



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 PM UTC

PDB ID : 1RVT / pdb_00001rvt
Title : 1930 H1 Hemagglutinin in complex with LSTC
Authors : Skehel, J.J.; Gamblin, S.J.; Haire, L.F.; Russell, R.J.; Stevens, D.J.; Xiao, B.;
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Deposited on : 2003-12-15
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

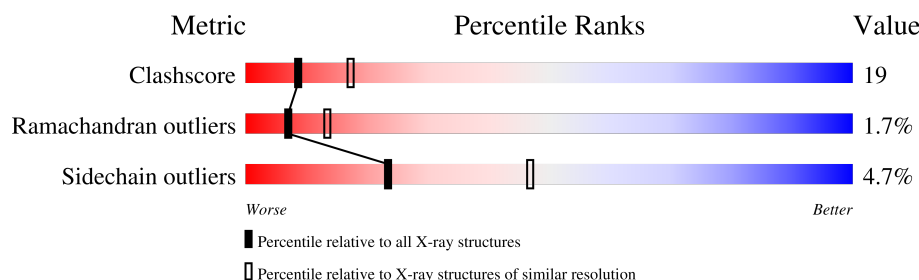
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	328	64% 31% . .
1	J	328	67% 29% . .
1	L	328	66% 29% 5% .
2	I	160	62% 31% . .
2	K	160	64% 29% 6% .
2	M	160	62% 32% 5% .
3	A	2	100%
3	C	2	100%

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Mol	Chain	Length	Quality of chain
4	B	5	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NDG	H	742	-	-	X	-
5	NDG	J	740	-	-	X	-
5	NDG	L	744	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12143 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.

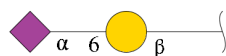
- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	324	Total	C	N	O	S	0	0	0
			2511	1580	436	484	11			
1	J	324	Total	C	N	O	S	0	0	0
			2511	1580	436	484	11			
1	L	324	Total	C	N	O	S	0	0	0
			2511	1580	436	484	11			

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	160	Total	C	N	O	S	0	0	0
			1281	801	223	252	5			
2	K	160	Total	C	N	O	S	0	0	0
			1281	801	223	252	5			
2	M	160	Total	C	N	O	S	0	0	0
			1281	801	223	252	5			

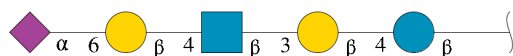
- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			31	17	1	13			
3	C	2	Total	C	N	O	0	0	0
			31	17	1	13			

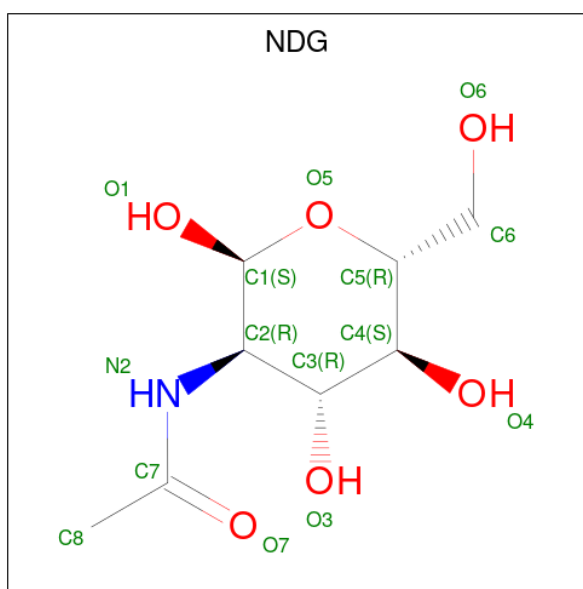
- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-

4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	5	Total	C	N	O	0	0	0
			68	37	2	29			

- Molecule 5 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	128	Total	O	0	0
			128	128		
6	I	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	151	Total 151	O 151	0	0
6	K	44	Total 44	O 44	0	0
6	L	191	Total 191	O 191	0	0
6	M	42	Total 42	O 42	0	0

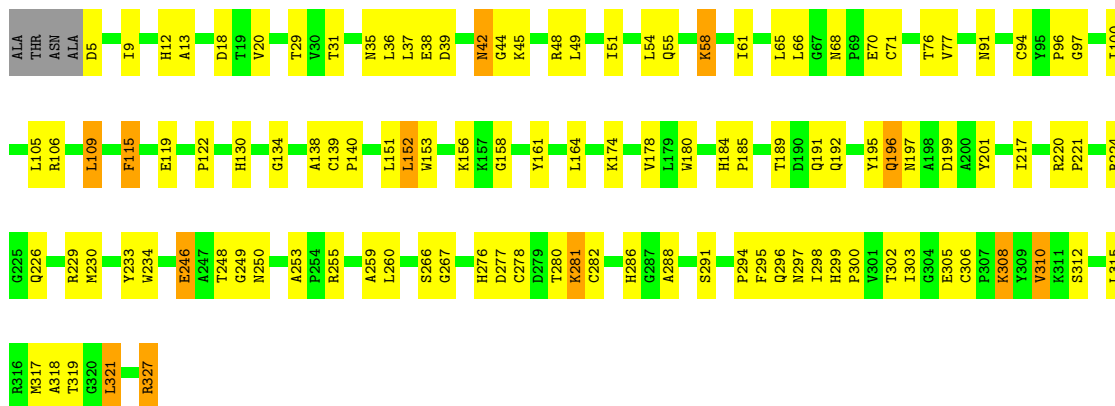
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

