	1	Total O 1 1	0	0
5	E	4	Total O 4 4	0	0
5	F	2	Total O 2 2	0	0
5	G	4	Total O 4 4	0	0
5	H	1	Total O 1 1	0	0

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.

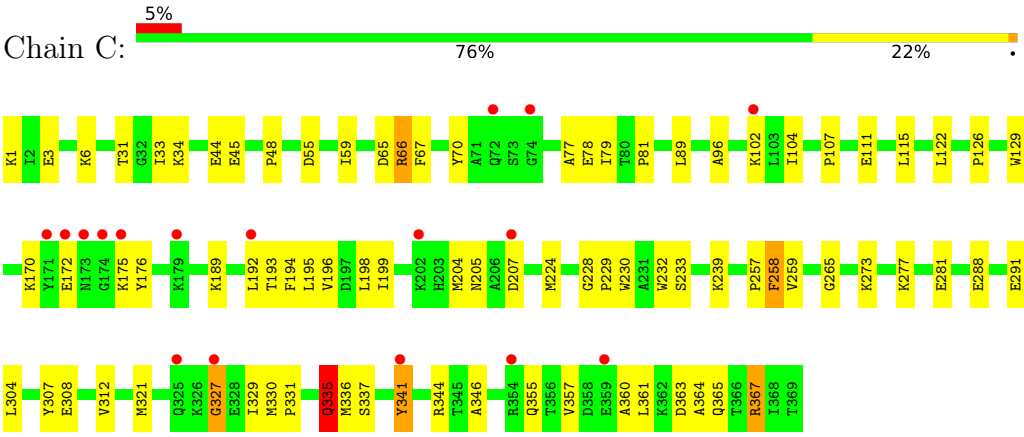
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein

Chain A:



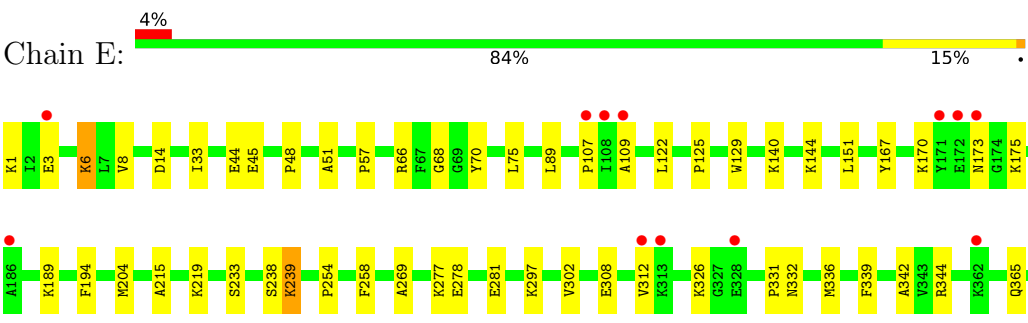
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein

Chain C:



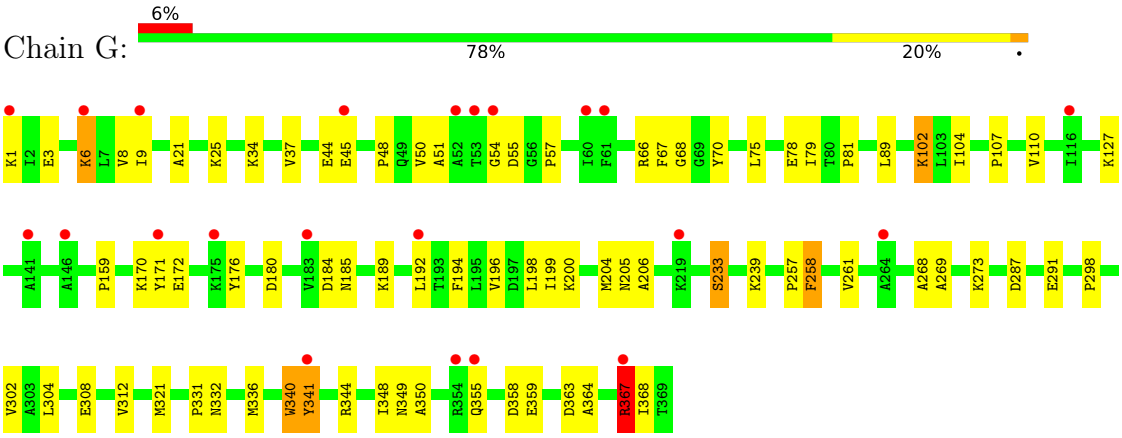
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein

Chain E:



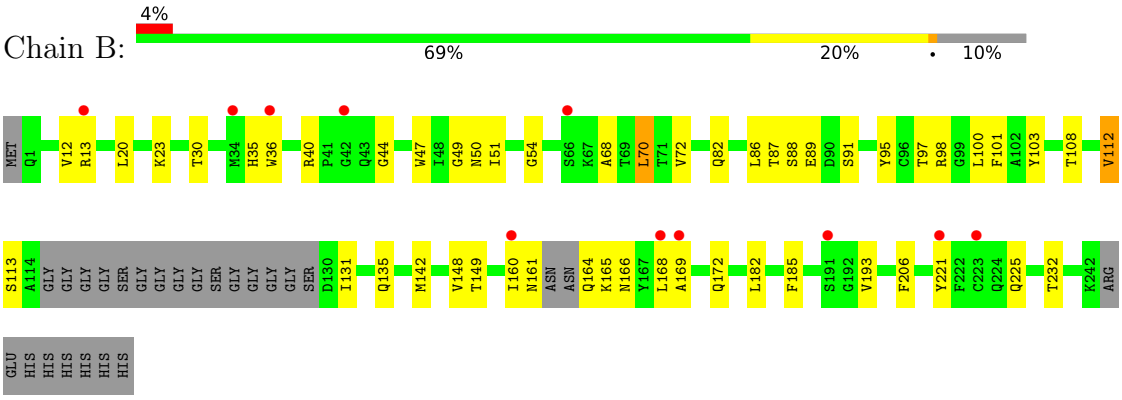
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein

Chain G:



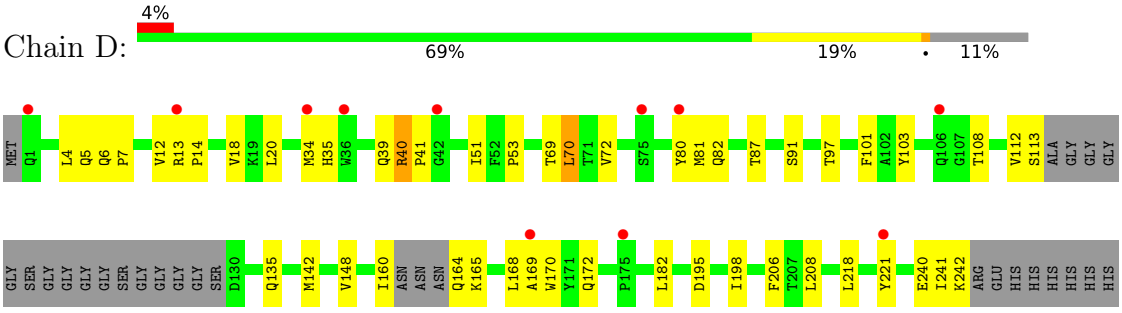
• Molecule 2: single-chain Fv antibody fragment (scFv)

Chain B:



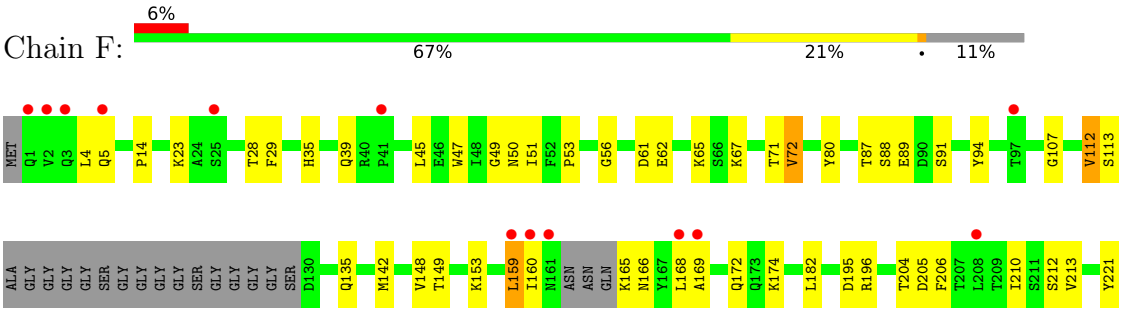
• Molecule 2: single-chain Fv antibody fragment (scFv)

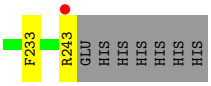
Chain D:



• Molecule 2: single-chain Fv antibody fragment (scFv)

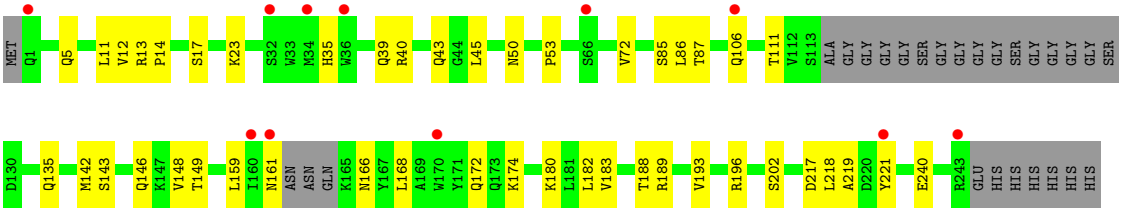
Chain F:





• Molecule 2: single-chain Fv antibody fragment (scFv)

Chain H:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

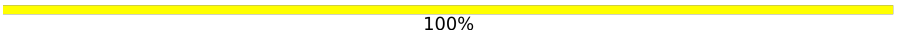
Chain J:

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.20Å 91.70Å 174.63Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.50) 98.4 (20.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.50Å)	Xtriage
Refinement program	PHENIX v1.11.1	Depositor
R, R_{free}	0.201 , 0.237 0.201 , 0.238	Depositor DCC
R_{free} test set	1980 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.851	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l 0.004 for -k,-h,-l 0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18514	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, GLC

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	0.51	2/2940 (0.1%)	0.74	9/3990 (0.2%)
1	C	0.53	1/2940 (0.0%)	0.83	12/3990 (0.3%)
1	E	0.50	1/2940 (0.0%)	0.73	5/3990 (0.1%)
1	G	0.51	1/2940 (0.0%)	0.77	13/3990 (0.3%)
2	B	0.49	0/1773	0.72	3/2403 (0.1%)
2	D	0.50	0/1760	0.96	8/2385 (0.3%)
2	F	0.51	0/1770	0.83	5/2398 (0.2%)
2	H	0.49	0/1770	0.75	3/2398 (0.1%)
All	All	0.51	5/18833 (0.0%)	0.79	58/25544 (0.2%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	179	LYS	CD-CE	6.21	1.66	1.51
1	A	359	GLU	CD-OE2	5.97	1.32	1.25
1	A	359	GLU	CD-OE1	5.72	1.31	1.25
1	C	34	LYS	CD-CE	5.67	1.65	1.51
1	G	367	ARG	CB-CG	-5.07	1.38	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	40	ARG	NE-CZ-NH1	-16.17	112.22	120.30
2	D	40	ARG	NE-CZ-NH2	13.70	127.15	120.30
2	D	70	LEU	CB-CG-CD2	-13.24	88.49	111.00
1	G	341	TYR	CA-CB-CG	-10.55	93.35	113.40
2	D	40	ARG	CG-CD-NE	9.56	131.88	111.80
1	C	341	TYR	CB-CG-CD2	-9.45	115.33	121.00
1	A	1	LYS	N-CA-C	8.95	135.16	111.00
2	F	159	LEU	CB-CG-CD2	8.58	125.59	111.00
1	G	367	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	F	5	GLN	C-N-CA	8.31	142.47	121.70
1	C	34	LYS	CB-CG-CD	-8.12	90.48	111.60
1	C	341	TYR	CB-CG-CD1	8.12	125.87	121.00
1	G	127	LYS	CB-CG-CD	-7.46	92.21	111.60
1	G	341	TYR	CB-CG-CD1	7.23	125.34	121.00
1	C	66	ARG	CG-CD-NE	7.21	126.94	111.80
2	F	72	VAL	CG1-CB-CG2	7.12	122.30	110.90
1	C	34	LYS	CA-CB-CG	7.10	129.02	113.40
2	H	180	LYS	CA-CB-CG	7.03	128.88	113.40
1	G	102	LYS	CD-CE-NZ	-6.91	95.80	111.70
1	A	1	LYS	CB-CA-C	-6.89	96.63	110.40
2	D	5	GLN	C-N-CA	6.87	138.87	121.70
1	A	175	LYS	CA-CB-CG	6.78	128.31	113.40
1	E	239	LYS	CA-CB-CG	6.72	128.18	113.40
1	A	179	LYS	CA-CB-CG	6.71	128.16	113.40
1	C	335	GLN	CA-CB-CG	6.65	128.03	113.40
2	D	39	GLN	C-N-CA	-6.62	105.15	121.70
1	G	102	LYS	CA-CB-CG	-6.56	98.96	113.40
1	E	33	ILE	CA-CB-CG1	-6.55	98.55	111.00
2	F	159	LEU	CA-CB-CG	6.55	130.37	115.30
1	G	200	LYS	CD-CE-NZ	-6.52	96.71	111.70
2	B	70	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	G	367	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	G	367	ARG	CB-CA-C	6.29	122.98	110.40
1	G	367	ARG	N-CA-CB	-6.29	99.28	110.60
1	G	50	VAL	CG1-CB-CG2	6.26	120.92	110.90
2	D	70	LEU	CA-CB-CG	-5.96	101.60	115.30
1	C	34	LYS	CD-CE-NZ	5.72	124.86	111.70
1	A	175	LYS	CB-CA-C	-5.59	99.22	110.40
1	E	239	LYS	N-CA-CB	-5.51	100.68	110.60
1	A	66	ARG	CG-CD-NE	5.50	123.36	111.80
1	A	175	LYS	N-CA-CB	5.49	120.49	110.60
2	F	112	VAL	CG1-CB-CG2	5.45	119.62	110.90
1	E	269	ALA	C-N-CA	-5.41	108.17	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	6	LYS	CB-CA-C	5.41	121.22	110.40
2	B	23	LYS	CA-CB-CG	5.39	125.27	113.40
1	C	138	GLU	N-CA-CB	-5.38	100.91	110.60
1	G	340	TRP	CA-CB-CG	5.35	123.86	113.70
1	A	1	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	A	359	GLU	CB-CA-C	5.34	121.08	110.40
2	H	43	GLN	C-N-CA	-5.31	111.15	122.30
1	C	327	GLY	C-N-CA	-5.30	108.45	121.70
1	G	102	LYS	CB-CG-CD	5.26	125.27	111.60
1	C	367	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	189	LYS	CD-CE-NZ	5.16	123.57	111.70
2	B	112	VAL	CG1-CB-CG2	-5.14	102.68	110.90
2	H	106	GLN	CA-CB-CG	5.09	124.61	113.40
2	D	198	ILE	CG1-CB-CG2	5.06	122.53	111.40
1	C	288	GLU	N-CA-CB	-5.03	101.56	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	335	GLN	Sidechain

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	2871	0	2850	44	0
1	C	2871	0	2850	62	2
1	E	2871	0	2850	37	2
1	G	2871	0	2850	64	0
2	B	1734	0	1676	37	0
2	D	1721	0	1665	50	0
2	F	1731	0	1675	40	0
2	H	1731	0	1676	24	0
3	J	23	0	21	0	0
3	K	23	0	21	4	0
3	L	23	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	23	0	21	2	0
4	B	1	0	0	0	0
4	F	1	0	0	1	0
4	H	1	0	0	0	0
5	A	4	0	0	1	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
5	G	4	0	0	0	0
5	H	1	0	0	0	0
All	All	18514	0	18176	350	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 10.

