



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:32 AM BST

PDB ID : 4XKE  
Title : Crystal structure of hemagglutinin from Taiwan (2013) H6N1 influenza virus  
in complex with 3'-SLN  
Authors : Tzarum, N.; Zhu, X.; Wilson, I.A.  
Deposited on : 2015-01-11  
Resolution : 2.36 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

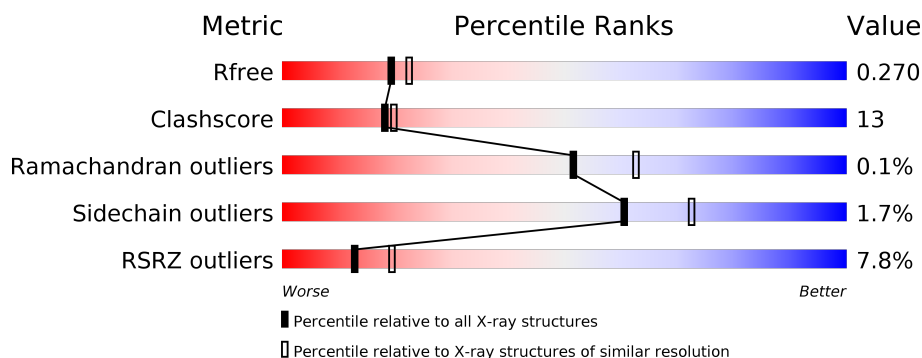
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	333	<div> <div>8%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	C	333	<div> <div>7%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
1	E	333	<div> <div>5%</div> <div>67%</div> <div>29%</div> <div>• •</div> </div>
2	B	180	<div> <div>9%</div> <div>75%</div> <div>21%</div> <div>•</div> </div>
2	D	180	<div> <div>10%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
2	F	180	<div> <div>8%</div> <div>73%</div> <div>23%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	401	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12144 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.

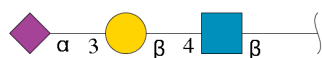
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2600	1648	443	496	13			
1	C	326	Total	C	N	O	S	0	0	0
			2569	1629	437	490	13			
1	E	325	Total	C	N	O	S	0	0	0
			2563	1626	437	487	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1393	868	244	274	7			
2	D	173	Total	C	N	O	S	0	0	0
			1393	868	244	274	7			
2	F	172	Total	C	N	O	S	0	0	0
			1385	862	243	273	7			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

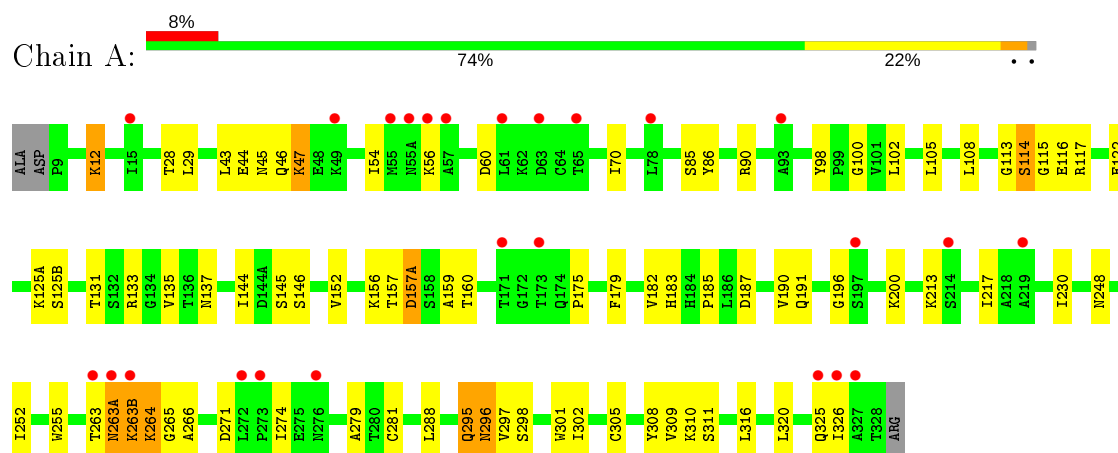
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	21	Total	O	0	0
			21	21		
5	C	25	Total	O	0	0
			25	25		
5	D	12	Total	O	0	0
			12	12		
5	E	19	Total	O	0	0
			19	19		
5	F	7	Total	O	0	0
			7	7		

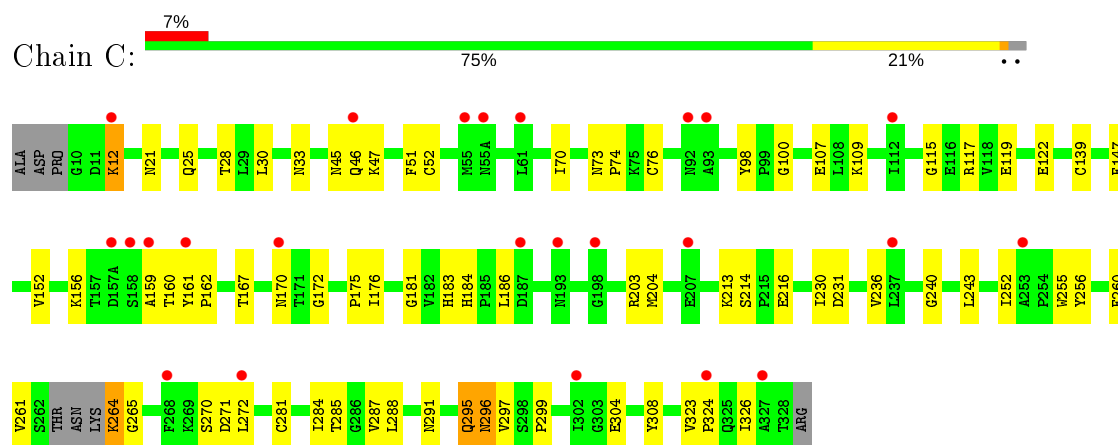
### 3 Residue-property plots

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.

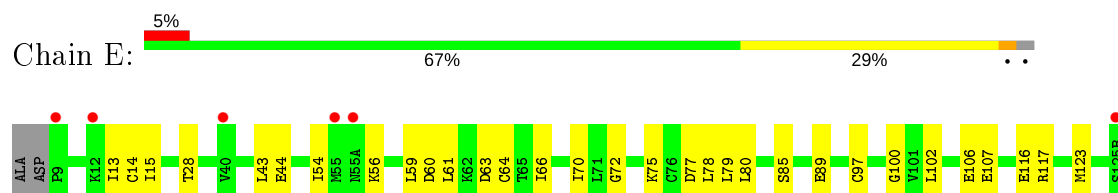
#### • Molecule 1: Hemagglutinin HA1 chain