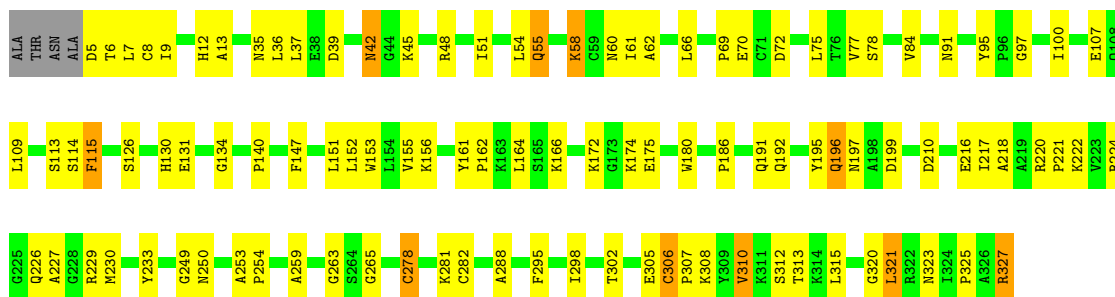
• Molecule 1: hemagglutinin

Chain H: 



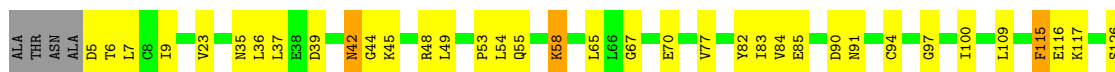
• Molecule 1: hemagglutinin

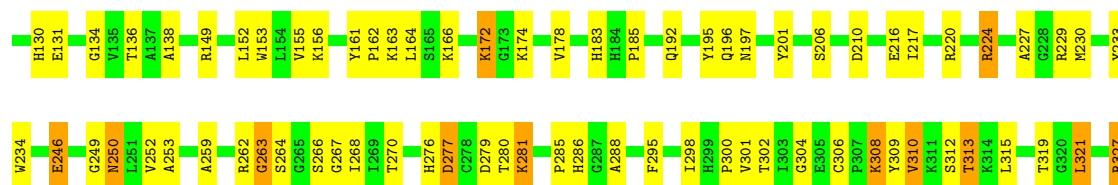
Chain J: 



• Molecule 1: hemagglutinin

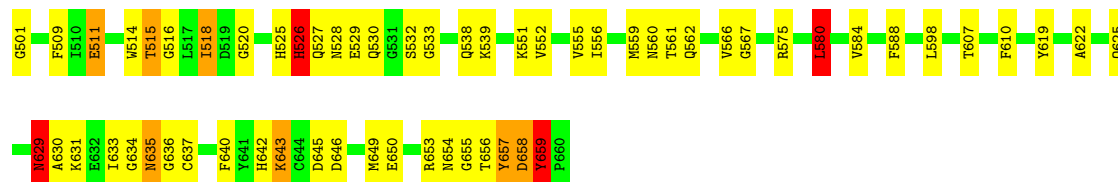
Chain L: 





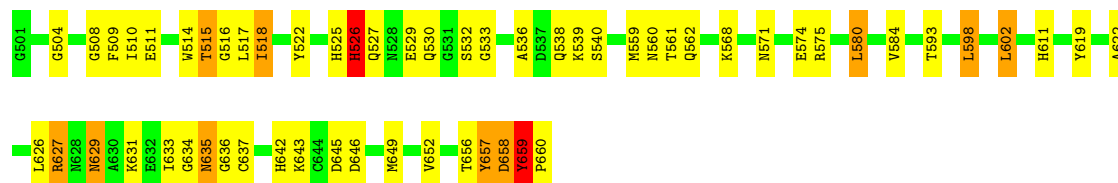
- Molecule 2: hemagglutinin

Chain I: 62% 31% . .



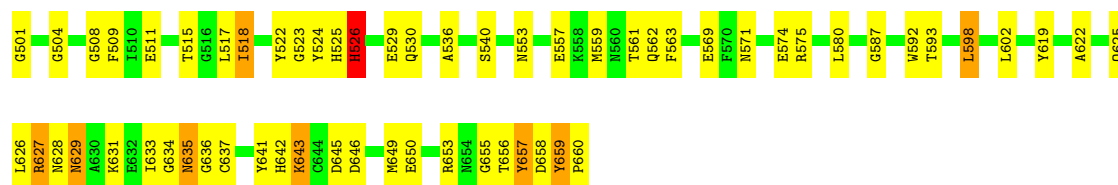
- Molecule 2: hemagglutinin

Chain K: 64% 29% 6% .



- Molecule 2: hemagglutinin

Chain M: 62% 32% 5% .



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain A: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain C: 100%



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

Chain B:

100%

BGC1
GAL2
NAG3
GAL4
SIA5

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.30Å 83.30Å 177.38Å 90.00° 106.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12143	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GAL, SIA, NDG, BGC