All (350) 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:G:1:LYS:HD2	1:G:54:GLY:C	1.72	1.09
1:C:170:LYS:HE2	1:C:172:GLU:CG	1.83	1.08
1:G:1:LYS:HD2	1:G:54:GLY:O	1.53	1.07
2:D:13:ARG:HG2	2:D:14:PRO:HD2	1.43	1.01
1:C:170:LYS:HE2	1:C:172:GLU:HG3	1.02	1.01
1:E:3:GLU:OE1	1:E:6:LYS:HE2	1.62	0.99
2:D:13:ARG:CG	2:D:14:PRO:HD2	1.94	0.98
1:E:3:GLU:CD	1:E:6:LYS:HE2	1.84	0.98
2:D:13:ARG:HB2	2:D:113:SER:C	1.86	0.94
1:G:355:GLN:OE1	1:G:359:GLU:OE1	1.88	0.91
2:D:13:ARG:CG	2:D:14:PRO:CD	2.50	0.90
1:C:170:LYS:CE	1:C:172:GLU:HG3	1.99	0.87
2:D:51:ILE:HD11	2:D:72:VAL:HB	1.55	0.85
1:G:341:TYR:HH	3:M:2:GLC:HO4	1.26	0.84
1:C:192:LEU:HD23	1:C:361:LEU:HD11	1.61	0.82
2:D:13:ARG:HG2	2:D:14:PRO:CD	2.09	0.82
1:A:89:LEU:HD12	1:A:94:TRP:CZ2	2.15	0.80
2:D:13:ARG:HG3	2:D:14:PRO:CD	2.11	0.80
2:D:51:ILE:CD1	2:D:72:VAL:HB	2.12	0.79
1:G:1:LYS:CD	1:G:54:GLY:HA3	2.16	0.76
2:F:135:GLN:NE2	2:F:221:TYR:O	2.18	0.75
2:F:174:LYS:NZ	4:F:301:CL:CL	2.57	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:HG23	2:B:112:VAL:HG12	1.70	0.74
1:C:1:LYS:N	1:C:55:ASP:OD1	2.18	0.74
1:A:48:PRO:HG3	1:A:70:TYR:HE1	1.51	0.74
2:H:5:GLN:HB3	2:H:23:LYS:HB3	1.70	0.73
2:H:135:GLN:NE2	2:H:221:TYR:O	2.23	0.72
1:G:1:LYS:HG2	1:G:55:ASP:OD2	1.91	0.71
2:F:142:MET:HG3	2:F:148:VAL:HG22	1.72	0.71
1:A:239:LYS:HG3	2:H:149:THR:HG21	1.73	0.70
1:G:1:LYS:HD2	1:G:54:GLY:CA	2.21	0.70
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.72	0.70
2:H:143:SER:O	2:H:146:GLN:HG3	1.92	0.69
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.28	0.68
1:C:344:ARG:NH2	3:K:2:GLC:H62	2.08	0.68
2:B:161:ASN:HA	2:B:164:GLN:HG3	1.75	0.68
1:E:238:SER:O	1:E:239:LYS:HB2	1.94	0.68
2:H:166:ASN:HD21	2:H:202:SER:HB2	1.58	0.68
1:E:48:PRO:HG3	1:E:70:TYR:HE1	1.60	0.67
2:D:160:ILE:HD11	2:D:164:GLN:HE22	1.59	0.67
2:B:87:THR:O	2:B:112:VAL:HG21	1.95	0.67
2:D:13:ARG:CB	2:D:113:SER:C	2.62	0.66
1:A:312:VAL:HG13	1:A:321:MET:HE1	1.77	0.66
2:D:13:ARG:HG3	2:D:14:PRO:HD3	1.78	0.66
2:B:142:MET:HG3	2:B:148:VAL:HG22	1.78	0.66
1:E:8:VAL:HG13	1:E:57:PRO:HA	1.79	0.65
2:B:160:ILE:HD11	2:B:165:LYS:HE3	1.77	0.65
1:E:308:GLU:O	1:E:312:VAL:HG23	1.97	0.65
1:G:89:LEU:HD23	1:G:107:PRO:HG2	1.79	0.65
1:C:96:ALA:HB2	1:C:329:ILE:HD11	1.78	0.65
2:D:13:ARG:HG3	2:D:14:PRO:HD2	1.71	0.65
1:A:89:LEU:HD23	1:A:304:LEU:HA	1.80	0.64
1:C:126:PRO:HD2	1:C:224:MET:HE3	1.79	0.64
2:D:12:VAL:O	2:D:112:VAL:HA	1.98	0.64
1:A:110:VAL:HG12	1:A:261:VAL:HG22	1.78	0.64
2:D:12:VAL:HG11	2:D:18:VAL:CG1	2.27	0.64
1:G:363:ASP:O	1:G:367:ARG:HB2	1.97	0.64
1:E:48:PRO:HG3	1:E:70:TYR:CE1	2.33	0.64
2:F:210:ILE:HB	2:F:213:VAL:HG12	1.79	0.64
1:G:1:LYS:CD	1:G:54:GLY:O	2.40	0.63
1:A:308:GLU:O	1:A:312:VAL:HG23	1.99	0.63
2:B:225:GLN:HE21	2:B:232:THR:HG22	1.63	0.63
2:B:13:ARG:HG2	2:B:113:SER:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LYS:HG3	2:F:149:THR:HG21	1.80	0.63
2:F:88:SER:HA	2:F:112:VAL:CG2	2.29	0.63
2:H:53:PRO:HB3	2:H:72:VAL:HG21	1.79	0.63
1:G:1:LYS:HD3	1:G:54:GLY:HA3	1.80	0.62
1:E:3:GLU:OE2	1:E:6:LYS:HE2	1.99	0.62
1:G:176:TYR:CZ	1:G:331:PRO:HG3	2.35	0.62
2:F:196:ARG:HD2	2:F:212:SER:O	2.00	0.62
1:G:78:GLU:CD	1:G:102:LYS:HD3	2.20	0.62
2:D:12:VAL:HG11	2:D:18:VAL:HG13	1.82	0.61
1:G:48:PRO:HG3	1:G:70:TYR:HE1	1.65	0.61
2:D:135:GLN:NE2	2:D:221:TYR:O	2.33	0.61
1:C:205:ASN:HB3	1:C:207:ASP:OD1	2.01	0.61
2:F:14:PRO:HD3	2:F:113:SER:C	2.21	0.61
1:G:110:VAL:HG22	1:G:261:VAL:HG22	1.83	0.61
2:F:142:MET:HG3	2:F:148:VAL:CG2	2.30	0.60
1:C:44:GLU:HG2	1:C:45:GLU:N	2.17	0.60
1:G:308:GLU:O	1:G:312:VAL:HG23	2.01	0.60
1:E:89:LEU:HD23	1:E:107:PRO:HG2	1.83	0.59
2:H:11:LEU:HD23	2:H:111:THR:HB	1.85	0.59
1:C:79:ILE:HG13	1:C:81:PRO:HD3	1.84	0.58
1:G:331:PRO:HD2	1:G:336:MET:HE3	1.83	0.58
1:A:238:SER:O	1:A:238:SER:OG	2.20	0.58
2:B:12:VAL:O	2:B:112:VAL:HA	2.03	0.58
1:C:259:VAL:HG13	1:C:329:ILE:HA	1.84	0.58
1:G:8:VAL:HG13	1:G:57:PRO:HA	1.86	0.57
2:D:87:THR:O	2:D:112:VAL:HG11	2.03	0.57
2:F:160:ILE:HD11	2:F:165:LYS:HE2	1.87	0.57
2:F:153:LYS:HE3	2:F:204:THR:OG1	2.05	0.57
1:C:65:ASP:OD2	3:K:2:GLC:O3	2.21	0.57
1:G:268:ALA:O	1:G:273:LYS:NZ	2.35	0.57
2:B:112:VAL:HG23	2:B:112:VAL:O	2.04	0.57
1:C:312:VAL:HG13	1:C:321:MET:HE1	1.86	0.57
2:B:131:ILE:O	2:B:232:THR:HG21	2.05	0.56
2:D:160:ILE:HD11	2:D:164:GLN:NE2	2.20	0.56
1:G:350:ALA:HA	1:G:355:GLN:O	2.05	0.56
2:B:51:ILE:HG12	2:B:72:VAL:HG23	1.87	0.56
2:F:168:LEU:HD22	2:F:206:PHE:CG	2.40	0.56
2:H:142:MET:HG3	2:H:148:VAL:HG22	1.87	0.56
1:C:89:LEU:HD23	1:C:107:PRO:HG2	1.87	0.56
1:C:45:GLU:O	1:C:48:PRO:HD2	2.06	0.56
1:E:277:LYS:HE3	1:E:281:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.71	0.56
2:D:12:VAL:O	2:D:113:SER:N	2.33	0.56
1:G:1:LYS:CG	1:G:55:ASP:OD2	2.54	0.56
1:G:45:GLU:O	1:G:48:PRO:HD2	2.06	0.56
1:G:192:LEU:O	1:G:196:VAL:HG23	2.06	0.56
1:G:312:VAL:HG13	1:G:321:MET:HE1	1.87	0.56
2:H:218:LEU:HD23	2:H:240:GLU:HA	1.88	0.56
1:A:286:THR:HB	1:A:289:GLY:H	1.71	0.55
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.87	0.55
1:E:44:GLU:HB2	1:E:66:ARG:HD3	1.88	0.55
1:E:278:GLU:OE2	2:F:28:THR:HB	2.06	0.55
2:H:196:ARG:NH2	2:H:217:ASP:OD1	2.38	0.55
1:C:122:LEU:HD21	1:C:126:PRO:HD3	1.88	0.55
2:D:142:MET:HG3	2:D:148:VAL:HG22	1.88	0.55
1:C:308:GLU:O	1:C:312:VAL:HG23	2.07	0.54
2:F:71:THR:OG1	2:F:80:TYR:HB2	2.07	0.54
2:F:112:VAL:HG23	2:F:112:VAL:O	2.08	0.54
1:E:342:ALA:HB3	1:E:368:ILE:HD11	1.90	0.54
1:E:68:GLY:HA3	1:E:332:ASN:O	2.07	0.54
2:D:4:LEU:HD12	2:D:103:TYR:HD1	1.73	0.54
2:D:172:GLN:HB2	2:D:182:LEU:HD11	1.89	0.54
1:C:115:LEU:HD11	1:C:224:MET:HE2	1.89	0.54
1:C:344:ARG:HH21	3:K:2:GLC:H62	1.72	0.54
2:D:35:HIS:HB2	2:D:97:THR:HG22	1.90	0.54
1:G:341:TYR:OH	3:M:2:GLC:O4	2.11	0.53
2:B:12:VAL:CG2	2:B:112:VAL:HG12	2.38	0.53
1:G:349:ASN:HB3	1:G:355:GLN:CG	2.39	0.53
2:B:87:THR:HG23	2:B:89:GLU:H	1.73	0.53
1:E:45:GLU:O	1:E:48:PRO:HD2	2.08	0.53
1:C:126:PRO:HD2	1:C:224:MET:CE	2.38	0.53
2:D:91:SER:OG	2:D:112:VAL:HG12	2.09	0.53
1:A:176:TYR:CZ	1:A:331:PRO:HG3	2.43	0.52
2:F:172:GLN:HB2	2:F:182:LEU:HD11	1.90	0.52
1:C:31:THR:HB	1:C:33:ILE:HD12	1.90	0.52
1:C:111:GLU:O	1:C:259:VAL:HG23	2.09	0.52
1:A:79:ILE:HG13	1:A:81:PRO:HD3	1.92	0.52
2:F:88:SER:HA	2:F:112:VAL:HG21	1.90	0.52
2:D:168:LEU:HD22	2:D:206:PHE:CG	2.44	0.52
1:G:48:PRO:HG3	1:G:70:TYR:CE1	2.44	0.52
1:C:199:ILE:HD13	1:C:204:MET:HB2	1.92	0.51
1:G:184:ASP:OD1	1:G:189:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.45	0.51
1:A:44:GLU:HG2	1:A:45:GLU:HG3	1.91	0.51
1:G:1:LYS:CD	1:G:54:GLY:CA	2.81	0.51
1:G:21:ALA:O	1:G:25:LYS:HG3	2.10	0.51
1:C:67:PHE:HB3	1:C:104:ILE:HD12	1.93	0.51
1:A:122:LEU:HD21	1:A:126:PRO:HD3	1.93	0.51
2:B:35:HIS:HB2	2:B:97:THR:HG22	1.93	0.51
2:D:6:GLN:HB3	2:D:108:THR:HG22	1.92	0.51
1:G:9:ILE:HB	1:G:37:VAL:HG12	1.93	0.50
1:G:68:GLY:HA3	1:G:332:ASN:O	2.10	0.50
2:B:172:GLN:HB2	2:B:182:LEU:HD11	1.92	0.50
1:C:176:TYR:CE2	1:C:331:PRO:HG3	2.47	0.50
2:D:70:LEU:HD21	2:D:81:MET:CB	2.41	0.50
1:A:185:ASN:O	1:A:189:LYS:HG3	2.11	0.50
1:C:257:PRO:HD2	1:C:327:GLY:HA3	1.93	0.50
2:D:70:LEU:HD23	2:D:80:TYR:O	2.12	0.50
2:D:218:LEU:HD13	2:D:240:GLU:HA	1.94	0.50
1:E:339:PHE:HA	1:E:368:ILE:HD12	1.93	0.50
2:D:51:ILE:HD11	2:D:72:VAL:CB	2.36	0.49
2:F:153:LYS:HD3	2:F:205:ASP:OD1	2.12	0.49
2:D:97:THR:HG21	2:D:101:PHE:CD2	2.47	0.49
1:C:365:GLN:O	1:C:365:GLN:HG3	2.12	0.49
2:F:67:LYS:HB2	2:H:87:THR:HG21	1.95	0.49
1:G:44:GLU:O	1:G:70:TYR:OH	2.30	0.49
2:D:6:GLN:HB3	2:D:108:THR:CG2	2.43	0.49
1:E:312:VAL:HG12	1:E:312:VAL:O	2.13	0.49
1:E:331:PRO:O	1:E:336:MET:HG3	2.12	0.49
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.95	0.49
1:A:62:TRP:CD1	1:A:66:ARG:HG3	2.47	0.49
2:D:53:PRO:HB3	2:D:72:VAL:HG21	1.94	0.49
1:C:361:LEU:HA	1:C:364:ALA:HB3	1.95	0.48