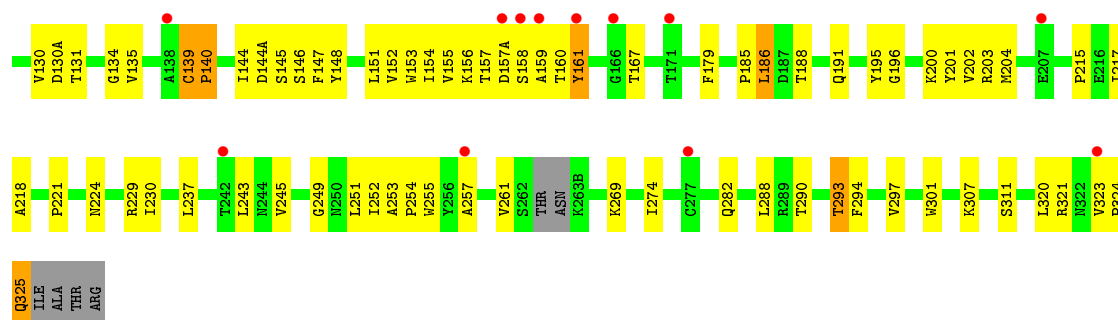


#### • Molecule 1: Hemagglutinin HA1 chain

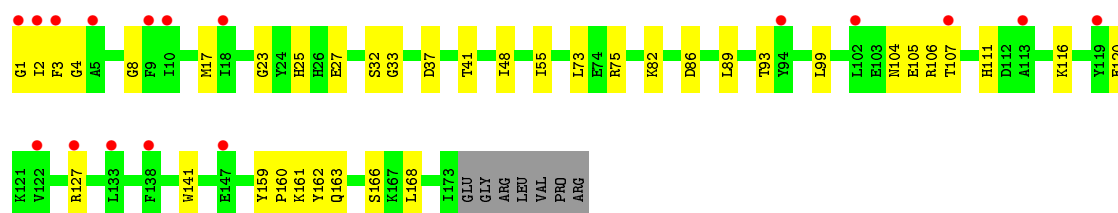
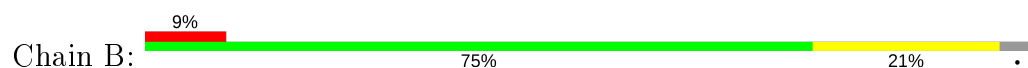


#### • Molecule 1: Hemagglutinin HA1 chain

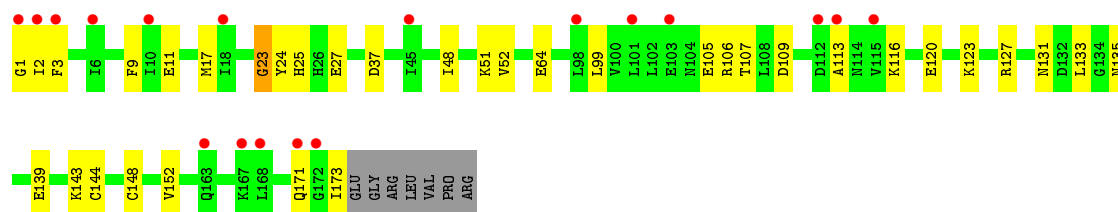
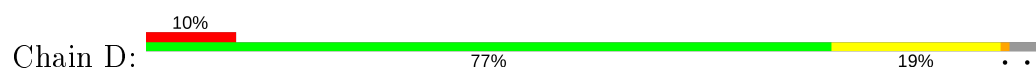




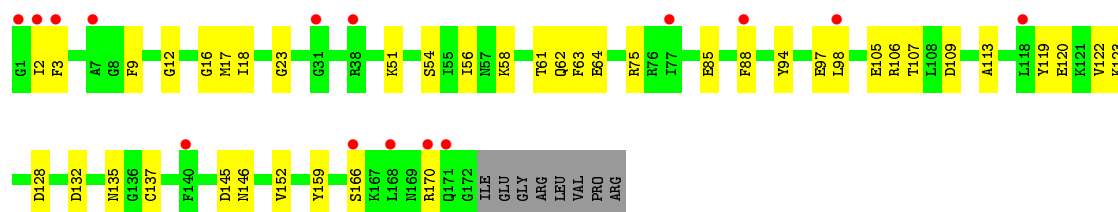
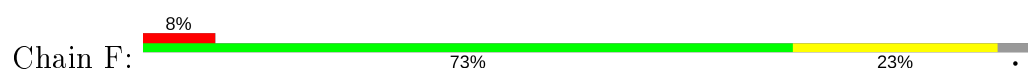
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.60Å 99.25Å 133.42Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	49.51 – 2.36 49.51 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.51-2.36) 91.9 (49.51-2.36)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.230 , 0.272 0.231 , 0.270	Depositor DCC
$R_{free}$ test set	3927 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: SIA, GAL, NAG

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	0.58	1/2662 (0.0%)	0.68	4/3622 (0.1%)
1	C	0.59	2/2629 (0.1%)	0.70	6/3576 (0.2%)
1	E	0.53	1/2624 (0.0%)	0.65	3/3567 (0.1%)
2	B	0.55	0/1421	0.66	1/1913 (0.1%)
2	D	0.49	0/1421	0.65	2/1913 (0.1%)
2	F	0.51	0/1413	0.78	3/1902 (0.2%)
All	All	0.55	4/12170 (0.0%)	0.68	19/16493 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	LYS	C-N	9.95	1.56	1.34
1	C	162	PRO	N-CD	5.48	1.55	1.47
1	C	324	PRO	N-CD	5.21	1.55	1.47
1	E	140	PRO	N-CD	5.02	1.54	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	62	GLN	O-C-N	-12.82	102.19	122.70
2	F	62	GLN	C-N-CA	10.38	147.64	121.70
1	A	12	LYS	CD-CE-NZ	9.26	133.01	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	LYS	O-C-N	-9.22	107.94	122.70
2	F	62	GLN	CA-C-N	8.80	136.56	117.20
2	B	1	GLY	N-CA-C	-6.47	96.93	113.10
1	A	47	LYS	CA-C-N	6.33	131.11	117.20
1	E	161	TYR	C-N-CD	6.29	141.61	128.40
1	C	12	LYS	CD-CE-NZ	6.25	126.07	111.70
1	E	253	ALA	C-N-CD	6.10	141.21	128.40
1	E	139	CYS	C-N-CD	6.08	141.16	128.40
1	C	139	CYS	C-N-CD	6.00	140.99	128.40
2	D	1	GLY	N-CA-C	-5.60	99.10	113.10
1	C	323	VAL	C-N-CD	5.55	140.06	128.40
1	C	161	TYR	C-N-CD	5.49	139.93	128.40
1	C	109	LYS	CD-CE-NZ	5.16	123.57	111.70
1	A	47	LYS	C-N-CA	5.16	134.60	121.70
2	D	23	GLY	N-CA-C	5.07	125.77	113.10
1	C	203	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	SER	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2600	0	2551	100	1
1	C	2569	0	2516	61	0
1	E	2563	0	2506	83	1
2	B	1393	0	1309	37	0
2	D	1393	0	1309	31	0
2	F	1385	0	1297	31	0
3	G	46	0	40	7	0
4	A	28	0	26	0	0
4	D	14	0	13	5	0
4	E	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	14	0	13	0	0
5	A	27	0	0	1	0
5	B	21	0	0	1	0
5	C	25	0	0	4	0
5	D	12	0	0	2	0
5	E	19	0	0	5	0
5	F	7	0	0	0	0
All	All	12144	0	11606	314	1

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 13.

