



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:22 AM UTC

PDB ID : 2WRG / pdb_00002wrg
Title : structure of H1 1918 hemagglutinin with human receptor
Authors : Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.;
Gamblin, S.J.; Skehel, J.J.
Deposited on : 2009-09-01
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

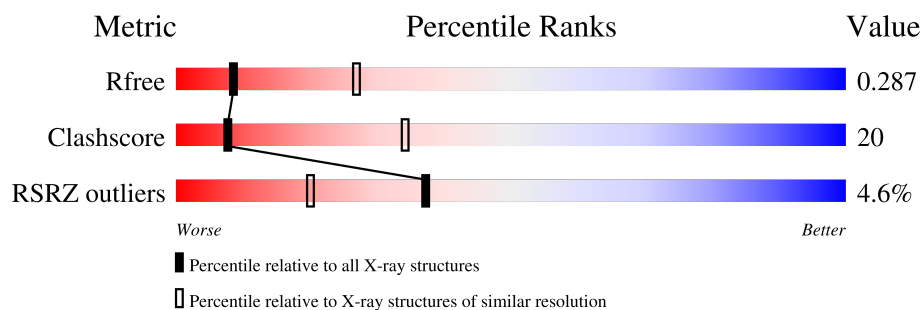
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	326	6% 66% 33%
1	J	326	4% 65% 33% .
1	L	326	3% 68% 30% .
2	I	222	5% 47% 24% . 27%
2	K	222	5% 49% 22% . 27%
2	M	222	3% 50% 20% . 27%
3	A	4	75% 25%

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
3	GAL	A	3	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11619 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	H	325	Total	C	N	O	S	0	0	1
			2517	1586	435	485	11			
1	J	325	Total	C	N	O	S	0	0	1
			2517	1586	435	485	11			
1	L	325	Total	C	N	O	S	0	0	1
			2517	1586	435	485	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	327	ARG	ILE	conflict	UNP Q9WFX3
J	327	ARG	ILE	conflict	UNP Q9WFX3
L	327	ARG	ILE	conflict	UNP Q9WFX3

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	161	Total	C	N	O	S	0	0	1
			1282	802	221	253	6			
2	K	161	Total	C	N	O	S	0	0	1
			1282	802	221	253	6			
2	M	161	Total	C	N	O	S	0	0	1
			1282	802	221	253	6			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	4	Total	C	N	O	0	0	0
			57	31	2	24			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	J	1	Total	C	N	O	0	0
			15	8	1	6		
4	J	1	Total	C	N	O	0	0
			15	8	1	6		
4	K	1	Total	C	N	O	0	0
			15	8	1	6		
4	L	1	Total	C	N	O	0	0
			15	8	1	6		
4	L	1	Total	C	N	O	0	0
			15	8	1	6		

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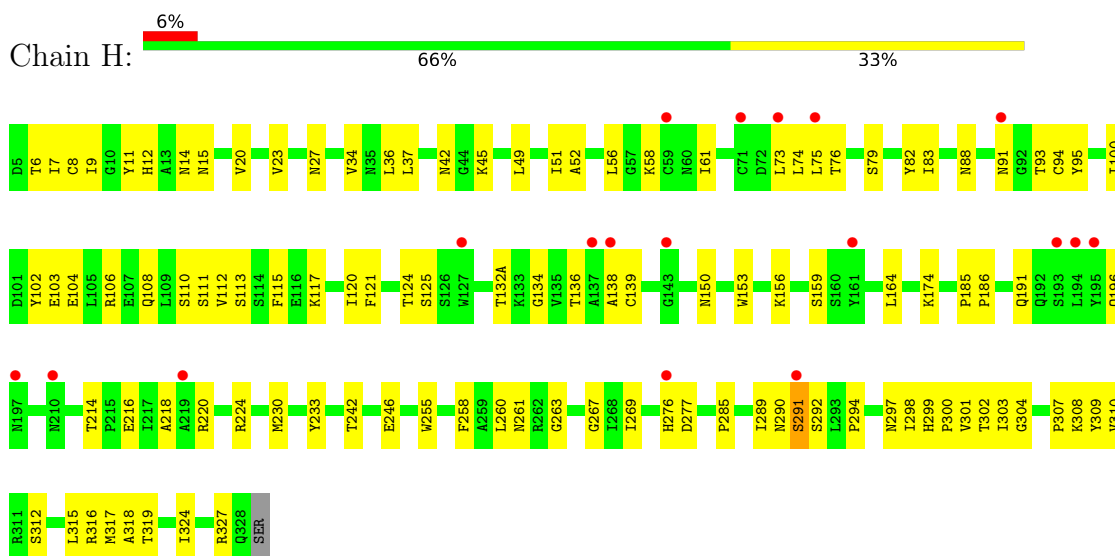
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	N	O	0	0
			15	8	1	6		