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	0.44	0/2574	0.97	9/3507 (0.3%)
1	J	0.43	0/2574	0.95	6/3507 (0.2%)
1	L	0.48	0/2574	0.98	11/3507 (0.3%)
2	I	0.38	0/1307	0.86	3/1761 (0.2%)
2	K	0.39	0/1307	0.86	4/1761 (0.2%)
2	M	0.40	0/1307	0.88	3/1761 (0.2%)
All	All	0.43	0/11643	0.94	36/15804 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	253	ALA	N-CA-C	8.15	121.32	110.08
2	M	515	THR	N-CA-C	-7.13	103.68	112.38
2	M	627	ARG	CB-CA-C	-6.96	107.76	117.23
1	J	227	ALA	N-CA-C	-6.96	104.94	113.50
2	K	627	ARG	CB-CA-C	-6.91	107.83	117.23
1	J	253	ALA	N-CA-C	6.86	119.37	109.84
2	K	515	THR	N-CA-C	-6.85	104.02	112.38
1	L	262	ARG	N-CA-C	-6.65	101.12	110.50
1	H	277	ASP	N-CA-C	-6.61	99.63	109.15
2	I	515	THR	N-CA-C	-6.61	104.32	112.38
1	L	253	ALA	N-CA-C	6.39	118.73	109.84
1	L	319	THR	N-CA-C	-6.23	105.69	113.55
1	L	281	LYS	N-CA-C	-6.08	106.18	113.97
1	L	172	LYS	N-CA-C	6.05	120.39	112.89
1	H	184	HIS	CA-C-N	5.95	123.94	119.66
1	H	184	HIS	C-N-CA	5.95	123.94	119.66
1	H	319	THR	N-CA-C	-5.90	106.11	113.55
1	H	248	THR	N-CA-C	-5.88	104.76	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	313	THR	N-CA-C	-5.87	106.25	113.41
2	K	593	THR	N-CA-C	-5.56	105.22	111.28
1	H	281	LYS	N-CA-C	-5.55	106.67	113.50
1	L	250	ASN	N-CA-C	5.48	119.79	113.38
1	L	227	ALA	N-CA-C	-5.46	106.46	113.23
1	J	84	VAL	N-CA-C	5.44	115.69	107.75
1	L	84	VAL	N-CA-C	5.35	115.55	107.80
1	J	307	PRO	N-CA-C	-5.33	102.90	111.38
1	L	277	ASP	N-CA-C	-5.32	99.27	108.52
1	L	252	VAL	N-CA-C	-5.32	97.76	106.32
1	H	260	LEU	N-CA-C	5.22	118.72	109.96
1	H	255	ARG	N-CA-C	-5.20	105.16	112.12
2	M	511	GLU	N-CA-C	5.17	121.80	110.80
2	I	511	GLU	N-CA-C	5.14	121.76	110.80
2	K	634	GLY	N-CA-C	-5.12	103.51	112.77
1	J	95	TYR	N-CA-C	-5.09	102.17	109.24
2	I	580	LEU	N-CA-C	-5.06	105.76	111.28
1	J	306	CYS	N-CA-C	5.00	116.36	108.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2511	0	2437	99	0
1	J	2511	0	2437	98	0
1	L	2511	0	2437	91	0
2	I	1281	0	1201	62	0
2	K	1281	0	1201	59	0
2	M	1281	0	1201	56	0
3	A	31	0	25	0	0
3	C	31	0	25	0	0
4	B	68	0	57	0	0
5	H	15	0	12	11	0
5	J	15	0	12	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	15	0	12	8	0
6	H	128	0	0	8	0
6	I	36	0	0	7	0
6	J	151	0	0	6	0
6	K	44	0	0	3	0
6	L	191	0	0	8	0
6	M	42	0	0	4	0
All	All	12143	0	11057	425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (425) 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:L:91:ASN:HD21	5:L:744:NDG:C1	1.55	1.19
1:J:58:LYS:H	1:J:58:LYS:HD3	1.06	1.11
1:L:58:LYS:H	1:L:58:LYS:HD3	1.16	1.09
1:H:58:LYS:H	1:H:58:LYS:HD3	1.17	1.04
1:J:224:ARG:NH2	5:J:740:NDG:H2	1.77	0.98
1:H:224:ARG:HH22	5:H:742:NDG:H2	1.26	0.96
1:L:224:ARG:NH2	5:L:744:NDG:H2	1.81	0.95
1:H:224:ARG:NH2	5:H:742:NDG:H2	1.82	0.93
1:L:91:ASN:ND2	5:L:744:NDG:C1	2.31	0.93
2:M:530:GLN:NE2	2:M:645:ASP:HB2	1.87	0.88
2:I:530:GLN:NE2	2:I:645:ASP:HB2	1.87	0.88
1:L:224:ARG:HH22	5:L:744:NDG:H2	1.36	0.87
1:H:139:CYS:HA	5:H:742:NDG:H8C2	1.57	0.86