All (314) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HD21	3:G:2:GAL:H4	1.05	1.17
2:F:2:ILE:CG2	2:F:109:ASP:OD1	1.96	1.12
2:F:2:ILE:HG22	2:F:109:ASP:OD1	1.52	1.09
1:A:137:ASN:HD21	3:G:2:GAL:C4	1.67	1.08
1:A:263:THR:HG21	1:A:263(B):LYS:HG2	1.33	1.07
2:F:51:LYS:NZ	2:F:107:THR:OG1	1.89	1.05
1:A:263:THR:CG2	1:A:263(B):LYS:HG2	1.90	1.01
1:A:12:LYS:HE2	2:B:27:GLU:OE1	1.62	1.00
1:E:293:THR:HG21	2:F:56:ILE:HG12	1.40	0.99
2:F:2:ILE:HG21	2:F:109:ASP:CG	1.83	0.98
1:A:137:ASN:ND2	3:G:2:GAL:H4	1.80	0.97
1:E:14:CYS:CB	2:F:137:CYS:SG	2.52	0.96
1:E:135:VAL:HG12	1:E:145:SER:HB3	1.46	0.96
1:A:133:ARG:O	3:G:3:SIA:H113	1.68	0.94
1:C:117:ARG:HB3	1:C:261:VAL:CG1	1.96	0.94
1:A:135:VAL:HG13	1:A:146:SER:N	1.83	0.93
1:A:86:TYR:CD1	1:A:302:ILE:HD11	2.03	0.93
2:F:17:MET:SD	2:F:23:GLY:HA3	2.11	0.91
1:A:86:TYR:CD1	1:A:302:ILE:CD1	2.54	0.91
1:A:295:GLN:OE1	1:A:298:SER:N	2.03	0.90
1:C:117:ARG:HB3	1:C:261:VAL:HG11	1.53	0.89
2:F:2:ILE:HG21	2:F:109:ASP:OD1	1.70	0.88
1:E:117:ARG:HB3	1:E:261:VAL:HG11	1.58	0.85
1:E:123:MET:HE2	1:E:257:ALA:HB2	1.63	0.80
1:E:135:VAL:CG1	1:E:145:SER:HB3	2.11	0.80
1:A:288:LEU:HD11	1:A:295:GLN:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:NZ	1:A:157:THR:O	2.15	0.79
4:D:201:NAG:H83	4:D:201:NAG:O3	1.82	0.79
1:E:117:ARG:HB3	1:E:261:VAL:CG1	2.14	0.77
1:E:155:VAL:HG22	5:E:510:HOH:O	1.84	0.77
1:E:135:VAL:HG13	1:E:146:SER:N	2.01	0.76
1:A:310:LYS:HE2	2:B:89:LEU:HD21	1.67	0.76
1:A:326:ILE:H	1:A:326:ILE:HD12	1.50	0.76
1:E:54:ILE:HD11	1:E:282:GLN:HB2	1.68	0.76
1:A:281:CYS:CB	1:A:305:CYS:HG	1.94	0.75
1:A:263:THR:HG21	1:A:263(B):LYS:CG	2.16	0.73
1:E:135:VAL:CG1	1:E:145:SER:C	2.57	0.72
1:C:326:ILE:N	1:C:326:ILE:HD12	2.05	0.72
1:C:46:GLN:OE1	5:C:401:HOH:O	2.05	0.72
1:C:117:ARG:HB3	1:C:261:VAL:HG12	1.71	0.72
1:A:326:ILE:N	1:A:326:ILE:HD12	2.04	0.72
1:A:12:LYS:CE	2:B:27:GLU:OE1	2.37	0.72
2:B:27:GLU:HG3	2:B:32:SER:HB3	1.72	0.70
1:A:135:VAL:HG13	1:A:146:SER:CA	2.22	0.70
1:C:45:ASN:HA	1:C:296:ASN:ND2	2.07	0.70
1:A:266:ALA:HB2	1:A:302:ILE:CG2	2.21	0.70
1:A:263(B):LYS:HG3	1:A:264:LYS:N	2.07	0.69
2:D:127:ARG:N	5:D:301:HOH:O	2.25	0.69
1:E:311:SER:OG	2:F:97:GLU:OE2	2.08	0.69
1:A:43:LEU:C	1:A:43:LEU:HD23	2.14	0.68
1:E:139:CYS:HB2	1:E:146:SER:O	1.94	0.68
4:D:201:NAG:H83	4:D:201:NAG:C3	2.24	0.67
1:A:263(B):LYS:HG3	1:A:265:GLY:N	2.09	0.67
1:A:86:TYR:CE1	1:A:302:ILE:HD11	2.29	0.67
1:A:135:VAL:CG1	1:A:146:SER:N	2.58	0.66
1:A:310:LYS:HG2	2:B:89:LEU:HD11	1.78	0.66
1:C:117:ARG:NH2	1:C:119:GLU:OE1	2.28	0.66
1:E:159:ALA:HB1	1:E:160:THR:CG2	2.26	0.66
2:D:143:LYS:HD3	2:D:144:CYS:N	2.10	0.66
2:B:163:GLN:HE22	2:D:171:GLN:HE22	1.43	0.65
1:C:45:ASN:HA	1:C:296:ASN:HD21	1.59	0.65
1:A:133:ARG:O	3:G:3:SIA:C11	2.44	0.65
1:A:266:ALA:CB	1:A:302:ILE:CG2	2.75	0.65
1:E:106:GLU:OE2	5:E:501:HOH:O	2.12	0.65
1:C:12:LYS:HG2	2:D:27:GLU:HB3	1.78	0.65
1:A:114:SER:O	1:A:263:THR:HG22	1.96	0.64
2:B:160:PRO:O	5:B:201:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:PRO:HB3	1:E:144(A):ASP:O	1.97	0.64
1:A:281:CYS:SG	1:A:305:CYS:CB	2.78	0.64
1:A:156:LYS:CE	1:A:159:ALA:HA	2.28	0.64
1:E:75:LYS:NZ	1:E:140:PRO:O	2.29	0.64
1:E:78:LEU:HD23	1:E:78:LEU:H	1.61	0.64
1:A:116:GLU:HB2	1:A:263:THR:HB	1.80	0.64
2:F:63:PHE:HE2	2:F:85:GLU:HG2	1.63	0.63
1:E:116:GLU:HG2	1:E:261:VAL:HG13	1.80	0.63
1:A:309:VAL:CG2	2:B:93:THR:HA	2.28	0.63
1:A:102:LEU:HD22	1:A:105:LEU:HD13	1.81	0.62
1:A:70:ILE:HD12	1:A:179:PHE:CZ	2.33	0.62
1:A:152:VAL:HG23	1:A:255:TRP:HB2	1.82	0.61
2:B:163:GLN:NE2	2:D:171:GLN:HE22	1.97	0.61
1:A:125(A):LYS:HD3	1:A:131:THR:HB	1.82	0.61
1:C:122:GLU:OE1	5:C:403:HOH:O	2.16	0.61
1:E:288:LEU:HD21	1:E:297:VAL:HG21	1.82	0.61
1:A:187:ASP:HB3	1:A:190:VAL:H	1.65	0.61
1:A:12:LYS:HG2	2:B:27:GLU:HB2	1.83	0.61
2:B:17:MET:SD	2:B:23:GLY:HA3	2.41	0.61
1:C:256:TYR:O	5:C:402:HOH:O	2.16	0.60
1:E:144:ILE:HD12	1:E:145:SER:O	2.01	0.60
3:G:1:NAG:H83	3:G:1:NAG:O1	2.02	0.60
2:D:17:MET:SD	2:D:23:GLY:HA3	2.41	0.60
1:E:221:PRO:O	1:E:229:ARG:NH2	2.34	0.60
1:C:107:GLU:OE2	2:F:75:ARG:N	2.36	0.59
2:D:133:LEU:HD11	2:D:139:GLU:HB2	1.85	0.59
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.85	0.59
1:A:156:LYS:HG2	1:A:157:THR:O	2.02	0.58
1:A:266:ALA:HB3	1:A:302:ILE:HG21	1.86	0.58
1:A:264:LYS:HG3	1:A:265:GLY:N	2.19	0.57
1:A:28:THR:HG22	2:B:104:ASN:HB3	1.86	0.57
1:A:264:LYS:HG3	1:A:265:GLY:H	1.69	0.57
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.15	0.57
2:F:54:SER:O	2:F:58:LYS:HG2	2.05	0.57
1:E:151:LEU:HD13	1:E:252:ILE:HG21	1.87	0.57
1:E:13:ILE:HD13	2:F:152:VAL:HG11	1.87	0.56
1:E:301:TRP:HH2	5:E:514:HOH:O	1.88	0.56