2:D:168:LEU:HD22	2:D:206:PHE:CD1	2.48	0.48
2:B:168:LEU:HD22	2:B:206:PHE:CG	2.47	0.48
1:A:362:LYS:O	1:A:366:THR:HG23	2.13	0.48
2:B:91:SER:OG	2:B:112:VAL:HG22	2.13	0.48
1:C:258:PHE:CD1	1:C:330:MET:HG2	2.49	0.48
1:E:170:LYS:HD2	1:E:180:ASP:OD2	2.13	0.48
1:E:185:ASN:O	1:E:189:LYS:HG3	2.14	0.48
2:F:35:HIS:CE1	2:F:50:ASN:HD22	2.31	0.48
2:F:159:LEU:HB2	2:F:166:ASN:OD1	2.14	0.48
2:F:87:THR:O	2:F:112:VAL:HG21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.49	0.48
1:E:3:GLU:OE2	1:E:6:LYS:CE	2.60	0.48
1:E:173:ASN:O	1:E:175:LYS:HD2	2.14	0.48
1:A:325:GLN:O	1:A:325:GLN:HG2	2.13	0.48
1:G:67:PHE:HB3	1:G:104:ILE:HD12	1.95	0.48
1:A:365:GLN:O	1:A:369:THR:OG1	2.31	0.47
2:F:91:SER:OG	2:F:112:VAL:HG22	2.14	0.47
1:G:185:ASN:O	1:G:189:LYS:HG3	2.13	0.47
1:G:205:ASN:OD1	1:G:206:ALA:N	2.47	0.47
1:G:170:LYS:HD2	1:G:180:ASP:OD2	2.14	0.47
2:B:68:ALA:HA	2:B:82:GLN:O	2.14	0.47
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.95	0.47
1:C:78:GLU:CD	1:C:102:LYS:HD3	2.35	0.47
1:C:66:ARG:NH2	3:K:2:GLC:O4	2.48	0.47
1:C:228:GLY:HA3	1:C:230:TRP:CH2	2.50	0.47
1:G:78:GLU:OE2	1:G:102:LYS:HD3	2.15	0.47
1:G:233:SER:HB2	1:G:298:PRO:HD3	1.97	0.47
1:G:302:VAL:HG12	1:G:304:LEU:H	1.79	0.47
2:H:159:LEU:HG	2:H:161:ASN:H	1.80	0.47
1:A:356:THR:OG1	1:A:359:GLU:HG2	2.14	0.47
1:C:357:VAL:O	1:C:361:LEU:HD12	2.15	0.47
1:G:344:ARG:HG2	1:G:348:ILE:HD12	1.95	0.47
2:F:89:GLU:OE2	2:H:40:ARG:NH1	2.48	0.47
2:B:35:HIS:CE1	2:B:50:ASN:HD22	2.33	0.46
2:B:98:ARG:HD3	2:B:103:TYR:HD1	1.81	0.46
1:A:189:LYS:HD3	1:A:358:ASP:OD1	2.14	0.46
2:F:51:ILE:HD11	2:F:56:GLY:HA2	1.97	0.46
1:G:341:TYR:CE1	1:G:344:ARG:NH2	2.84	0.46
2:F:53:PRO:HB3	2:F:72:VAL:HG21	1.98	0.46
1:E:344:ARG:NH2	3:L:2:GLC:H62	2.30	0.45
1:G:199:ILE:HA	1:G:204:MET:O	2.16	0.45
1:C:363:ASP:O	1:C:367:ARG:HG3	2.16	0.45
2:B:35:HIS:HB2	2:B:97:THR:CG2	2.46	0.45
1:C:229:PRO:HB3	1:C:232:TRP:CH2	2.51	0.45
1:C:193:THR:O	1:C:196:VAL:HG22	2.16	0.45
1:C:277:LYS:HE3	1:C:281:GLU:OE2	2.17	0.45
1:E:140:LYS:HD3	1:E:144:LYS:O	2.17	0.45
1:A:29:LYS:HA	2:B:100:LEU:HD12	1.99	0.45
1:C:331:PRO:HB2	1:C:336:MET:HE3	1.97	0.45
1:G:78:GLU:OE1	1:G:102:LYS:HD3	2.16	0.45
1:A:229:PRO:HB3	1:A:232:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LEU:HD21	2:D:81:MET:HB2	1.98	0.45
2:D:70:LEU:CD2	2:D:81:MET:HA	2.47	0.45
2:D:70:LEU:HD23	2:D:70:LEU:HA	1.64	0.45
1:E:66:ARG:HG2	1:E:66:ARG:HH11	1.81	0.45
1:G:258:PHE:HD2	1:G:340:TRP:CH2	2.35	0.45
1:C:77:ALA:HB2	1:C:273:LYS:HE3	1.98	0.45
1:G:176:TYR:CE1	1:G:331:PRO:HG3	2.52	0.45
1:A:45:GLU:O	1:A:48:PRO:HD2	2.16	0.44
2:D:40:ARG:HH11	2:D:40:ARG:HD2	1.40	0.44
1:A:158:TRP:CE2	1:A:258:PHE:CE2	3.05	0.44
2:B:40:ARG:NH1	2:B:91:SER:O	2.48	0.44
2:D:35:HIS:HB2	2:D:97:THR:CG2	2.48	0.44
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.52	0.44
1:C:312:VAL:HG12	1:C:312:VAL:O	2.17	0.44
2:B:97:THR:HG21	2:B:101:PHE:CD2	2.52	0.44
1:A:270:SER:O	1:A:273:LYS:NZ	2.50	0.44
1:E:167:TYR:CZ	1:E:170:LYS:HE3	2.53	0.44
2:H:189:ARG:HG2	2:H:193:VAL:CG2	2.47	0.44
1:A:220:GLY:HA2	5:A:401:HOH:O	2.18	0.44
2:D:242:LYS:HA	2:D:242:LYS:HD3	1.78	0.44
2:F:39:GLN:HB2	2:F:45:LEU:CD2	2.44	0.44
2:H:172:GLN:HB2	2:H:182:LEU:HD11	2.00	0.44
1:C:159:PRO:HG3	1:C:257:PRO:HA	2.00	0.44
2:D:168:LEU:HG	2:D:169:ALA:N	2.33	0.44
1:E:44:GLU:HG2	1:E:45:GLU:HG3	1.99	0.44
2:F:168:LEU:HG	2:F:169:ALA:N	2.32	0.44
1:G:44:GLU:HG2	1:G:45:GLU:HG3	1.99	0.44
1:C:59:ILE:HA	1:C:265:GLY:O	2.18	0.44
1:C:193:THR:HA	1:C:196:VAL:HG22	2.00	0.43
1:E:179:LYS:HD3	1:E:179:LYS:HA	1.67	0.43
2:F:210:ILE:CB	2:F:213:VAL:HG12	2.46	0.43
2:H:85:SER:O	2:H:85:SER:OG	2.30	0.43
2:D:170:TRP:CD2	2:D:208:LEU:HB2	2.53	0.43
1:G:6:LYS:NZ	1:G:34:LYS:NZ	2.66	0.43
2:H:35:HIS:CE1	2:H:50:ASN:HD22	2.36	0.43
1:G:171:TYR:O	1:G:172:GLU:HG3	2.19	0.43
2:B:88:SER:HA	2:B:112:VAL:CG2	2.49	0.43
1:C:129:TRP:HB3	1:C:194:PHE:CE1	2.53	0.43
2:F:153:LYS:HD2	2:F:204:THR:O	2.18	0.43
1:G:194:PHE:CE2	1:G:198:LEU:HD11	2.54	0.43
1:A:215:ALA:O	1:A:219:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:OE1	1:C:6:LYS:HE2	2.18	0.43
1:C:346:ALA:HB2	1:C:364:ALA:HB2	2.01	0.43
1:E:365:GLN:O	1:E:369:THR:OG1	2.33	0.43
2:F:62:GLU:HA	2:F:65:LYS:HD2	1.99	0.43
1:G:308:GLU:OE1	1:G:312:VAL:HG22	2.19	0.43
2:F:47:TRP:CZ2	2:F:49:GLY:HA2	2.54	0.43
1:G:79:ILE:HG13	1:G:81:PRO:HD3	2.00	0.43
2:H:174:LYS:HG2	2:H:219:ALA:HB2	1.99	0.43
1:A:175:LYS:HE2	1:A:175:LYS:HB3	1.67	0.43
1:A:233:SER:O	1:A:237:THR:HG23	2.19	0.43
2:D:34:MET:HB3	2:D:51:ILE:HG23	2.00	0.43
1:A:97:VAL:O	1:A:104:ILE:HG13	2.19	0.42
2:B:30:THR:HG22	2:B:54:GLY:HA2	2.01	0.42
1:G:51:ALA:HB3	1:G:75:LEU:HD13	2.00	0.42
1:G:287:ASP:O	1:G:291:GLU:HG3	2.18	0.42
2:B:149:THR:HG21	1:G:239:LYS:HD3	2.01	0.42
2:F:45:LEU:HD12	2:F:233:PHE:CE1	2.54	0.42
2:B:182:LEU:HA	2:B:193:VAL:HG21	2.01	0.42
1:C:204:MET:HE2	1:C:204:MET:HB3	1.71	0.42
1:G:1:LYS:HE3	1:G:269:ALA:HB1	2.02	0.42
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.78	0.42
1:C:195:LEU:HA	1:C:198:LEU:HD12	2.02	0.42
1:C:302:VAL:HG21	1:C:307:TYR:HD2	1.84	0.42
2:D:195:ASP:OD1	2:D:195:ASP:N	2.53	0.42
1:A:331:PRO:HD2	1:A:336:MET:CE	2.49	0.42
1:E:129:TRP:HB3	1:E:194:PHE:CE2	2.55	0.42
2:H:13:ARG:HD3	2:H:13:ARG:HA	1.67	0.42
1:A:277:LYS:HE3	1:A:281:GLU:OE2	2.18	0.42
2:B:20:LEU:HD22	2:B:108:THR:HG21	2.01	0.42
1:G:159:PRO:HG3	1:G:257:PRO:HA	2.01	0.42
2:B:36:TRP:HA	2:B:95:TYR:O	2.20	0.42
2:D:240:GLU:HG2	2:D:241:ILE:N	2.34	0.42
1:E:122:LEU:HD21	1:E:125:PRO:HA	2.01	0.42
1:E:254:PRO:HB3	1:E:326:LYS:HD3	2.02	0.42
2:F:94:TYR:O	2:F:107:GLY:HA2	2.20	0.42
1:A:110:VAL:HG22	1:A:301:ALA:HB3	2.00	0.42
1:E:215:ALA:O	1:E:219:LYS:HG3	2.19	0.42
2:B:88:SER:HA	2:B:112:VAL:HG23	2.01	0.42
2:B:168:LEU:HG	2:B:169:ALA:N	2.33	0.42
2:B:36:TRP:CD1	2:B:70:LEU:HD21	2.55	0.41
1:C:115:LEU:HD21	1:C:224:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:VAL:HG21	1:C:307:TYR:CD2	2.55	0.41
2:F:4:LEU:HA	2:F:23:LYS:O	2.20	0.41
1:A:46:LYS:O	1:A:50:VAL:HG22	2.19	0.41
1:C:355:GLN:OE1	1:C:360:ALA:HA	2.20	0.41
1:E:14:ASP:O	1:E:297:LYS:HD2	2.20	0.41
1:G:171:TYR:HB2	1:G:176:TYR:CE1	2.55	0.41
2:H:183:VAL:HG23	2:H:188:THR:O	2.20	0.41
1:A:68:GLY:HA3	1:A:332:ASN:O	2.19	0.41
2:D:170:TRP:CE2	2:D:208:LEU:HB2	2.55	0.41
1:E:51:ALA:HB3	1:E:75:LEU:HD13	2.02	0.41
1:G:66:ARG:HH12	1:G:341:TYR:HE2	1.62	0.41
1:A:158:TRP:CD1	1:A:258:PHE:CD2	3.09	0.41
2:F:47:TRP:CE3	2:F:61:ASP:HB2	2.56	0.41
2:D:40:ARG:HA	2:D:41:PRO:HD3	1.91	0.41
2:F:89:GLU:OE1	2:H:40:ARG:NH1	2.53	0.41
1:E:151:LEU:HD11	1:E:204:MET:HE2	2.03	0.41
1:G:331:PRO:CD	1:G:336:MET:HE3	2.47	0.41
2:H:13:ARG:HD2	2:H:14:PRO:HD3	2.02	0.41
1:C:192:LEU:CD2	1:C:361:LEU:HD11	2.42	0.41
1:G:331:PRO:O	1:G:336:MET:HG3	2.20	0.41
2:D:7:PRO:O	2:D:108:THR:HG22	2.21	0.41
2:D:69:THR:HG23	2:D:82:GLN:HB3	2.02	0.41
2:F:112:VAL:CG2	2:F:112:VAL:O	2.68	0.41
1:A:168:ALA:O	1:A:181:VAL:HA	2.21	0.41
2:B:135:GLN:NE2	2:B:221:TYR:O	2.47	0.41
1:C:205:ASN:ND2	1:C:207:ASP:CG	2.75	0.41
1:C:291:GLU:O	1:C:295:LYS:HB2	2.21	0.41
1:G:341:TYR:HE1	1:G:344:ARG:NH2	2.19	0.41
1:A:52:ALA:C	1:A:54:GLY:H	2.23	0.41
2:B:166:ASN:O	2:B:185:PHE:HA	2.21	0.41
1:C:304:LEU:HD23	1:C:307:TYR:HB2	2.03	0.41
1:E:109:ALA:HA	1:E:302:VAL:HA	2.04	0.40
1:A:61:PHE:HA	1:A:263:SER:O	2.22	0.40
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.57	0.40
1:C:66:ARG:NH2	1:C:341:TYR:CZ	2.89	0.40
1:G:302:VAL:CG1	1:G:304:LEU:H	2.34	0.40
1:A:349:ASN:HB3	1:A:355:GLN:HB2	2.04	0.40
2:D:20:LEU:O	2:D:80:TYR:HA	2.21	0.40
1:G:364:ALA:O	1:G:368:ILE:HG13	2.22	0.40
1:A:59:ILE:HA	1:A:265:GLY:O	2.21	0.40
2:F:29:PHE:CZ	2:F:72:VAL:CG2	3.05	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:C:175:LYS:NZ	1:E:219:LYS:NZ[2_957]	1.06	1.14
1:C:175:LYS:NZ	1:E:219:LYS:CE[2_957]	2.14	0.06

