



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 09:39 AM BST

PDB ID : 2WRG
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 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

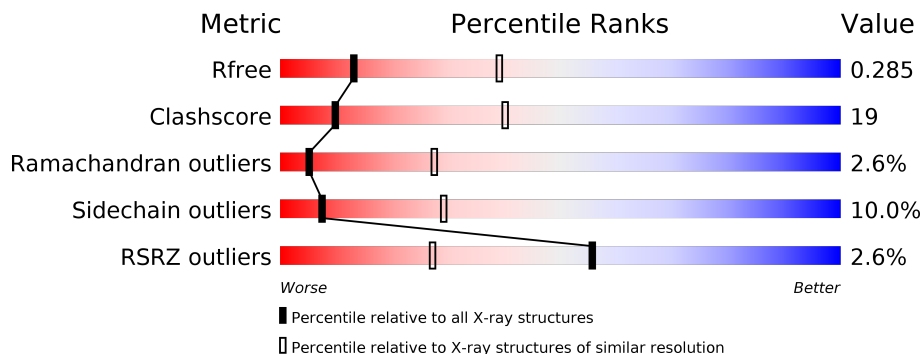
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



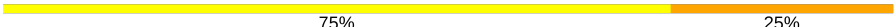
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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% 64% 31% .
1	J	326	 2% 63% 33% .
1	L	326	 2% 66% 29% 5%
2	I	222	 % 46% 21% . . 27%
2	K	222	 % 46% 21% . . 27%
2	M	222	 % 49% 18% 5% . 27%

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Mol	Chain	Length	Quality of chain
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	-	-	-
4	NAG	H	1330	-	-	-	X
4	NAG	H	1332	-	-	-	X
4	NAG	K	1661	-	-	-	X
4	NAG	M	1661	-	-	-	X

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	H	325	2517	1586	435	485	11	0	0	1
1	J	325	2517	1586	435	485	11	0	0	1
1	L	325	2517	1586	435	485	11	0	0	1

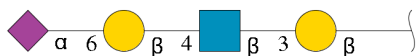
There are 3 discrepancies between the modelled and reference sequences:

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.

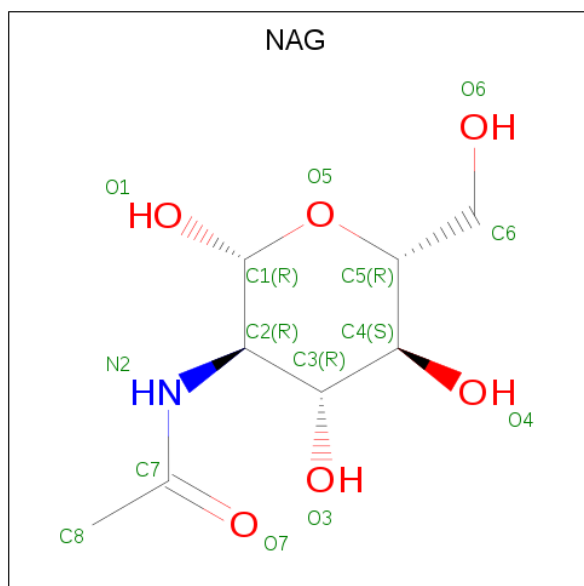
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	161	1282	802	221	253	6	0	0	1
2	K	161	1282	802	221	253	6	0	0	1
2	M	161	1282	802	221	253	6	0	0	1

- 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
			Total	C	N	O			
3	A	4	57	31	2	24	0	0	0

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

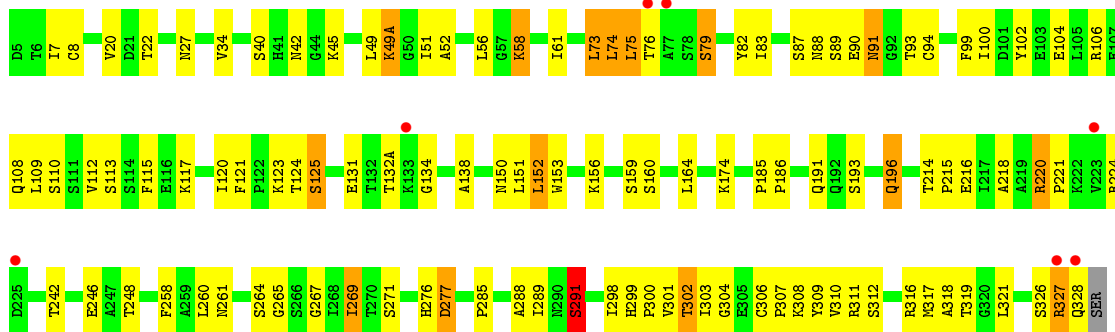


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	J	1	Total	C	N	O	0	0
			15	8	1	6		
4	J	1	Total	C	N	O	0	0
	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