1:A:47:LYS:HD3	1:A:297:VAL:HG13	1.86	0.56
1:C:28:THR:HG22	1:C:30:LEU:H	1.71	0.56
1:A:263(B):LYS:CD	1:A:265:GLY:HA2	2.36	0.56
1:E:135:VAL:HG13	1:E:145:SER:C	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:GLN:HA	2:D:173:ILE:HG22	1.88	0.56
1:E:159:ALA:HB1	1:E:160:THR:HG23	1.87	0.56
2:B:116:LYS:NZ	2:F:120:GLU:OE1	2.35	0.56
2:D:51:LYS:NZ	2:D:107:THR:OG1	2.34	0.56
1:A:200:LYS:NZ	1:A:248:ASN:O	2.33	0.56
1:E:135:VAL:HG13	1:E:146:SER:CA	2.35	0.56
1:E:97:CYS:O	1:E:224:ASN:ND2	2.37	0.56
1:E:135:VAL:HG11	1:E:145:SER:O	2.06	0.56
2:F:2:ILE:CG2	2:F:109:ASP:CG	2.54	0.56
1:A:47:LYS:HD3	1:A:297:VAL:CG1	2.36	0.55
2:F:145:ASP:OD1	2:F:146:ASN:N	2.39	0.55
2:F:63:PHE:CE1	2:F:88:PHE:CD2	2.94	0.55
1:A:326:ILE:CD1	1:A:326:ILE:H	2.16	0.55
1:E:56:LYS:HB3	1:E:85:SER:HB3	1.88	0.55
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.89	0.55
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.89	0.55
1:A:102:LEU:HD22	1:A:105:LEU:CD1	2.37	0.55
2:B:2:ILE:HG23	2:B:3:PHE:CD1	2.41	0.54
2:F:123:LYS:NZ	2:F:132:ASP:OD2	2.40	0.54
1:E:185:PRO:O	1:E:217:ILE:HG23	2.07	0.54
1:E:179:PHE:O	1:E:254:PRO:HB3	2.07	0.54
1:A:135:VAL:HG12	1:A:145:SER:HB3	1.90	0.54
2:D:9:PHE:O	2:D:135:ASN:HA	2.07	0.54
1:E:140:PRO:HD2	5:E:519:HOH:O	2.07	0.54
1:A:60:ASP:HB2	1:A:274:ILE:HD12	1.88	0.54
1:C:326:ILE:HD12	1:C:326:ILE:H	1.71	0.54
4:D:201:NAG:C8	4:D:201:NAG:C3	2.86	0.54
1:E:152:VAL:HG23	1:E:255:TRP:HB2	1.90	0.54
2:B:116:LYS:HE3	2:B:120:GLU:OE2	2.09	0.53
1:E:77:ASP:O	1:E:80:LEU:HB2	2.08	0.53
1:E:186:LEU:HA	1:E:218:ALA:O	2.09	0.53
1:A:298:SER:C	1:A:308:TYR:CD1	2.82	0.53
1:A:86:TYR:CD1	1:A:302:ILE:HD13	2.43	0.53
1:C:159:ALA:HB1	1:C:160:THR:HA	1.89	0.53
1:E:204:MET:HG2	1:E:245:VAL:HG22	1.90	0.53
1:A:156:LYS:HE2	1:A:159:ALA:HA	1.90	0.53
2:B:75:ARG:N	1:E:107:GLU:OE2	2.39	0.52
1:A:266:ALA:CB	1:A:302:ILE:HG21	2.40	0.52
1:E:54:ILE:HD11	1:E:282:GLN:CB	2.39	0.52
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.90	0.52
1:A:90:ARG:HH11	1:A:271:ASP:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LYS:HE2	2:D:27:GLU:OE1	2.08	0.52
1:E:325:GLN:OE1	2:F:12:GLY:HA3	2.08	0.52
1:C:326:ILE:N	1:C:326:ILE:CD1	2.73	0.52
1:A:137:ASN:ND2	3:G:2:GAL:C4	2.50	0.52
2:B:106:ARG:HH22	2:D:105:GLU:CD	2.13	0.52
1:A:263(B):LYS:HD2	1:A:265:GLY:HA2	1.91	0.51
1:C:159:ALA:HB1	1:C:160:THR:HG22	1.91	0.51
1:A:295:GLN:HG2	1:A:297:VAL:H	1.75	0.51
1:E:307:LYS:NZ	2:F:61:THR:O	2.42	0.51
2:B:161:LYS:HE2	2:B:162:TYR:CZ	2.46	0.51
1:C:288:LEU:HD11	1:C:297:VAL:HG21	1.93	0.50
1:E:151:LEU:HB3	1:E:252:ILE:CG2	2.41	0.50
1:A:263:THR:HG23	1:A:263(B):LYS:HG2	1.88	0.50
1:A:12:LYS:HE2	2:B:27:GLU:CD	2.29	0.50
1:C:170:ASN:HB3	1:C:240:GLY:H	1.77	0.50
2:D:3:PHE:CE2	2:D:113:ALA:HB2	2.47	0.50
2:D:143:LYS:HD3	2:D:143:LYS:C	2.32	0.50
1:C:184:HIS:CE1	1:C:216:GLU:HG3	2.46	0.50
1:E:135:VAL:HG11	1:E:145:SER:C	2.32	0.50
1:E:60:ASP:HB2	1:E:274:ILE:HD12	1.94	0.50
1:C:45:ASN:CA	1:C:296:ASN:HD21	2.24	0.50
1:A:263:THR:OG1	1:A:263(A):ASN:N	2.45	0.49
1:E:117:ARG:O	1:E:261:VAL:HG12	2.12	0.49
1:A:263(A):ASN:ND2	1:A:263(A):ASN:H	2.10	0.49
1:A:135:VAL:CG1	1:A:145:SER:C	2.81	0.49
1:E:167:THR:HA	1:E:243:LEU:O	2.12	0.49
1:C:51:PHE:CE2	1:C:272:LEU:HB2	2.48	0.49
1:C:170:ASN:O	1:C:172:GLY:N	2.36	0.48
2:D:2:ILE:HG22	2:D:109:ASP:OD1	2.12	0.48
1:A:12:LYS:HG2	2:B:27:GLU:CB	2.42	0.48
1:A:196:GLY:O	1:A:200:LYS:HE2	2.12	0.48
2:B:105:GLU:CD	2:F:106:ARG:HH22	2.17	0.48
2:B:37:ASP:O	2:B:41:THR:HG23	2.13	0.48
1:E:100:GLY:HA3	1:E:230:ILE:O	2.13	0.48
1:E:156:LYS:HB3	1:E:156:LYS:HE3	1.67	0.48
1:E:159:ALA:HB1	1:E:160:THR:HG22	1.95	0.48
1:C:115:GLY:HA3	1:C:260:PHE:CZ	2.49	0.48
1:C:176:ILE:O	1:C:236:VAL:HA	2.14	0.48
1:A:113:GLY:C	1:A:115:GLY:HA3	2.34	0.48
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.78	0.48
1:A:144:ILE:HG22	1:A:145:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:OE2	1:A:46:GLN:HB2	2.13	0.47
1:C:284:ILE:HG23	1:C:285:THR:HG23	1.96	0.47
2:F:3:PHE:CE1	2:F:113:ALA:HB2	2.49	0.47
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.29	0.47
2:B:2:ILE:HG23	2:B:3:PHE:N	2.29	0.47
1:C:186:LEU:H	1:C:186:LEU:HD23	1.79	0.47
1:A:100:GLY:HA3	1:A:230:ILE:O	2.14	0.47
1:A:122:GLU:OE1	1:A:255:TRP:NE1	2.46	0.47
1:E:157:THR:HG22	1:E:157(A):ASP:N	2.30	0.47
2:D:123:LYS:O	5:D:301:HOH:O	2.20	0.47
1:C:74:PRO:HG3	1:C:147:PHE:O	2.13	0.47
1:E:201:TYR:HD2	1:E:203:ARG:HG3	1.79	0.47
2:D:17:MET:CE	2:D:23:GLY:HA3	2.44	0.47
2:B:4:GLY:O	2:B:8:GLY:HA3	2.16	0.46
1:A:114:SER:C	1:A:263:THR:HG22	2.35	0.46
2:D:2:ILE:CG2	2:D:109:ASP:OD1	2.64	0.46
2:B:2:ILE:HG23	2:B:3:PHE:HD1	1.80	0.46
2:B:127:ARG:NH2	2:D:131:ASN:OD1	2.33	0.46