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	367/369 (100%)	359 (98%)	8 (2%)	0	100	100
1	C	367/369 (100%)	359 (98%)	7 (2%)	1 (0%)	41	61
1	E	367/369 (100%)	360 (98%)	7 (2%)	0	100	100
1	G	367/369 (100%)	359 (98%)	8 (2%)	0	100	100
2	B	219/251 (87%)	209 (95%)	9 (4%)	1 (0%)	29	48
2	D	217/251 (86%)	207 (95%)	9 (4%)	1 (0%)	29	48
2	F	218/251 (87%)	211 (97%)	7 (3%)	0	100	100
2	H	218/251 (87%)	207 (95%)	11 (5%)	0	100	100
All	All	2340/2480 (94%)	2271 (97%)	66 (3%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	337	SER
2	D	165	LYS
2	B	44	GLY

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	297/297 (100%)	291 (98%)	6 (2%)	55 79
1	C	297/297 (100%)	294 (99%)	3 (1%)	76 90
1	E	297/297 (100%)	294 (99%)	3 (1%)	76 90
1	G	297/297 (100%)	291 (98%)	6 (2%)	55 79
2	B	192/206 (93%)	192 (100%)	0	100 100
2	D	191/206 (93%)	191 (100%)	0	100 100
2	F	192/206 (93%)	190 (99%)	2 (1%)	76 90
2	H	192/206 (93%)	190 (99%)	2 (1%)	76 90
All	All	1955/2012 (97%)	1933 (99%)	22 (1%)	73 89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	88	LYS
1	A	229	PRO
1	A	233	SER
1	A	313	LYS
1	A	336	MET
1	C	233	SER
1	C	258	PHE
1	C	335	GLN
1	E	1	LYS
1	E	233	SER
1	E	258	PHE
2	F	195	ASP
2	F	243	ARG
1	G	3	GLU
1	G	6	LYS
1	G	233	SER
1	G	258	PHE
1	G	358	ASP
1	G	367	ARG
2	H	17	SER
2	H	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	D	164	GLN
2	F	50	ASN
2	F	59	ASN
1	G	355	GLN
2	H	50	ASN
2	H	214	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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	J	1	3	12,12,12	0.57	0	17,17,17	0.64	0
3	GLC	J	2	3	11,11,12	0.60	0	15,15,17	1.16	1 (6%)
3	GLC	K	1	3	12,12,12	0.65	0	17,17,17	1.05	1 (5%)
3	GLC	K	2	3	11,11,12	1.11	0	15,15,17	2.82	5 (33%)
3	GLC	L	1	3	12,12,12	0.58	0	17,17,17	1.27	2 (11%)
3	GLC	L	2	3	11,11,12	0.57	0	15,15,17	0.96	0
3	GLC	M	1	3	12,12,12	0.62	0	17,17,17	1.05	1 (5%)
3	GLC	M	2	3	11,11,12	0.92	0	15,15,17	1.84	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	1/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	2/2/19/22	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	GLC	O3-C3-C2	-8.00	94.67	109.99
3	K	2	GLC	O5-C5-C6	-4.63	99.94	107.20
3	M	2	GLC	O4-C4-C3	-3.90	101.34	110.35
3	M	2	GLC	O4-C4-C5	3.07	116.91	109.30
3	K	2	GLC	C1-C2-C3	2.90	113.23	109.67
3	L	1	GLC	C1-C2-C3	2.74	116.00	110.31
3	K	2	GLC	C6-C5-C4	2.68	119.27	113.00
3	K	2	GLC	C1-O5-C5	2.60	115.71	112.19
3	L	1	GLC	C3-C4-C5	2.53	114.75	110.24
3	M	2	GLC	C2-C3-C4	-2.45	106.66	110.89
3	M	1	GLC	O5-C5-C4	-2.41	105.31	109.69
3	K	1	GLC	C1-C2-C3	2.25	114.99	110.31
3	J	2	GLC	O5-C5-C6	2.01	110.36	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	GLC	C4-C5-C6-O6
3	M	2	GLC	O5-C5-C6-O6
3	L	2	GLC	C4-C5-C6-O6
3	K	2	GLC	O5-C5-C6-O6
3	L	2	GLC	O5-C5-C6-O6

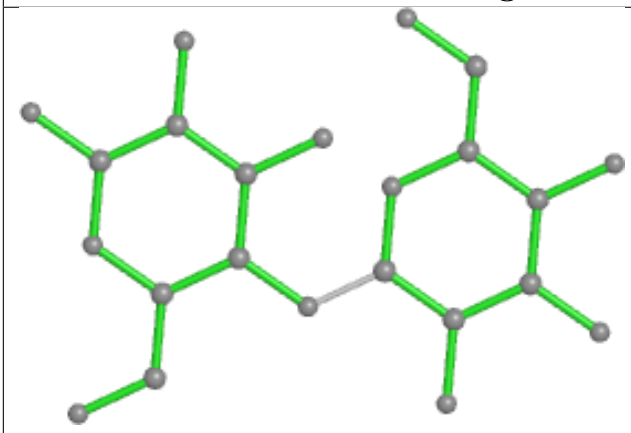
There are no ring outliers.