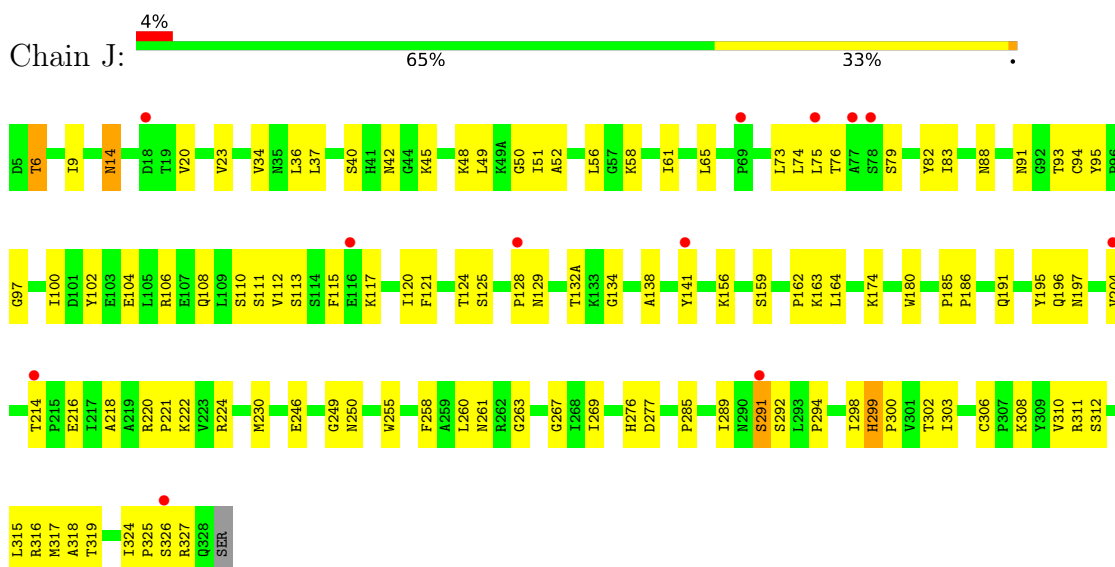
3 Residue-property plots

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

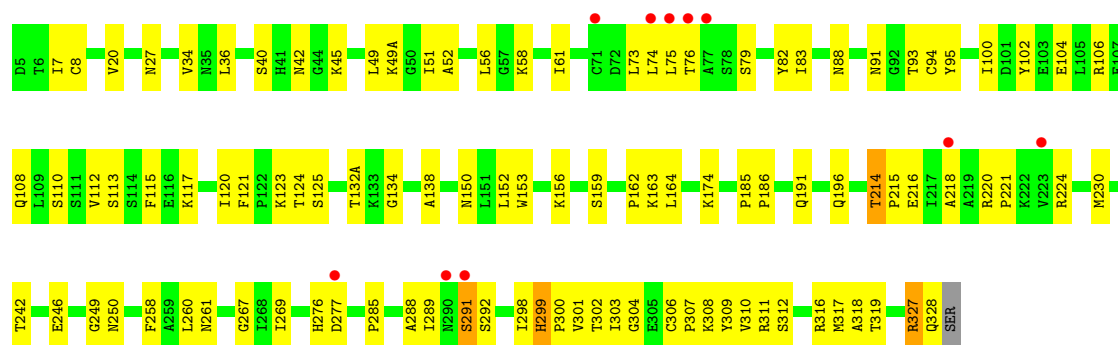


• Molecule 1: HEMAGGLUTININ HA1 CHAIN

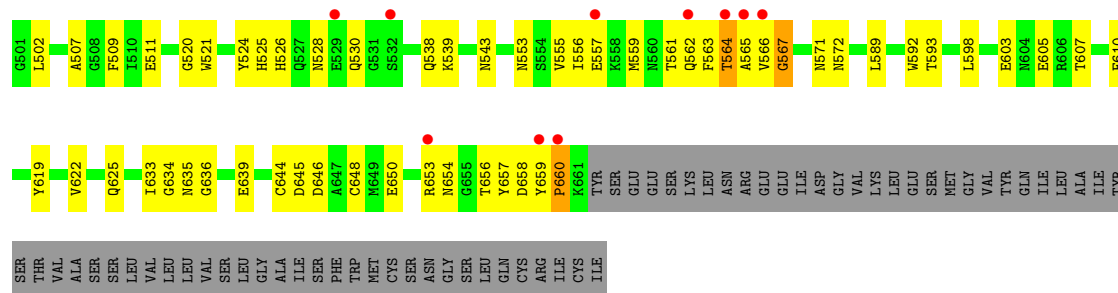


• Molecule 1: HEMAGGLUTININ HA1 CHAIN

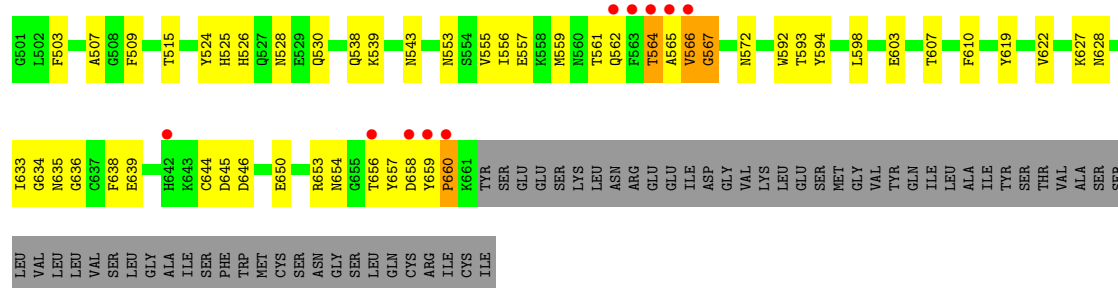




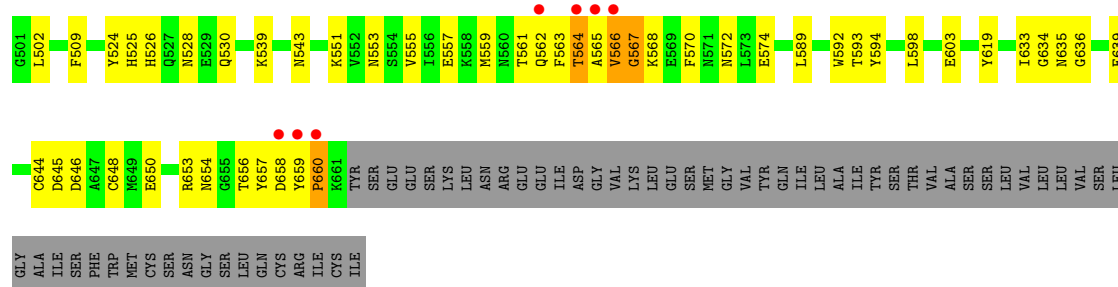
• Molecule 2: HEMAGGLUTININ HA2 CHAIN



• Molecule 2: HEMAGGLUTININ HA2 CHAIN



• Molecule 2: HEMAGGLUTININ HA2 CHAIN



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain A:



GAL1	GAL3
NAG2	STIA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.76Å 156.84Å 157.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 3.00 29.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.8 (29.68-3.00) 97.8 (29.68-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.268 , 0.308 0.258 , 0.287	Depositor DCC
R_{free} test set	2646 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11619	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	H	0.49	1/2581 (0.0%)	0.89	6/3516 (0.2%)
1	J	0.53	1/2581 (0.0%)	0.91	9/3516 (0.3%)
1	L	0.55	1/2581 (0.0%)	0.90	6/3516 (0.2%)
2	I	0.65	2/1308 (0.2%)	0.90	3/1764 (0.2%)
2	K	0.74	4/1308 (0.3%)	0.92	1/1764 (0.1%)
2	M	0.70	3/1308 (0.2%)	0.93	2/1764 (0.1%)
All	All	0.59	12/11667 (0.1%)	0.91	27/15840 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	660	PRO	C-N	-7.19	1.23	1.33
2	K	660	PRO	C-N	-7.09	1.23	1.33
2	M	564	THR	CA-CB	7.01	1.65	1.53
2	I	660	PRO	C-N	-6.95	1.23	1.33
1	H	327	ARG	C-N	-6.74	1.24	1.33
1	L	327	ARG	C-N	-6.63	1.24	1.33
1	J	327	ARG	C-N	-6.63	1.24	1.33
2	K	564	THR	CA-CB	6.62	1.64	1.53
2	M	566	VAL	CA-CB	6.61	1.63	1.54
2	I	564	THR	CA-CB	5.95	1.63	1.53
2	K	564	THR	CA-C	5.09	1.59	1.52
2	K	566	VAL	CA-CB	5.08	1.61	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	291	SER	N-CA-C	9.11	124.81	108.69
1	L	291	SER	N-CA-C	9.07	124.74	108.69
1	H	291	SER	N-CA-C	8.49	123.72	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	568	LYS	CB-CG-CD	6.84	127.03	111.30
2	M	567	GLY	N-CA-C	-6.76	101.81	111.42
1	H	214	THR	CA-C-N	6.66	128.17	119.84
1	H	214	THR	C-N-CA	6.66	128.17	119.84
1	L	214	THR	CA-C-N	6.42	127.87	119.84
1	L	214	THR	C-N-CA	6.42	127.87	119.84
1	J	214	THR	CA-C-N	6.35	127.77	119.84
1	J	214	THR	C-N-CA	6.35	127.77	119.84
1	J	292	SER	N-CA-C	-6.30	106.56	114.56
1	H	292	SER	N-CA-C	-5.93	107.02	114.56
2	I	567	GLY	N-CA-C	-5.79	102.44	112.06
1	H	255	TRP	N-CA-C	-5.74	105.54	113.18
2	K	567	GLY	N-CA-C	-5.53	102.89	112.06
1	J	6	THR	N-CA-C	5.38	117.15	108.32
2	I	625	GLN	N-CA-C	-5.38	106.77	113.55
1	L	299	HIS	CA-C-N	5.36	124.54	118.97
1	L	299	HIS	C-N-CA	5.36	124.54	118.97
1	H	14	ASN	N-CA-C	5.35	115.30	108.24
1	J	14	ASN	N-CA-C	5.30	115.23	108.24
1	L	292	SER	N-CA-C	-5.24	107.90	114.56
1	J	255	TRP	N-CA-C	-5.18	106.90	113.43
1	J	299	HIS	CA-C-N	5.18	124.80	119.05
1	J	299	HIS	C-N-CA	5.18	124.80	119.05
2	I	511	GLU	N-CA-C	5.07	116.81	111.28

There are no chirality outliers.

There are no planarity outliers.

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	H	2517	0	2439	122	0
1	J	2517	0	2439	100	1
1	L	2517	0	2439	107	2
2	I	1282	0	1200	69	0
2	K	1282	0	1198	60	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1282	0	1200	64	1
3	A	57	0	44	1	0
4	H	75	0	75	17	0
4	J	30	0	30	3	0
4	K	15	0	15	3	0
4	L	30	0	30	4	0
4	M	15	0	15	5	0
All	All	11619	0	11124	453	3

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 20.