1:C:152:VAL:HG23	1:C:255:TRP:HB2	1.98	0.46
4:D:201:NAG:C8	4:D:201:NAG:H3	2.46	0.46
1:C:12:LYS:NZ	2:D:25:HIS:NE2	2.57	0.46
2:B:141:TRP:O	2:B:166:SER:HA	2.15	0.46
2:F:9:PHE:O	2:F:135:ASN:HA	2.15	0.46
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.15	0.46
1:C:175:PRO:HD2	1:C:260:PHE:O	2.16	0.46
2:D:106:ARG:NH2	2:F:105:GLU:OE2	2.37	0.46
1:A:288:LEU:HD21	1:A:297:VAL:HG21	1.98	0.46
2:F:94:TYR:CZ	2:F:98:LEU:HD22	2.50	0.46
1:A:114:SER:N	1:A:115:GLY:HA3	2.31	0.45
2:D:24:TYR:HE1	2:D:37:ASP:HB2	1.81	0.45
1:A:298:SER:O	1:A:308:TYR:CD1	2.69	0.45
1:C:281:CYS:HB2	1:C:304:GLU:O	2.16	0.45
2:B:73:LEU:HA	2:B:73:LEU:HD23	1.87	0.45
1:E:200:LYS:O	1:E:215:PRO:HD2	2.16	0.45
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.99	0.45
1:A:45:ASN:OD1	1:A:46:GLN:HG2	2.17	0.45
1:E:130(A):ASP:OD1	1:E:131:THR:N	2.50	0.45
1:C:117:ARG:CB	1:C:261:VAL:HG12	2.44	0.45
1:C:326:ILE:H	1:C:326:ILE:CD1	2.29	0.45
1:C:21:ASN:ND2	5:C:408:HOH:O	2.49	0.44
1:E:70:ILE:HD13	1:E:179:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ILE:O	2:D:52:VAL:HG23	2.18	0.44
1:A:182:VAL:HG21	1:A:213:LYS:HB3	1.99	0.44
1:C:12:LYS:HG2	2:D:27:GLU:CB	2.44	0.44
1:E:72:GLY:O	1:E:148:TYR:HA	2.17	0.44
1:C:291:ASN:OD1	1:C:291:ASN:N	2.51	0.44
1:C:47:LYS:HD2	1:C:297:VAL:HG13	1.99	0.44
1:E:237:LEU:HA	1:E:237:LEU:HD12	1.84	0.44
1:E:66:ILE:O	1:E:70:ILE:HG13	2.17	0.44
1:E:15:ILE:HD11	2:F:122:VAL:HG21	2.00	0.44
1:C:25:GLN:OE1	1:C:33:ASN:HB3	2.18	0.44
1:C:70:ILE:HA	1:C:70:ILE:HD12	1.89	0.44
1:E:89:GLU:O	1:E:269:LYS:HA	2.18	0.44
1:A:295:GLN:OE1	1:A:308:TYR:HD1	2.01	0.44
2:F:166:SER:HB3	2:F:170:ARG:HH21	1.83	0.44
1:E:196:GLY:N	1:E:200:LYS:HZ1	2.16	0.43
1:A:217:ILE:O	1:E:203:ARG:HD2	2.17	0.43
1:C:159:ALA:HB1	1:C:160:THR:CG2	2.48	0.43
1:C:261:VAL:O	1:C:261:VAL:HG13	2.17	0.43
1:E:107:GLU:HB2	5:E:503:HOH:O	2.18	0.43
1:E:156:LYS:HE2	1:E:195:TYR:O	2.19	0.43
1:E:252:ILE:HD12	1:E:252:ILE:N	2.33	0.43
4:D:201:NAG:H83	4:D:201:NAG:H3	1.98	0.43
1:C:299:PRO:HB3	1:C:308:TYR:CD2	2.53	0.43
1:E:158:SER:C	1:E:159:ALA:O	2.55	0.43
1:E:59:LEU:HD11	1:E:79:LEU:HD22	2.00	0.43
1:A:43:LEU:C	1:A:43:LEU:CD2	2.86	0.43
1:C:156:LYS:HD2	1:C:159:ALA:HA	2.00	0.43
1:C:52:CYS:SG	1:C:287:VAL:HG21	2.59	0.43
1:E:196:GLY:H	1:E:200:LYS:HZ1	1.66	0.43
1:A:125(A):LYS:HD3	1:A:131:THR:CB	2.48	0.43
1:A:43:LEU:HD23	1:A:44:GLU:N	2.34	0.43
2:B:25:HIS:ND1	2:B:33:GLY:O	2.52	0.43
2:B:82:LYS:HE3	2:B:86:ASP:OD2	2.19	0.43
1:E:144:ILE:CD1	1:E:145:SER:O	2.67	0.42
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.79	0.42
1:C:12:LYS:HE3	2:D:25:HIS:NE2	2.34	0.42
1:C:45:ASN:CB	1:C:296:ASN:HD21	2.32	0.42
1:E:185:PRO:HG2	1:E:191:GLN:OE1	2.18	0.42
1:E:293:THR:OG1	1:E:294:PHE:CD2	2.73	0.42
1:A:320:LEU:HB3	2:B:111:HIS:CG	2.54	0.42
1:C:73:ASN:O	1:C:76:CYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.55	0.42
1:E:202:VAL:HG22	1:E:251:LEU:HB2	2.02	0.42
1:A:98:TYR:CE1	1:A:230:ILE:HG13	2.55	0.42
1:E:252:ILE:CD1	1:E:252:ILE:N	2.82	0.42
1:A:160:THR:O	1:A:160:THR:HG23	2.20	0.42
1:C:100:GLY:HA3	1:C:230:ILE:O	2.19	0.42
1:C:264:LYS:HE2	1:C:265:GLY:O	2.20	0.41
1:E:61:LEU:HB3	1:E:64:CYS:O	2.20	0.41
1:E:44:GLU:HG2	1:E:290:THR:HG21	2.01	0.41
1:A:56:LYS:HB3	1:A:85:SER:HB3	2.02	0.41
2:D:3:PHE:CD2	2:D:113:ALA:HB2	2.55	0.41
1:A:296:ASN:OD1	1:A:311:SER:O	2.38	0.41
1:C:295:GLN:NE2	1:C:308:TYR:HB2	2.34	0.41
1:E:130:VAL:HG21	1:E:154:ILE:HG22	2.02	0.41
1:E:70:ILE:HD13	1:E:179:PHE:CE2	2.54	0.41
2:D:148:CYS:O	2:D:152:VAL:HG23	2.20	0.41
1:E:70:ILE:H	1:E:70:ILE:HG13	1.74	0.41
1:C:213:LYS:HG3	1:C:214:SER:N	2.36	0.41
1:C:167:THR:HA	1:C:243:LEU:O	2.20	0.41
1:E:323:VAL:HA	1:E:324:PRO:HD2	1.96	0.41
1:A:29:LEU:HB2	2:B:105:GLU:OE2	2.20	0.41
2:B:55:ILE:HG12	2:B:99:LEU:HD21	2.03	0.41
1:C:204:MET:HE3	1:C:243:LEU:HD11	2.02	0.41
2:D:116:LYS:HE3	2:D:120:GLU:OE2	2.20	0.41
1:C:98:TYR:CE1	1:C:230:ILE:HG13	2.56	0.41
1:A:54:ILE:HD13	1:A:279:ALA:O	2.21	0.41
1:A:310:LYS:CG	2:B:89:LEU:HD11	2.49	0.41
2:F:16:GLY:O	2:F:18:ILE:HG12	2.20	0.41
1:C:181:GLY:HA2	1:C:231:ASP:O	2.21	0.40
2:D:99:LEU:HD13	2:F:98:LEU:HD21	2.04	0.40
1:A:70:ILE:HD11	1:A:108:LEU:HD21	2.04	0.40
2:B:48:ILE:CD1	2:B:107:THR:HG23	2.52	0.40
1:C:117:ARG:O	1:C:261:VAL:HG12	2.21	0.40
2:D:11:GLU:O	2:D:11:GLU:HG2	2.21	0.40
1:E:130:VAL:HG22	1:E:155:VAL:O	2.20	0.40
1:A:175:PRO:CD	5:A:513:HOH:O	2.69	0.40
1:A:264:LYS:HE3	1:A:301:TRP:O	2.21	0.40
2:B:168:LEU:HA	2:B:168:LEU:HD23	1.93	0.40
1:C:270:SER:OG	1:C:271:ASP:N	2.55	0.40
1:E:43:LEU:HA	1:E:294:PHE:O	2.21	0.40
2:F:64:GLU:OE2	2:F:64:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:CYS:SG	1:C:288:LEU:HB2	2.61	0.40