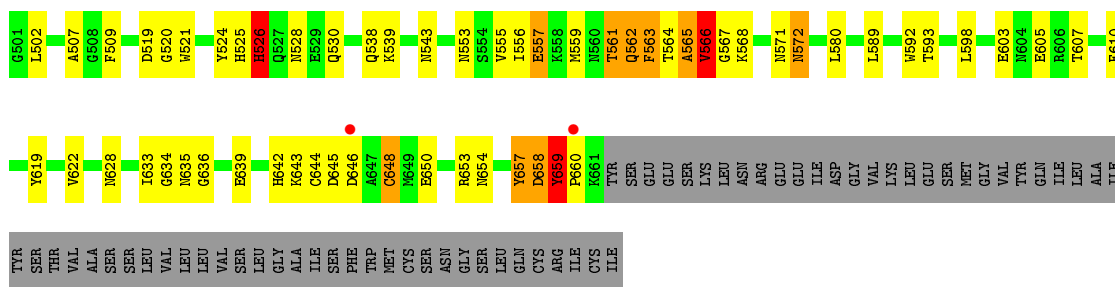
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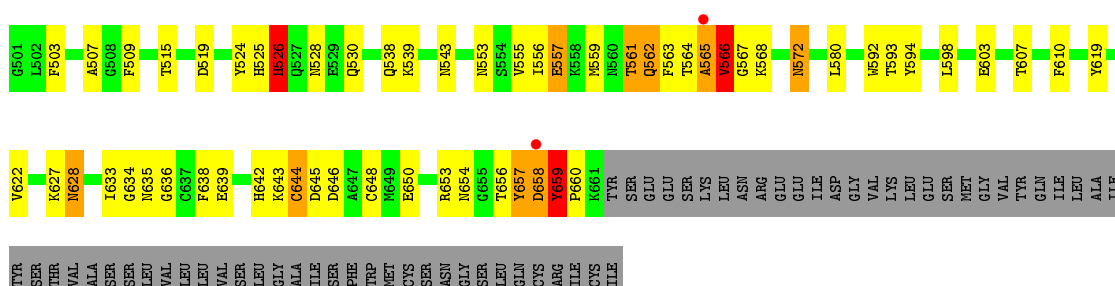
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	M	1	15	8	1	6	0	0



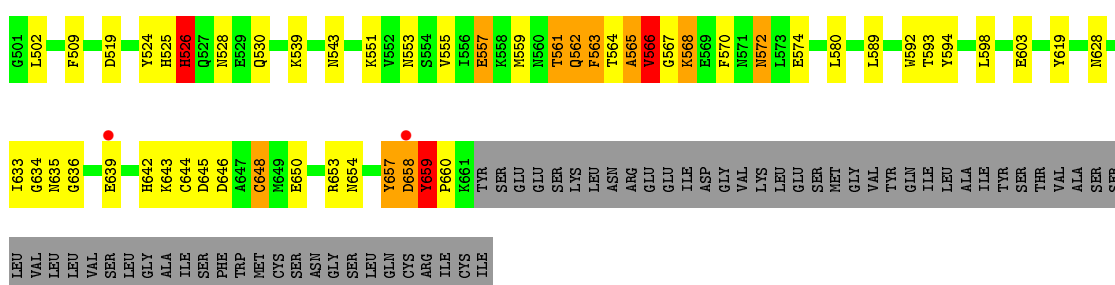
• Molecule 2: HEMAGGLUTININ HA2 CHAIN




• 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:  75% 25%

GAL1
MAG2
GAL3
SIA4

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) 98.0 (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)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.268 , 0.308 0.256 , 0.285	Depositor DCC
R_{free} test set	2646 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
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

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.*

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	0.38	0/2581	0.54	0/3516
1	J	0.43	0/2581	0.58	1/3516 (0.0%)
1	L	0.44	0/2581	0.58	1/3516 (0.0%)
2	I	0.50	0/1308	0.60	0/1764
2	K	0.58	0/1308	0.64	0/1764
2	M	0.55	0/1308	0.63	1/1764 (0.1%)
All	All	0.46	0/11667	0.59	3/15840 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	568	LYS	CB-CG-CD	5.94	127.03	111.60
1	J	291	SER	N-CA-C	5.12	124.81	111.00
1	L	291	SER	N-CA-C	5.09	124.74	111.00

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	116	0
1	J	2517	0	2439	95	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2517	0	2439	99	2
2	I	1282	0	1200	69	0
2	K	1282	0	1198	60	2
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	4	0
4	K	15	0	15	3	0
4	L	30	0	30	4	0
4	M	15	0	15	6	0
All	All	11619	0	11124	435	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 19.

