



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 05:50 AM EST

PDB ID : 1TEX  
Title : Mycobacterium smegmatis Stf0 Sulfotransferase with Trehalose  
Authors : Mougous, J.D.; Petzold, C.J.; Senaratne, R.H.; Lee, D.H.; Akey, D.L.; Lin, F.L.; Munchel, S.E.; Pratt, M.R.; Riley, L.W.; Leary, J.A.; Berger, J.M.; Bertozzi, C.R.  
Deposited on : 2004-05-25  
Resolution : 2.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

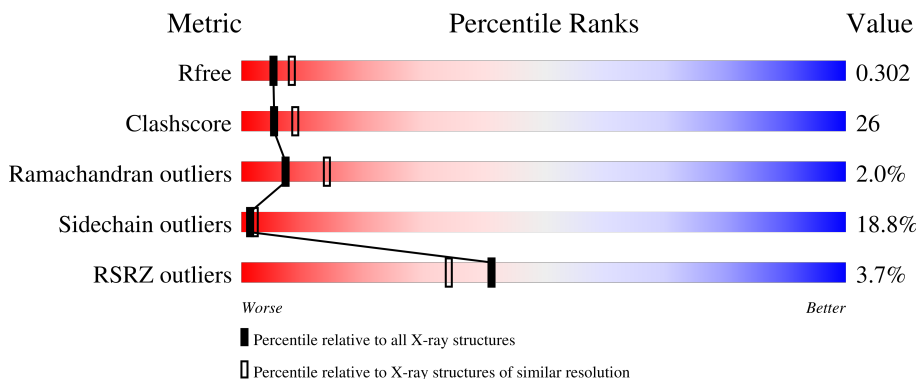
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.




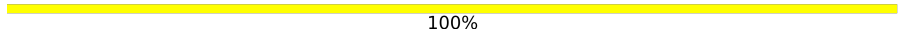
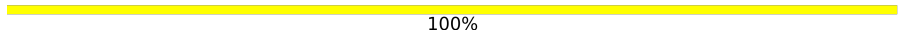
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	287	
1	B	287	
1	C	287	
1	D	287	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 100%
2	H	2	 100%

## 2 Entry composition [i](#)

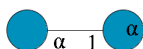
There are 3 unique types of molecules in this entry. The entry contains 7919 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Stf0 Sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	Total 1794	C 1145	N 312	O 334	S 3	0	0	0
1	B	243	Total 1853	C 1183	N 327	O 340	S 3	0	0	0
1	C	244	Total 1883	C 1205	N 326	O 349	S 3	0	0	0
1	D	247	Total 1887	C 1212	N 329	O 343	S 3	0	0	0

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	63	Total 63	O 63	0	0
3	B	113	Total 113	O 113	0	0

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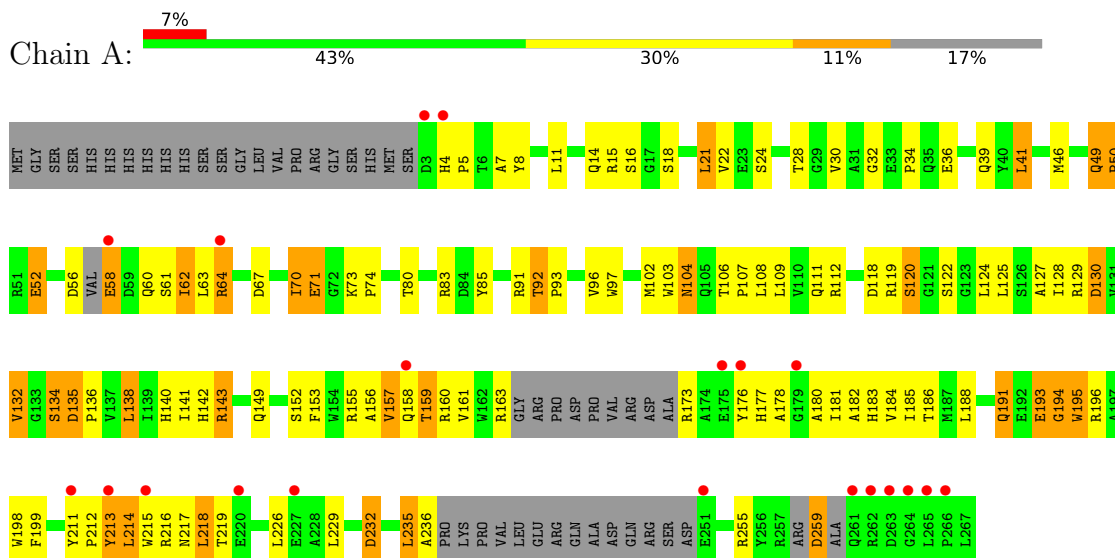
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	C	138	Total 138	O 138	0	0
3	D	96	Total 96	O 96	0	0

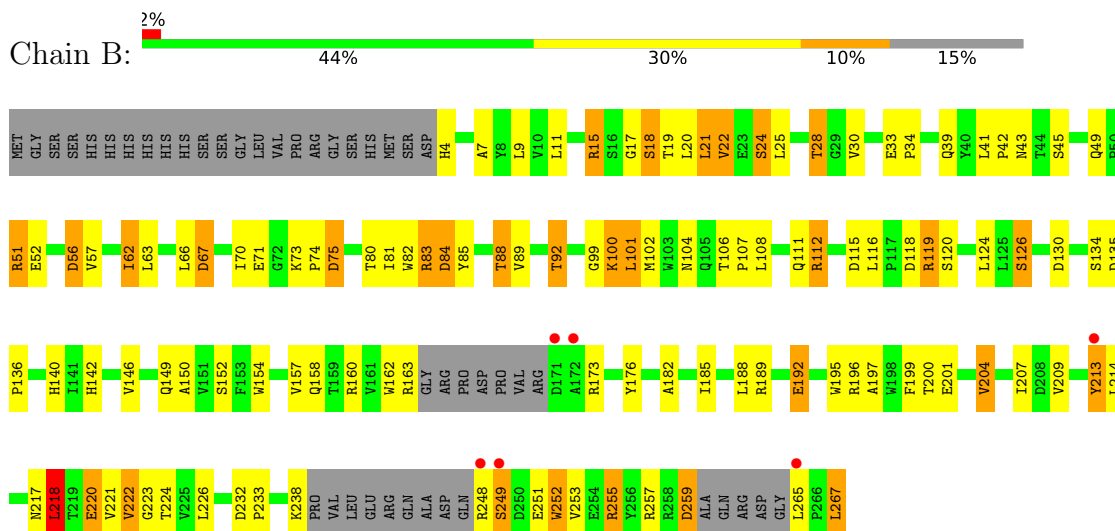
### 3 Residue-property plots i

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: Stf0 Sulfotransferase

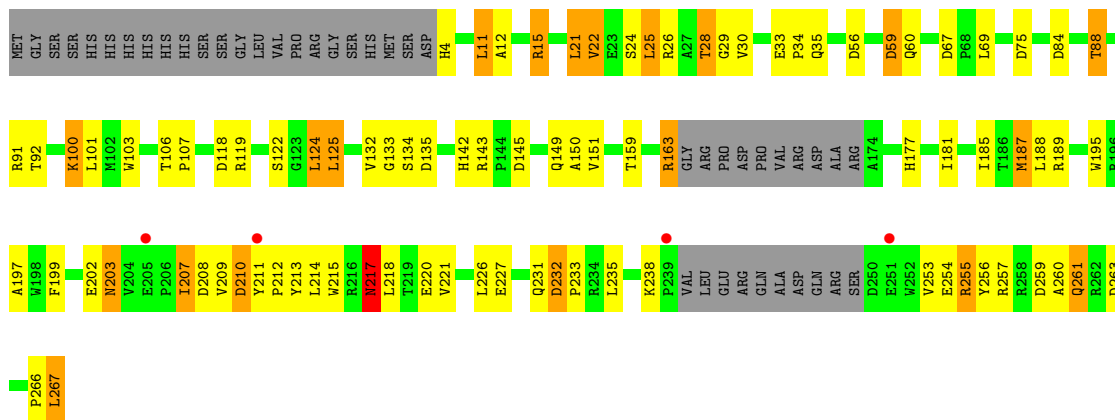


- Molecule 1: Stf0 Sulfotransferase

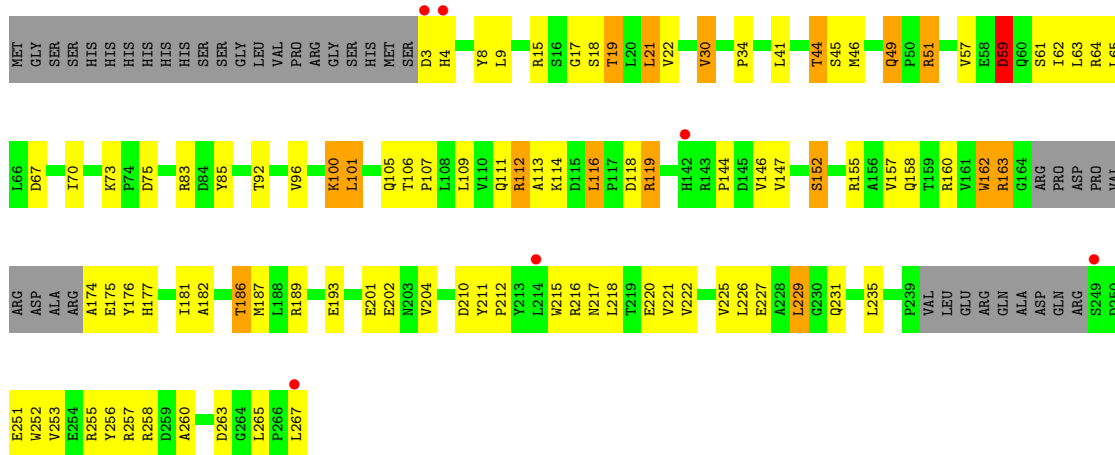


- Molecule 1: Stf0 Sulfotransferase





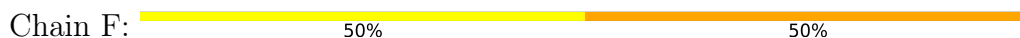
• Molecule 1: Stf0 Sulfotransferase



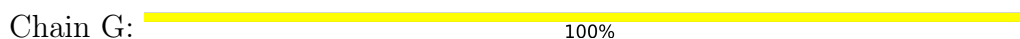
• Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



• Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



• Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain H:

100%

GLC1  
GLC2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.93Å 101.93Å 228.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.60 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.60) 97.6 (14.99-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.218 , 0.274 0.255 , 0.302	Depositor DCC
$R_{free}$ test set	2106 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.6	Xtrriage
Anisotropy	0.002	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.75	0/1839	0.83	5/2520 (0.2%)
1	B	0.85	1/1899 (0.1%)	0.89	4/2601 (0.2%)
1	C	0.91	0/1933	1.01	11/2650 (0.4%)
1	D	0.86	2/1939 (0.1%)	0.90	4/2662 (0.2%)
All	All	0.85	3/7610 (0.0%)	0.91	24/10433 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	TYR	CD2-CE2	5.44	1.47	1.39
1	B	252	TRP	CB-CG	5.43	1.60	1.50
1	D	162	TRP	CB-CG	-5.24	1.40	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	ASP	CB-CG-OD2	10.32	127.58	118.30
1	B	84	ASP	CB-CG-OD2	7.61	125.15	118.30
1	D	59	ASP	CB-CG-OD2	7.30	124.87	118.30
1	C	84	ASP	CB-CG-OD2	6.96	124.57	118.30
1	C	259	ASP	CB-CG-OD2	6.84	124.46	118.30
1	D	67	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	67	ASP	CB-CG-OD2	6.59	124.23	118.30
1	C	75	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	A	259	ASP	CB-CG-OD2	6.04	123.74	118.30
1	C	263	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	67	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	56	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	135	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	59	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	LEU	CB-CG-CD2	5.59	120.51	111.00
1	D	75	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	135	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	145	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	56	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	67	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	263	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	232	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	75	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	130	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1794	0	1647	93	0
1	B	1853	0	1765	121	0
1	C	1883	0	1801	100	0
1	D	1887	0	1805	74	0
2	E	23	0	21	5	0
2	F	23	0	21	2	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	63	0	0	24	0
3	B	113	0	0	38	0
3	C	138	0	0	29	0
3	D	96	0	0	18	0
All	All	7919	0	7102	383	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 26.