All (453) 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:H:58:LYS:H	1:H:58:LYS:HE2	1.07	1.18
1:L:58:LYS:HE2	1:L:58:LYS:H	1.06	1.11
1:J:58:LYS:HE2	1:J:58:LYS:H	1.11	1.08
1:L:27:ASN:ND2	4:L:1329:NAG:H4	1.70	1.07
1:H:27:ASN:ND2	4:H:1332:NAG:H4	1.73	1.02
1:H:290:ASN:HB3	4:H:1330:NAG:H83	1.50	0.92
1:L:58:LYS:HE2	1:L:58:LYS:N	1.86	0.89
1:H:8:CYS:O	2:I:524:TYR:HA	1.73	0.89
1:H:58:LYS:HE2	1:H:58:LYS:N	1.88	0.87
1:H:91:ASN:N	1:H:91:ASN:HD22	1.71	0.87
1:J:58:LYS:HE2	1:J:58:LYS:N	1.91	0.85
1:L:73:LEU:HD23	1:L:73:LEU:H	1.42	0.85
1:L:156:LYS:HD2	1:L:196:GLN:HG2	1.60	0.83
1:H:73:LEU:H	1:H:73:LEU:HD23	1.44	0.83
1:H:289:ILE:HG22	1:H:291:SER:HB2	1.59	0.83
1:H:224:ARG:NH2	4:H:1328:NAG:O3	2.12	0.83
1:J:73:LEU:HD23	1:J:73:LEU:H	1.42	0.82
1:J:289:ILE:HG22	1:J:291:SER:HB2	1.62	0.82
1:L:91:ASN:HD22	1:L:91:ASN:N	1.76	0.82
1:L:289:ILE:HG22	1:L:291:SER:HB2	1.62	0.81
1:H:156:LYS:HD2	1:H:196:GLN:HG2	1.63	0.80
1:J:156:LYS:HD2	1:J:196:GLN:HG2	1.63	0.80
1:J:185:PRO:HG2	1:J:191:GLN:NE2	1.99	0.78
1:H:9:ILE:HD11	2:I:622:VAL:HG21	1.66	0.77
2:M:530:GLN:NE2	2:M:645:ASP:HB2	2.01	0.76
1:H:267:GLY:HA3	2:I:566:VAL:HG21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:PRO:HG2	1:H:191:GLN:NE2	2.01	0.75
2:K:572:ASN:HD22	2:K:572:ASN:H	1.33	0.75
1:H:91:ASN:CG	4:H:1328:NAG:O1	2.28	0.75
1:L:58:LYS:H	1:L:58:LYS:CE	1.95	0.75
1:J:91:ASN:N	1:J:91:ASN:HD22	1.84	0.75
2:M:572:ASN:HD22	2:M:572:ASN:H	1.35	0.74
2:I:572:ASN:HD22	2:I:572:ASN:H	1.33	0.74
2:I:530:GLN:NE2	2:I:645:ASP:HB2	2.02	0.74
2:K:654:ASN:HD21	4:K:1661:NAG:HN2	1.32	0.74
2:M:553:ASN:O	2:M:557:GLU:HB3	1.88	0.74
2:K:564:THR:O	2:K:565:ALA:CB	2.37	0.73
1:H:91:ASN:HD22	1:H:91:ASN:H	1.36	0.73
4:H:1328:NAG:H61	4:H:1329:NAG:O5	1.90	0.71
1:L:185:PRO:HG2	1:L:191:GLN:NE2	2.05	0.71
1:H:58:LYS:H	1:H:58:LYS:CE	1.97	0.71
2:K:553:ASN:O	2:K:557:GLU:HB3	1.91	0.71
1:H:91:ASN:ND2	4:H:1328:NAG:O1	2.24	0.70
2:K:530:GLN:NE2	2:K:645:ASP:HB2	2.06	0.70
2:M:530:GLN:HE22	2:M:645:ASP:HB2	1.57	0.70
2:K:658:ASP:O	2:K:659:TYR:HB2	1.92	0.69
1:J:269:ILE:HD12	1:J:285:PRO:HA	1.74	0.69
2:I:644:CYS:HB2	2:I:648:CYS:SG	2.33	0.69
2:I:633:ILE:HD11	2:I:639:GLU:HB2	1.75	0.68
1:L:267:GLY:HA3	2:M:566:VAL:HG21	1.75	0.68
1:L:27:ASN:CG	4:L:1329:NAG:H4	2.16	0.68
1:J:9:ILE:HD11	2:K:622:VAL:HG21	1.75	0.68
1:L:308:LYS:HD3	2:M:559:MET:HE1	1.75	0.68
2:M:564:THR:O	2:M:565:ALA:CB	2.42	0.68
2:I:553:ASN:O	2:I:557:GLU:HB3	1.92	0.68
2:I:658:ASP:O	2:I:659:TYR:HB2	1.92	0.68
2:M:658:ASP:O	2:M:659:TYR:HB2	1.93	0.68
2:I:564:THR:O	2:I:565:ALA:CB	2.41	0.67
1:H:269:ILE:HD12	1:H:285:PRO:HA	1.75	0.67
2:I:530:GLN:HE22	2:I:645:ASP:HB2	1.59	0.67
2:M:525:HIS:O	2:M:526:HIS:HB3	1.94	0.67
1:L:327:ARG:C	1:L:327:ARG:HD2	2.21	0.66
2:I:539:LYS:HE2	2:I:543:ASN:HD21	1.59	0.66
1:H:303:ILE:CG1	2:I:566:VAL:HG13	2.26	0.66
1:L:58:LYS:HA	1:L:88:ASN:O	1.96	0.65
1:H:15:ASN:ND2	4:H:1331:NAG:N2	2.43	0.65
1:H:91:ASN:OD1	4:H:1328:NAG:O1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:633:ILE:HD11	2:M:639:GLU:HB2	1.78	0.65
1:H:58:LYS:HA	1:H:88:ASN:O	1.95	0.65
1:L:91:ASN:HD22	1:L:91:ASN:H	1.42	0.65
1:H:302:THR:O	2:I:566:VAL:HA	1.96	0.65
1:J:58:LYS:H	1:J:58:LYS:CE	2.00	0.65
1:L:269:ILE:HD12	1:L:285:PRO:HA	1.79	0.65
1:J:308:LYS:HD3	2:K:559:MET:HE1	1.79	0.65
2:M:644:CYS:HB2	2:M:648:CYS:SG	2.37	0.65
1:J:58:LYS:HA	1:J:88:ASN:O	1.96	0.65
1:H:308:LYS:HD3	2:I:559:MET:HE1	1.79	0.64
2:I:603:GLU:OE2	2:I:603:GLU:HA	1.97	0.64
2:I:525:HIS:O	2:I:526:HIS:HB3	1.99	0.63
1:H:290:ASN:ND2	4:H:1330:NAG:N2	2.45	0.63
2:K:633:ILE:HD11	2:K:639:GLU:HB2	1.80	0.63
2:M:603:GLU:OE2	2:M:603:GLU:HA	1.99	0.63
2:K:525:HIS:O	2:K:526:HIS:HB3	1.97	0.63
1:J:185:PRO:HG2	1:J:191:GLN:HE21	1.63	0.63
2:K:603:GLU:OE2	2:K:603:GLU:HA	1.97	0.62
2:K:654:ASN:ND2	4:K:1661:NAG:HN2	1.96	0.62
2:M:539:LYS:HE2	2:M:543:ASN:HD21	1.64	0.62
1:J:73:LEU:H	1:J:73:LEU:CD2	2.12	0.62
1:L:289:ILE:CG2	1:L:291:SER:HB2	2.28	0.62
1:J:267:GLY:HA3	2:K:566:VAL:HG21	1.82	0.61
1:H:289:ILE:CG2	1:H:291:SER:HB2	2.29	0.61
2:M:654:ASN:ND2	4:M:1661:NAG:O1	2.32	0.61
1:J:20:VAL:HG12	1:J:316:ARG:HG2	1.83	0.61
2:K:634:GLY:O	2:K:635:ASN:HB2	2.01	0.61
1:L:73:LEU:H	1:L:73:LEU:CD2	2.13	0.61
1:H:20:VAL:HG12	1:H:316:ARG:HG2	1.81	0.60
1:J:102:TYR:CZ	1:J:106:ARG:HD2	2.37	0.60
1:H:185:PRO:HG2	1:H:191:GLN:HE21	1.66	0.60
1:H:15:ASN:HD22	4:H:1331:NAG:HN2	1.48	0.60
1:J:221:PRO:HG3	1:L:242:THR:HB	1.84	0.59
2:K:530:GLN:HE22	2:K:645:ASP:HB2	1.65	0.59
1:H:74:LEU:C	1:H:76:THR:H	2.11	0.59
1:J:289:ILE:CG2	1:J:291:SER:HB2	2.31	0.59
1:L:302:THR:O	2:M:566:VAL:HA	2.02	0.59
1:H:317:MET:HE1	2:I:555:VAL:HG21	1.85	0.59
2:K:539:LYS:HE2	2:K:543:ASN:HD21	1.68	0.58
1:H:304:GLY:CA	2:I:564:THR:HA	2.33	0.58
2:I:572:ASN:H	2:I:572:ASN:ND2	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:LEU:HD11	1:H:317:MET:HE3	1.86	0.58
2:K:572:ASN:H	2:K:572:ASN:ND2	2.00	0.58
1:H:6:THR:O	2:I:526:HIS:HA	2.04	0.57
1:L:74:LEU:C	1:L:76:THR:H	2.12	0.57
2:I:644:CYS:CB	2:I:648:CYS:SG	2.92	0.57
1:J:174:LYS:HB2	1:J:260:LEU:O	2.05	0.57
1:J:74:LEU:C	1:J:76:THR:H	2.11	0.57
1:L:301:VAL:HG13	2:M:566:VAL:HG12	1.87	0.57
1:H:15:ASN:ND2	4:H:1331:NAG:HN2	2.03	0.57
1:H:303:ILE:HG13	2:I:566:VAL:HG13	1.86	0.57
1:J:120:ILE:HG23	1:J:121:PHE:H	1.69	0.57
1:H:174:LYS:HB2	1:H:260:LEU:O	2.03	0.57
2:K:530:GLN:NE2	2:K:646:ASP:H	2.02	0.57
2:K:654:ASN:ND2	4:K:1661:NAG:N2	2.53	0.57
1:H:45:LYS:HG2	1:H:276:HIS:ND1	2.19	0.57
1:H:73:LEU:H	1:H:73:LEU:CD2	2.15	0.57
1:J:310:VAL:HG13	1:J:312:SER:H	1.70	0.57
2:M:530:GLN:NE2	2:M:646:ASP:H	2.03	0.57
1:L:20:VAL:HG12	1:L:316:ARG:HG2	1.85	0.57
1:H:104:GLU:O	1:H:108:GLN:HG2	2.04	0.56
1:J:317:MET:HE1	2:K:555:VAL:HG21	1.87	0.56
1:L:303:ILE:HG13	2:M:566:VAL:HG13	1.86	0.56
2:I:563:PHE:CE2	1:L:311:ARG:NH2	2.74	0.56
1:L:58:LYS:HZ1	1:L:73:LEU:HD21	1.71	0.56
2:M:572:ASN:H	2:M:572:ASN:ND2	2.02	0.56
2:M:644:CYS:CB	2:M:648:CYS:SG	2.93	0.56
2:M:654:ASN:HD21	4:M:1661:NAG:H82	1.71	0.56
1:H:308:LYS:HG2	2:I:592:TRP:CE2	2.40	0.56
1:L:310:VAL:HG13	1:L:312:SER:H	1.70	0.56
1:L:102:TYR:CZ	1:L:106:ARG:HD2	2.41	0.56
1:L:303:ILE:CG1	2:M:566:VAL:HG13	2.36	0.56
2:K:564:THR:O	2:K:565:ALA:HB2	2.06	0.56
1:L:156:LYS:HD2	1:L:196:GLN:CG	2.34	0.56
1:H:7:ILE:HA	2:I:526:HIS:HA	1.86	0.55
2:K:530:GLN:HE22	2:K:646:ASP:H	1.53	0.55
1:L:164:LEU:O	1:L:246:GLU:HA	2.06	0.55
1:J:94:CYS:HB3	4:J:1328:NAG:O7	2.06	0.55
1:H:290:ASN:HD22	4:H:1330:NAG:C8	2.20	0.55
1:J:75:LEU:HD21	1:J:117:LYS:HZ2	1.71	0.55
2:I:530:GLN:NE2	2:I:646:ASP:H	2.05	0.55
1:L:79:SER:HB2	1:L:113:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:216:GLU:O	1:L:220:ARG:NH2	2.40	0.55