All (435) 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:HE2	1:H:58:LYS:H	1.07	1.18
1:L:58:LYS:H	1:L:58:LYS:HE2	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:HD22	1:H:91:ASN:N	1.71	0.87
1:J:58:LYS:HE2	1:J:58:LYS:N	1.91	0.85
2:I:644:CYS:CB	2:I:648:CYS:HG	1.90	0.85
1:L:73:LEU:H	1:L:73:LEU:HD23	1.42	0.85
1:L:156:LYS:HD2	1:L:196:GLN:HG2	1.60	0.83
1:H:73:LEU:HD23	1:H:73:LEU:H	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:289:ILE:HG22	1:J:291:SER:HB2	1.62	0.82
1:J:73:LEU:H	1:J:73:LEU:HD23	1.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:308:LYS:HD3	2:K:559:MET:HE1	1.66	0.76
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
1:H:185:PRO:HG2	1:H:191:GLN:NE2	2.01	0.75
2:K:572:ASN:H	2:K:572:ASN:HD22	1.33	0.75
1:L:58:LYS:H	1:L:58:LYS:CE	1.95	0.75
1:J:91:ASN:HD22	1:J:91:ASN:N	1.84	0.75
2:M:572:ASN:HD22	2:M:572:ASN:H	1.35	0.74
2:I:572:ASN:H	2:I:572:ASN:HD22	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:H	1:H:91:ASN:HD22	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
1:H:91:ASN:CG	4:H:1328:NAG:O1	2.28	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:H:308:LYS:HD3	2:I:559:MET:HE1	1.75	0.68
1:J:9:ILE:HD11	2:K:622:VAL:HG21	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:308:LYS:HD3	2:M:559:MET:HE1	1.76	0.67
2:I:539:LYS:HE2	2:I:543:ASN:HD21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:MET:HE1	2:I:555:VAL:HG11	1.76	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:91:ASN:OD1	4:H:1328:NAG:O1	2.14	0.65
1:H:15:ASN:ND2	4:H:1331:NAG:N2	2.43	0.65
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:CE	1:J:58:LYS:H	2.00	0.65
1:L:269:ILE:HD12	1:L:285:PRO:HA	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
2:I:603:GLU:HA	2:I:603:GLU:OE2	1.97	0.64
1:L:27:ASN:CG	4:L:1329:NAG:H4	2.16	0.63
1:H:58:LYS:HZ1	1:H:73:LEU:HD21	1.63	0.63
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:CD2	1:J:73:LEU:H	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:327:ARG:C	1:L:327:ARG:HD2	2.21	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
1:L:91:ASN:N	1:L:91:ASN:ND2	2.49	0.59
2:K:530:GLN:HE22	2:K:645:ASP:HB2	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:539:LYS:HE2	2:K:543:ASN:HD21	1.68	0.58
1:L:317:MET:HE1	2:M:555:VAL:HG11	1.85	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
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:J:174:LYS:HB2	1:J:260:LEU:O	2.05	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:CD2	1:H:73:LEU:H	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:L:303:ILE:HG13	2:M:566:VAL:HG13	1.86	0.56
1:H:104:GLU:O	1:H:108:GLN:HG2	2.04	0.56
1:J:317:MET:HE1	2:K:555:VAL:HG11	1.87	0.56
2:I:644:CYS:HB2	2:I:648:CYS:HG	1.65	0.56
2:I:563:PHE:CE2	1:L:311:ARG:NH2	2.74	0.56
2:M:654:ASN:HD21	4:M:1661:NAG:H82	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
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:I:644:CYS:CB	2:I:648:CYS:SG	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:530:GLN:NE2	2:I:646:ASP:H	2.05	0.55
1:L:216:GLU:O	1:L:220:ARG:NH2	2.40	0.55
1:L:79:SER:HB2	1:L:113:SER:O	2.07	0.55
1:H:120:ILE:HG23	1:H:121:PHE:H	1.71	0.55
1:L:113:SER:OG	1:L:261:ASN:HB2	2.07	0.55
1:L:45:LYS:HG2	1:L:276:HIS:ND1	2.22	0.55
1:J:91:ASN:H	1:J:91:ASN:HD22	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:74:LEU:C	1:H:76:THR:H	2.11	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: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:ND2	1:H:91:ASN:N	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
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: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:82:TYR:HA	1:J:110:SER:O	2.09	0.53
1:J:58:LYS:NZ	1:J:73:LEU:HD21	2.24	0.53
1:J:74:LEU:C	1:J:76:THR:H	2.11	0.53
1:L:185:PRO:HG2	1:L:191:GLN:HE21	1.74	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:82:TYR:HA	1:L:110:SER:O	2.10	0.52
1:L:58:LYS:NZ	1:L:73:LEU:HD21	2.25	0.52
1:H:82:TYR:HA	1:H:110:SER:O	2.09	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:75:LEU:HD21	1:J:117:LYS:HZ2	1.75	0.51
1:H:58:LYS:NZ	1:H:73:LEU:HD21	2.25	0.51
1:L:74:LEU:C	1:L:76:THR:H	2.12	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
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
2:M:564:THR:O	2:M:565:ALA:HB2	2.11	0.50
1:L:58:LYS:HZ1	1:L:73:LEU:HD21	1.77	0.50
2:M:561:THR:O	2:M:562:GLN:O	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:74:LEU:C	1:H:76:THR:N	2.66	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:289:ILE:HD11	1:L:298:ILE:HB	1.93	0.49
1:L:42:ASN:OD1	1:L:45:LYS:HB2	2.12	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:M:654:ASN:CG	4:M:1661:NAG:O1	2.51	0.49
1:L:74:LEU:C	1:L:76:THR:N	2.67	0.48
2:I:650:GLU:O	2:I:654:ASN:CB	2.61	0.48
1:J:74:LEU:C	1:J:76:THR:N	2.67	0.48
1:J:302:THR:HG23	1:J:306:CYS:SG	2.53	0.48