All (383) 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:C:122:SER:HB3	3:C:580:HOH:O	1.29	1.28
1:D:44:THR:CG2	1:D:46:MET:HB2	1.75	1.16
1:C:15:ARG:HG3	1:C:15:ARG:HH11	1.06	1.11
1:C:28:THR:HG22	1:C:30:VAL:H	1.18	1.07
1:B:249:SER:HA	3:B:513:HOH:O	1.53	1.06
1:B:257:ARG:NH1	1:C:197:ALA:HB2	1.75	1.00
1:B:74:PRO:HD2	3:B:557:HOH:O	1.64	0.97
1:B:49:GLN:HE22	1:B:70:ILE:H	1.13	0.95
1:D:158:GLN:HE22	1:D:175:GLU:H	0.97	0.94
1:B:51:ARG:HG3	1:B:51:ARG:HH11	1.29	0.94
1:A:156:ALA:HA	1:A:159:THR:CG2	1.96	0.94
1:A:104:ASN:HB3	1:A:191:GLN:HE21	1.30	0.94
1:D:44:THR:HG22	1:D:46:MET:HB2	1.51	0.91
1:B:238:LYS:HA	3:B:508:HOH:O	1.69	0.91
1:C:217:ASN:N	1:C:217:ASN:HD22	1.68	0.90
1:A:85:TYR:CE2	3:A:524:HOH:O	2.26	0.88
1:B:207:ILE:HG22	1:B:207:ILE:O	1.73	0.88
1:C:15:ARG:HG3	1:C:15:ARG:NH1	1.89	0.87
1:C:25:LEU:O	1:C:28:THR:HB	1.75	0.87
1:C:91:ARG:HD3	3:C:540:HOH:O	1.73	0.85
1:D:19:THR:HG22	1:D:100:LYS:HE3	1.57	0.84
1:C:28:THR:HG23	1:C:30:VAL:HB	1.60	0.83
1:D:44:THR:HG21	1:D:46:MET:HB2	1.58	0.83
1:C:15:ARG:HH11	1:C:15:ARG:CG	1.91	0.83
1:C:142:HIS:HE1	1:C:208:ASP:OD2	1.62	0.82
1:A:103:TRP:HB3	1:A:191:GLN:HG2	1.61	0.81
1:A:156:ALA:HA	1:A:159:THR:HG22	1.62	0.81
1:B:73:LYS:HB2	3:B:557:HOH:O	1.79	0.81
1:C:266:PRO:HA	3:C:606:HOH:O	1.81	0.81
1:B:20:LEU:O	1:B:24:SER:HB2	1.81	0.80
1:B:119:ARG:HH12	1:B:126:SER:HB2	1.48	0.79
1:B:118:ASP:O	1:B:119:ARG:C	2.20	0.79
1:A:122:SER:HB3	3:A:549:HOH:O	1.83	0.79
1:A:91:ARG:CB	3:A:563:HOH:O	2.30	0.78
1:B:49:GLN:NE2	1:B:70:ILE:H	1.80	0.78
1:B:257:ARG:HH11	1:C:197:ALA:HB2	1.48	0.78
1:D:44:THR:HG22	1:D:46:MET:N	1.98	0.78
1:C:21:LEU:HD22	1:C:25:LEU:HD22	1.66	0.77
1:A:85:TYR:HB2	3:A:547:HOH:O	1.83	0.77
1:D:30:VAL:HG13	1:D:231:GLN:HG3	1.66	0.77
1:B:22:VAL:HG11	1:B:100:LYS:HZ2	1.50	0.76
1:C:28:THR:HG22	1:C:30:VAL:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PRO:HD2	3:D:565:HOH:O	1.85	0.75
1:B:51:ARG:HH11	1:B:51:ARG:CG	1.99	0.75
1:B:259:ASP:C	3:B:610:HOH:O	2.25	0.75
1:D:158:GLN:HE22	1:D:175:GLU:N	1.81	0.75
1:B:115:ASP:HB2	3:B:549:HOH:O	1.86	0.75
1:B:57:VAL:HG11	1:B:62:ILE:HG12	1.69	0.74
1:B:25:LEU:O	1:B:28:THR:HG23	1.88	0.74
1:B:80:THR:HG23	3:B:564:HOH:O	1.87	0.74
1:B:118:ASP:C	1:B:119:ARG:O	2.24	0.74
1:B:108:LEU:HA	3:B:562:HOH:O	1.88	0.73
1:C:217:ASN:N	1:C:217:ASN:ND2	2.34	0.73
3:A:521:HOH:O	2:E:2:GLC:C6	2.37	0.73
1:C:142:HIS:CE1	1:C:208:ASP:OD2	2.42	0.72
1:C:163:ARG:HG3	1:C:163:ARG:NH1	2.05	0.72
1:C:202:GLU:HB3	3:C:598:HOH:O	1.90	0.72
1:B:257:ARG:NH2	3:B:524:HOH:O	2.22	0.72
1:D:22:VAL:HG13	1:D:34:PRO:HG2	1.72	0.72
1:D:160:ARG:CB	3:D:600:HOH:O	2.37	0.71
1:A:155:ARG:O	1:A:159:THR:HG22	1.90	0.71
1:A:143:ARG:HG3	1:A:211:TYR:CD2	2.24	0.71
1:C:227:GLU:HG2	1:C:233:PRO:HG3	1.70	0.71
1:B:118:ASP:O	1:B:119:ARG:O	2.09	0.70
1:B:43:ASN:CB	3:B:517:HOH:O	2.39	0.70
1:B:217:ASN:O	1:B:218:LEU:C	2.29	0.69
1:C:125:LEU:HD11	3:C:583:HOH:O	1.92	0.69
1:A:158:GLN:HA	3:A:519:HOH:O	1.93	0.69
1:C:100:LYS:CE	3:C:539:HOH:O	2.40	0.69
1:C:207:ILE:H	1:C:207:ILE:CD1	2.06	0.68
1:A:5:PRO:HD2	3:A:506:HOH:O	1.93	0.68
1:B:112:ARG:NE	3:B:529:HOH:O	2.27	0.68
1:C:266:PRO:HB3	3:C:588:HOH:O	1.93	0.68
1:B:176:TYR:HD1	1:B:252:TRP:CD1	2.12	0.67
1:D:252:TRP:CZ2	3:D:519:HOH:O	2.46	0.67
1:C:163:ARG:HG3	1:C:163:ARG:HH11	1.59	0.66
1:A:62:ILE:O	1:A:64:ARG:N	2.29	0.66
1:C:28:THR:CG2	1:C:30:VAL:H	2.02	0.66
1:B:140:HIS:CE1	3:B:615:HOH:O	2.48	0.66
1:C:261:GLN:HG2	3:C:633:HOH:O	1.95	0.65
1:B:62:ILE:HG13	1:B:63:LEU:N	2.12	0.65
1:B:83:ARG:HD3	3:B:613:HOH:O	1.97	0.65
1:C:4:HIS:CB	3:C:513:HOH:O	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLN:NE2	1:B:188:LEU:HD13	2.12	0.65
1:C:177:HIS:O	1:C:181:ILE:HD12	1.97	0.64
1:C:215:TRP:CB	3:C:586:HOH:O	2.45	0.64
3:A:521:HOH:O	2:E:2:GLC:H61	1.95	0.64
1:C:28:THR:CG2	1:C:30:VAL:HB	2.28	0.64
1:B:100:LYS:HE2	3:B:561:HOH:O	1.98	0.64
1:B:207:ILE:O	1:B:207:ILE:CG2	2.44	0.64
1:C:151:VAL:CB	3:C:630:HOH:O	2.44	0.64
1:B:146:VAL:HG21	1:B:189:ARG:CZ	2.27	0.64
3:A:547:HOH:O	1:B:85:TYR:CE1	2.50	0.63
1:D:44:THR:HG22	1:D:46:MET:CB	2.25	0.63
1:A:85:TYR:CZ	3:A:524:HOH:O	2.50	0.63
1:C:11:LEU:HG	1:C:195:TRP:CH2	2.34	0.63
1:A:62:ILE:CG2	1:A:180:ALA:HB2	2.30	0.62
1:C:210:ASP:HB3	3:C:613:HOH:O	1.99	0.62
1:B:112:ARG:HD3	3:B:608:HOH:O	1.99	0.62
1:D:51:ARG:HH11	1:D:51:ARG:HG2	1.63	0.62
1:B:22:VAL:HG11	1:B:100:LYS:NZ	2.15	0.62
1:C:125:LEU:CD1	3:C:583:HOH:O	2.47	0.62
1:C:217:ASN:ND2	1:C:217:ASN:H	1.96	0.62
1:A:11:LEU:HB3	1:A:195:TRP:CZ2	2.35	0.62
1:D:112:ARG:NH1	3:D:598:HOH:O	2.31	0.62
1:D:155:ARG:CZ	3:D:519:HOH:O	2.47	0.62
1:B:82:TRP:CE2	1:B:112:ARG:HD2	2.34	0.61
1:A:41:LEU:HB3	3:A:532:HOH:O	2.00	0.61
1:C:100:LYS:HE3	3:C:539:HOH:O	2.00	0.61
3:A:511:HOH:O	2:E:2:GLC:H2	1.99	0.61
1:D:44:THR:HG22	1:D:46:MET:H	1.63	0.61
1:A:153:PHE:O	1:A:157:VAL:HB	2.01	0.60
1:A:143:ARG:HG3	1:A:211:TYR:HB3	1.84	0.60
1:D:158:GLN:NE2	1:D:175:GLU:H	1.82	0.60
1:A:120:SER:HB3	1:A:130:ASP:OD2	2.02	0.60
1:B:18:SER:HB2	1:B:100:LYS:HD3	1.82	0.60
1:B:19:THR:HG21	1:B:163:ARG:HD3	1.83	0.60
1:C:260:ALA:HB1	1:C:267:LEU:HD21	1.84	0.60
1:B:21:LEU:HB2	1:B:214:LEU:HD21	1.82	0.60
1:C:226:LEU:CD2	1:C:231:GLN:HB2	2.32	0.59
1:C:253:VAL:HB	3:C:632:HOH:O	2.02	0.59
1:B:257:ARG:HH12	1:C:197:ALA:HB2	1.63	0.59
1:B:119:ARG:NH1	1:B:126:SER:HB2	2.18	0.59
1:C:88:THR:HG22	3:C:533:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:VAL:HG12	1:C:132:VAL:O	2.02	0.59
1:A:156:ALA:HA	1:A:159:THR:HG23	1.81	0.59
1:B:238:LYS:HA	3:B:530:HOH:O	2.01	0.59
1:B:56:ASP:HB3	3:B:551:HOH:O	2.03	0.59
1:C:212:PRO:HA	3:C:566:HOH:O	2.03	0.59
1:D:260:ALA:HA	1:D:265:LEU:HB2	1.85	0.59
1:A:218:LEU:HD12	1:A:218:LEU:C	2.22	0.59
1:B:253:VAL:O	1:B:257:ARG:HG3	2.02	0.59
1:B:49:GLN:HE22	1:B:70:ILE:N	1.93	0.58
1:A:49:GLN:O	1:A:52:GLU:HB2	2.03	0.58
1:C:26:ARG:NH2	1:C:35:GLN:OE1	2.36	0.58
1:A:140:HIS:C	1:A:140:HIS:CD2	2.76	0.58
1:B:160:ARG:NH1	3:B:506:HOH:O	2.36	0.58
1:C:133:GLY:O	1:C:134:SER:HB3	2.04	0.57
1:D:210:ASP:CB	3:D:561:HOH:O	2.52	0.57
1:A:7:ALA:O	1:A:136:PRO:HA	2.04	0.57
1:D:252:TRP:CH2	3:D:519:HOH:O	2.58	0.57
3:A:547:HOH:O	1:B:85:TYR:CD1	2.58	0.57
1:C:33:GLU:HG2	3:D:553:HOH:O	2.04	0.57
1:C:187:MET:HE2	3:C:575:HOH:O	2.05	0.57
1:D:113:ALA:HA	1:D:116:LEU:HD22	1.86	0.57
1:A:125:LEU:O	1:A:129:ARG:HG2	2.04	0.56
1:A:22:VAL:HG13	1:A:34:PRO:HB2	1.87	0.56
1:A:62:ILE:C	1:A:64:ARG:H	2.08	0.56
1:D:19:THR:HG21	3:D:574:HOH:O	2.05	0.56
1:C:118:ASP:OD2	1:C:118:ASP:N	2.34	0.56
1:D:15:ARG:NH1	1:D:152:SER:OG	2.38	0.56
1:A:143:ARG:HG3	1:A:211:TYR:CB	2.36	0.55
1:C:132:VAL:O	1:C:132:VAL:CG1	2.55	0.55
1:C:207:ILE:CD1	1:C:207:ILE:N	2.67	0.55
1:B:257:ARG:NH1	1:C:197:ALA:CB	2.60	0.55
1:B:56:ASP:HA	3:B:592:HOH:O	2.07	0.55
1:B:176:TYR:HB2	1:B:252:TRP:NE1	2.21	0.55
1:D:163:ARG:NH1	1:D:163:ARG:HG3	2.22	0.55
1:D:251:GLU:HG3	3:D:580:HOH:O	2.05	0.55
1:A:161:VAL:HG22	1:B:30:VAL:CG1	2.37	0.55
1:B:83:ARG:CD	3:B:613:HOH:O	2.54	0.55
1:A:118:ASP:HA	3:A:562:HOH:O	2.07	0.55
1:D:176:TYR:HB2	1:D:252:TRP:CE2	2.42	0.55
1:B:106:THR:N	1:B:107:PRO:CD	2.70	0.55
1:C:210:ASP:OD1	1:C:213:TYR:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:OH	1:A:178:ALA:HB2	2.07	0.54
1:B:142:HIS:CB	3:B:609:HOH:O	2.55	0.54
1:D:220:GLU:CB	3:D:551:HOH:O	2.55	0.54
1:A:235:LEU:O	1:A:236:ALA:HB2	2.07	0.54
1:C:88:THR:HG21	1:D:45:SER:HB3	1.89	0.54
1:D:212:PRO:O	1:D:216:ARG:HD2	2.07	0.54
1:B:176:TYR:CD1	1:B:252:TRP:CD1	2.96	0.54
1:B:238:LYS:CA	3:B:508:HOH:O	2.39	0.54
1:C:163:ARG:HH11	1:C:163:ARG:CG	2.20	0.54
1:A:71:GLU:O	1:A:71:GLU:HG2	2.08	0.53
1:B:176:TYR:HB2	1:B:252:TRP:CD1	2.44	0.53
1:B:84:ASP:O	1:B:88:THR:HG23	2.08	0.53
1:C:207:ILE:N	1:C:207:ILE:HD12	2.23	0.53
1:D:182:ALA:O	1:D:186:THR:HG22	2.09	0.53
1:D:44:THR:HG21	3:D:509:HOH:O	2.08	0.53
1:B:49:GLN:O	1:B:52:GLU:HB2	2.09	0.52
1:C:59:ASP:OD2	1:C:59:ASP:C	2.47	0.52
1:B:221:VAL:C	1:B:223:GLY:N	2.63	0.52
1:D:19:THR:CG2	3:D:574:HOH:O	2.57	0.52
1:D:62:ILE:HG13	1:D:177:HIS:CE1	2.45	0.52
1:B:51:ARG:NH1	1:B:67:ASP:O	2.43	0.52
1:D:112:ARG:CZ	3:D:598:HOH:O	2.58	0.52
1:D:163:ARG:HG3	1:D:163:ARG:HH11	1.75	0.51
1:B:19:THR:HG23	3:B:573:HOH:O	2.09	0.51
1:D:49:GLN:HE22	1:D:70:ILE:H	1.57	0.51
1:B:259:ASP:OD1	1:B:259:ASP:N	2.44	0.51
1:B:217:ASN:HB3	1:B:220:GLU:HB2	1.93	0.51
1:D:46:MET:SD	3:D:576:HOH:O	2.59	0.51
1:A:106:THR:OG1	1:A:107:PRO:HD3	2.11	0.51
1:A:193:GLU:O	1:A:195:TRP:N	2.44	0.51