1:J:224:ARG:HH22	5:J:740:NDG:H2	1.38	0.86
1:J:58:LYS:H	1:J:58:LYS:CD	1.86	0.85
1:H:65:LEU:HD11	1:H:109:LEU:HD21	1.61	0.83
2:K:530:GLN:NE2	2:K:645:ASP:HB2	1.93	0.82
1:J:58:LYS:HD3	1:J:58:LYS:N	1.92	0.80
1:L:65:LEU:HD11	1:L:109:LEU:HD21	1.62	0.80
1:J:55:GLN:HG3	6:J:811:HOH:O	1.82	0.80
2:I:530:GLN:HE21	2:I:645:ASP:HB2	1.47	0.79
1:H:220:ARG:HD2	1:H:229:ARG:HG2	1.65	0.79
1:L:192:GLN:HG2	6:L:854:HOH:O	1.82	0.78
1:J:310:VAL:HG12	1:J:312:SER:H	1.50	0.77
1:J:156:LYS:HD2	1:J:196:GLN:HG2	1.67	0.76
1:H:100:ILE:HG13	1:H:233:TYR:CE2	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:501:GLY:HA3	6:M:661:HOH:O	1.86	0.76
2:M:629:ASN:N	2:M:629:ASN:HD22	1.83	0.75
1:L:100:ILE:HG13	1:L:233:TYR:CE2	2.22	0.74
1:H:192:GLN:HG2	6:H:813:HOH:O	1.88	0.74
2:K:526:HIS:HB2	2:K:649:MET:HE3	1.70	0.74
1:H:156:LYS:HD2	1:H:196:GLN:HG2	1.69	0.74
1:L:58:LYS:HD3	1:L:58:LYS:N	1.99	0.74
1:H:158:GLY:HA3	6:H:830:HOH:O	1.88	0.73
2:I:526:HIS:HB2	2:I:649:MET:HE3	1.71	0.72
1:J:199:ASP:HB2	6:J:856:HOH:O	1.89	0.72
1:L:58:LYS:HG3	6:L:887:HOH:O	1.89	0.71
2:I:561:THR:HG22	2:I:562:GLN:H	1.54	0.71
1:H:42:ASN:C	1:H:42:ASN:HD22	1.99	0.70
1:H:224:ARG:HH22	5:H:742:NDG:C2	2.00	0.70
2:K:518:ILE:HD13	2:K:518:ILE:H	1.57	0.69
1:J:35:ASN:ND2	1:J:37:LEU:H	1.89	0.69
2:K:571:ASN:OD1	2:K:574:GLU:HG3	1.93	0.69
2:I:629:ASN:N	2:I:629:ASN:HD22	1.88	0.69
1:J:5:ASP:OD2	2:K:529:GLU:HG3	1.93	0.69
1:J:113:SER:HB3	1:J:263:GLY:HA3	1.76	0.68
1:J:221:PRO:HG2	1:L:206:SER:HA	1.73	0.68
1:H:295:PHE:CZ	2:I:559:MET:HG3	2.29	0.68
1:J:42:ASN:C	1:J:42:ASN:HD22	2.02	0.68
2:K:629:ASN:N	2:K:629:ASN:HD22	1.90	0.68
1:L:224:ARG:HH22	5:L:744:NDG:C2	2.05	0.68
1:H:9:ILE:HD11	2:I:622:ALA:CB	2.25	0.67
1:H:5:ASP:OD2	2:I:529:GLU:HG3	1.93	0.67
1:J:42:ASN:ND2	1:J:45:LYS:H	1.93	0.66
1:J:100:ILE:HG13	1:J:233:TYR:CE2	2.30	0.66
2:M:530:GLN:NE2	2:M:646:ASP:H	1.94	0.66
2:M:530:GLN:HE21	2:M:645:ASP:HB2	1.59	0.66
1:H:61:ILE:HD13	1:H:106:ARG:NH1	2.10	0.66
2:I:516:GLY:O	2:I:518:ILE:HG23	1.95	0.65
1:H:139:CYS:HA	5:H:742:NDG:C8	2.27	0.65
2:I:561:THR:HG22	2:I:562:GLN:N	2.11	0.65
2:I:560:ASN:HA	6:I:687:HOH:O	1.96	0.64
1:L:35:ASN:ND2	1:L:37:LEU:H	1.94	0.64
2:K:561:THR:HG22	2:K:562:GLN:N	2.12	0.64
1:J:310:VAL:CG1	1:J:312:SER:H	2.11	0.64
2:M:569:GLU:HG3	6:M:675:HOH:O	1.97	0.64
1:J:9:ILE:HD11	2:K:622:ALA:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:575:ARG:HD2	6:K:690:HOH:O	1.97	0.64
1:H:35:ASN:HD22	1:H:36:LEU:N	1.96	0.63
1:J:224:ARG:HH22	5:J:740:NDG:C2	2.11	0.63
1:L:5:ASP:OD2	2:M:529:GLU:HG3	1.99	0.63
2:K:518:ILE:HD13	2:K:518:ILE:N	2.14	0.63
1:J:156:LYS:NZ	1:J:196:GLN:HE21	1.97	0.63
1:L:220:ARG:HD2	1:L:229:ARG:CG	2.28	0.63
2:K:530:GLN:NE2	2:K:646:ASP:H	1.97	0.62
1:H:156:LYS:NZ	1:H:196:GLN:HE21	1.98	0.62
2:K:530:GLN:HE21	2:K:645:ASP:HB2	1.62	0.62
2:K:517:LEU:HD11	2:K:536:ALA:HB2	1.81	0.61
1:L:220:ARG:HD2	1:L:229:ARG:HG2	1.82	0.61
1:H:35:ASN:ND2	1:H:37:LEU:H	1.99	0.61
2:I:515:THR:HG23	6:I:669:HOH:O	2.00	0.61
1:H:140:PRO:HD2	5:H:742:NDG:H8C1	1.83	0.61