1:H:120:ILE:HG23	1:H:121:PHE:H	1.71	0.55
1:L:45:LYS:HG2	1:L:276:HIS:ND1	2.22	0.55
1:L:113:SER:OG	1:L:261:ASN:HB2	2.07	0.55
2:M:654:ASN:CG	4:M:1661:NAG:HO1	2.14	0.55
1:J:91:ASN:HD22	1:J:91:ASN:H	1.53	0.55
1:H:102:TYR:CZ	1:H:106:ARG:HD2	2.41	0.54
1:H:310:VAL:HG13	1:H:312:SER:H	1.71	0.54
1:J:308:LYS:HD3	2:K:559:MET:CE	2.36	0.54
1:L:104:GLU:O	1:L:108:GLN:HG2	2.07	0.54
1:H:290:ASN:CB	4:H:1330:NAG:H3	2.37	0.54
1:H:12:HIS:HB2	2:I:520:GLY:O	2.07	0.54
1:H:164:LEU:O	1:H:246:GLU:HA	2.07	0.54
1:J:104:GLU:O	1:J:108:GLN:HG2	2.07	0.54
1:H:74:LEU:C	1:H:76:THR:N	2.66	0.54
1:H:156:LYS:HD2	1:H:196:GLN:CG	2.37	0.54
1:J:164:LEU:O	1:J:246:GLU:HA	2.07	0.54
1:H:91:ASN:N	1:H:91:ASN:ND2	2.44	0.54
2:I:650:GLU:O	2:I:654:ASN:HB2	2.08	0.54
1:J:94:CYS:O	1:J:224:ARG:HD3	2.08	0.53
1:L:75:LEU:HD21	1:L:117:LYS:HZ2	1.74	0.53
2:M:654:ASN:CG	4:M:1661:NAG:O1	2.51	0.53
1:H:94:CYS:O	1:H:224:ARG:HD3	2.08	0.53
1:J:120:ILE:HG23	1:J:121:PHE:N	2.23	0.53
1:L:74:LEU:C	1:L:76:THR:N	2.67	0.53
1:J:74:LEU:C	1:J:76:THR:N	2.67	0.53
1:J:222:LYS:NZ	3:A:3:GAL:O3	2.22	0.53
1:J:75:LEU:HD21	1:J:117:LYS:NZ	2.23	0.53
2:M:525:HIS:O	2:M:526:HIS:CB	2.56	0.53
1:H:113:SER:OG	1:H:261:ASN:HB2	2.09	0.53
1:H:310:VAL:CG1	1:H:312:SER:H	2.21	0.53
1:J:58:LYS:NZ	1:J:73:LEU:HD21	2.24	0.53
1:J:82:TYR:HA	1:J:110:SER:O	2.09	0.53
1:L:317:MET:HE1	2:M:555:VAL:HG21	1.90	0.53
1:L:185:PRO:HG2	1:L:191:GLN:HE21	1.74	0.52
1:J:325:PRO:O	1:J:326:SER:C	2.52	0.52
2:I:564:THR:O	2:I:565:ALA:HB2	2.09	0.52
1:H:75:LEU:HD21	1:H:117:LYS:NZ	2.25	0.52
1:L:58:LYS:NZ	1:L:73:LEU:HD21	2.25	0.52
1:L:82:TYR:HA	1:L:110:SER:O	2.10	0.52
1:H:82:TYR:HA	1:H:110:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:525:HIS:O	2:K:526:HIS:CB	2.57	0.52
2:M:650:GLU:O	2:M:654:ASN:HB2	2.10	0.52
1:J:289:ILE:HD11	1:J:298:ILE:HB	1.92	0.52
1:L:94:CYS:O	1:L:224:ARG:HD3	2.09	0.52
1:H:20:VAL:HG21	1:H:318:ALA:HB2	1.91	0.52
1:J:310:VAL:CG1	1:J:312:SER:H	2.23	0.52
1:L:327:ARG:HD2	1:L:328:GLN:N	2.25	0.52
1:L:174:LYS:HB2	1:L:260:LEU:O	2.10	0.52
2:I:634:GLY:O	2:I:635:ASN:HB2	2.10	0.51
1:H:23:VAL:HG12	2:I:605:GLU:HB2	1.92	0.51
1:H:75:LEU:HD21	1:H:117:LYS:HZ2	1.75	0.51
1:J:97:GLY:HA3	1:J:230:MET:O	2.10	0.51
2:K:561:THR:O	2:K:562:GLN:O	2.27	0.51
1:J:113:SER:OG	1:J:261:ASN:HB2	2.10	0.51
1:L:302:THR:HG23	1:L:306:CYS:SG	2.51	0.51
1:J:56:LEU:HA	1:J:74:LEU:HD13	1.93	0.51
1:H:58:LYS:NZ	1:H:73:LEU:HD21	2.25	0.51
1:H:289:ILE:HD11	1:H:298:ILE:HB	1.92	0.51
1:J:42:ASN:OD1	1:J:45:LYS:HB2	2.11	0.51
2:K:528:ASN:HD21	2:K:645:ASP:HA	1.75	0.51
2:K:650:GLU:O	2:K:654:ASN:HB2	2.09	0.51
2:M:634:GLY:O	2:M:635:ASN:HB2	2.09	0.51
1:H:42:ASN:OD1	1:H:45:LYS:HB2	2.11	0.51
1:H:303:ILE:HG12	2:I:566:VAL:HG13	1.92	0.51
1:H:216:GLU:O	1:H:220:ARG:NH2	2.45	0.50
2:K:561:THR:C	2:K:562:GLN:O	2.53	0.50
1:H:103:GLU:OE2	2:I:571:ASN:HB3	2.11	0.50
1:H:120:ILE:HG23	1:H:121:PHE:N	2.25	0.50
1:H:290:ASN:ND2	4:H:1330:NAG:H1	2.26	0.50
2:K:650:GLU:O	2:K:654:ASN:CB	2.59	0.50
1:L:7:ILE:HA	2:M:526:HIS:HA	1.91	0.50
1:H:49:LEU:HD21	1:H:303:ILE:HG22	1.93	0.50
1:L:49:LEU:HD21	1:L:303:ILE:HG22	1.92	0.50
1:J:156:LYS:HD2	1:J:196:GLN:CG	2.38	0.50
1:L:75:LEU:HD21	1:L:117:LYS:NZ	2.27	0.50
2:I:502:LEU:HG	2:K:503:PHE:CZ	2.47	0.50
2:I:525:HIS:O	2:I:526:HIS:CB	2.59	0.50
1:J:224:ARG:NH2	4:J:1328:NAG:O3	2.45	0.50
1:L:304:GLY:CA	2:M:564:THR:HA	2.42	0.50
1:L:308:LYS:HD3	2:M:559:MET:CE	2.40	0.50
1:J:58:LYS:HZ1	1:J:73:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:564:THR:O	2:M:565:ALA:HB2	2.11	0.50
1:J:36:LEU:HD11	1:J:317:MET:HE3	1.93	0.50
1:L:36:LEU:HD11	1:L:317:MET:HE3	1.93	0.50
2:M:561:THR:O	2:M:562:GLN:O	2.29	0.49
1:H:8:CYS:HB2	2:I:525:HIS:HB3	1.93	0.49
1:J:9:ILE:HG12	2:K:619:TYR:HA	1.93	0.49
1:H:8:CYS:O	2:I:524:TYR:CA	2.54	0.49
2:I:658:ASP:O	2:I:659:TYR:CB	2.60	0.49
1:J:14:ASN:HA	2:K:515:THR:HG22	1.94	0.49
1:L:42:ASN:OD1	1:L:45:LYS:HB2	2.12	0.49
1:L:289:ILE:HD11	1:L:298:ILE:HB	1.93	0.49
1:H:308:LYS:HD3	2:I:559:MET:CE	2.43	0.49
1:L:91:ASN:N	1:L:91:ASN:ND2	2.49	0.49
1:J:20:VAL:HG21	1:J:318:ALA:HB2	1.93	0.49
1:L:138:ALA:O	1:L:224:ARG:NH1	2.43	0.49
1:L:152:LEU:HD23	1:L:153:TRP:N	2.28	0.49
2:I:650:GLU:O	2:I:654:ASN:CB	2.61	0.48
1:J:302:THR:HG23	1:J:306:CYS:SG	2.53	0.48
2:M:561:THR:C	2:M:562:GLN:O	2.54	0.48
1:H:51:ILE:HG22	1:H:52:ALA:N	2.27	0.48
2:I:561:THR:C	2:I:562:GLN:O	2.56	0.48
2:I:559:MET:HG2	2:M:594:TYR:CE1	2.49	0.48
1:L:100:ILE:N	1:L:100:ILE:HD12	2.29	0.48
2:M:658:ASP:O	2:M:659:TYR:CB	2.61	0.48
1:J:51:ILE:HG22	1:J:52:ALA:N	2.28	0.48
1:J:216:GLU:O	1:J:220:ARG:NH2	2.46	0.48
2:K:659:TYR:O	2:K:660:PRO:C	2.57	0.48
1:L:164:LEU:HD12	1:L:164:LEU:C	2.39	0.48
1:J:310:VAL:HG22	2:K:593:THR:HA	1.96	0.48
1:L:20:VAL:HG21	1:L:318:ALA:HB2	1.95	0.48
1:L:267:GLY:HA3	2:M:566:VAL:CG2	2.41	0.48
1:J:132(A):THR:C	1:J:134:GLY:H	2.22	0.48
1:L:61:ILE:HD11	1:L:83:ILE:HG21	1.95	0.48
4:L:1328:NAG:O3	4:L:1328:NAG:H83	2.14	0.48
2:K:566:VAL:HB	2:K:567:GLY:O	2.14	0.47
2:K:657:TYR:O	2:K:658:ASP:CB	2.61	0.47
1:H:61:ILE:HD11	1:H:83:ILE:HG21	1.96	0.47
1:J:128:PRO:O	1:J:129:ASN:HB2	2.15	0.47
1:H:324:ILE:HD11	2:I:507:ALA:HB2	1.97	0.47
1:J:23:VAL:CG2	2:M:551:LYS:HG3	2.44	0.47
1:J:45:LYS:HG2	1:J:276:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:138:ALA:O	1:J:224:ARG:NH1	2.46	0.47
1:L:120:ILE:HG23	1:L:121:PHE:H	1.79	0.47
1:H:267:GLY:HA3	2:I:566:VAL:CG2	2.42	0.47
1:J:74:LEU:O	1:J:76:THR:N	2.40	0.47
2:K:658:ASP:O	2:K:659:TYR:CB	2.62	0.47
1:H:91:ASN:H	1:H:91:ASN:ND2	2.07	0.47
1:L:95:TYR:CD2	1:L:230:MET:HE3	2.50	0.47
1:J:79:SER:HB2	1:J:113:SER:O	2.15	0.47
1:J:102:TYR:O	1:J:106:ARG:HG3	2.14	0.47
2:K:564:THR:O	2:K:565:ALA:HB3	2.13	0.47
1:H:34:VAL:HG13	1:H:319:THR:HG21	1.97	0.46
1:J:49:LEU:HD21	1:J:303:ILE:HG22	1.97	0.46
2:M:530:GLN:HE22	2:M:646:ASP:H	1.61	0.46
2:M:659:TYR:O	2:M:660:PRO:C	2.56	0.46
1:H:115:PHE:CZ	1:H:258:PHE:CD2	3.04	0.46
2:M:566:VAL:HB	2:M:567:GLY:O	2.16	0.46
2:M:657:TYR:O	2:M:658:ASP:CB	2.63	0.46
2:K:566:VAL:HB	2:K:567:GLY:H	1.35	0.46
1:L:310:VAL:CG1	1:L:312:SER:H	2.28	0.46
2:M:524:TYR:CE1	2:M:653:ARG:HB2	2.49	0.46
1:J:91:ASN:HA	4:J:1328:NAG:O1	2.16	0.46
1:H:242:THR:HB	1:L:221:PRO:HG3	1.96	0.46
1:L:8:CYS:O	2:M:524:TYR:HA	2.16	0.46
1:H:56:LEU:HA	1:H:74:LEU:HD13	1.97	0.46
1:H:61:ILE:CD1	1:H:83:ILE:HD13	2.45	0.46
1:J:294:PRO:HD3	2:K:556:ILE:HG23	1.98	0.46
1:H:138:ALA:O	1:H:224:ARG:NH1	2.49	0.46
1:H:304:GLY:HA2	2:I:564:THR:HA	1.97	0.46
1:J:112:VAL:HG11	1:J:115:PHE:HB2	1.98	0.46
2:M:528:ASN:HD21	2:M:530:GLN:NE2	2.14	0.46