1:B:39:GLN:NE2	2:F:2:GLC:O4	2.43	0.51
1:D:193:GLU:CB	3:D:558:HOH:O	2.59	0.50
1:C:4:HIS:N	3:C:513:HOH:O	2.43	0.50
1:D:118:ASP:OD1	1:D:118:ASP:N	2.42	0.50
1:A:62:ILE:HG21	1:A:180:ALA:HB2	1.94	0.50
1:B:7:ALA:O	1:B:136:PRO:HA	2.12	0.50
1:A:214:LEU:HD23	1:A:218:LEU:HB2	1.93	0.50
1:C:142:HIS:HB2	3:C:564:HOH:O	2.11	0.50
1:D:22:VAL:HG13	1:D:34:PRO:CG	2.41	0.50
1:A:104:ASN:HB3	1:A:191:GLN:NE2	2.12	0.50
1:A:140:HIS:HD1	1:A:199:PHE:HZ	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HB	1:A:124:LEU:HD13	1.94	0.50
1:D:22:VAL:CG1	1:D:34:PRO:HB2	2.42	0.50
1:B:192:GLU:HG3	3:B:595:HOH:O	2.11	0.49
1:C:211:TYR:HB3	1:C:212:PRO:HD3	1.94	0.49
1:B:199:PHE:HA	1:B:204:VAL:HG23	1.94	0.49
1:B:192:GLU:HA	1:B:192:GLU:OE1	2.03	0.49
1:C:210:ASP:OD1	1:C:213:TYR:CB	2.61	0.49
1:B:222:VAL:O	1:B:226:LEU:HD12	2.12	0.49
1:D:177:HIS:O	1:D:181:ILE:HD12	2.11	0.49
1:A:92:THR:HB	1:A:93:PRO:CD	2.43	0.49
1:A:124:LEU:O	1:A:127:ALA:HB3	2.12	0.49
1:D:62:ILE:O	1:D:65:LEU:HB2	2.13	0.49
1:A:134:SER:OG	1:A:135:ASP:N	2.45	0.48
1:D:218:LEU:O	1:D:221:VAL:N	2.45	0.48
1:A:193:GLU:HA	1:A:196:ARG:NH1	2.28	0.48
1:C:207:ILE:H	1:C:207:ILE:HD13	1.76	0.48
1:B:101:LEU:HD13	1:B:195:TRP:HH2	1.77	0.48
1:C:150:ALA:CB	1:C:185:ILE:HG13	2.43	0.48
1:B:112:ARG:NH2	3:B:529:HOH:O	2.47	0.48
1:B:267:LEU:C	3:B:527:HOH:O	2.51	0.48
1:C:119:ARG:O	3:C:629:HOH:O	2.20	0.48
1:A:125:LEU:HB2	1:A:198:TRP:HZ2	1.79	0.48
1:C:187:MET:HE3	1:C:187:MET:HB2	1.69	0.48
1:B:75:ASP:OD2	1:B:112:ARG:NH1	2.39	0.48
1:C:150:ALA:HB2	1:C:185:ILE:HG13	1.94	0.48
1:C:214:LEU:HD12	1:C:221:VAL:HG21	1.96	0.48
1:D:118:ASP:O	1:D:119:ARG:C	2.51	0.48
1:B:221:VAL:O	1:B:223:GLY:N	2.47	0.47
1:B:248:ARG:C	3:B:554:HOH:O	2.52	0.47
1:B:251:GLU:O	1:B:255:ARG:HB2	2.13	0.47
1:C:26:ARG:NH2	1:C:34:PRO:O	2.47	0.47
1:C:226:LEU:HD22	1:C:231:GLN:HB2	1.96	0.47
1:A:30:VAL:O	1:A:30:VAL:HG13	2.14	0.47
1:A:91:ARG:HA	1:A:96:VAL:O	2.14	0.47
1:C:142:HIS:CD2	3:C:564:HOH:O	2.68	0.47
1:D:101:LEU:HD23	1:D:105:GLN:HE21	1.79	0.47
1:A:70:ILE:CG2	1:A:71:GLU:N	2.76	0.47
1:B:42:PRO:O	1:B:74:PRO:HA	2.15	0.47
1:B:83:ARG:HH11	1:B:116:LEU:HD22	1.80	0.47
1:B:182:ALA:HB2	1:B:265:LEU:HD22	1.96	0.47
1:C:28:THR:HG22	1:C:29:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASP:OD2	1:D:61:SER:OG	2.28	0.47
1:A:36:GLU:O	1:A:39:GLN:HG2	2.14	0.47
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.67	0.47
1:B:221:VAL:C	1:B:223:GLY:H	2.16	0.47
1:D:96:VAL:HG11	1:D:229:LEU:HD13	1.96	0.47
1:B:146:VAL:HG12	1:B:185:ILE:HG12	1.97	0.47
1:B:189:ARG:HA	3:B:597:HOH:O	2.14	0.47
1:A:143:ARG:HG3	1:A:211:TYR:HD2	1.78	0.47
1:A:194:GLY:HA2	3:A:561:HOH:O	2.15	0.47
1:B:28:THR:OG1	1:B:30:VAL:HG22	2.15	0.47
1:A:70:ILE:HG22	1:A:71:GLU:N	2.30	0.46
1:B:34:PRO:C	3:B:598:HOH:O	2.53	0.46
1:B:162:TRP:CD2	2:F:2:GLC:H1	2.51	0.46
1:D:163:ARG:HD2	1:D:163:ARG:HA	1.50	0.46
1:B:21:LEU:HD12	3:B:539:HOH:O	2.14	0.46
1:B:213:TYR:CE2	1:B:217:ASN:HB2	2.50	0.46
1:C:142:HIS:HD2	3:C:564:HOH:O	1.98	0.46
1:A:14:GLN:O	1:A:15:ARG:HB2	2.15	0.46
1:A:73:LYS:HB2	1:A:74:PRO:CD	2.45	0.46
1:C:232:ASP:HA	1:C:233:PRO:HD3	1.67	0.46
1:D:51:ARG:HG2	1:D:51:ARG:NH1	2.30	0.46
1:D:59:ASP:HB3	1:D:62:ILE:HD12	1.98	0.46
1:A:16:SER:OG	1:A:18:SER:HB2	2.16	0.46
1:A:28:THR:HG21	1:A:226:LEU:HD21	1.96	0.46
1:C:28:THR:CG2	1:C:30:VAL:N	2.72	0.46
1:D:255:ARG:O	1:D:258:ARG:HB3	2.15	0.46
1:B:257:ARG:HH12	1:C:197:ALA:CB	2.25	0.46
3:C:634:HOH:O	1:D:73:LYS:HE3	2.16	0.46
1:A:4:HIS:CB	3:A:506:HOH:O	2.63	0.46
1:A:11:LEU:HD11	1:A:138:LEU:HG	1.97	0.46
1:D:176:TYR:OH	1:D:256:TYR:HA	2.16	0.46
1:C:238:LYS:HD2	1:C:238:LYS:HA	1.70	0.46
1:D:22:VAL:HG13	1:D:34:PRO:HB2	1.98	0.46
1:A:4:HIS:HA	3:A:506:HOH:O	2.14	0.45
1:B:82:TRP:CZ2	1:B:112:ARG:HD2	2.51	0.45
1:A:4:HIS:CA	3:A:506:HOH:O	2.64	0.45
1:B:17:GLY:O	1:B:18:SER:C	2.53	0.45
1:A:163:ARG:HD2	1:A:163:ARG:HA	1.80	0.45
1:D:147:VAL:HG12	1:D:253:VAL:HG13	1.99	0.45
1:A:11:LEU:HB3	1:A:195:TRP:CH2	2.52	0.45
3:A:511:HOH:O	2:E:2:GLC:C2	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD22	1:B:195:TRP:CH2	2.51	0.45
1:C:231:GLN:HB3	3:C:608:HOH:O	2.16	0.45
1:A:218:LEU:C	1:A:218:LEU:CD1	2.85	0.45
1:B:92:THR:HB	3:B:548:HOH:O	2.17	0.45
1:B:154:TRP:CE2	1:B:158:GLN:NE2	2.85	0.45
1:A:143:ARG:HG3	1:A:211:TYR:CG	2.50	0.45
1:A:157:VAL:O	1:A:157:VAL:HG13	2.17	0.45
1:D:22:VAL:HG13	1:D:34:PRO:CB	2.47	0.45
1:A:58:GLU:N	3:A:505:HOH:O	2.50	0.45
1:A:211:TYR:N	1:A:212:PRO:HD2	2.32	0.45
1:B:4:HIS:N	3:B:522:HOH:O	2.50	0.45
1:B:51:ARG:CG	1:B:51:ARG:NH1	2.66	0.44
1:C:21:LEU:HD22	1:C:25:LEU:CD2	2.43	0.44
1:A:61:SER:OG	1:A:177:HIS:NE2	2.49	0.44
1:B:150:ALA:CB	1:B:185:ILE:HG13	2.47	0.44
1:B:265:LEU:N	3:B:605:HOH:O	2.49	0.44
1:D:119:ARG:HD2	1:D:119:ARG:HA	1.71	0.44
1:C:233:PRO:C	1:C:235:LEU:H	2.19	0.44
1:C:261:GLN:CG	3:C:633:HOH:O	2.62	0.44
1:D:21:LEU:HD22	1:D:21:LEU:O	2.18	0.44
1:B:85:TYR:CE2	1:B:89:VAL:HG21	2.52	0.44
1:A:7:ALA:HA	1:A:97:TRP:O	2.18	0.44
1:A:92:THR:HB	1:A:93:PRO:HD2	2.00	0.44
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.74	0.44
1:C:226:LEU:HD23	1:C:231:GLN:HB2	1.99	0.44
1:B:85:TYR:CZ	1:B:89:VAL:HG21	2.53	0.44
1:A:128:ILE:O	1:A:132:VAL:HG13	2.17	0.44
1:B:34:PRO:HA	1:B:99:GLY:HA2	2.00	0.44
1:C:29:GLY:HA3	1:D:163:ARG:HB2	2.00	0.44
1:C:103:TRP:CE3	1:C:106:THR:HG21	2.53	0.44
1:A:30:VAL:O	1:A:30:VAL:CG1	2.66	0.43
1:A:50:PRO:C	1:A:52:GLU:H	2.20	0.43
1:A:213:TYR:HD1	1:A:217:ASN:OD1	2.00	0.43
1:B:56:ASP:C	3:B:592:HOH:O	2.55	0.43
1:D:226:LEU:O	1:D:227:GLU:C	2.55	0.43
1:C:118:ASP:O	1:C:119:ARG:C	2.55	0.43
1:C:208:ASP:O	1:C:209:VAL:HG22	2.18	0.43
1:D:162:TRP:CD1	1:D:162:TRP:N	2.86	0.43
1:D:217:ASN:O	1:D:218:LEU:C	2.56	0.43
1:D:19:THR:HG23	3:D:533:HOH:O	2.18	0.43
1:B:104:ASN:HA	3:B:593:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:HA2	1:A:92:THR:HG23	2.01	0.43
1:A:156:ALA:CA	1:A:159:THR:HG22	2.40	0.43
1:C:22:VAL:HG22	1:C:34:PRO:HG3	2.01	0.43
1:C:255:ARG:CB	3:C:530:HOH:O	2.67	0.43
1:B:15:ARG:O	1:B:149:GLN:HG3	2.19	0.43
1:C:106:THR:N	1:C:107:PRO:CD	2.82	0.43
1:B:62:ILE:HD12	1:B:154:TRP:CH2	2.54	0.42
1:B:120:SER:N	1:B:130:ASP:OD2	2.50	0.42
1:C:254:GLU:O	1:C:256:TYR:N	2.52	0.42
1:A:149:GLN:NE2	1:A:188:LEU:HD22	2.34	0.42
1:C:213:TYR:CE2	1:C:220:GLU:OE1	2.71	0.42
1:A:193:GLU:O	1:A:194:GLY:C	2.58	0.42
1:B:146:VAL:CG2	1:B:189:ARG:CZ	2.98	0.42
1:A:255:ARG:C	3:A:541:HOH:O	2.58	0.42
1:D:17:GLY:O	1:D:18:SER:C	2.55	0.42
1:D:158:GLN:NE2	1:D:174:ALA:HA	2.35	0.42
1:B:218:LEU:HD22	1:B:222:VAL:CG2	2.50	0.42
1:D:106:THR:N	1:D:107:PRO:CD	2.82	0.42
1:C:163:ARG:HD2	1:C:163:ARG:HA	1.49	0.42
1:D:3:ASP:O	1:D:4:HIS:C	2.58	0.42
1:A:143:ARG:CG	1:A:211:TYR:HB3	2.49	0.42
1:A:191:GLN:HG3	3:A:551:HOH:O	2.20	0.42
1:B:9:LEU:HD11	1:B:101:LEU:HB2	2.01	0.42
1:A:8:TYR:CD2	1:A:229:LEU:HD11	2.55	0.42
1:A:143:ARG:NH1	1:A:149:GLN:HA	2.34	0.42
1:B:100:LYS:HZ2	1:B:100:LYS:HG3	1.59	0.42
1:A:232:ASP:HB3	1:A:235:LEU:HD12	2.02	0.41
1:A:181:ILE:O	1:A:181:ILE:HG22	2.19	0.41
1:C:189:ARG:HH21	1:C:267:LEU:C	2.23	0.41
1:C:213:TYR:C	1:C:213:TYR:CD2	2.94	0.41
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.86	0.41
1:B:112:ARG:CZ	3:B:529:HOH:O	2.65	0.41
1:A:149:GLN:HG2	1:A:188:LEU:HD13	2.03	0.41
1:C:143:ARG:HG3	1:C:211:TYR:CD2	2.55	0.41
1:A:194:GLY:N	3:A:561:HOH:O	2.53	0.41
1:B:197:ALA:O	1:B:201:GLU:HB2	2.20	0.41
1:C:199:PHE:O	1:C:203:ASN:N	2.54	0.41
1:A:56:ASP:O	3:A:505:HOH:O	2.22	0.41
1:A:108:LEU:HA	1:A:108:LEU:HD23	1.84	0.41
1:D:112:ARG:HA	3:D:544:HOH:O	2.20	0.41
1:B:196:ARG:NH2	1:C:257:ARG:CZ	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLN:CB	3:C:571:HOH:O	2.68	0.41
1:C:149:GLN:HG2	1:C:188:LEU:HD13	2.03	0.41
1:C:267:LEU:HB2	3:C:599:HOH:O	2.20	0.41
1:D:211:TYR:HB3	1:D:212:PRO:HD3	2.03	0.41
1:B:51:ARG:HD2	3:B:575:HOH:O	2.21	0.41
1:B:232:ASP:HA	1:B:233:PRO:HD3	1.96	0.41
1:D:229:LEU:HD12	1:D:231:GLN:HG2	2.03	0.40
1:B:15:ARG:HA	3:B:606:HOH:O	2.20	0.40
1:B:17:GLY:O	1:B:19:THR:N	2.55	0.40
1:D:8:TYR:CD2	1:D:8:TYR:N	2.90	0.40
1:A:21:LEU:HD12	1:A:141:ILE:HD11	2.04	0.40
1:B:33:GLU:OE2	2:E:2:GLC:H4	2.21	0.40
1:D:222:VAL:O	1:D:225:VAL:N	2.55	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	228/287 (79%)	181 (79%)	38 (17%)	9 (4%)	3	4
1	B	235/287 (82%)	217 (92%)	14 (6%)	4 (2%)	9	18
1	C	238/287 (83%)	222 (93%)	12 (5%)	4 (2%)	9	18
1	D	241/287 (84%)	220 (91%)	19 (8%)	2 (1%)	19	39
All	All	942/1148 (82%)	840 (89%)	83 (9%)	19 (2%)	7	14