2:I:526:HIS:HD2	2:I:649:MET:HG3	1.66	0.61
2:K:509:PHE:O	2:K:635:ASN:HA	2.01	0.60
2:M:619:TYR:CE1	2:M:636:GLY:HA2	2.36	0.60
2:M:625:GLN:HE22	2:M:655:GLY:HA2	1.66	0.60
1:J:97:GLY:HA3	1:J:230:MET:O	2.02	0.60
1:H:308:LYS:HD2	6:I:689:HOH:O	2.02	0.60
1:H:134:GLY:HA3	1:H:153:TRP:HB3	1.83	0.60
1:L:302:THR:HB	1:L:306:CYS:SG	2.42	0.60
2:I:518:ILE:HD13	2:I:518:ILE:H	1.67	0.60
2:I:530:GLN:NE2	2:I:646:ASP:H	2.00	0.60
2:I:631:LYS:HE3	2:I:633:ILE:CD1	2.31	0.59
1:L:49:LEU:HD23	1:L:280:THR:O	2.02	0.59
1:H:42:ASN:ND2	1:H:45:LYS:H	2.01	0.59
1:H:220:ARG:HD2	1:H:229:ARG:CG	2.31	0.59
1:J:220:ARG:HD2	1:J:229:ARG:CG	2.32	0.59
2:M:629:ASN:N	2:M:629:ASN:ND2	2.49	0.59
1:H:94:CYS:HB2	1:H:138:ALA:O	2.02	0.59
2:K:619:TYR:CE1	2:K:636:GLY:HA2	2.38	0.59
2:M:559:MET:HA	2:M:559:MET:HE3	1.83	0.59
1:L:42:ASN:ND2	1:L:288:ALA:H	2.01	0.59
1:J:54:LEU:HD13	1:J:77:VAL:HG11	1.85	0.59
1:L:310:VAL:HG13	1:L:312:SER:H	1.67	0.58
1:H:13:ALA:O	2:I:515:THR:HA	2.04	0.58
2:K:658:ASP:O	2:K:659:TYR:HB2	2.04	0.58
1:L:39:ASP:C	1:L:298:ILE:HD11	2.29	0.57
2:I:635:ASN:OD1	2:I:637:CYS:SG	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:ILE:HD12	2:K:619:TYR:HA	1.86	0.57
1:L:7:LEU:HD11	2:M:524:TYR:HB3	1.86	0.57
2:K:635:ASN:HB2	6:K:698:HOH:O	2.03	0.57
1:J:48:ARG:HB2	1:J:51:ILE:O	2.03	0.57
1:J:321:LEU:HD23	1:J:321:LEU:N	2.20	0.57
2:K:627:ARG:NH1	2:K:660:PRO:HB3	2.18	0.57
1:J:295:PHE:CE2	2:K:559:MET:HE2	2.40	0.57
1:H:66:LEU:HD22	1:H:151:LEU:HD11	1.87	0.57
1:H:189:THR:HG23	6:H:901:HOH:O	2.04	0.57
2:M:517:LEU:HD11	2:M:536:ALA:HB2	1.87	0.57
1:J:174:LYS:HD2	1:J:259:ALA:HB1	1.86	0.56
1:H:174:LYS:HD2	1:H:259:ALA:HB1	1.86	0.56
1:H:220:ARG:HE	1:J:210:ASP:CG	2.12	0.56
1:H:295:PHE:CE2	2:I:559:MET:HE2	2.40	0.56
1:J:91:ASN:ND2	5:J:740:NDG:O1	2.38	0.56
2:K:631:LYS:HE3	2:K:633:ILE:HD13	1.88	0.56
1:L:172:LYS:HE2	6:L:825:HOH:O	2.05	0.56
2:M:525:HIS:O	2:M:526:HIS:ND1	2.36	0.56
1:J:42:ASN:HD21	1:J:288:ALA:H	1.54	0.55
1:J:156:LYS:NZ	1:J:196:GLN:NE2	2.55	0.55
2:K:526:HIS:HD2	2:K:649:MET:HG3	1.71	0.55
1:H:119:GLU:CD	1:H:122:PRO:HA	2.32	0.55
2:M:518:ILE:HD13	2:M:518:ILE:H	1.72	0.55
1:J:327:ARG:NE	1:J:327:ARG:C	2.65	0.55
1:L:48:ARG:NH2	1:L:277:ASP:HA	2.22	0.55
1:H:70:GLU:HG3	5:H:742:NDG:O1	2.07	0.55
1:J:295:PHE:HE2	2:K:559:MET:HE2	1.72	0.55
1:H:302:THR:HB	1:H:306:CYS:SG	2.47	0.54
1:H:138:ALA:O	1:H:224:ARG:NH1	2.40	0.54
1:J:164:LEU:C	1:J:164:LEU:HD12	2.32	0.54
1:H:295:PHE:HE2	2:I:559:MET:HE2	1.71	0.54
2:I:631:LYS:HE3	2:I:633:ILE:HD13	1.90	0.54
1:J:35:ASN:HD22	1:J:36:LEU:N	2.04	0.54
2:K:516:GLY:O	2:K:518:ILE:HG23	2.07	0.54
1:J:220:ARG:HD2	1:J:229:ARG:HG3	1.90	0.54
1:H:321:LEU:N	1:H:321:LEU:HD23	2.23	0.54
1:L:35:ASN:HD22	1:L:36:LEU:N	2.05	0.53
1:L:70:GLU:HG3	5:L:744:NDG:O1	2.08	0.53
2:I:629:ASN:N	2:I:629:ASN:ND2	2.56	0.53
1:H:58:LYS:HD3	1:H:58:LYS:N	2.02	0.53
1:J:42:ASN:ND2	1:J:288:ALA:H	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:ASN:HB3	1:H:71:CYS:SG	2.48	0.53