3 monomers are involved in 7 short contacts:

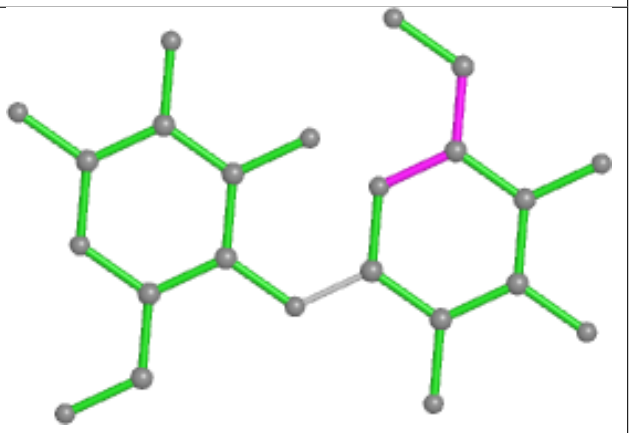
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	GLC	2	0
3	L	2	GLC	1	0
3	K	2	GLC	4	0

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

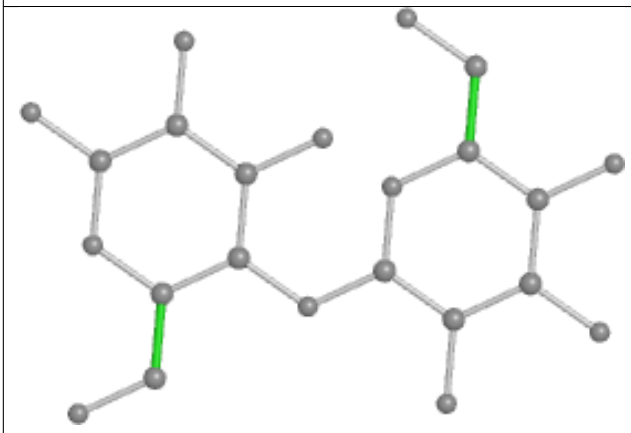
Oligosaccharide Chain J



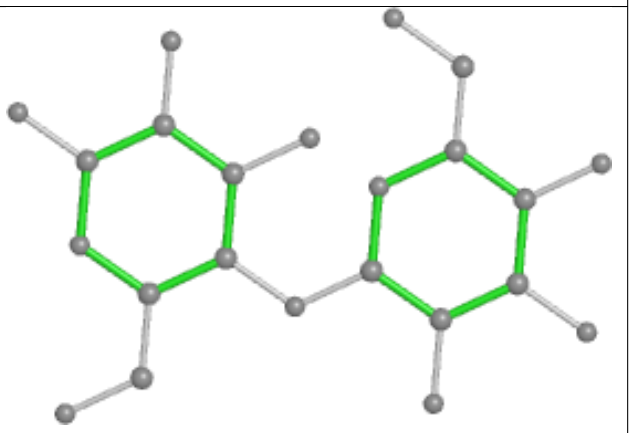
Bond lengths



Bond angles

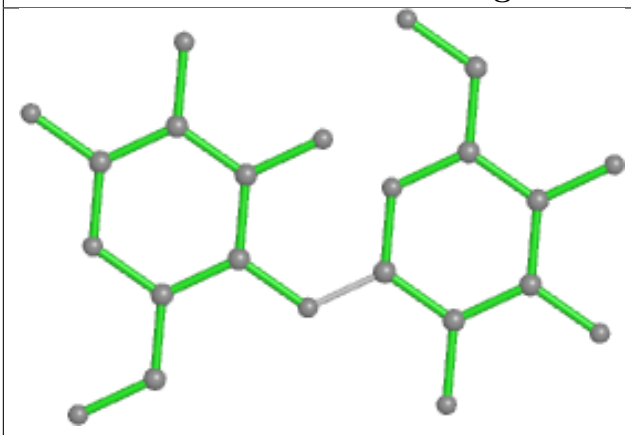


Torsions

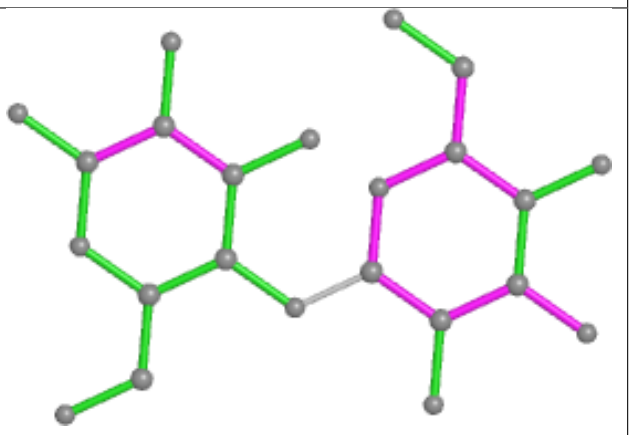


Rings

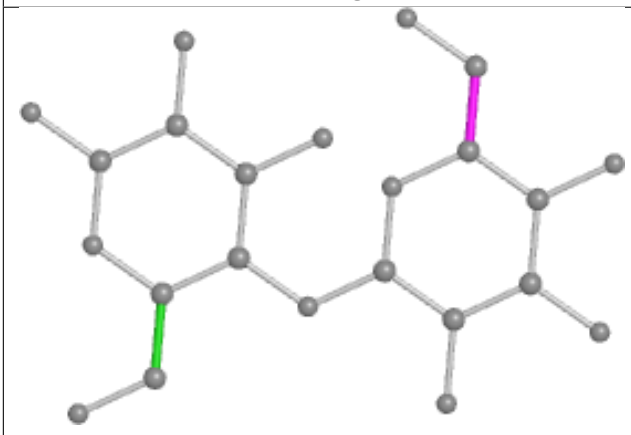
Oligosaccharide Chain K



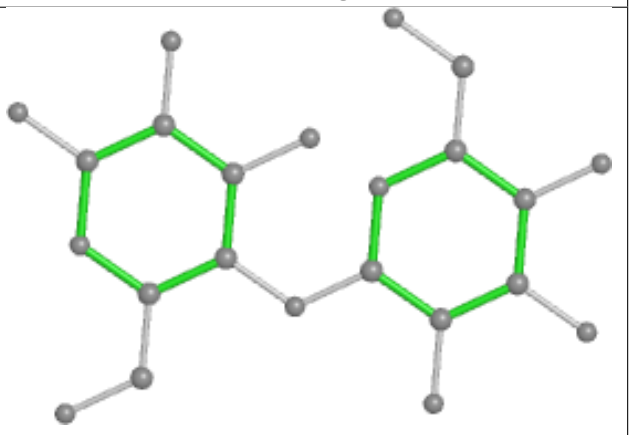
Bond lengths



Bond angles

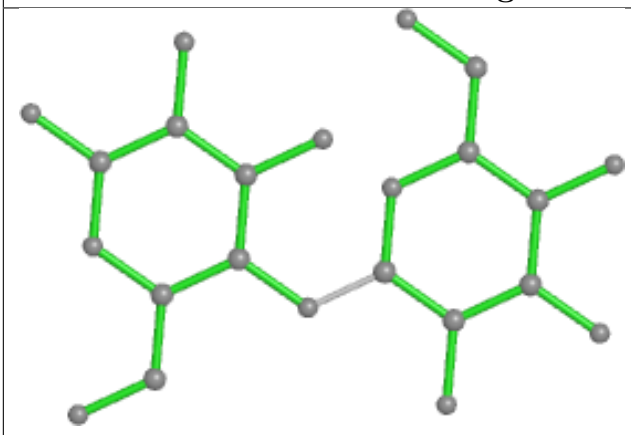


Torsions

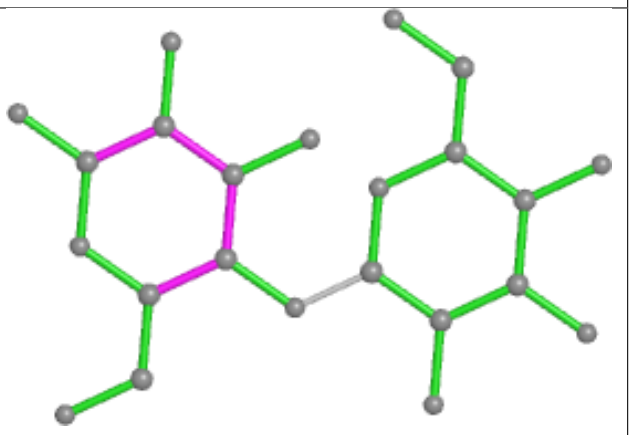


Rings

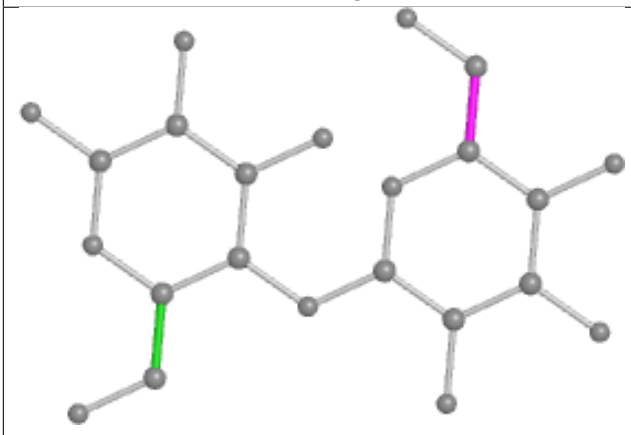
Oligosaccharide Chain L



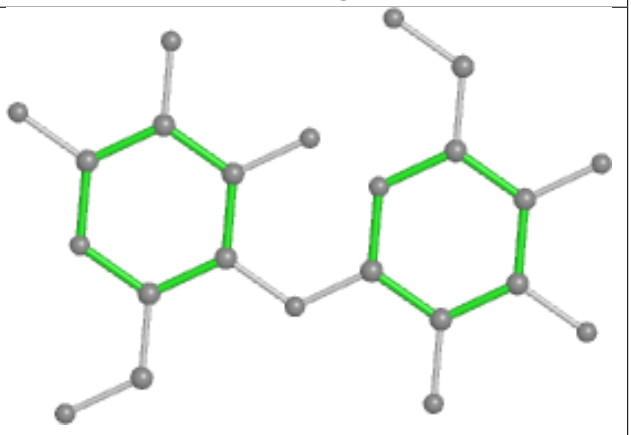
Bond lengths



Bond angles

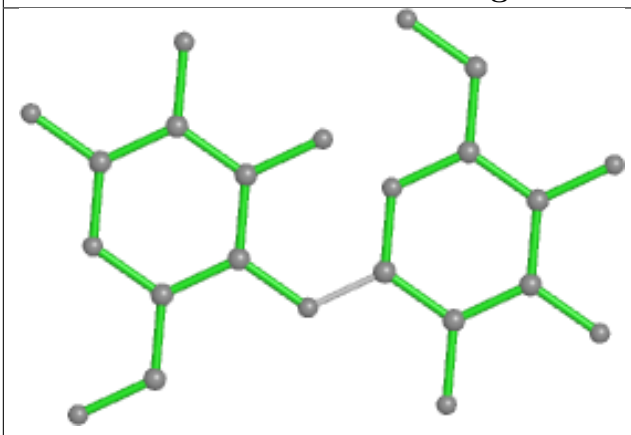


Torsions

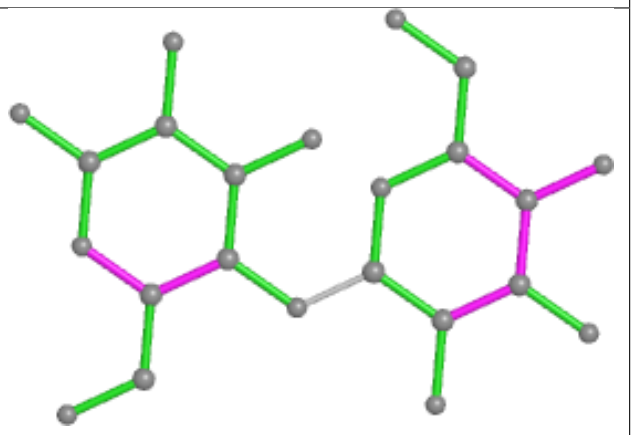


Rings

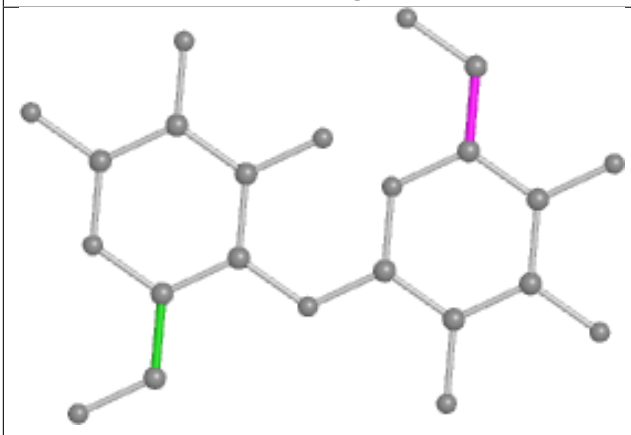
Oligosaccharide Chain M



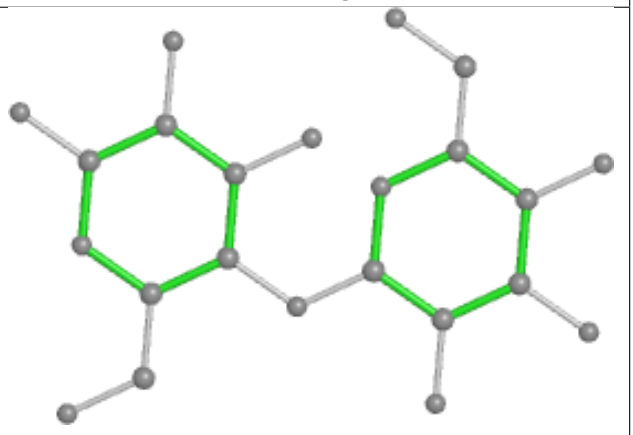
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

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, 95^{th} 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	369/369 (100%)	0.02	10 (2%)	54	58	47, 61, 78, 106	0
1	C	369/369 (100%)	0.21	18 (4%)	29	31	50, 66, 97, 110	0
1	E	369/369 (100%)	0.02	13 (3%)	44	47	45, 59, 77, 101	0
1	G	369/369 (100%)	0.12	22 (5%)	21	22	49, 68, 88, 97	0
2	B	225/251 (89%)	0.19	11 (4%)	29	31	53, 65, 83, 97	0
2	D	223/251 (88%)	0.35	11 (4%)	29	31	54, 69, 90, 113	0
2	F	224/251 (89%)	0.20	14 (6%)	20	21	50, 65, 82, 111	0
2	H	224/251 (89%)	0.27	11 (4%)	29	31	55, 69, 84, 113	0
All	All	2372/2480 (95%)	0.15	110 (4%)	32	34	45, 65, 87, 113	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	341	TYR	5.1
2	F	243	ARG	4.7
2	D	13	ARG	4.3
2	H	1	GLN	4.3
1	G	1	LYS	4.3
2	H	161	ASN	4.2
1	C	354	ARG	4.0