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	194	GLY

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Mol	Chain	Res	Type
1	B	119	ARG
1	B	218	LEU
1	A	182	ALA
1	A	193	GLU
1	D	59	ASP
1	D	64	ARG
1	C	203	ASN
1	A	60	GLN
1	A	183	HIS
1	B	209	VAL
1	C	217	ASN
1	A	184	VAL
1	C	12	ALA
1	C	255	ARG
1	B	222	VAL
1	A	185	ILE
1	A	50	PRO

### 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	172/245 (70%)	131 (76%)	41 (24%)	<b>0</b> <b>1</b>
1	B	185/245 (76%)	146 (79%)	39 (21%)	<b>1</b> <b>2</b>
1	C	192/245 (78%)	168 (88%)	24 (12%)	<b>4</b> <b>8</b>
1	D	190/245 (78%)	155 (82%)	35 (18%)	<b>1</b> <b>2</b>
All	All	739/980 (75%)	600 (81%)	139 (19%)	<b>1</b> <b>2</b>

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	24	SER
1	A	41	LEU
1	A	46	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	49	GLN
1	A	52	GLU
1	A	58	GLU
1	A	62	ILE
1	A	64	ARG
1	A	70	ILE
1	A	71	GLU
1	A	80	THR
1	A	83	ARG
1	A	92	THR
1	A	102	MET
1	A	104	ASN
1	A	109	LEU
1	A	111	GLN
1	A	112	ARG
1	A	119	ARG
1	A	120	SER
1	A	132	VAL
1	A	134	SER
1	A	138	LEU
1	A	142	HIS
1	A	143	ARG
1	A	152	SER
1	A	157	VAL
1	A	159	THR
1	A	160	ARG
1	A	173	ARG
1	A	186	THR
1	A	191	GLN
1	A	195	TRP
1	A	213	TYR
1	A	214	LEU
1	A	215	TRP
1	A	218	LEU
1	A	219	THR
1	A	235	LEU
1	A	259	ASP
1	B	15	ARG
1	B	18	SER
1	B	21	LEU
1	B	22	VAL
1	B	24	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	28	THR
1	B	41	LEU
1	B	45	SER
1	B	51	ARG
1	B	62	ILE
1	B	66	LEU
1	B	71	GLU
1	B	81	ILE
1	B	83	ARG
1	B	88	THR
1	B	92	THR
1	B	100	LYS
1	B	101	LEU
1	B	102	MET
1	B	111	GLN
1	B	112	ARG
1	B	124	LEU
1	B	126	SER
1	B	134	SER
1	B	135	ASP
1	B	152	SER
1	B	157	VAL
1	B	173	ARG
1	B	192	GLU
1	B	200	THR
1	B	204	VAL
1	B	213	TYR
1	B	218	LEU
1	B	220	GLU
1	B	224	THR
1	B	249	SER
1	B	255	ARG
1	B	259	ASP
1	B	267	LEU
1	C	11	LEU
1	C	15	ARG
1	C	21	LEU
1	C	22	VAL
1	C	24	SER
1	C	25	LEU
1	C	28	THR
1	C	69	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	88	THR
1	C	92	THR
1	C	100	LYS
1	C	101	LEU
1	C	124	LEU
1	C	125	LEU
1	C	159	THR
1	C	163	ARG
1	C	187	MET
1	C	207	ILE
1	C	210	ASP
1	C	217	ASN
1	C	218	LEU
1	C	232	ASP
1	C	261	GLN
1	C	267	LEU
1	D	9	LEU
1	D	19	THR
1	D	21	LEU
1	D	30	VAL
1	D	41	LEU
1	D	44	THR
1	D	49	GLN
1	D	51	ARG
1	D	57	VAL
1	D	63	LEU
1	D	83	ARG
1	D	92	THR
1	D	100	LYS
1	D	101	LEU
1	D	109	LEU
1	D	111	GLN
1	D	112	ARG
1	D	114	LYS
1	D	116	LEU
1	D	119	ARG
1	D	146	VAL
1	D	152	SER
1	D	157	VAL
1	D	163	ARG
1	D	186	THR
1	D	187	MET

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Mol	Chain	Res	Type
1	D	189	ARG
1	D	201	GLU
1	D	202	GLU
1	D	204	VAL
1	D	215	TRP
1	D	229	LEU
1	D	235	LEU
1	D	257	ARG
1	D	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	105	GLN
1	A	149	GLN
1	A	191	GLN
1	B	39	GLN
1	B	49	GLN
1	B	87	GLN
1	B	111	GLN
1	B	149	GLN
1	B	183	HIS
1	C	105	GLN
1	C	142	HIS
1	C	217	ASN
1	D	35	GLN
1	D	39	GLN
1	D	49	GLN
1	D	105	GLN
1	D	158	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
2	GLC	E	1	2	11,11,12	0.77	0	15,15,17	4.19	9 (60%)
2	GLC	E	2	2	12,12,12	1.00	0	17,17,17	3.10	10 (58%)
2	GLC	F	1	2	11,11,12	1.28	2 (18%)	15,15,17	4.63	12 (80%)
2	GLC	F	2	2	12,12,12	0.72	0	17,17,17	3.12	11 (64%)
2	GLC	G	1	2	11,11,12	1.57	2 (18%)	15,15,17	4.25	10 (66%)
2	GLC	G	2	2	12,12,12	0.78	0	17,17,17	3.14	12 (70%)
2	GLC	H	1	2	11,11,12	1.13	0	15,15,17	4.02	7 (46%)
2	GLC	H	2	2	12,12,12	0.94	1 (8%)	17,17,17	3.10	10 (58%)