1:H:96:PRO:HG3	1:H:226:GLN:HB2	1.89	0.53
1:L:42:ASN:HD21	1:L:288:ALA:H	1.56	0.53
2:I:518:ILE:HD13	2:I:518:ILE:N	2.24	0.53
1:J:192:GLN:HG2	6:J:838:HOH:O	2.08	0.53
1:L:224:ARG:HH22	5:L:744:NDG:C3	2.22	0.53
1:J:42:ASN:HD22	1:J:45:LYS:H	1.56	0.53
1:L:115:PHE:C	1:L:115:PHE:CD1	2.87	0.53
1:L:164:LEU:HD12	1:L:164:LEU:C	2.33	0.53
1:H:310:VAL:HG13	1:H:312:SER:H	1.74	0.52
1:J:70:GLU:HB2	1:J:91:ASN:ND2	2.24	0.52
2:K:627:ARG:HH11	2:K:660:PRO:HB3	1.75	0.52
2:M:627:ARG:NH1	2:M:660:PRO:HB3	2.25	0.52
2:K:525:HIS:O	2:K:533:GLY:O	2.27	0.52
2:K:629:ASN:N	2:K:629:ASN:ND2	2.57	0.52
2:M:634:GLY:O	2:M:636:GLY:N	2.42	0.52
1:H:42:ASN:C	1:H:42:ASN:ND2	2.66	0.52
2:I:514:TRP:C	2:I:516:GLY:N	2.64	0.52
2:M:631:LYS:HE3	2:M:633:ILE:CD1	2.40	0.52
1:H:9:ILE:HD11	2:I:622:ALA:HB3	1.90	0.52
1:J:156:LYS:CD	1:J:196:GLN:HG2	2.39	0.52
1:J:302:THR:HB	1:J:306:CYS:SG	2.50	0.52
2:K:525:HIS:O	2:K:526:HIS:ND1	2.40	0.52
2:K:561:THR:CG2	2:K:562:GLN:N	2.73	0.52
1:L:91:ASN:ND2	5:L:744:NDG:O1	2.28	0.52
1:L:197:ASN:ND2	6:L:920:HOH:O	2.42	0.52
2:M:530:GLN:HE22	2:M:645:ASP:HB2	1.71	0.52
2:M:575:ARG:NE	6:M:673:HOH:O	2.43	0.52
1:H:217:ILE:N	1:H:217:ILE:HD12	2.25	0.52
2:K:509:PHE:CD1	2:K:510:ILE:HG13	2.45	0.51
2:I:656:THR:O	2:I:657:TYR:C	2.53	0.51
1:J:140:PRO:HD2	5:J:740:NDG:H8C1	1.92	0.51
2:M:625:GLN:NE2	2:M:655:GLY:HA2	2.25	0.51
1:H:36:LEU:HD11	1:H:317:MET:HG3	1.93	0.51
1:H:185:PRO:HG2	1:H:191:GLN:HE21	1.75	0.51
1:H:97:GLY:HA3	1:H:230:MET:O	2.10	0.51
2:M:559:MET:HE1	2:M:592:TRP:CE3	2.45	0.51
2:I:634:GLY:O	2:I:636:GLY:N	2.44	0.51
2:M:642:HIS:O	2:M:643:LYS:O	2.29	0.51
2:I:566:VAL:HG22	6:I:675:HOH:O	2.11	0.51
2:K:504:GLY:O	2:K:508:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:PHE:HZ	2:I:559:MET:HG3	1.75	0.51
1:J:66:LEU:HD22	1:J:151:LEU:HD11	1.93	0.51
1:H:35:ASN:HD22	1:H:36:LEU:H	1.58	0.50
2:I:650:GLU:HA	2:I:653:ARG:HD2	1.93	0.50
1:J:249:GLY:C	1:J:250:ASN:HD22	2.20	0.50
2:M:561:THR:HG22	2:M:562:GLN:N	2.26	0.50
1:H:115:PHE:CD1	1:H:115:PHE:C	2.90	0.50
1:J:220:ARG:HD2	1:J:229:ARG:HG2	1.94	0.50
1:J:265:GLY:HA2	6:J:850:HOH:O	2.09	0.50
1:L:115:PHE:C	1:L:115:PHE:HD1	2.18	0.50
2:I:630:ALA:HB2	2:I:640:PHE:HA	1.92	0.50
1:L:216:GLU:O	1:L:220:ARG:NH2	2.43	0.50
1:J:172:LYS:HD2	6:J:896:HOH:O	2.11	0.50
2:K:530:GLN:HE22	2:K:645:ASP:HB2	1.76	0.50
1:L:246:GLU:HG3	6:L:952:HOH:O	2.10	0.50
1:H:44:GLY:HA2	1:H:286:HIS:O	2.12	0.50
1:H:115:PHE:C	1:H:115:PHE:HD1	2.20	0.50
1:L:217:ILE:N	1:L:217:ILE:HD12	2.27	0.50
1:H:58:LYS:H	1:H:58:LYS:CD	2.00	0.49
2:M:622:ALA:O	2:M:626:LEU:HG	2.12	0.49
2:I:501:GLY:HA3	6:I:663:HOH:O	2.11	0.49
1:H:246:GLU:HG3	6:H:894:HOH:O	2.12	0.49
1:L:58:LYS:H	1:L:58:LYS:CD	1.96	0.49
1:L:220:ARG:HG3	1:L:220:ARG:HH11	1.76	0.49
2:M:627:ARG:HH11	2:M:660:PRO:HB3	1.77	0.49
1:H:18:ASP:O	1:H:29:THR:HA	2.13	0.49
2:I:635:ASN:OD1	2:I:635:ASN:C	2.56	0.49
1:H:310:VAL:CG1	1:H:312:SER:H	2.26	0.49
1:L:9:ILE:HD11	2:M:622:ALA:CB	2.43	0.49
1:J:39:ASP:C	1:J:298:ILE:HD11	2.38	0.49