1:H:164:LEU:C	1:H:164:LEU:HD12	2.41	0.46
2:M:509:PHE:O	2:M:635:ASN:HA	2.16	0.46
1:H:100:ILE:HD12	1:H:100:ILE:N	2.31	0.46
2:I:566:VAL:HB	2:I:567:GLY:O	2.15	0.46
1:H:93:THR:HG22	1:H:93:THR:O	2.15	0.46
2:K:524:TYR:CE1	2:K:653:ARG:HB2	2.51	0.45
2:K:594:TYR:CE1	2:M:559:MET:HG2	2.50	0.45
2:I:509:PHE:O	2:I:635:ASN:HA	2.17	0.45
1:J:164:LEU:C	1:J:164:LEU:HD12	2.40	0.45
1:L:34:VAL:HG13	1:L:319:THR:HG21	1.97	0.45
1:L:277:ASP:OD2	1:L:277:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:294:PRO:HD3	2:I:556:ILE:HG23	1.98	0.45
1:L:120:ILE:HG23	1:L:121:PHE:N	2.31	0.45
1:L:309:TYR:CD2	2:M:589:LEU:HD13	2.52	0.45
1:H:45:LYS:HG2	1:H:276:HIS:CE1	2.51	0.45
1:L:51:ILE:HG22	1:L:52:ALA:N	2.31	0.45
2:K:528:ASN:OD1	2:K:644:CYS:O	2.34	0.45
2:I:619:TYR:CE1	2:I:636:GLY:HA2	2.51	0.45
2:I:659:TYR:O	2:I:660:PRO:C	2.59	0.45
1:L:159:SER:C	1:L:196:GLN:HG3	2.42	0.45
2:M:650:GLU:O	2:M:654:ASN:CB	2.64	0.45
2:K:656:THR:O	2:K:657:TYR:C	2.58	0.45
1:L:214:THR:HA	1:L:215:PRO:HD3	1.87	0.45
1:H:27:ASN:HD21	4:H:1332:NAG:H4	1.71	0.45
2:I:598:LEU:HA	2:I:598:LEU:HD23	1.76	0.45
1:H:294:PRO:HB3	2:I:559:MET:HG3	1.98	0.44
1:L:224:ARG:NH2	4:L:1328:NAG:O3	2.50	0.44
1:J:9:ILE:HD13	2:K:638:PHE:HE1	1.82	0.44
2:I:524:TYR:CE1	2:I:653:ARG:HB2	2.53	0.44
1:J:186:PRO:O	1:J:218:ALA:O	2.34	0.44
1:L:156:LYS:CD	1:L:196:GLN:HG2	2.40	0.44
1:L:327:ARG:O	1:L:327:ARG:NH1	2.39	0.44
2:M:654:ASN:HD21	4:M:1661:NAG:C8	2.30	0.44
1:H:27:ASN:HD22	4:H:1332:NAG:H4	1.71	0.44
2:K:619:TYR:CE1	2:K:636:GLY:HA2	2.52	0.44
1:H:37:LEU:HB2	1:H:315:LEU:HB2	2.00	0.44
1:H:95:TYR:CD2	1:H:230:MET:HE3	2.53	0.44
1:L:95:TYR:CE2	1:L:230:MET:HE3	2.53	0.44
1:L:115:PHE:CZ	1:L:258:PHE:CD2	3.06	0.44
1:L:310:VAL:HG22	2:M:593:THR:HA	1.99	0.44
1:H:79:SER:HB2	1:H:113:SER:O	2.17	0.44
1:J:34:VAL:HG13	1:J:319:THR:HG21	2.00	0.44
1:J:48:LYS:HD2	1:J:50:GLY:O	2.17	0.44
1:L:93:THR:O	1:L:93:THR:HG22	2.16	0.44
1:J:95:TYR:CD2	1:J:230:MET:HB2	2.53	0.43
2:I:530:GLN:HE22	2:I:646:ASP:H	1.65	0.43
1:J:95:TYR:CD2	1:J:230:MET:HE3	2.53	0.43
1:J:162:PRO:O	1:J:163:LYS:C	2.59	0.43
1:H:132(A):THR:C	1:H:134:GLY:H	2.26	0.43
2:I:561:THR:O	2:I:562:GLN:O	2.35	0.43
1:J:93:THR:O	1:J:93:THR:HG22	2.17	0.43
1:J:311:ARG:NH2	2:M:563:PHE:CE2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:HIS:CE1	1:H:301:VAL:HB	2.54	0.43
1:L:304:GLY:H	2:M:564:THR:HA	1.82	0.43
1:H:164:LEU:O	1:H:164:LEU:HD12	2.18	0.43
2:I:564:THR:O	2:I:565:ALA:HB3	2.18	0.43
1:J:159:SER:C	1:J:196:GLN:HG3	2.44	0.43
2:M:502:LEU:HD12	2:M:502:LEU:HA	1.83	0.43
1:H:324:ILE:CD1	2:I:507:ALA:HB2	2.48	0.43
2:I:524:TYR:CD1	2:I:524:TYR:N	2.86	0.43
2:K:528:ASN:HD21	2:K:530:GLN:NE2	2.17	0.43
1:J:49:LEU:HD12	1:J:49:LEU:HA	1.90	0.43
1:J:100:ILE:HD12	1:J:100:ILE:N	2.33	0.43
1:J:308:LYS:HG2	2:K:592:TRP:CE2	2.54	0.43
1:J:6:THR:O	2:K:526:HIS:HA	2.19	0.43
1:H:277:ASP:OD2	1:H:277:ASP:N	2.52	0.43
2:I:538:GLN:HA	2:I:538:GLN:OE1	2.19	0.43
1:L:291:SER:HB3	1:L:307:PRO:CG	2.49	0.43
1:H:100:ILE:HG12	1:H:233:TYR:CE2	2.53	0.42
1:H:111:SER:OG	1:H:263:GLY:HA3	2.18	0.42
1:H:112:VAL:HG11	1:H:115:PHE:HB2	2.01	0.42
1:J:65:LEU:HD23	1:J:65:LEU:HA	1.79	0.42
1:L:40:SER:N	1:L:298:ILE:HD11	2.33	0.42
1:L:49:LEU:O	1:L:49(A):LYS:CB	2.67	0.42
1:L:117:LYS:HE3	1:L:150:ASN:OD1	2.18	0.42
1:H:74:LEU:O	1:H:76:THR:N	2.39	0.42
1:J:91:ASN:N	1:J:91:ASN:ND2	2.55	0.42
2:M:619:TYR:CE1	2:M:636:GLY:HA2	2.55	0.42
2:M:656:THR:O	2:M:657:TYR:C	2.62	0.42
1:J:277:ASP:OD2	1:J:277:ASP:N	2.50	0.42
1:J:324:ILE:CD1	2:K:507:ALA:HB2	2.49	0.42
2:K:528:ASN:ND2	2:K:530:GLN:NE2	2.67	0.42
1:H:317:MET:HE1	2:I:555:VAL:HG11	2.01	0.42
1:L:49:LEU:HD12	1:L:49:LEU:HA	1.83	0.42
1:L:299:HIS:HA	1:L:300:PRO:HD2	1.87	0.42
1:H:37:LEU:HD21	1:H:297:ASN:ND2	2.34	0.42
1:H:117:LYS:HE3	1:H:150:ASN:OD1	2.19	0.42
1:L:112:VAL:HG11	1:L:115:PHE:HB2	2.01	0.42
2:I:607:THR:O	2:I:610:PHE:HB3	2.19	0.42
2:I:657:TYR:O	2:I:658:ASP:CB	2.67	0.42
1:J:115:PHE:CZ	1:J:258:PHE:CD2	3.08	0.42
1:L:74:LEU:O	1:L:76:THR:N	2.38	0.42
1:J:195:TYR:O	1:J:197:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:538:GLN:OE1	2:K:538:GLN:HA	2.18	0.42
1:L:186:PRO:O	1:L:218:ALA:O	2.38	0.42
1:J:299:HIS:HA	1:J:300:PRO:HD2	1.87	0.42
2:K:627:LYS:HB3	2:K:628:ASN:H	1.66	0.42
1:L:164:LEU:O	1:L:164:LEU:HD12	2.19	0.42
1:L:309:TYR:CE2	2:M:589:LEU:HD13	2.54	0.42
1:L:153:TRP:CD1	1:L:153:TRP:C	2.98	0.42
2:M:564:THR:O	2:M:565:ALA:HB3	2.18	0.42
2:M:598:LEU:HD23	2:M:598:LEU:HA	1.80	0.42
1:J:95:TYR:CE2	1:J:230:MET:HE3	2.55	0.42
1:J:124:THR:O	1:J:125:SER:CB	2.67	0.42
2:K:607:THR:O	2:K:610:PHE:HB3	2.20	0.42
1:H:11:TYR:HA	2:I:521:TRP:O	2.19	0.41
2:I:528:ASN:HD21	2:I:530:GLN:NE2	2.18	0.41
2:K:509:PHE:O	2:K:635:ASN:HA	2.20	0.41
1:L:304:GLY:N	2:M:564:THR:HA	2.35	0.41
1:L:42:ASN:HB3	1:L:288:ALA:N	2.35	0.41
1:L:249:GLY:C	1:L:250:ASN:HD22	2.27	0.41
1:H:153:TRP:CD1	1:H:153:TRP:C	2.98	0.41
1:J:36:LEU:HD11	1:J:317:MET:CE	2.50	0.41
1:J:180:TRP:CZ2	1:J:204:VAL:HG21	2.55	0.41
1:J:267:GLY:HA3	2:K:566:VAL:CG2	2.47	0.41
1:L:308:LYS:HG2	2:M:592:TRP:CE2	2.55	0.41
1:J:249:GLY:C	1:J:250:ASN:HD22	2.29	0.41
1:L:302:THR:CG2	1:L:306:CYS:SG	3.08	0.41
1:H:310:VAL:HG22	2:I:593:THR:HA	2.02	0.41
1:J:40:SER:N	1:J:298:ILE:HD11	2.35	0.41
1:J:61:ILE:HD11	1:J:83:ILE:HG21	2.03	0.41
1:L:162:PRO:O	1:L:163:LYS:C	2.62	0.41
2:M:524:TYR:CD1	2:M:524:TYR:N	2.88	0.41
1:L:56:LEU:HA	1:L:74:LEU:HD13	2.02	0.41
1:L:124:THR:O	1:L:125:SER:CB	2.69	0.41
1:H:58:LYS:HZ1	1:H:73:LEU:HD21	1.83	0.41
1:H:186:PRO:O	1:H:218:ALA:O	2.38	0.41
1:J:303:ILE:CG1	2:K:566:VAL:HG13	2.51	0.41
1:L:132(A):THR:C	1:L:134:GLY:H	2.28	0.41
1:L:134:GLY:HA3	1:L:153:TRP:HB3	2.03	0.41
1:L:289:ILE:HG21	1:L:289:ILE:HD13	1.84	0.41
1:H:159:SER:C	1:H:196:GLN:HG3	2.46	0.41
1:H:291:SER:HB3	1:H:307:PRO:CG	2.51	0.41
1:H:299:HIS:HA	1:H:300:PRO:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:524:TYR:CD1	2:K:524:TYR:N	2.88	0.41
1:L:152:LEU:C	1:L:152:LEU:CD2	2.94	0.41
2:M:570:PHE:HB3	2:M:574:GLU:HB2	2.03	0.41
2:K:598:LEU:HA	2:K:598:LEU:HD23	1.84	0.41
2:M:563:PHE:CD1	2:M:563:PHE:N	2.88	0.41
1:H:94:CYS:HB3	4:H:1328:NAG:O7	2.21	0.40
1:H:309:TYR:CD2	2:I:589:LEU:HD13	2.56	0.40
1:J:37:LEU:HB2	1:J:315:LEU:HB2	2.03	0.40
2:I:528:ASN:HD21	2:I:645:ASP:HA	1.86	0.40
1:H:124:THR:O	1:H:125:SER:CB	2.70	0.40
1:H:242:THR:O	1:L:221:PRO:HG2	2.20	0.40
2:I:656:THR:O	2:I:657:TYR:C	2.65	0.40
1:H:136:THR:HG23	1:H:139:CYS:H	1.87	0.40
1:H:156:LYS:CD	1:H:196:GLN:HG2	2.43	0.40
1:J:111:SER:OG	1:J:263:GLY:HA3	2.21	0.40
1:H:134:GLY:HA3	1:H:153:TRP:HB3	2.04	0.40
2:K:559:MET:HE3	2:K:559:MET:HB3	1.85	0.40