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	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	GLC	E	2	2	-	1/2/22/22	0/1/1/1
2	GLC	F	1	2	-	1/2/19/22	0/1/1/1
2	GLC	F	2	2	-	0/2/22/22	0/1/1/1
2	GLC	G	1	2	-	1/2/19/22	0/1/1/1
2	GLC	G	2	2	-	2/2/22/22	0/1/1/1
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLC	C2-C3	-3.55	1.47	1.52
2	F	1	GLC	O5-C1	-2.31	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	GLC	C2-C3	-2.11	1.49	1.52
2	G	1	GLC	C4-C3	-2.04	1.47	1.52
2	H	2	GLC	C3-C2	-2.02	1.47	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	GLC	C1-O5-C5	11.16	127.32	112.19
2	H	1	GLC	C1-O5-C5	10.14	125.94	112.19
2	E	1	GLC	C1-O5-C5	9.95	125.67	112.19
2	F	1	GLC	C1-C2-C3	9.09	120.84	109.67
2	G	1	GLC	C1-O5-C5	9.06	124.47	112.19
2	H	1	GLC	C1-C2-C3	8.23	119.78	109.67
2	G	2	GLC	C1-O5-C5	7.50	127.82	113.66
2	E	1	GLC	C1-C2-C3	7.29	118.62	109.67
2	G	1	GLC	C1-C2-C3	7.14	118.44	109.67
2	G	1	GLC	C6-C5-C4	-6.21	98.47	113.00
2	F	2	GLC	C1-O5-C5	5.96	124.92	113.66
2	H	2	GLC	C1-O5-C5	5.57	124.18	113.66
2	E	1	GLC	C3-C4-C5	5.46	119.97	110.24
2	F	2	GLC	C4-C3-C2	5.45	120.34	110.82
2	F	2	GLC	O5-C5-C4	5.23	119.19	109.69
2	F	1	GLC	O5-C5-C6	-5.14	99.15	107.20
2	E	2	GLC	C1-O5-C5	5.12	123.33	113.66
2	E	1	GLC	O3-C3-C2	5.06	119.69	109.99
2	E	2	GLC	C3-C4-C5	4.99	119.14	110.24
2	G	1	GLC	O2-C2-C1	4.85	119.08	109.15
2	H	1	GLC	C3-C4-C5	4.70	118.61	110.24
2	H	2	GLC	O1-C1-O5	-4.59	96.61	110.38
2	E	2	GLC	O5-C1-C2	4.54	118.39	110.28
2	H	2	GLC	O2-C2-C1	4.53	119.66	109.16
2	E	2	GLC	O5-C5-C4	4.48	117.83	109.69
2	E	2	GLC	C1-C2-C3	4.47	119.59	110.31
2	F	1	GLC	C3-C4-C5	4.38	118.05	110.24
2	H	2	GLC	C4-C3-C2	4.34	118.41	110.82
2	E	1	GLC	O5-C1-C2	4.18	117.22	110.77
2	H	1	GLC	O2-C2-C1	4.13	117.59	109.15
2	H	2	GLC	O5-C5-C4	3.99	116.94	109.69
2	G	2	GLC	O1-C1-O5	-3.88	98.73	110.38
2	H	2	GLC	O5-C1-C2	3.85	117.15	110.28
2	G	1	GLC	O3-C3-C4	3.84	119.22	110.35
2	G	1	GLC	C3-C4-C5	3.83	117.08	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GLC	C2-C3-C4	3.82	117.51	110.89
2	H	2	GLC	C3-C4-C5	3.78	116.99	110.24
2	G	2	GLC	C4-C3-C2	3.76	117.38	110.82
2	F	2	GLC	O5-C1-C2	3.64	116.77	110.28
2	E	2	GLC	O1-C1-O5	-3.54	99.74	110.38
2	G	1	GLC	O3-C3-C2	3.53	116.75	109.99
2	G	2	GLC	O2-C2-C1	3.45	117.16	109.16
2	F	1	GLC	C6-C5-C4	-3.44	104.94	113.00
2	H	2	GLC	C1-C2-C3	3.37	117.30	110.31
2	G	2	GLC	C1-C2-C3	3.35	117.27	110.31
2	F	2	GLC	O3-C3-C2	3.31	118.00	110.35
2	G	2	GLC	O5-C5-C4	3.28	115.65	109.69
2	F	1	GLC	O2-C2-C1	3.22	115.75	109.15
2	G	2	GLC	O2-C2-C3	3.17	117.68	110.35
2	E	2	GLC	O2-C2-C1	3.16	116.49	109.16
2	G	2	GLC	C3-C4-C5	3.12	115.81	110.24
2	E	1	GLC	O2-C2-C3	3.08	116.31	110.14
2	G	1	GLC	O5-C5-C4	3.06	118.26	110.83
2	E	2	GLC	O1-C1-C2	-3.00	100.58	109.03
2	F	1	GLC	O5-C5-C4	2.96	118.02	110.83
2	F	2	GLC	O1-C1-C2	-2.95	100.73	109.03
2	E	1	GLC	O5-C5-C6	-2.91	102.64	107.20
2	G	2	GLC	O3-C3-C4	2.91	117.08	110.35
2	E	1	GLC	O5-C5-C4	2.85	117.77	110.83
2	F	2	GLC	C1-C2-C3	2.84	116.20	110.31
2	E	2	GLC	C4-C3-C2	2.82	115.75	110.82
2	E	1	GLC	C2-C3-C4	2.79	115.72	110.89
2	H	1	GLC	O3-C3-C2	2.73	115.22	109.99
2	F	2	GLC	C3-C4-C5	2.72	115.09	110.24
2	F	1	GLC	C2-C3-C4	2.69	115.54	110.89
2	H	1	GLC	O2-C2-C3	2.68	115.51	110.14
2	F	1	GLC	O3-C3-C4	2.65	116.48	110.35
2	F	1	GLC	O2-C2-C3	2.63	115.40	110.14
2	F	1	GLC	O5-C1-C2	2.57	114.74	110.77
2	E	2	GLC	O3-C3-C2	-2.47	104.64	110.35
2	H	2	GLC	O1-C1-C2	-2.46	102.11	109.03
2	G	2	GLC	O4-C4-C3	2.43	115.98	110.35
2	G	2	GLC	O5-C1-C2	2.40	114.56	110.28
2	F	2	GLC	O1-C1-O5	-2.33	103.37	110.38
2	F	1	GLC	O3-C3-C2	2.29	114.38	109.99
2	G	1	GLC	O5-C1-C2	2.27	114.28	110.77
2	F	2	GLC	O3-C3-C4	2.27	115.59	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	GLC	O1-C1-C2	-2.19	102.88	109.03
2	F	2	GLC	O5-C5-C6	2.10	111.65	106.44
2	H	2	GLC	O3-C3-C4	2.04	115.06	110.35
2	H	1	GLC	O4-C4-C5	2.03	114.34	109.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

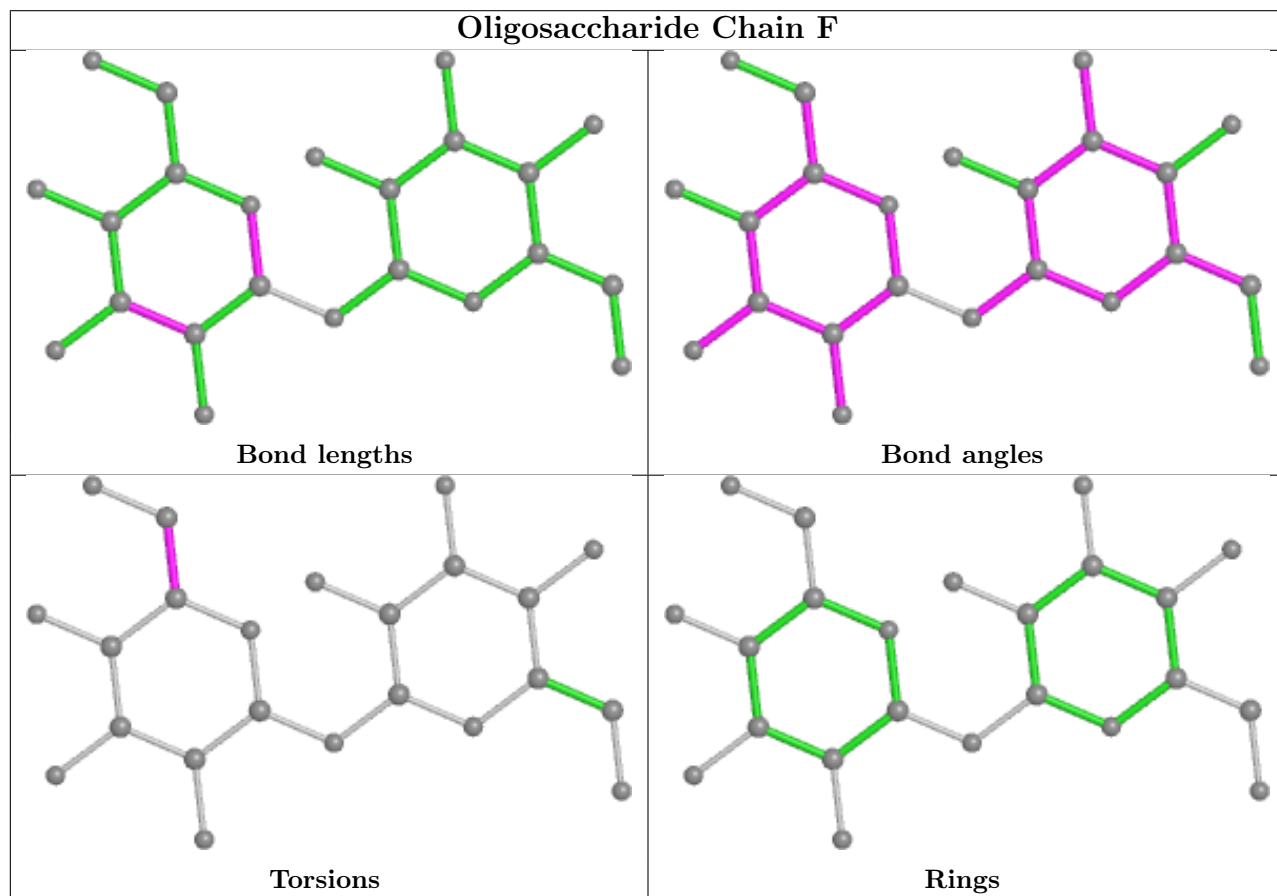
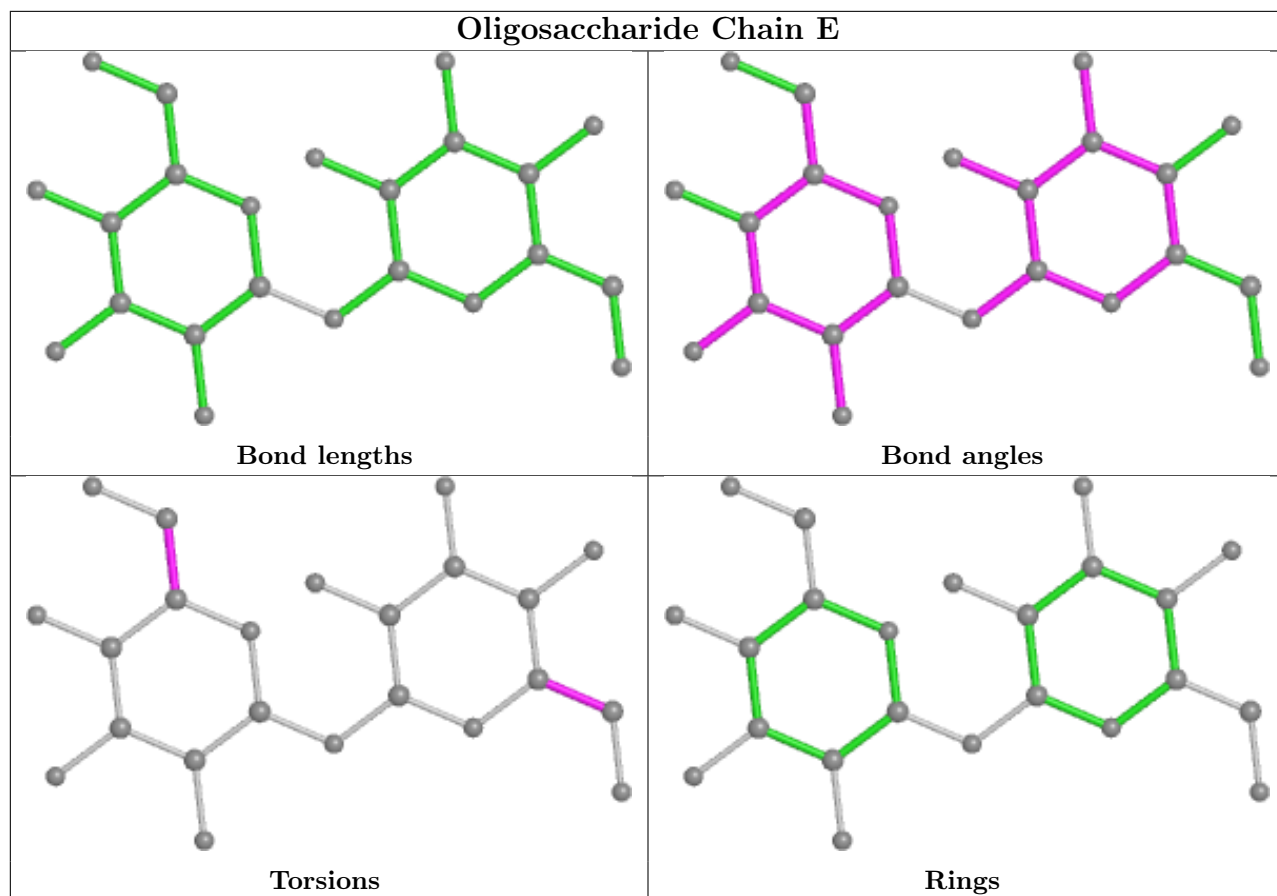
Mol	Chain	Res	Type	Atoms
2	E	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6