1:H:51:ILE:HG22	1:H:52:ALA:N	2.27	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:216:GLU:O	1:J:220:ARG:NH2	2.46	0.48
1:J:51:ILE:HG22	1:J:52:ALA:N	2.28	0.48
1:L:74:LEU:O	1:L:76:THR:N	2.38	0.48
1:J:308:LYS:CD	2:K:559:MET:HE1	2.40	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:325:PRO:O	1:J:326:SER:C	2.52	0.48
4:L:1328:NAG:O3	4:L:1328:NAG:H83	2.14	0.48
1:L:61:ILE:HD11	1:L:83:ILE:HG21	1.95	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:138:ALA:O	1:J:224:ARG:NH1	2.46	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
1:L:120:ILE:HG23	1:L:121:PHE:H	1.79	0.47
1:J:58:LYS:HZ1	1:J:73:LEU:HD21	1.78	0.47
1:H:267:GLY:HA3	2:I:566:VAL:CG2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:658:ASP:O	2:K:659:TYR:CB	2.62	0.47
1:J:74:LEU:O	1:J:76:THR:N	2.40	0.47
1:H:91:ASN:H	1:H:91:ASN:ND2	2.07	0.47
1:J:102:TYR:O	1:J:106:ARG:HG3	2.14	0.47
1:J:79:SER:HB2	1:J:113:SER:O	2.15	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
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:51:ILE:HG22	1:L:52:ALA:N	2.31	0.46
1:L:8:CYS:O	2:M:524:TYR:HA	2.16	0.46
2:M:654:ASN:OD1	4:M:1661:NAG:O1	2.27	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
2:M:654:ASN:CG	4:M:1661:NAG:HO1	2.17	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
2:K:561:THR:C	2:K:562:GLN:O	2.53	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:L:277:ASP:OD2	1:L:277:ASP:N	2.49	0.45
1:L:34:VAL:HG13	1:L:319:THR:HG21	1.97	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:LYS:HG2	1:H:276:HIS:CE1	2.51	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:M:561:THR:C	2:M:562:GLN:O	2.54	0.45
2:M:650:GLU:O	2:M:654:ASN:CB	2.64	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
1:H:308:LYS:HD3	2:I:559:MET:CE	2.43	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
4:J:1328:NAG:C7	4:J:1328:NAG:HO1	2.30	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:NH1	1:L:327:ARG:O	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: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:HG22	1:L:93:THR:O	2.16	0.44
2:I:561:THR:C	2:I:562:GLN:O	2.56	0.43
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
2:I:561:THR:O	2:I:562:GLN:O	2.35	0.43
1:J:93:THR:HG22	1:J:93:THR:O	2.17	0.43
2:K:659:TYR:O	2:K:660:PRO:C	2.57	0.43
1:J:311:ARG:NH2	2:M:563:PHE:CE2	2.87	0.43
1:L:164:LEU:HD12	1:L:164:LEU:C	2.39	0.43
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
2:M:502:LEU:HA	2:M:502:LEU:HD12	1.83	0.43
1:H:324:ILE:CD1	2:I:507:ALA:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:524:TYR:N	2:I:524:TYR:CD1	2.86	0.43
2:K:528:ASN:HD21	2:K:530:GLN:NE2	2.17	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:49:LEU:HA	1:J:49:LEU:HD12	1.90	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:OE1	2:I:538:GLN:HA	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:HA	1:J:65:LEU:HD23	1.79	0.42
1:L:117:LYS:HE3	1:L:150:ASN:OD1	2.18	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:H:74:LEU:O	1:H:76:THR:N	2.39	0.42
1:J:91:ASN:ND2	1:J:91:ASN:N	2.55	0.42
2:M:619:TYR:CE1	2:M:636:GLY:HA2	2.55	0.42
1:J:277:ASP:N	1:J:277:ASP:OD2	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:L:299:HIS:HA	1:L:300:PRO:HD2	1.87	0.42
1:L:49:LEU:HA	1:L:49:LEU:HD12	1.83	0.42
1:H:117:LYS:HE3	1:H:150:ASN:OD1	2.19	0.42
1:H:37:LEU:HD21	1:H:297:ASN:ND2	2.34	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:J:164:LEU:C	1:J:164:LEU:HD12	2.40	0.42
1:J:195:TYR:O	1:J:197:ASN:N	2.53	0.42
2:K:538:GLN:HA	2:K:538:GLN:OE1	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
2:M:659:TYR:O	2:M:660:PRO:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:THR:O	1:J:125:SER:CB	2.67	0.42
1:J:132(A):THR:C	1:J:134:GLY:H	2.22	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:J:180:TRP:CZ2	1:J:204:VAL:HG21	2.55	0.41
1:J:36:LEU:HD11	1:J:317:MET:CE	2.50	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: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
2:M:524:TYR:CD1	2:M:524:TYR:N	2.88	0.41
1:H:164:LEU:HD12	1:H:164:LEU:C	2.41	0.41
1:L:124:THR:O	1:L:125:SER:CB	2.69	0.41
1:L:56:LEU:HA	1:L:74:LEU:HD13	2.02	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: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:299:HIS:HA	1:H:300:PRO:HD2	1.88	0.41
1:H:291:SER:HB3	1:H:307:PRO:CG	2.51	0.41
2:K:656:THR:O	2:K:657:TYR:C	2.58	0.41
2:K:524:TYR:N	2:K:524:TYR:CD1	2.88	0.41
2:M:570:PHE:HB3	2:M:574:GLU:HB2	2.03	0.41
2:K:598:LEU:HD23	2:K:598:LEU:HA	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:L:159:SER:C	1:L:196:GLN:HG3	2.42	0.40
1:H:242:THR:O	1:L:221:PRO:HG2	2.20	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
2:I:659:TYR:O	2:I:660:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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](#)