All (1) 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:A:157(A):ASP:OD1	1:E:188:THR:OG1[2_757]	1.88	0.32

## 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	328/333 (98%)	314 (96%)	13 (4%)	1 (0%)	41	47
1	C	322/333 (97%)	312 (97%)	10 (3%)	0	100	100
1	E	321/333 (96%)	306 (95%)	15 (5%)	0	100	100
2	B	171/180 (95%)	170 (99%)	1 (1%)	0	100	100
2	D	171/180 (95%)	166 (97%)	5 (3%)	0	100	100
2	F	170/180 (94%)	167 (98%)	3 (2%)	0	100	100
All	All	1483/1539 (96%)	1435 (97%)	47 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263(B)	LYS

### 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	289/291 (99%)	281 (97%)	8 (3%)	43	53
1	C	285/291 (98%)	282 (99%)	3 (1%)	73	84
1	E	284/291 (98%)	275 (97%)	9 (3%)	39	47
2	B	147/153 (96%)	147 (100%)	0	100	100
2	D	147/153 (96%)	146 (99%)	1 (1%)	84	91
2	F	146/153 (95%)	145 (99%)	1 (1%)	84	91
All	All	1298/1332 (97%)	1276 (98%)	22 (2%)	60	72

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

Mol	Chain	Res	Type
1	A	125(B)	SER
1	A	157(A)	ASP
1	A	263(A)	ASN
1	A	264	LYS
1	A	295	GLN
1	A	296	ASN
1	A	316	LEU
1	A	325	GLN
1	C	264	LYS
1	C	295	GLN
1	C	296	ASN
2	D	64	GLU
1	E	28	THR
1	E	63	ASP
1	E	102	LEU
1	E	147	PHE
1	E	186	LEU
1	E	293	THR
1	E	320	LEU
1	E	321	ARG
1	E	325	GLN
2	F	119	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	226	GLN
1	A	263(A)	ASN
2	B	60	ASN
2	B	117	ASN
2	B	163	GLN
1	C	170	ASN
1	C	296	ASN
1	C	325	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

3 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	NAG	G	1	3	15,15,15	0.58	0	21,21,21	1.68	3 (14%)
3	GAL	G	2	3	11,11,12	1.62	2 (18%)	15,15,17	1.54	5 (33%)
3	SIA	G	3	3	17,20,21	0.72	0	21,28,31	1.32	3 (14%)

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	NAG	G	1	3	-	5/6/26/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
3	SIA	G	3	3	-	2/14/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	GAL	O5-C1	-3.74	1.37	1.43
3	G	2	GAL	C1-C2	3.27	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O5-C1-C2	-4.01	105.48	109.52
3	G	3	SIA	O9-C9-C8	-3.43	103.59	111.07
3	G	1	NAG	O4-C4-C3	-3.40	102.48	110.35
3	G	1	NAG	C1-C2-N2	3.22	114.46	110.73
3	G	2	GAL	C1-O5-C5	-3.21	107.84	112.19
3	G	3	SIA	C6-C5-N5	-3.06	105.83	110.91
3	G	2	GAL	O5-C1-C2	-2.48	106.95	110.77
3	G	3	SIA	C6-O6-C2	2.33	116.33	111.34
3	G	2	GAL	O2-C2-C1	2.16	113.57	109.15
3	G	2	GAL	C6-C5-C4	2.15	118.03	113.00
3	G	2	GAL	O5-C5-C6	-2.01	104.05	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