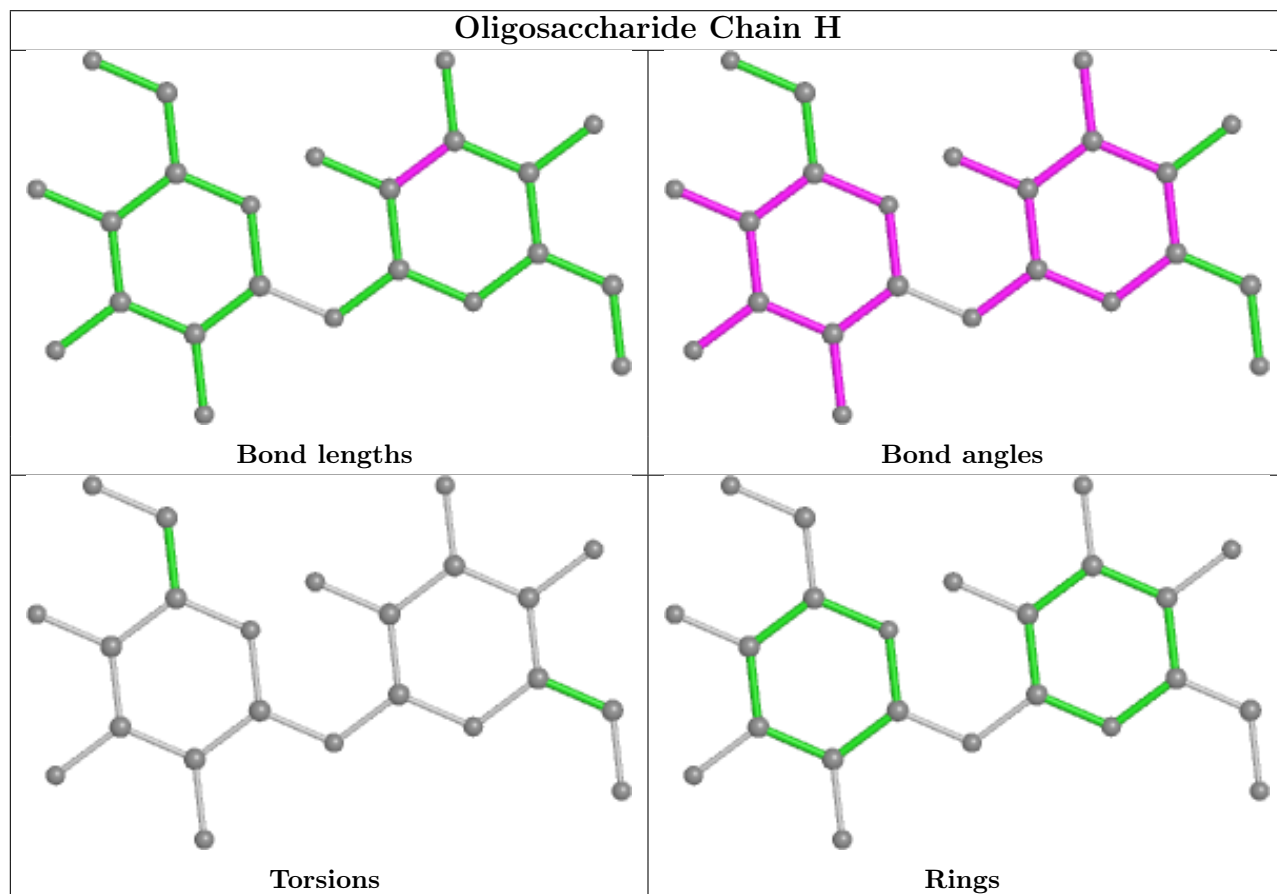
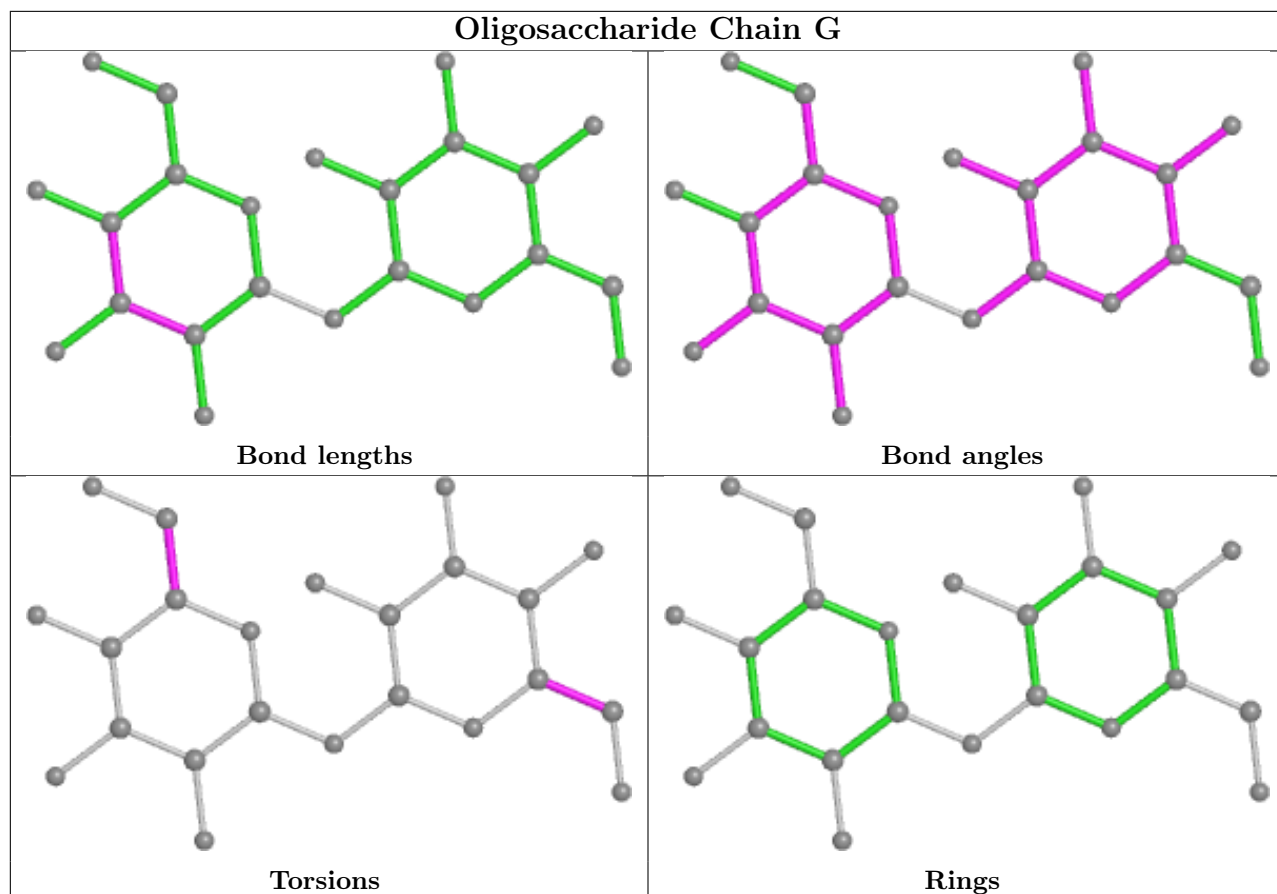
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GLC	5	0
2	F	2	GLC	2	0

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







## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	239/287 (83%)	0.21	20 (8%) <b>11</b> <b>7</b>	20, 54, 93, 97	0
1	B	243/287 (84%)	-0.18	6 (2%) 57 51	19, 40, 76, 89	0
1	C	244/287 (85%)	-0.19	4 (1%) 72 68	12, 35, 62, 81	0
1	D	247/287 (86%)	-0.18	6 (2%) 59 53	17, 34, 58, 70	1 (0%)
All	All	973/1148 (84%)	-0.09	36 (3%) 41 34	12, 38, 79, 97	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	GLY	5.4
1	D	3	ASP	4.5
1	A	265	LEU	4.4
1	B	249	SER	4.3
1	B	171	ASP	4.1
1	A	266	PRO	3.9
1	A	262	ARG	3.9
1	A	211	TYR	3.7
1	A	263	ASP	3.6
1	A	3	ASP	3.4
1	A	261	GLN	3.3
1	A	179	GLY	3.2
1	A	4	HIS	3.1
1	A	64	ARG	3.0
1	A	213	TYR	2.9
1	A	175	GLU	2.9
1	D	249	SER	2.8
1	B	265	LEU	2.8
1	A	251	GLU	2.7
1	D	4	HIS	2.7
1	A	176	TYR	2.7

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	D	142	HIS	2.6
1	A	158	GLN	2.6
1	C	239	PRO	2.5
1	A	220	GLU	2.5
1	C	211	TYR	2.5
1	C	251	GLU	2.2
1	C	205	GLU	2.2
1	A	215	TRP	2.2
1	A	58	GLU	2.1
1	B	172	ALA	2.1
1	B	248	ARG	2.1
1	D	214	LEU	2.1
1	D	267	LEU	2.1
1	A	227	GLU	2.0
1	B	213	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](#)