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	H	323/326 (99%)	289 (90%)	29 (9%)	5 (2%)	10	42
1	J	323/326 (99%)	287 (89%)	31 (10%)	5 (2%)	10	42
1	L	323/326 (99%)	288 (89%)	29 (9%)	6 (2%)	8	36
2	I	159/222 (72%)	144 (91%)	8 (5%)	7 (4%)	2	15
2	K	159/222 (72%)	144 (91%)	8 (5%)	7 (4%)	2	15
2	M	159/222 (72%)	143 (90%)	9 (6%)	7 (4%)	2	15
All	All	1446/1644 (88%)	1295 (90%)	114 (8%)	37 (3%)	5	27

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	125	SER
2	I	562	GLN
2	I	565	ALA
2	I	657	TYR

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Mol	Chain	Res	Type
2	I	659	TYR
1	J	125	SER
2	K	562	GLN
2	K	565	ALA
2	K	659	TYR
1	L	125	SER
2	M	562	GLN
2	M	565	ALA
2	M	657	TYR
2	M	659	TYR
2	I	526	HIS
2	I	643	LYS
1	J	196	GLN
2	K	526	HIS
2	K	657	TYR
1	L	75	LEU
2	M	526	HIS
2	M	643	LYS
1	H	75	LEU
1	H	196	GLN
1	J	75	LEU
2	K	643	LYS
1	L	196	GLN
1	L	326	SER
2	I	566	VAL
2	K	566	VAL
1	L	79	SER
2	M	566	VAL
1	J	79	SER
1	H	79	SER
1	L	265	GLY
1	H	265	GLY
1	J	265	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	279/282 (99%)	253 (91%)	26 (9%)	9	33
1	J	279/282 (99%)	251 (90%)	28 (10%)	7	29
1	L	279/282 (99%)	252 (90%)	27 (10%)	8	31
2	I	135/190 (71%)	121 (90%)	14 (10%)	7	27
2	K	135/190 (71%)	120 (89%)	15 (11%)	6	25
2	M	135/190 (71%)	121 (90%)	14 (10%)	7	27
All	All	1242/1416 (88%)	1118 (90%)	124 (10%)	7	29

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	49(A)	LYS
1	H	58	LYS
1	H	73	LEU
1	H	74	LEU
1	H	87	SER
1	H	89	SER
1	H	90	GLU
1	H	91	ASN
1	H	99	PHE
1	H	109	LEU
1	H	131	GLU
1	H	132(A)	THR
1	H	151	LEU
1	H	152	LEU
1	H	160	SER
1	H	193	SER
1	H	220	ARG
1	H	248	THR
1	H	264	SER
1	H	269	ILE
1	H	271	SER
1	H	277	ASP
1	H	290	ASN
1	H	291	SER
1	H	302	THR
1	H	321	LEU
2	I	519	ASP
2	I	526	HIS
2	I	557	GLU
2	I	561	THR