1	C	174	GLY	3.8
2	H	243	ARG	3.8
1	C	341	TYR	3.8
1	C	172	GLU	3.4
1	E	173	ASN	3.3
2	F	1	GLN	3.3
1	A	173	ASN	3.2
2	D	221	TYR	3.1
2	F	159	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	186	ALA	3.1
1	A	312	VAL	3.0
2	F	161	ASN	3.0
2	D	1	GLN	2.9
1	A	179	LYS	2.9
1	G	116	ILE	2.9
2	B	36	TRP	2.8
1	C	173	ASN	2.8
1	G	355	GLN	2.8
2	B	160	ILE	2.8
1	A	52	ALA	2.8
2	B	13	ARG	2.8
1	C	359	GLU	2.7
1	G	175	LYS	2.7
2	B	168	LEU	2.7
2	H	160	ILE	2.7
1	C	202	LYS	2.7
2	H	106	GLN	2.6
1	E	172	GLU	2.6
1	A	172	GLU	2.6
1	A	171	TYR	2.6
1	E	109	ALA	2.5
2	B	223	CYS	2.5
2	D	75	SER	2.5
2	D	36	TRP	2.5
1	C	175	LYS	2.5
2	D	169	ALA	2.5
2	B	169	ALA	2.5
1	G	171	TYR	2.4
2	H	36	TRP	2.4
1	E	362	LYS	2.4
1	E	171	TYR	2.4
1	E	108	ILE	2.4
1	A	1	LYS	2.4
1	G	53	THR	2.4
2	B	66	SER	2.4
1	C	207	ASP	2.4
1	A	264	ALA	2.4
2	F	169	ALA	2.4
1	G	54	GLY	2.3
2	H	66	SER	2.3
1	C	179	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	3	GLU	2.3
1	G	146	ALA	2.3
1	E	312	VAL	2.3
2	B	34	MET	2.3
2	B	42	GLY	2.3
1	C	158	TRP	2.3
2	H	34	MET	2.2
2	H	170	TRP	2.2
1	E	313	LYS	2.2
1	C	327	GLY	2.2
2	D	106	GLN	2.2
2	D	34	MET	2.2
2	F	2	VAL	2.2
1	C	102	LYS	2.2
1	G	141	ALA	2.2
2	F	97	THR	2.2
1	G	9	ILE	2.2
1	G	45	GLU	2.2
1	G	6	LYS	2.2
2	F	208	LEU	2.2
2	F	5	GLN	2.2
1	A	108	ILE	2.2
2	D	42	GLY	2.2
1	G	192	LEU	2.2
2	F	3	GLN	2.1
2	F	25	SER	2.2
1	G	264	ALA	2.1
2	F	160	ILE	2.1
2	F	41	PRO	2.1
1	G	354	ARG	2.1
1	G	61	PHE	2.1
2	H	221	TYR	2.1
1	A	87	ASP	2.1
1	G	52	ALA	2.1
1	G	60	ILE	2.1
2	F	168	LEU	2.1
1	C	72	GLN	2.1
2	D	175	PRO	2.0
1	G	183	VAL	2.0
2	B	191	SER	2.0
2	D	80	TYR	2.0
2	H	32	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	192	LEU	2.0
1	E	107	PRO	2.0
1	E	179	LYS	2.0
1	G	219	LYS	2.0
1	C	74	GLY	2.0
1	G	367	ARG	2.0
1	E	328	GLU	2.0
1	C	325	GLN	2.0
1	C	171	TYR	2.0
2	B	221	TYR	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)

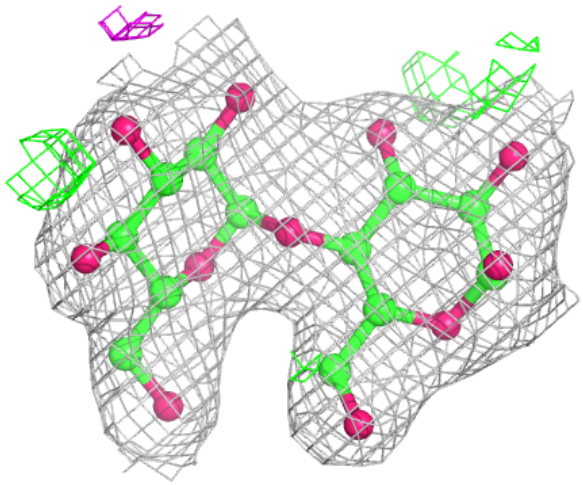
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