1:J:107:GLU:OE2	2:K:568:LYS:NZ	2.42	0.49
1:H:49:LEU:CD1	1:H:303:ILE:HG22	2.42	0.48
1:H:266:SER:OG	1:H:267:GLY:N	2.46	0.48
1:L:48:ARG:HH22	1:L:277:ASP:CG	2.22	0.48
1:L:131:GLU:HB3	1:L:155:VAL:HG23	1.94	0.48
1:J:175:GLU:HG2	6:J:879:HOH:O	2.14	0.48
1:L:134:GLY:HA3	1:L:153:TRP:HB3	1.94	0.48
2:I:526:HIS:CB	2:I:649:MET:HE3	2.43	0.48
1:H:42:ASN:HD21	1:H:288:ALA:H	1.61	0.48
1:H:199:ASP:HB2	6:H:888:HOH:O	2.13	0.48
2:K:560:ASN:N	6:K:664:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:ILE:O	1:L:268:ILE:HA	2.13	0.48
2:M:628:ASN:O	2:M:641:TYR:CD1	2.67	0.48
1:L:54:LEU:HD13	1:L:77:VAL:HG11	1.95	0.48
1:L:97:GLY:HA3	1:L:230:MET:O	2.14	0.48
1:L:249:GLY:C	1:L:250:ASN:HD22	2.20	0.48
1:H:38:GLU:OE1	1:H:291:SER:HB2	2.14	0.48
1:J:156:LYS:HZ2	1:J:196:GLN:NE2	2.11	0.48
1:J:9:ILE:HD11	2:K:622:ALA:HB3	1.96	0.48
1:J:115:PHE:CD1	1:J:115:PHE:C	2.92	0.48
2:K:518:ILE:N	2:K:518:ILE:CD1	2.77	0.48
2:K:538:GLN:O	2:K:539:LYS:C	2.56	0.48
1:L:183:HIS:CE1	1:L:185:PRO:HG3	2.48	0.48
1:J:42:ASN:C	1:J:42:ASN:ND2	2.70	0.48
1:J:78:SER:O	1:J:114:SER:HB2	2.14	0.48
1:J:282:CYS:HB2	1:J:305:GLU:O	2.12	0.47
1:L:295:PHE:CZ	2:M:559:MET:HG3	2.49	0.47
1:L:321:LEU:HD23	1:L:321:LEU:N	2.29	0.47
2:M:656:THR:O	2:M:657:TYR:C	2.57	0.47
1:L:90:ASP:HB2	6:L:921:HOH:O	2.15	0.47
2:M:518:ILE:HD13	2:M:518:ILE:N	2.30	0.47
2:M:635:ASN:OD1	2:M:637:CYS:SG	2.72	0.47
1:H:42:ASN:ND2	1:H:288:ALA:H	2.12	0.47
1:H:161:TYR:CZ	1:H:249:GLY:HA2	2.50	0.47
5:H:742:NDG:C1	5:H:742:NDG:O7	2.63	0.47
2:I:634:GLY:C	2:I:636:GLY:N	2.72	0.47
1:L:156:LYS:NZ	1:L:196:GLN:HE21	2.12	0.47
2:I:580:LEU:O	2:I:584:VAL:HG23	2.15	0.47
1:J:9:ILE:HD11	2:K:622:ALA:HB2	1.96	0.47
1:J:8:CYS:HA	2:K:637:CYS:HA	1.97	0.47
1:L:220:ARG:HD2	1:L:229:ARG:HG3	1.96	0.47
1:H:9:ILE:HD11	2:I:622:ALA:HB2	1.96	0.47
1:H:48:ARG:HB2	1:H:51:ILE:O	2.15	0.47
1:L:53:PRO:HB3	1:L:82:TYR:CZ	2.50	0.47
2:M:522:TYR:HD1	2:M:540:SER:HB3	1.79	0.47
2:I:634:GLY:C	2:I:636:GLY:H	2.22	0.47
1:H:224:ARG:HH22	5:H:742:NDG:C3	2.28	0.46
1:H:105:LEU:HD12	1:H:105:LEU:O	2.15	0.46
1:H:294:PRO:HG2	1:H:295:PHE:CD1	2.50	0.46
1:J:115:PHE:C	1:J:115:PHE:HD1	2.23	0.46
1:J:134:GLY:HA3	1:J:153:TRP:HB3	1.96	0.46
1:L:266:SER:OG	1:L:267:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:310:VAL:HG22	2:M:593:THR:HA	1.96	0.46
1:J:91:ASN:ND2	5:J:740:NDG:C1	2.79	0.46
1:J:216:GLU:O	1:J:220:ARG:NH2	2.49	0.46
1:J:131:GLU:HB3	1:J:155:VAL:HG23	1.98	0.46
1:L:161:TYR:CZ	1:L:249:GLY:HA2	2.50	0.46
2:M:523:GLY:HA3	2:M:536:ALA:HA	1.98	0.46
2:M:571:ASN:OD1	2:M:574:GLU:HG3	2.15	0.46
2:I:526:HIS:O	2:I:526:HIS:ND1	2.48	0.46
1:J:295:PHE:CZ	2:K:559:MET:HG3	2.51	0.46
2:K:526:HIS:CB	2:K:649:MET:HE3	2.40	0.46
1:L:174:LYS:HD2	1:L:259:ALA:HB1	1.97	0.46
2:M:553:ASN:O	2:M:557:GLU:HG3	2.16	0.46
1:H:31:THR:HG23	1:H:321:LEU:O	2.15	0.46
1:J:91:ASN:HD21	5:J:740:NDG:C1	2.28	0.46
1:J:217:ILE:N	1:J:217:ILE:HD12	2.31	0.46
2:M:598:LEU:HD13	2:M:602:LEU:HD22	1.98	0.46
1:H:249:GLY:C	1:H:250:ASN:HD22	2.24	0.45
2:I:658:ASP:O	2:I:659:TYR:HB2	2.15	0.45