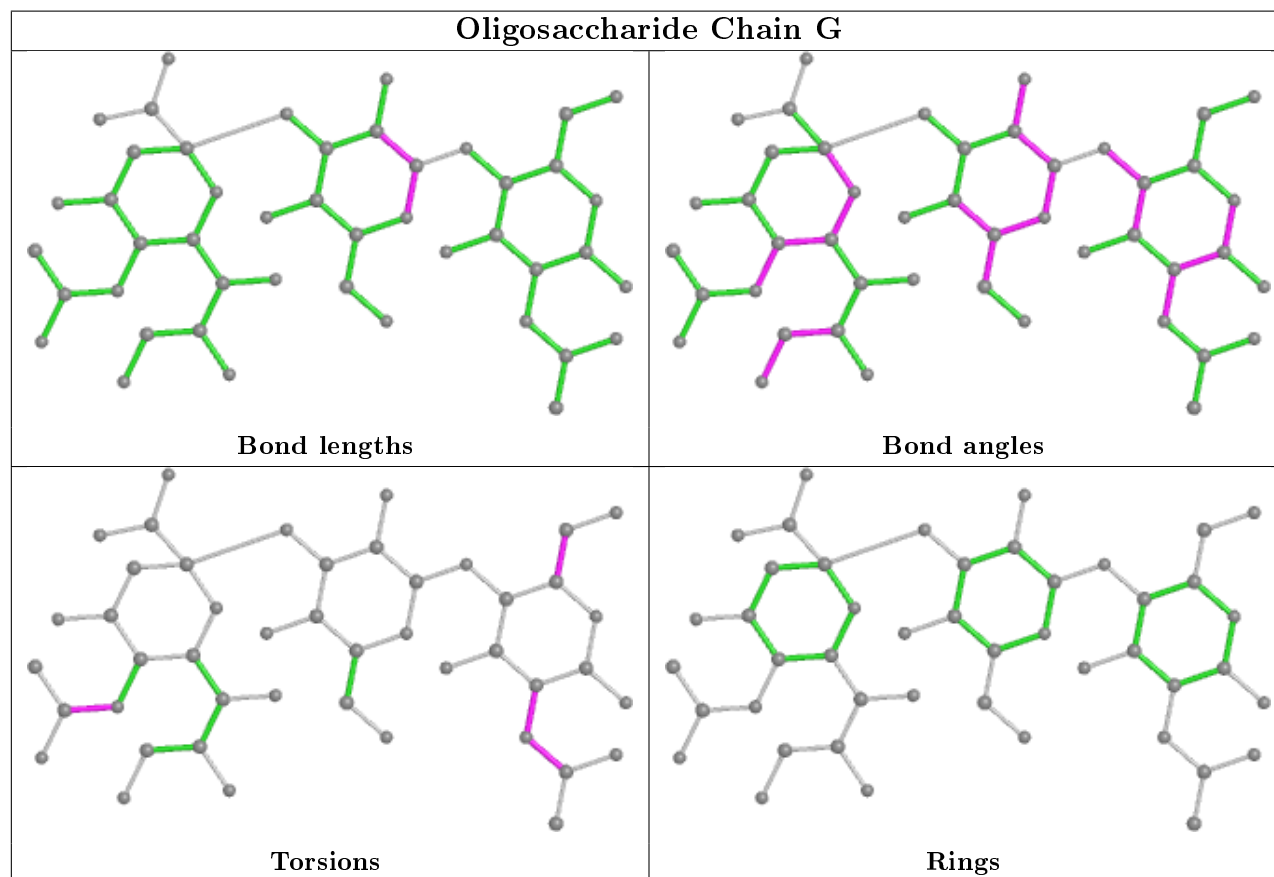
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	3	SIA	C11-C10-N5-C5
3	G	3	SIA	O10-C10-N5-C5

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	GAL	4	0
3	G	3	SIA	2	0
3	G	1	NAG	1	0

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



## 5.6 Ligand geometry [i](#)

6 ligands 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	$\# Z  > 2$
4	NAG	D	201	2	14,14,15	0.60	0	17,19,21	2.66	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	F	201	2	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
4	NAG	E	402	1	14,14,15	0.73	0	17,19,21	2.00	5 (29%)
4	NAG	A	402	1	14,14,15	0.41	0	17,19,21	0.47	0
4	NAG	E	401	1	14,14,15	0.45	0	17,19,21	1.67	3 (17%)
4	NAG	A	401	1	14,14,15	0.54	0	17,19,21	1.10	1 (5%)

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
4	NAG	D	201	2	-	4/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1
4	NAG	E	402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1
4	NAG	E	401	1	-	4/6/23/26	0/1/1/1
4	NAG	A	401	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	NAG	C1-C2-N2	-7.81	97.14	110.49
4	E	402	NAG	C1-C2-N2	-4.64	102.56	110.49
4	E	402	NAG	O5-C5-C6	-4.51	100.14	107.20
4	D	201	NAG	O5-C5-C6	-4.45	100.23	107.20
4	E	401	NAG	O5-C5-C6	-4.06	100.84	107.20
4	D	201	NAG	C6-C5-C4	-3.63	104.49	113.00
4	A	401	NAG	O5-C5-C6	-3.42	101.84	107.20
4	E	401	NAG	C6-C5-C4	-3.16	105.61	113.00
4	E	401	NAG	C1-O5-C5	2.83	116.02	112.19
4	E	402	NAG	C6-C5-C4	-2.79	106.48	113.00
4	F	201	NAG	C1-O5-C5	2.74	115.91	112.19
4	D	201	NAG	C2-N2-C7	2.69	126.74	122.90
4	D	201	NAG	O6-C6-C5	-2.65	102.19	111.29
4	D	201	NAG	C1-O5-C5	2.65	115.78	112.19
4	E	402	NAG	C1-O5-C5	2.14	115.09	112.19
4	E	402	NAG	O3-C3-C2	2.02	113.65	109.47