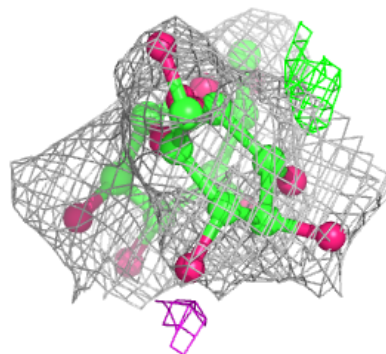
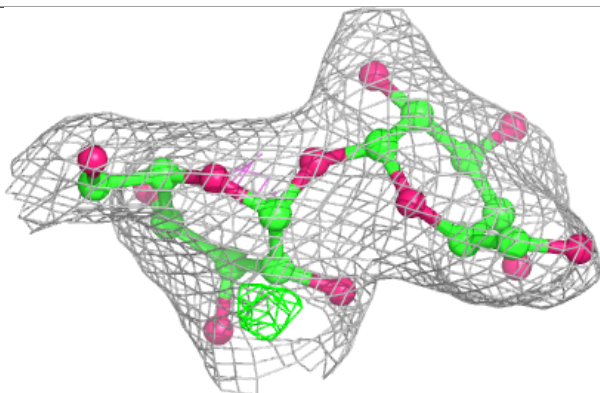
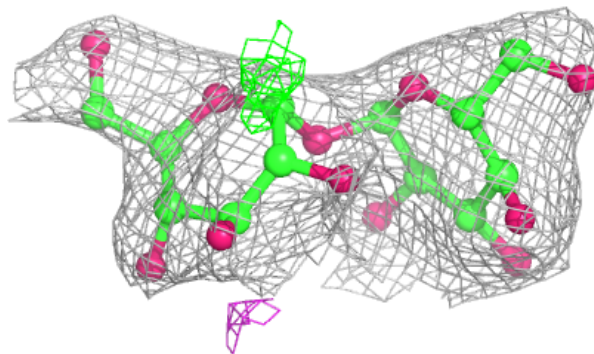
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	E	2	12/12	0.91	0.13	33,39,42,42	0
2	GLC	E	1	11/12	0.93	0.14	28,30,33,36	0
2	GLC	H	1	11/12	0.93	0.20	24,26,31,31	0
2	GLC	H	2	12/12	0.94	0.19	25,29,32,37	0
2	GLC	G	2	12/12	0.95	0.17	26,34,36,38	0
2	GLC	F	1	11/12	0.95	0.20	27,31,42,49	0
2	GLC	G	1	11/12	0.95	0.19	24,26,31,35	0
2	GLC	F	2	12/12	0.96	0.18	23,28,32,32	0

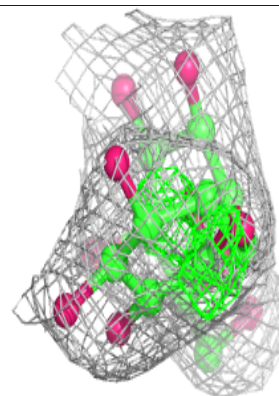
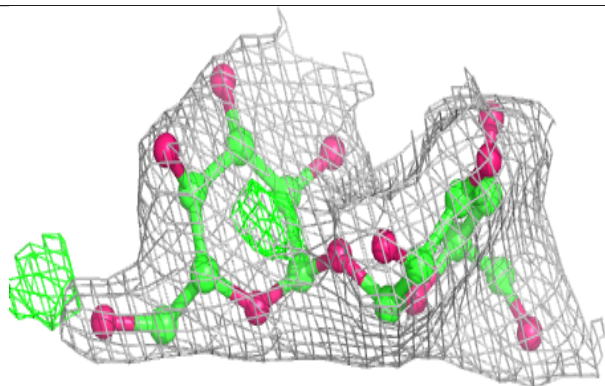
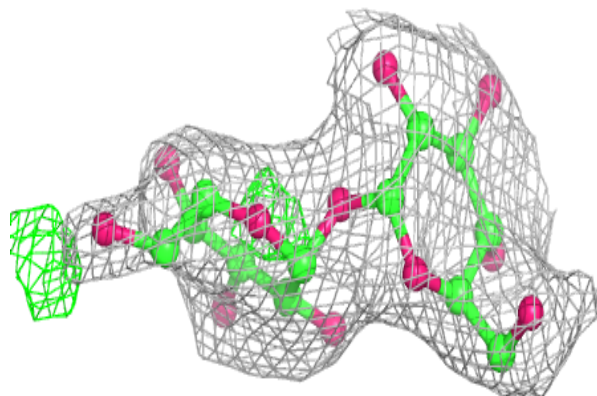
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

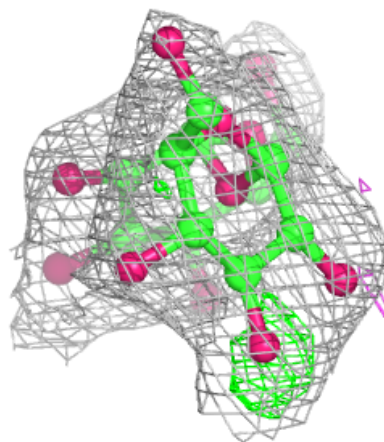
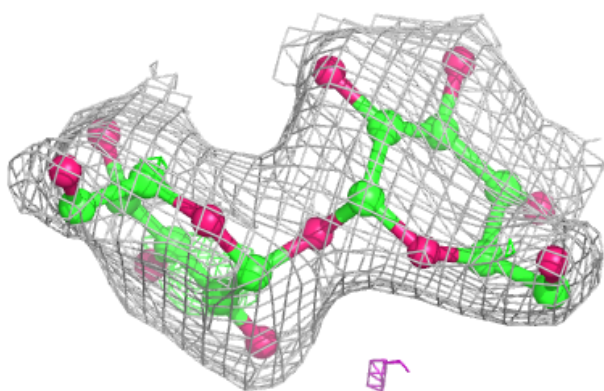
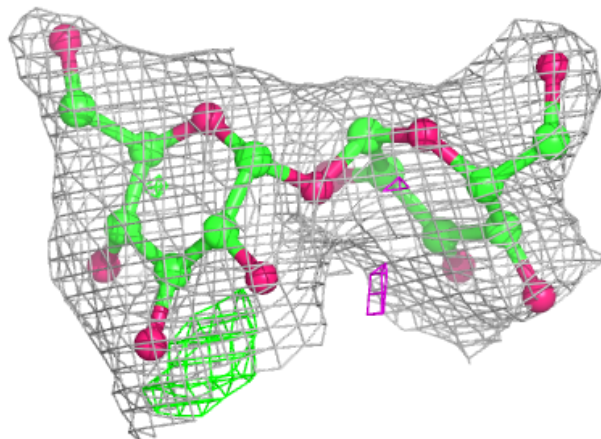
**Electron density around Chain F:**

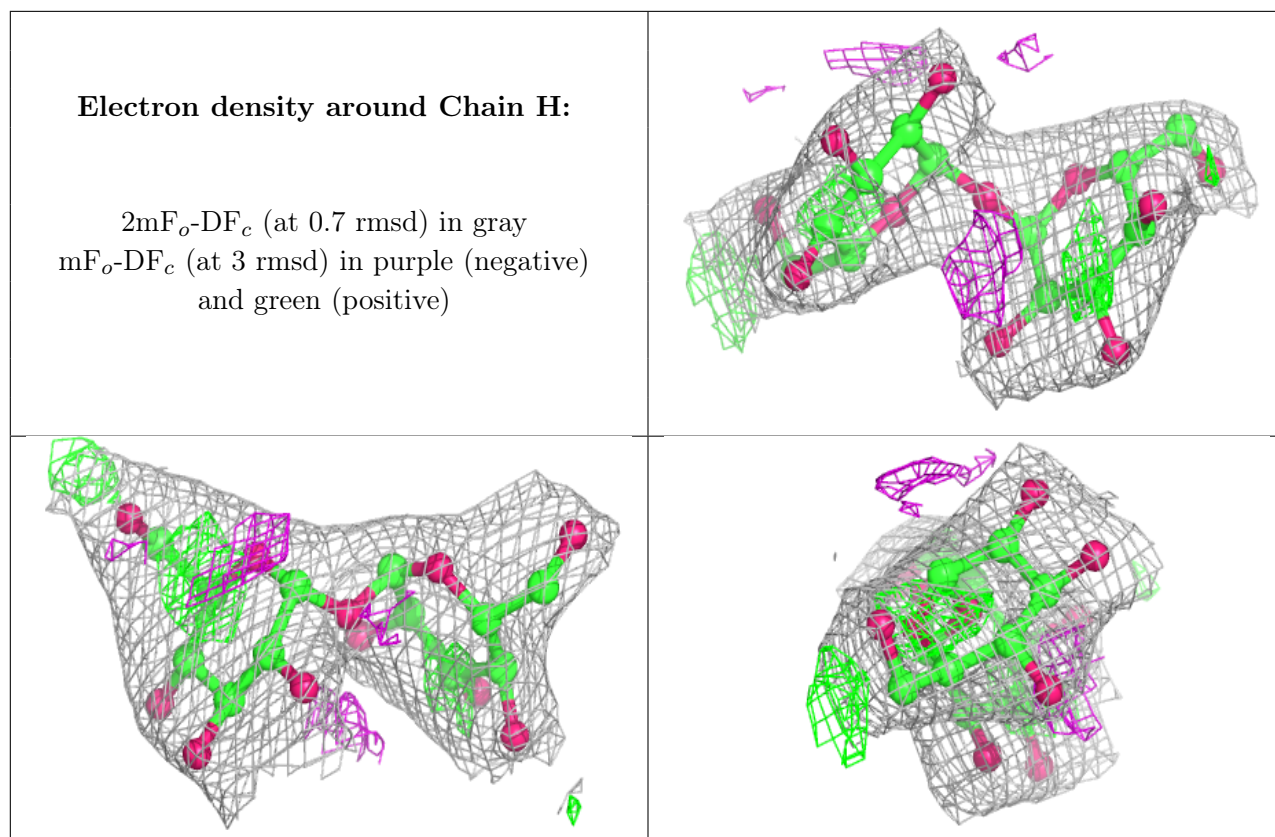
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.