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Mol	Chain	Res	Type
2	I	563	PHE
2	I	566	VAL
2	I	568	LYS
2	I	572	ASN
2	I	580	LEU
2	I	628	ASN
2	I	642	HIS
2	I	648	CYS
2	I	658	ASP
2	I	659	TYR
1	J	5	ASP
1	J	6	THR
1	J	49(A)	LYS
1	J	58	LYS
1	J	73	LEU
1	J	74	LEU
1	J	87	SER
1	J	89	SER
1	J	90	GLU
1	J	91	ASN
1	J	99	PHE
1	J	109	LEU
1	J	131	GLU
1	J	132(A)	THR
1	J	151	LEU
1	J	152	LEU
1	J	160	SER
1	J	193	SER
1	J	220	ARG
1	J	248	THR
1	J	264	SER
1	J	269	ILE
1	J	271	SER
1	J	277	ASP
1	J	290	ASN
1	J	291	SER
1	J	302	THR
1	J	321	LEU
2	K	519	ASP
2	K	526	HIS
2	K	557	GLU
2	K	561	THR

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Mol	Chain	Res	Type
2	K	563	PHE
2	K	566	VAL
2	K	568	LYS
2	K	572	ASN
2	K	580	LEU
2	K	628	ASN
2	K	642	HIS
2	K	644	CYS
2	K	648	CYS
2	K	658	ASP
2	K	659	TYR
1	L	22	THR
1	L	49(A)	LYS
1	L	58	LYS
1	L	73	LEU
1	L	74	LEU
1	L	87	SER
1	L	89	SER
1	L	90	GLU
1	L	91	ASN
1	L	99	PHE
1	L	109	LEU
1	L	131	GLU
1	L	132(A)	THR
1	L	151	LEU
1	L	152	LEU
1	L	160	SER
1	L	193	SER
1	L	220	ARG
1	L	248	THR
1	L	264	SER
1	L	269	ILE
1	L	271	SER
1	L	277	ASP
1	L	291	SER
1	L	302	THR
1	L	321	LEU
1	L	327	ARG
2	M	519	ASP
2	M	526	HIS
2	M	557	GLU
2	M	561	THR

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Mol	Chain	Res	Type
2	M	563	PHE
2	M	566	VAL
2	M	568	LYS
2	M	572	ASN
2	M	580	LEU
2	M	628	ASN
2	M	642	HIS
2	M	648	CYS
2	M	658	ASP
2	M	659	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	27	ASN
1	H	35	ASN
1	H	55	GLN
1	H	91	ASN
1	H	130	HIS
1	H	191	GLN
1	H	250	ASN
1	H	290	ASN
2	I	530	GLN
2	I	543	ASN
2	I	562	GLN
2	I	572	ASN
2	I	625	GLN
2	I	629	ASN
2	I	642	HIS
1	J	35	ASN
1	J	55	GLN
1	J	130	HIS
1	J	191	GLN
1	J	196	GLN
1	J	250	ASN
2	K	528	ASN
2	K	530	GLN
2	K	543	ASN
2	K	562	GLN
2	K	572	ASN
2	K	595	ASN
2	K	625	GLN

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Mol	Chain	Res	Type
2	K	629	ASN
2	K	642	HIS
2	K	654	ASN
1	L	35	ASN
1	L	55	GLN
1	L	91	ASN
1	L	130	HIS
1	L	191	GLN
1	L	196	GLN
1	L	250	ASN
2	M	530	GLN
2	M	543	ASN
2	M	562	GLN
2	M	572	ASN
2	M	625	GLN
2	M	629	ASN
2	M	642	HIS
2	M	654	ASN

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](#)

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	2.10	4 (33%)	17,17,17	2.97	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	2	3	14,14,15	1.96	6 (42%)	17,19,21	1.32	1 (5%)
3	GAL	A	3	3	11,11,12	2.91	7 (63%)	15,15,17	2.75	6 (40%)
3	SIA	A	4	3	17,20,21	5.60	8 (47%)	21,28,31	3.09	6 (28%)