There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	201	NAG	C3-C2-N2-C7
4	D	201	NAG	C8-C7-N2-C2
4	D	201	NAG	O7-C7-N2-C2
4	E	401	NAG	C8-C7-N2-C2
4	E	401	NAG	O7-C7-N2-C2
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	E	402	NAG	O5-C5-C6-O6
4	A	401	NAG	C1-C2-N2-C7
4	E	401	NAG	O5-C5-C6-O6
4	A	401	NAG	O5-C5-C6-O6
4	E	402	NAG	C4-C5-C6-O6
4	E	401	NAG	C4-C5-C6-O6
4	A	401	NAG	C4-C5-C6-O6
4	D	201	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	NAG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/333 (99%)	0.68	25 (7%) 13 21	48, 64, 81, 96	0
1	C	326/333 (97%)	0.65	24 (7%) 14 22	49, 62, 80, 99	0
1	E	325/333 (97%)	0.65	18 (5%) 25 36	50, 63, 79, 98	0
2	B	173/180 (96%)	0.84	17 (9%) 7 12	47, 58, 72, 85	0
2	D	173/180 (96%)	0.84	18 (10%) 6 10	49, 62, 78, 91	0
2	F	172/180 (95%)	0.87	15 (8%) 10 15	48, 62, 78, 95	0
All	All	1499/1539 (97%)	0.73	117 (7%) 13 19	47, 62, 79, 99	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	GLY	8.8
2	F	1	GLY	7.7
2	B	1	GLY	7.5
2	F	38	ARG	5.3
1	A	61	LEU	4.8
1	A	55	MET	4.8
1	C	157(A)	ASP	4.7
1	A	263	THR	4.6
2	F	171	GLN	4.6
1	C	158	SER	4.5
2	F	2	ILE	4.5
1	C	92	ASN	4.2
2	B	2	ILE	4.2
1	E	171	THR	4.1
2	D	2	ILE	4.1
1	A	325	GLN	4.1
1	E	207	GLU	3.7
2	D	163	GLN	3.4
1	A	326	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	10	ILE	3.1
1	A	93	ALA	3.0
1	C	93	ALA	3.0
1	C	46	GLN	3.0
2	F	98	LEU	3.0
1	C	12	LYS	3.0
1	C	324	PRO	3.0
1	C	327	ALA	2.9
2	D	171	GLN	2.9
2	F	170	ARG	2.9
2	D	168	LEU	2.9
1	A	273	PRO	2.9
2	B	9	PHE	2.8
1	A	219	ALA	2.8
2	B	18	ILE	2.8
2	D	18	ILE	2.8
1	C	61	LEU	2.8
2	D	167	LYS	2.8
1	C	268	PHE	2.8
1	C	170	ASN	2.8
1	E	9	PRO	2.7
1	A	171	THR	2.7
1	A	263(B)	LYS	2.7
1	A	55(A)	ASN	2.7
1	E	40	VAL	2.7
2	B	147	GLU	2.7
1	E	166	GLY	2.7
2	D	103	GLU	2.6
1	E	125(B)	SER	2.6
1	A	327	ALA	2.6
2	B	122	VAL	2.6
1	A	263(A)	ASN	2.6
1	C	55	MET	2.6
1	E	277	CYS	2.6
2	F	3	PHE	2.5
2	F	7	ALA	2.5
2	B	107	THR	2.5
2	D	112	ASP	2.5
2	B	3	PHE	2.5
2	F	168	LEU	2.5
1	E	157(A)	ASP	2.5
2	F	140	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	161	TYR	2.4
1	A	78	LEU	2.4
1	E	55(A)	ASN	2.4
2	B	5	ALA	2.4
2	F	88	PHE	2.4
1	A	65	THR	2.4
2	D	3	PHE	2.3
1	E	159	ALA	2.3
1	C	187	ASP	2.3
2	D	172	GLY	2.3
1	A	49	LYS	2.3
2	B	127	ARG	2.3
1	A	276	ASN	2.3
1	A	56	LYS	2.3
1	A	57	ALA	2.3
1	C	253	ALA	2.3
2	B	94	TYR	2.3
1	C	272	LEU	2.2
2	F	77	ILE	2.2
1	C	198	GLY	2.2
1	C	302	ILE	2.2
1	E	242	THR	2.2
2	B	113	ALA	2.2
2	D	6	ILE	2.2
2	F	118	LEU	2.2
1	A	63	ASP	2.2
2	B	119	TYR	2.2
2	D	115	VAL	2.2
2	B	138	PHE	2.2
2	D	113	ALA	2.1
1	C	237	LEU	2.1
2	D	98	LEU	2.1
1	A	214	SER	2.1
1	E	12	LYS	2.1
2	F	166	SER	2.1
1	C	193	ASN	2.1
1	E	161	TYR	2.1
1	A	173	THR	2.1
2	D	45	ILE	2.1
2	F	31	GLY	2.1
1	C	159	ALA	2.1
1	A	15	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	55(A)	ASN	2.1
1	E	55	MET	2.1
1	E	323	VAL	2.1
1	A	272	LEU	2.1
2	B	10	ILE	2.1
1	E	257	ALA	2.1
1	E	158	SER	2.0
2	B	133	LEU	2.0
2	D	101	LEU	2.0
1	A	197	SER	2.0
1	E	138	ALA	2.0
1	C	112	ILE	2.0
1	C	207	GLU	2.0
2	B	102	LEU	2.0

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

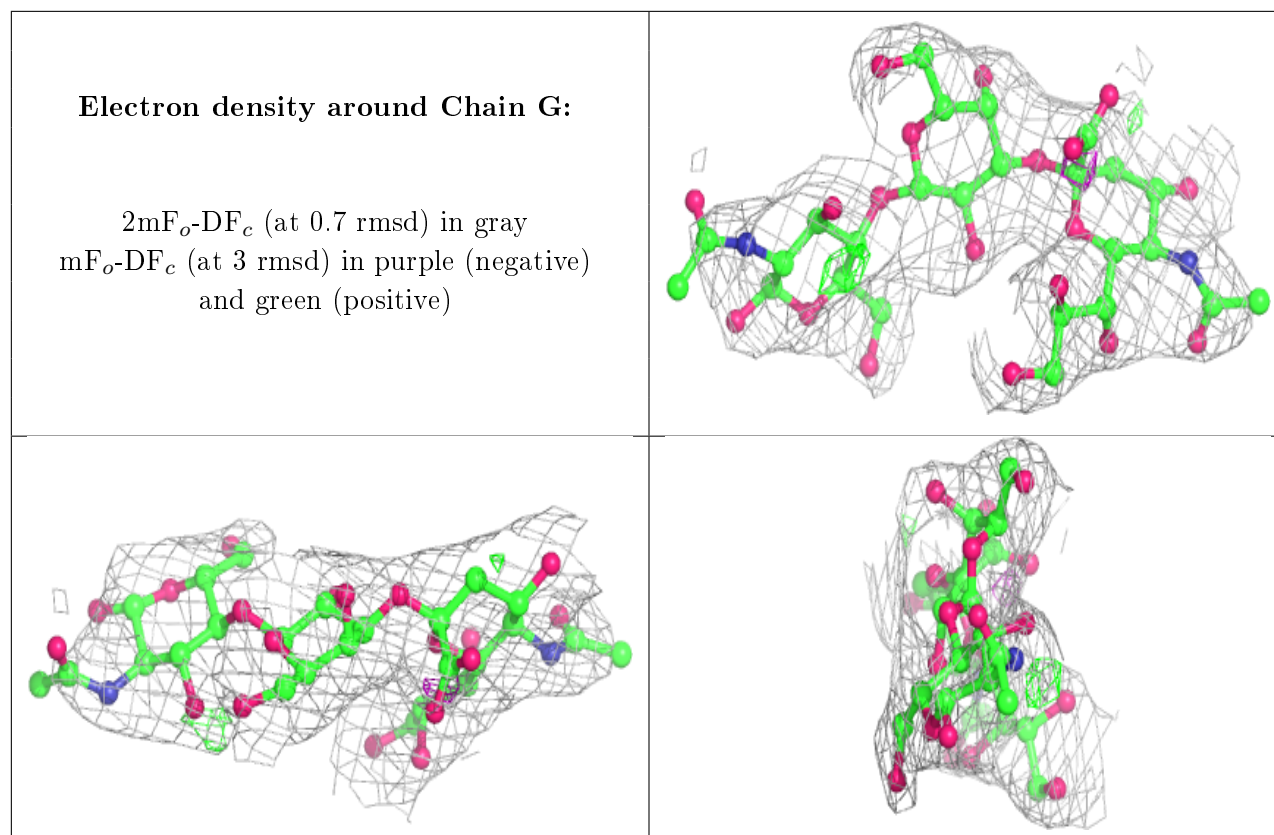
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	SIA	G	3	20/21	0.83	0.17	62,69,74,75	1
3	NAG	G	1	15/15	0.84	0.20	83,87,99,105	0
3	GAL	G	2	11/12	0.94	0.09	72,76,78,81	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.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	NAG	A	401	14/15	0.64	0.24	89,96,104,105	0
4	NAG	D	201	14/15	0.65	0.25	91,100,105,110	0
4	NAG	E	401	14/15	0.68	0.47	102,111,118,118	0
4	NAG	F	201	14/15	0.72	0.21	85,89,95,98	0
4	NAG	A	402	14/15	0.83	0.16	76,84,88,88	0
4	NAG	E	402	14/15	0.86	0.19	91,97,103,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.