All (3) 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:L:123:LYS:NZ	2:M:659:TYR:OH[2_454]	2.11	0.09
1:J:141:TYR:OH	2:K:658:ASP:OD1[3_555]	2.14	0.06
2:K:639:GLU:OE2	1:L:75:LEU:O[2_455]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

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 ⓘ

4 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	GAL	A	1	3	12,12,12	2.08	4 (33%)	17,17,17	2.92	5 (29%)
3	NAG	A	2	3	14,14,15	1.96	7 (50%)	17,19,21	1.29	1 (5%)
3	GAL	A	3	3	11,11,12	2.87	7 (63%)	15,15,17	2.32	5 (33%)
3	SIA	A	4	3	20,20,21	5.65	9 (45%)	21,28,31	2.17	5 (23%)

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	GAL	A	1	3	-	0/2/22/22	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	GAL	A	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	SIA	A	4	3	-	0/18/34/38	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	SIA	C11-C10	-13.36	1.22	1.50
3	A	4	SIA	O10-C10	13.17	1.52	1.23
3	A	4	SIA	C2-C1	9.96	1.64	1.52
3	A	4	SIA	O4-C4	-7.47	1.27	1.43
3	A	4	SIA	C6-C5	6.09	1.62	1.53
3	A	4	SIA	C3-C4	5.60	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	SIA	C4-C5	5.35	1.58	1.53
3	A	1	GAL	O5-C5	4.96	1.56	1.44
3	A	3	GAL	O5-C5	4.36	1.51	1.43
3	A	4	SIA	O6-C6	-4.21	1.37	1.44
3	A	3	GAL	C2-C3	3.89	1.58	1.52
3	A	3	GAL	C4-C5	3.69	1.60	1.53
3	A	3	GAL	C1-C2	3.48	1.60	1.52
3	A	3	GAL	C4-C3	3.41	1.61	1.52
3	A	3	GAL	O5-C1	2.85	1.48	1.43
3	A	2	NAG	O5-C1	2.84	1.48	1.43
3	A	2	NAG	C4-C3	2.72	1.59	1.52
3	A	1	GAL	O1-C1	2.61	1.47	1.39
3	A	2	NAG	C2-N2	2.60	1.50	1.46
3	A	1	GAL	O5-C1	2.54	1.49	1.42
3	A	4	SIA	C7-C6	-2.54	1.49	1.52
3	A	2	NAG	C4-C5	2.46	1.58	1.53
3	A	3	GAL	O4-C4	2.38	1.48	1.43
3	A	2	NAG	C6-C5	2.35	1.59	1.51
3	A	2	NAG	O4-C4	2.31	1.48	1.43
3	A	1	GAL	O3-C3	-2.09	1.37	1.43
3	A	2	NAG	O5-C5	2.06	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	GAL	O1-C1-C2	9.30	135.99	108.98
3	A	1	GAL	O1-C1-O5	-5.19	95.00	110.41
3	A	3	GAL	C1-O5-C5	5.00	118.89	112.19
3	A	3	GAL	O5-C1-C2	4.64	121.85	110.79
3	A	4	SIA	C6-C5-N5	-4.61	103.54	110.91
3	A	4	SIA	O6-C2-C3	-4.59	104.39	110.56
3	A	4	SIA	O1B-C1-C2	4.16	123.54	112.71
3	A	4	SIA	O1A-C1-C2	-3.99	114.22	122.85
3	A	3	GAL	C3-C4-C5	-3.22	104.39	110.23
3	A	1	GAL	C3-C4-C5	-2.79	105.17	110.23
3	A	4	SIA	C5-N5-C10	2.51	128.98	123.11
3	A	1	GAL	C1-C2-C3	-2.49	105.28	110.36
3	A	2	NAG	O6-C6-C5	2.46	119.72	111.33
3	A	3	GAL	O2-C2-C3	2.45	115.22	110.15
3	A	3	GAL	C2-C3-C4	-2.40	106.65	110.86
3	A	1	GAL	O5-C5-C6	2.05	111.51	106.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	3	GAL	C1