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	-	0/14/34/38	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	SIA	C11-C10	-13.33	1.22	1.50
3	A	4	SIA	O10-C10	13.03	1.52	1.23
3	A	4	SIA	O4-C4	-7.40	1.27	1.43
3	A	4	SIA	C3-C4	6.11	1.63	1.52
3	A	4	SIA	C6-C5	5.87	1.62	1.53
3	A	4	SIA	C4-C5	5.54	1.58	1.53
3	A	1	GAL	O5-C5	5.01	1.56	1.44
3	A	3	GAL	O5-C5	4.19	1.51	1.43
3	A	4	SIA	O6-C6	-4.16	1.37	1.44
3	A	3	GAL	C2-C3	4.03	1.58	1.52
3	A	3	GAL	C4-C5	3.73	1.60	1.53
3	A	3	GAL	C1-C2	3.65	1.60	1.52
3	A	3	GAL	C4-C3	3.48	1.61	1.52
3	A	3	GAL	O5-C1	2.98	1.48	1.43
3	A	2	NAG	O5-C1	2.97	1.48	1.43
3	A	2	NAG	C4-C3	2.78	1.59	1.52
3	A	1	GAL	O1-C1	2.57	1.47	1.39
3	A	2	NAG	C2-N2	2.50	1.50	1.46
3	A	4	SIA	C7-C6	-2.49	1.49	1.53
3	A	2	NAG	C4-C5	2.49	1.58	1.53
3	A	3	GAL	O4-C4	2.49	1.48	1.43
3	A	1	GAL	O5-C1	2.48	1.49	1.42
3	A	2	NAG	O4-C4	2.42	1.48	1.43
3	A	2	NAG	C6-C5	2.34	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	GAL	O3-C3	-2.21	1.37	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	SIA	C6-O6-C2	11.61	136.17	111.34
3	A	1	GAL	O1-C1-C2	9.57	135.99	109.03
3	A	3	GAL	O5-C1-C2	7.18	121.85	110.77
3	A	1	GAL	O1-C1-O5	-5.12	95.00	110.38
3	A	3	GAL	C1-O5-C5	4.94	118.89	112.19
3	A	4	SIA	C6-C5-N5	-4.44	103.54	110.91
3	A	3	GAL	C3-C4-C5	-3.28	104.39	110.24
3	A	4	SIA	O6-C2-C3	-3.13	104.39	109.87
3	A	4	SIA	C3-C4-C5	-2.85	108.01	111.46
3	A	1	GAL	C3-C4-C5	-2.84	105.17	110.24
3	A	3	GAL	O2-C2-C3	2.54	115.22	110.14
3	A	2	NAG	O6-C6-C5	2.46	119.72	111.29
3	A	3	GAL	C2-C3-C4	-2.45	106.65	110.89
3	A	1	GAL	C1-C2-C3	-2.43	105.28	110.31
3	A	4	SIA	C5-N5-C10	2.38	128.98	123.18
3	A	3	GAL	C1-C2-C3	2.29	112.48	109.67
3	A	1	GAL	O5-C5-C6	2.04	111.51	106.44
3	A	4	SIA	O4-C4-C3	-2.04	104.89	109.94

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

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	1.60	7 (33%)
4	NAG	H	1330	-	15,15,15	0.41	0	21,21,21	0.93	1 (4%)
4	NAG	M	1661	-	15,15,15	0.69	0	21,21,21	2.59	5 (23%)
4	NAG	L	1328	-	15,15,15	0.49	0	21,21,21	1.46	3 (14%)
4	NAG	K	1661	-	15,15,15	0.41	0	21,21,21	0.89	1 (4%)
4	NAG	J	1328	-	15,15,15	0.64	0	21,21,21	2.44	6 (28%)
4	NAG	L	1329	-	15,15,15	0.52	0	21,21,21	0.96	1 (4%)
4	NAG	H	1328	-	15,15,15	0.82	0	21,21,21	3.06	4 (19%)
4	NAG	H	1329	-	15,15,15	0.45	0	21,21,21	1.12	2 (9%)
4	NAG	J	1329	-	15,15,15	0.61	0	21,21,21	2.18	4 (19%)
4	NAG	H	1331	-	15,15,15	0.43	0	21,21,21	1.18	1 (4%)

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	H	1330	-	-	6/6/26/26	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	K	1661	-	-	4/6/26/26	0/1/1/1
4	NAG	J	1328	-	-	0/6/26/26	0/1/1/1
4	NAG	L	1329	-	-	4/6/26/26	0/1/1/1
4	NAG	H	1328	-	-	4/6/26/26	0/1/1/1
4	NAG	H	1329	-	-	3/6/26/26	0/1/1/1
4	NAG	J	1329	-	-	3/6/26/26	0/1/1/1
4	NAG	H	1331	-	-	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	-5.69	102.01	110.34
4	J	1329	NAG	C1-C2-C3	-4.87	103.90	110.54
4	H	1328	NAG	C1-O5-C5	-4.50	105.18	113.66
4	J	1329	NAG	C3-C4-C5	3.81	117.03	110.24
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	C1-O5-C5	-3.46	107.14	113.66
4	M	1661	NAG	O5-C1-C2	-3.42	106.08	109.52
4	J	1328	NAG	O1-C1-C2	-3.00	102.99	109.22
4	H	1332	NAG	C1-C2-N2	2.97	114.17	110.73
4	M	1661	NAG	C3-C4-C5	2.95	115.50	110.24
4	H	1331	NAG	O5-C5-C4	2.95	115.05	109.69
4	M	1661	NAG	C3-C2-N2	2.93	116.15	110.62
4	L	1328	NAG	O5-C5-C6	2.91	113.67	106.44
4	J	1329	NAG	O5-C5-C4	2.85	114.86	109.69
4	H	1328	NAG	C3-C4-C5	2.78	115.19	110.24
4	J	1328	NAG	C3-C2-N2	2.75	115.80	110.62
4	H	1328	NAG	O4-C4-C3	-2.73	104.05	110.35
4	L	1329	NAG	O5-C1-C2	2.59	112.12	109.52
4	H	1332	NAG	O5-C5-C4	2.54	114.31	109.69
4	H	1330	NAG	O5-C5-C4	2.36	113.97	109.69
4	L	1328	NAG	O7-C7-C8	-2.27	117.84	122.06
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	K	1661	NAG	O5-C5-C4	2.08	113.47	109.69
4	H	1332	NAG	C3-C4-C5	2.06	113.92	110.24
4	J	1328	NAG	O4-C4-C5	2.06	114.41	109.30
4	H	1332	NAG	O7-C7-C8	-2.05	118.24	122.06