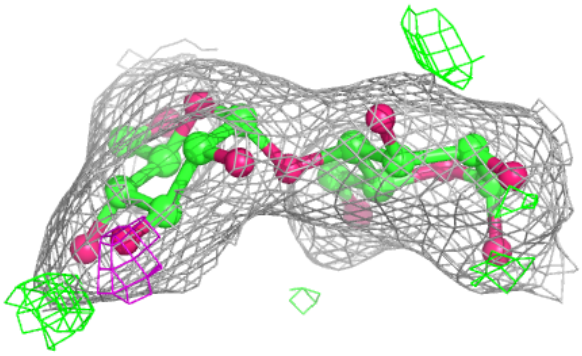
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	K	2	11/12	0.90	0.14	53,65,77,78	0
3	GLC	K	1	12/12	0.96	0.12	54,56,61,64	0
3	GLC	L	1	12/12	0.96	0.10	47,52,58,59	0
3	GLC	L	2	11/12	0.96	0.13	52,54,59,64	0
3	GLC	M	1	12/12	0.96	0.11	60,63,67,69	0
3	GLC	M	2	11/12	0.96	0.12	62,65,71,73	0
3	GLC	J	2	11/12	0.97	0.13	51,58,61,61	0
3	GLC	J	1	12/12	0.98	0.09	51,58,62,62	0

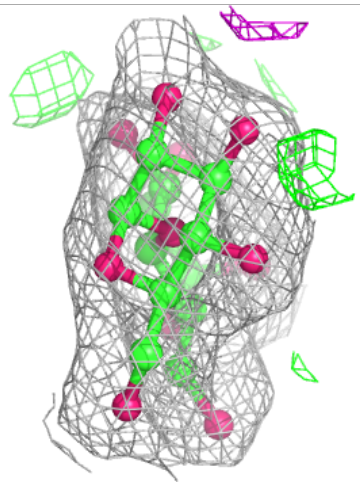
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

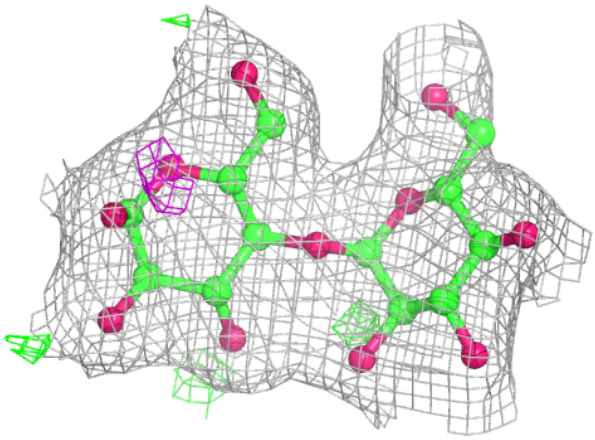


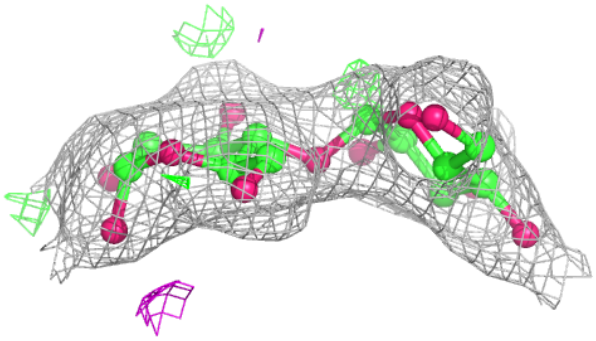


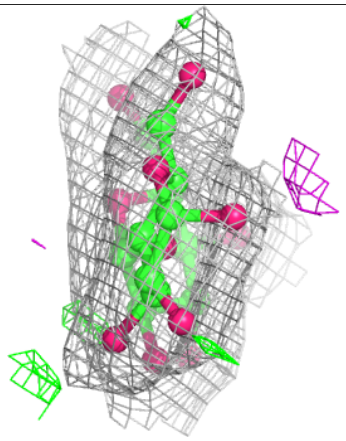


Electron density around Chain K:

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

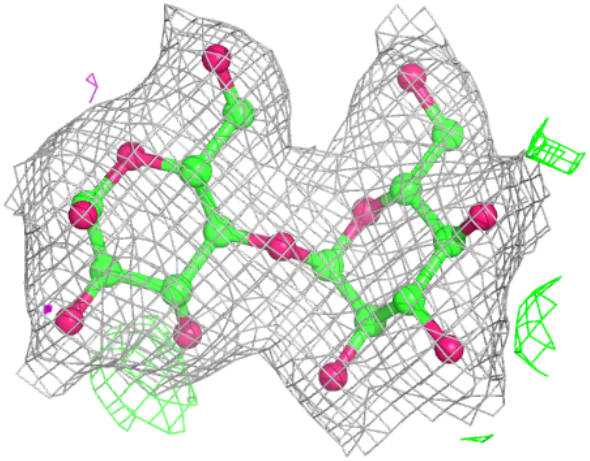


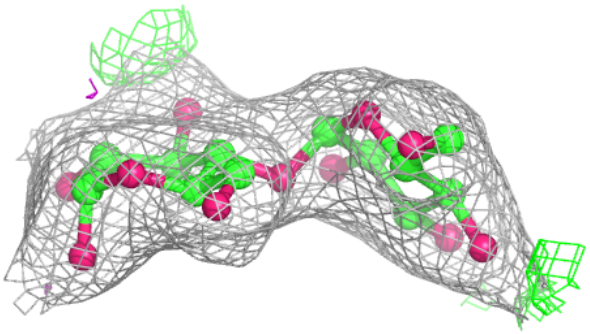


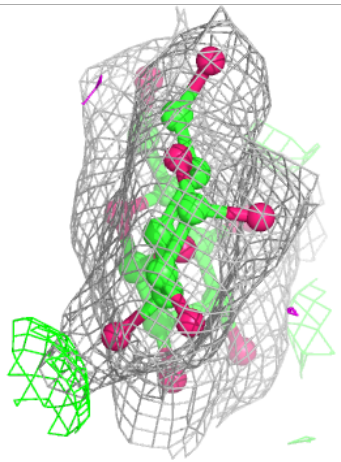


Electron density around Chain L:

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

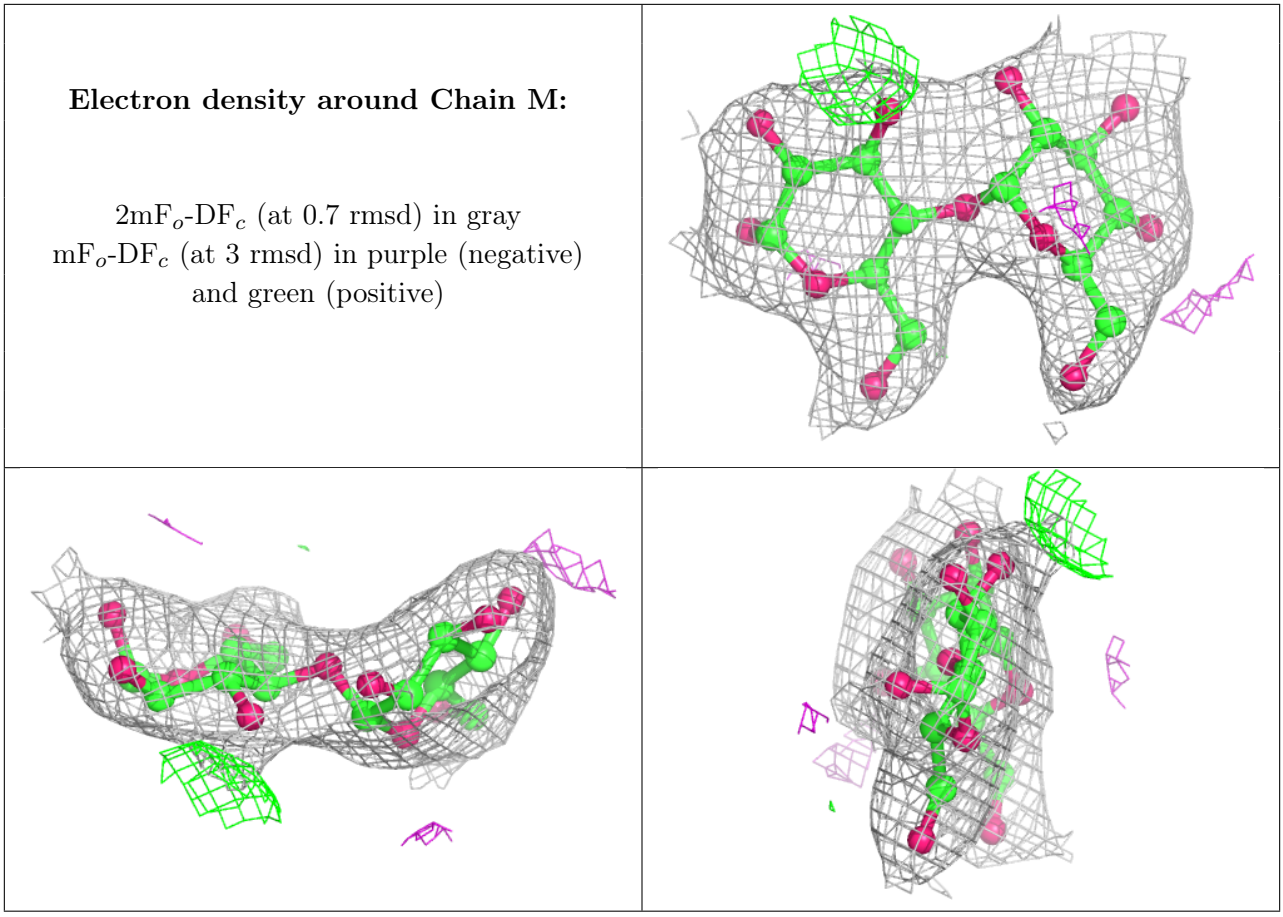






Electron density around Chain M:

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



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, 95^{th} 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
4	CL	H	301	1/1	0.90	0.18	75,75,75,75	0
4	CL	F	301	1/1	0.91	0.07	81,81,81,81	0
4	CL	B	301	1/1	0.91	0.08	79,79,79,79	0

6.5 Other polymers

There are no such residues in this entry.