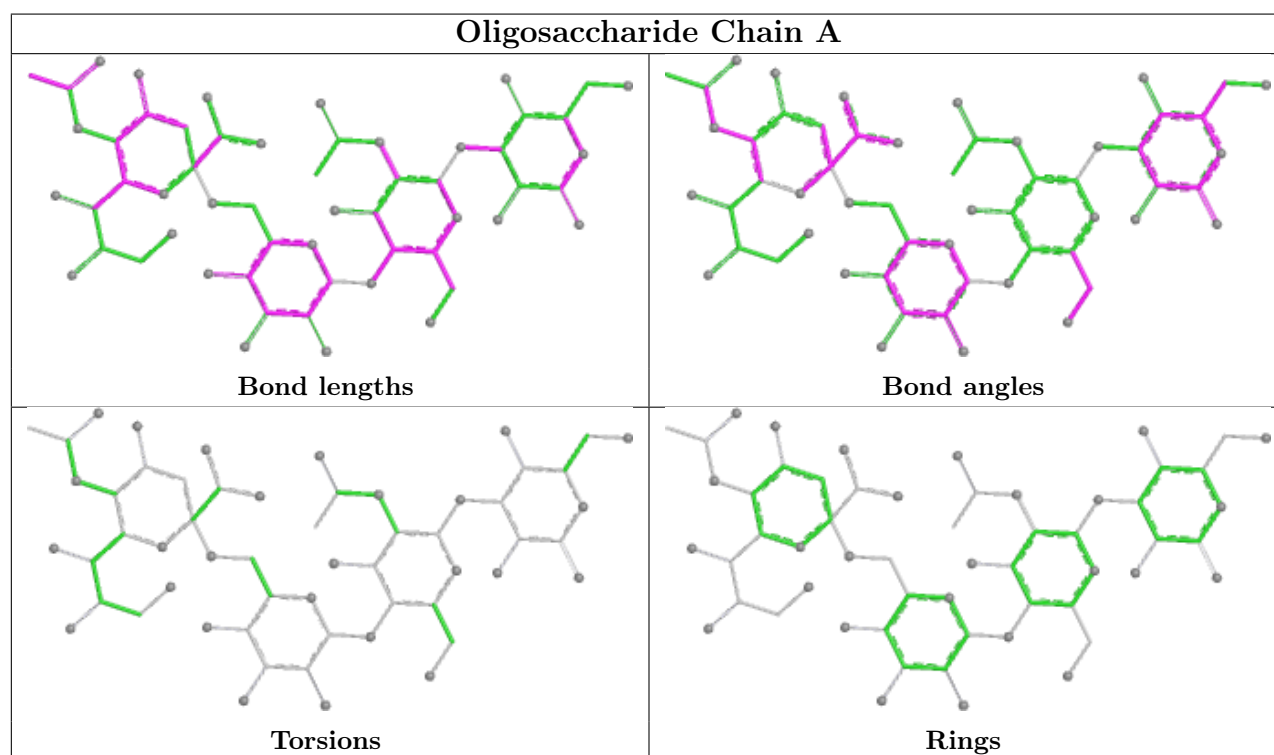
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	GAL	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](#)

11 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	H	1332	-	15,15,15	0.55	0	21,21,21	1.61	7 (33%)
4	NAG	J	1328	-	15,15,15	0.64	0	21,21,21	2.46	6 (28%)
4	NAG	J	1329	-	15,15,15	0.61	0	21,21,21	2.17	4 (19%)
4	NAG	K	1661	-	15,15,15	0.41	0	21,21,21	0.90	1 (4%)
4	NAG	M	1661	-	15,15,15	0.69	0	21,21,21	2.60	5 (23%)
4	NAG	L	1328	-	15,15,15	0.48	0	21,21,21	1.46	3 (14%)
4	NAG	L	1329	-	15,15,15	0.52	0	21,21,21	0.96	1 (4%)
4	NAG	H	1329	-	15,15,15	0.45	0	21,21,21	1.12	2 (9%)
4	NAG	H	1331	-	15,15,15	0.42	0	21,21,21	1.18	1 (4%)
4	NAG	H	1330	-	15,15,15	0.41	0	21,21,21	0.94	1 (4%)
4	NAG	H	1328	-	15,15,15	0.81	0	21,21,21	3.05	4 (19%)

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	H	1332	-	-	3/6/26/26	0/1/1/1
4	NAG	J	1328	-	-	0/6/26/26	0/1/1/1
4	NAG	J	1329	-	-	4/6/26/26	0/1/1/1
4	NAG	K	1661	-	-	4/6/26/26	0/1/1/1
4	NAG	M	1661	-	-	4/6/26/26	0/1/1/1
4	NAG	L	1328	-	-	6/6/26/26	0/1/1/1
4	NAG	L	1329	-	-	4/6/26/26	0/1/1/1
4	NAG	H	1329	-	-	3/6/26/26	0/1/1/1
4	NAG	H	1331	-	-	4/6/26/26	0/1/1/1
4	NAG	H	1330	-	-	6/6/26/26	0/1/1/1
4	NAG	H	1328	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1328	NAG	C1-C2-C3	-11.88	94.34	110.54
4	M	1661	NAG	C1-C2-C3	-9.08	98.16	110.54
4	J	1328	NAG	O5-C1-C2	6.54	116.09	109.52
4	J	1329	NAG	O5-C1-C2	-6.18	103.30	109.52
4	J	1328	NAG	C4-C3-C2	-5.76	102.01	110.40
4	J	1329	NAG	C1-C2-C3	-4.87	103.90	110.54
4	H	1328	NAG	C1-O5-C5	-4.38	105.18	113.65
4	J	1329	NAG	C3-C4-C5	3.75	117.03	110.23
4	J	1328	NAG	C1-C2-N2	-3.75	106.39	110.73
4	H	1329	NAG	O5-C1-C2	3.66	113.19	109.52
4	L	1328	NAG	C1-C2-C3	-3.47	105.81	110.54
4	M	1661	NAG	O5-C1-C2	-3.42	106.08	109.52
4	M	1661	NAG	C1-O5-C5	-3.37	107.14	113.65
4	M	1661	NAG	C3-C2-N2	3.00	116.15	110.62
4	J	1328	NAG	O1-C1-C2	-3.00	102.99	109.22
4	H	1331	NAG	O5-C5-C4	2.97	115.05	109.70
4	H	1332	NAG	C1-C2-N2	2.97	114.17	110.73
4	L	1328	NAG	O5-C5-C6	2.92	113.67	106.44
4	M	1661	NAG	C3-C4-C5	2.91	115.50	110.23
4	J	1329	NAG	O5-C5-C4	2.87	114.86	109.70
4	J	1328	NAG	C3-C2-N2	2.82	115.80	110.62
4	H	1328	NAG	C3-C4-C5	2.74	115.19	110.23
4	H	1328	NAG	O4-C4-C3	-2.68	104.05	110.38
4	L	1329	NAG	O5-C1-C2	2.59	112.12	109.52
4	H	1332	NAG	O5-C5-C4	2.56	114.31	109.70
4	H	1330	NAG	O5-C5-C4	2.37	113.97	109.70
4	L	1328	NAG	O7-C7-C8	-2.37	117.84	122.05
4	H	1332	NAG	O5-C1-C2	-2.26	107.24	109.52
4	H	1332	NAG	C1-C2-C3	-2.25	107.47	110.54
4	H	1329	NAG	C1-C2-C3	2.21	113.55	110.54
4	H	1332	NAG	O1-C1-C2	2.20	113.79	109.22
4	H	1332	NAG	O7-C7-C8	-2.14	118.24	122.05
4	K	1661	NAG	O5-C5-C4	2.09	113.47	109.70
4	J	1328	NAG	O4-C4-C5	2.07	114.41	109.32
4	H	1332	NAG	C3-C4-C5	2.03	113.92	110.23