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1332	NAG	C8-C7-N2-C2

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

There are no ring outliers.

10 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1332	NAG	3	0
4	H	1330	NAG	5	0
4	M	1661	NAG	6	0
4	L	1328	NAG	2	0
4	K	1661	NAG	3	0
4	J	1328	NAG	4	0
4	L	1329	NAG	2	0
4	H	1328	NAG	6	0
4	H	1329	NAG	1	0
4	H	1331	NAG	3	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%)	0.30	19 (5%) 23 7	40, 92, 141, 207	0
1	J	325/326 (99%)	-0.10	6 (1%) 68 40	35, 68, 118, 182	0
1	L	325/326 (99%)	-0.03	7 (2%) 62 33	33, 63, 122, 166	0
2	I	161/222 (72%)	0.02	2 (1%) 79 54	36, 69, 120, 176	0
2	K	161/222 (72%)	-0.23	2 (1%) 79 54	33, 54, 90, 162	0
2	M	161/222 (72%)	-0.16	2 (1%) 79 54	32, 61, 109, 195	0
All	All	1458/1644 (88%)	-0.01	38 (2%) 56 27	32, 69, 129, 207	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	328	GLN	9.3
2	I	660	PRO	4.9
1	H	327	ARG	4.7
1	J	328	GLN	4.2
1	J	159	SER	3.9
1	J	90	GLU	3.6
2	K	658	ASP	3.5
1	L	328	GLN	3.5
1	H	156	LYS	3.3
1	H	150	ASN	3.1
1	H	197	ASN	3.1
1	H	162	PRO	3.1
1	H	143	GLY	3.0
1	H	91	ASN	2.9
1	L	77	ALA	2.9
1	H	193	SER	2.9
1	J	160	SER	2.9
1	L	76	THR	2.7
2	I	646	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	225	ASP	2.6
2	M	658	ASP	2.5
1	H	199	ASP	2.5
1	J	88	ASN	2.4
1	L	327	ARG	2.4
1	L	223	VAL	2.3
1	H	144	ALA	2.3
1	L	133	LYS	2.3
1	H	137	ALA	2.3
1	H	161	TYR	2.2
1	H	171	ASN	2.2
1	H	196	GLN	2.2
1	H	173	GLY	2.2
1	H	114	SER	2.2
1	H	254	PRO	2.1
2	K	565	ALA	2.1
1	H	157	LYS	2.0
1	J	141	TYR	2.0
2	M	639	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GAL	A	3	11/12	0.75	0.29	114,121,124,124	0
3	GAL	A	1	12/12	0.78	0.40	136,140,143,143	0
3	SIA	A	4	20/21	0.84	0.24	101,106,113,114	0
3	NAG	A	2	14/15	0.86	0.22	128,131,132,133	0

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, 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(\AA^2)	Q<0.9
4	NAG	L	1329	15/15	0.52	0.38	125,130,131,131	0
4	NAG	M	1661	15/15	0.58	0.60	155,161,162,162	0
4	NAG	H	1330	15/15	0.58	0.48	133,136,138,138	0
4	NAG	H	1332	15/15	0.68	0.49	127,128,130,130	0
4	NAG	J	1329	15/15	0.75	0.36	128,128,129,129	0
4	NAG	H	1331	15/15	0.76	0.34	151,153,154,154	0
4	NAG	K	1661	15/15	0.77	0.49	138,142,144,144	0
4	NAG	L	1328	15/15	0.81	0.27	76,81,83,83	0
4	NAG	H	1329	15/15	0.89	0.44	128,129,131,132	0
4	NAG	H	1328	15/15	0.92	0.23	102,103,104,104	0
4	NAG	J	1328	15/15	0.96	0.24	68,71,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.