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1328	NAG	C1-C2-N2-C7
4	H	1328	NAG	C8-C7-N2-C2
4	H	1328	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	H	1329	NAG	C1-C2-N2-C7
4	H	1329	NAG	C8-C7-N2-C2
4	H	1329	NAG	O7-C7-N2-C2
4	H	1330	NAG	C1-C2-N2-C7
4	H	1330	NAG	C3-C2-N2-C7
4	H	1330	NAG	C8-C7-N2-C2
4	H	1330	NAG	O7-C7-N2-C2
4	H	1332	NAG	C8-C7-N2-C2
4	H	1332	NAG	O7-C7-N2-C2
4	K	1661	NAG	C8-C7-N2-C2
4	K	1661	NAG	O7-C7-N2-C2
4	L	1328	NAG	C8-C7-N2-C2
4	L	1328	NAG	O7-C7-N2-C2
4	L	1329	NAG	C8-C7-N2-C2
4	L	1329	NAG	O7-C7-N2-C2
4	M	1661	NAG	C8-C7-N2-C2
4	M	1661	NAG	O7-C7-N2-C2
4	L	1329	NAG	O5-C5-C6-O6
4	M	1661	NAG	O5-C5-C6-O6
4	K	1661	NAG	O5-C5-C6-O6
4	J	1329	NAG	O5-C5-C6-O6
4	H	1330	NAG	O5-C5-C6-O6
4	M	1661	NAG	C4-C5-C6-O6
4	H	1331	NAG	C8-C7-N2-C2
4	H	1331	NAG	O7-C7-N2-C2
4	H	1331	NAG	O5-C5-C6-O6
4	L	1328	NAG	O5-C5-C6-O6
4	H	1331	NAG	C4-C5-C6-O6
4	L	1328	NAG	C4-C5-C6-O6
4	H	1330	NAG	C4-C5-C6-O6
4	K	1661	NAG	C4-C5-C6-O6
4	L	1329	NAG	C4-C5-C6-O6
4	J	1329	NAG	C4-C5-C6-O6
4	L	1328	NAG	C1-C2-N2-C7
4	H	1328	NAG	C3-C2-N2-C7
4	J	1329	NAG	C8-C7-N2-C2
4	L	1328	NAG	C3-C2-N2-C7
4	H	1332	NAG	C4-C5-C6-O6
4	J	1329	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1332	NAG	3	0
4	J	1328	NAG	3	0
4	K	1661	NAG	3	0
4	M	1661	NAG	5	0
4	L	1328	NAG	2	0
4	L	1329	NAG	2	0
4	H	1329	NAG	1	0
4	H	1331	NAG	3	0
4	H	1330	NAG	5	0
4	H	1328	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	H	325/326 (99%)	0.50	18 (5%)	30 15	40, 92, 141, 207	0
1	J	325/326 (99%)	0.18	12 (3%)	45 25	35, 68, 118, 182	0
1	L	325/326 (99%)	0.15	10 (3%)	51 30	32, 63, 122, 166	0
2	I	161/222 (72%)	0.27	10 (6%)	26 14	36, 69, 120, 176	0
2	K	161/222 (72%)	-0.01	10 (6%)	26 14	33, 54, 90, 162	0
2	M	161/222 (72%)	0.05	7 (4%)	40 21	32, 61, 109, 195	0
All	All	1458/1644 (88%)	0.22	67 (4%)	37 20	32, 69, 128, 207	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	562	GLN	5.4
2	K	658	ASP	5.0
1	L	77	ALA	4.9
2	M	659	TYR	4.7
2	I	529	GLU	4.5
2	K	659	TYR	4.5
1	L	75	LEU	4.4
2	K	562	GLN	4.2
2	M	565	ALA	4.1
2	K	565	ALA	3.8
2	I	566	VAL	3.8
2	I	659	TYR	3.6
2	I	562	GLN	3.6
1	H	75	LEU	3.5
1	L	223	VAL	3.5
1	L	277	ASP	3.5
1	L	74	LEU	3.3
2	K	660	PRO	3.3
2	K	566	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	75	LEU	3.2
2	I	660	PRO	3.1
1	H	91	ASN	3.0
1	L	290	ASN	3.0
2	M	564	THR	3.0
1	L	71	CYS	2.9
1	H	276	HIS	2.9
1	H	195	TYR	2.9
1	L	76	THR	2.9
2	M	658	ASP	2.8
2	M	566	VAL	2.8
1	H	291	SER	2.8
1	L	218	ALA	2.8
1	H	194	LEU	2.7
1	H	197	ASN	2.6
1	H	137	ALA	2.6
1	J	291	SER	2.6
1	J	78	SER	2.6
1	J	77	ALA	2.6
1	H	59	CYS	2.5
1	L	291	SER	2.5
1	J	69	PRO	2.5
1	H	210	ASN	2.5
1	J	141	TYR	2.5
1	H	143	GLY	2.5
1	H	73	LEU	2.4
2	I	565	ALA	2.4
2	M	660	PRO	2.4
1	J	326	SER	2.4
2	I	564	THR	2.4
1	H	219	ALA	2.3
2	K	642	HIS	2.3
1	J	116	GLU	2.3
1	J	204	VAL	2.3
1	H	127	TRP	2.2
2	I	532	SER	2.2
2	I	653	ARG	2.2
1	J	214	THR	2.2
1	J	128	PRO	2.2
2	K	564	THR	2.1
1	H	193	SER	2.1
1	H	71	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	557	GLU	2.1
2	K	656	THR	2.1
1	H	138	ALA	2.1
1	H	161	TYR	2.0
1	J	18	ASP	2.0
2	K	563	PHE	2.0

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

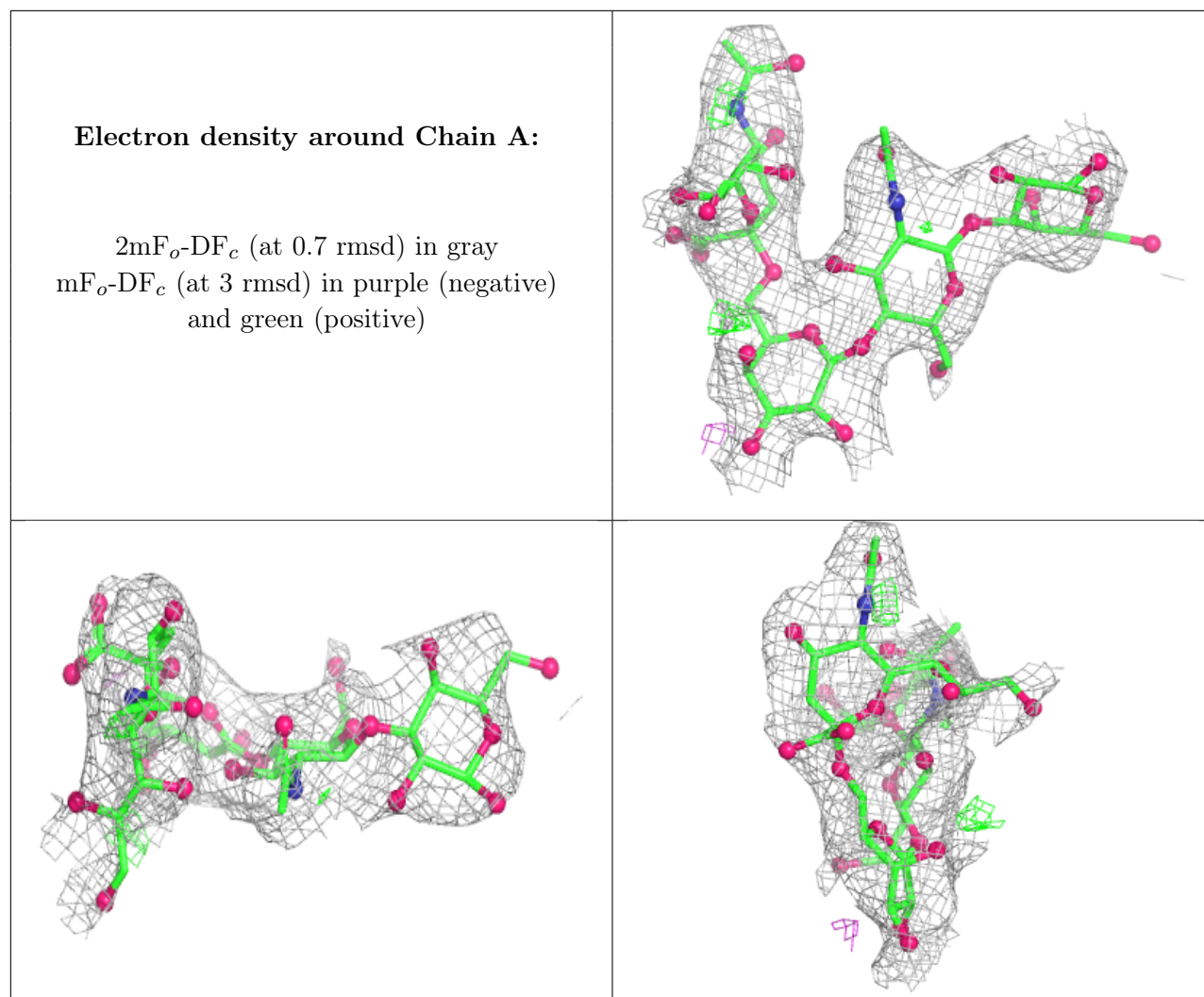
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAL	A	1	12/12	-	-	136,140,143,143	0
3	NAG	A	2	14/15	-	-	128,131,132,133	0
3	GAL	A	3	11/12	-	-	114,121,124,124	0
3	SIA	A	4	20/21	-	-	101,106,113,114	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	L	1329	15/15	0.19	0.17	125,130,131,131	0
4	NAG	M	1661	15/15	0.29	0.21	155,161,162,162	0
4	NAG	H	1331	15/15	0.34	0.15	151,153,154,154	0
4	NAG	H	1329	15/15	0.52	0.13	128,129,131,132	0
4	NAG	H	1330	15/15	0.54	0.15	133,136,138,138	0
4	NAG	H	1332	15/15	0.57	0.15	127,128,130,130	0
4	NAG	K	1661	15/15	0.61	0.15	138,142,144,144	0
4	NAG	J	1329	15/15	0.66	0.16	128,128,129,129	0
4	NAG	L	1328	15/15	0.74	0.14	76,81,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	1328	15/15	0.89	0.10	102,103,104,104	0
4	NAG	J	1328	15/15	0.92	0.09	68,71,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.