1:L:42:ASN:ND2	1:L:45:LYS:H	2.14	0.45
1:L:45:LYS:HD2	1:L:276:HIS:CG	2.51	0.45
1:L:310:VAL:CG1	1:L:312:SER:H	2.28	0.45
1:J:130:HIS:CE1	1:J:162:PRO:HD2	2.51	0.45
2:K:598:LEU:HD13	2:K:602:LEU:HD22	1.99	0.45
1:H:276:HIS:HB3	6:H:846:HOH:O	2.15	0.45
1:H:54:LEU:HD13	1:H:77:VAL:HG11	1.99	0.45
1:H:37:LEU:HB2	1:H:315:LEU:HB2	1.97	0.45
1:H:130:HIS:HD2	6:H:852:HOH:O	1.99	0.45
1:J:13:ALA:O	2:K:515:THR:HA	2.16	0.45
1:J:58:LYS:O	1:J:91:ASN:HB2	2.16	0.45
2:I:525:HIS:O	2:I:533:GLY:O	2.35	0.45
1:J:222:LYS:HA	1:J:226:GLN:O	2.17	0.45
1:J:323:ASN:C	1:J:325:PRO:HD3	2.41	0.45
2:K:559:MET:HE3	2:K:559:MET:HA	1.99	0.45
1:L:42:ASN:C	1:L:42:ASN:HD22	2.24	0.45
2:I:514:TRP:C	2:I:516:GLY:H	2.23	0.45
1:J:323:ASN:O	1:J:325:PRO:HD3	2.17	0.45
2:I:588:PHE:CZ	2:M:587:GLY:HA3	2.52	0.45
1:J:191:GLN:HA	1:J:191:GLN:HE21	1.82	0.45
1:J:195:TYR:O	1:J:196:GLN:HB2	2.17	0.45
2:K:509:PHE:CE1	2:K:510:ILE:HG13	2.51	0.45
2:M:522:TYR:CD1	2:M:540:SER:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:575:ARG:HD2	6:I:661:HOH:O	2.16	0.45
2:I:619:TYR:CE1	2:I:636:GLY:HA2	2.52	0.45
1:H:9:ILE:HD12	2:I:619:TYR:HA	1.98	0.44
1:J:60:ASN:OD1	1:J:62:ALA:HB3	2.18	0.44
2:M:625:GLN:HE22	2:M:655:GLY:CA	2.31	0.44
2:I:538:GLN:O	2:I:539:LYS:C	2.60	0.44
1:J:69:PRO:HG3	1:J:147:PHE:O	2.17	0.44
2:K:580:LEU:O	2:K:584:VAL:HG23	2.17	0.44
1:L:308:LYS:HD2	6:M:677:HOH:O	2.17	0.44
1:H:49:LEU:HD23	1:H:280:THR:O	2.17	0.44
1:J:35:ASN:HD22	1:J:36:LEU:H	1.65	0.44
1:H:224:ARG:CZ	5:H:742:NDG:H2	2.44	0.44
1:H:327:ARG:C	1:H:327:ARG:NE	2.76	0.44
2:K:642:HIS:HD1	2:K:642:HIS:C	2.25	0.44
1:J:320:GLY:O	2:K:611:HIS:CD2	2.70	0.44
2:I:561:THR:CG2	2:I:562:GLN:H	2.27	0.44
2:K:514:TRP:C	2:K:516:GLY:N	2.72	0.44
2:K:527:GLN:HG3	2:K:532:SER:OG	2.18	0.44
1:L:156:LYS:HD2	1:L:196:GLN:HG2	1.99	0.44
1:L:327:ARG:C	1:L:327:ARG:NE	2.75	0.44
1:J:131:GLU:HB3	1:J:155:VAL:CG2	2.47	0.44
1:H:91:ASN:ND2	5:H:742:NDG:C1	2.81	0.43
1:H:156:LYS:HZ2	1:H:196:GLN:HE21	1.66	0.43
1:H:37:LEU:HD21	1:H:297:ASN:ND2	2.33	0.43
2:M:559:MET:HE1	2:M:592:TRP:CZ3	2.53	0.43
2:M:625:GLN:HE22	2:M:655:GLY:C	2.25	0.43
2:I:509:PHE:O	2:I:635:ASN:HA	2.19	0.43
2:K:522:TYR:HD1	2:K:540:SER:HB3	1.84	0.43
1:L:263:GLY:O	1:L:264:SER:HB3	2.18	0.43
1:H:164:LEU:C	1:H:164:LEU:HD12	2.42	0.43
2:K:656:THR:O	2:K:658:ASP:N	2.51	0.43
1:L:285:PRO:HD3	1:L:301:VAL:O	2.18	0.43
1:L:94:CYS:HB2	1:L:138:ALA:O	2.19	0.43
1:H:201:TYR:CD1	1:H:201:TYR:C	2.96	0.43
1:L:315:LEU:HD23	1:L:315:LEU:HA	1.88	0.43
2:M:634:GLY:C	2:M:636:GLY:N	2.74	0.43
1:H:20:VAL:HG21	1:H:318:ALA:HB2	2.01	0.43
2:M:526:HIS:O	2:M:526:HIS:CG	2.72	0.43
1:H:39:ASP:C	1:H:298:ILE:HD11	2.44	0.43
2:I:561:THR:CG2	2:I:562:GLN:N	2.80	0.43
1:J:12:HIS:CG	1:J:13:ALA:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:SER:HB3	1:J:166:LYS:HE2	2.00	0.43
1:J:220:ARG:O	1:J:221:PRO:C	2.62	0.43
1:L:300:PRO:HB3	1:L:309:TYR:CD2	2.54	0.43
1:H:299:HIS:ND1	1:H:300:PRO:HD2	2.34	0.42
2:K:622:ALA:O	2:K:626:LEU:HG	2.18	0.42
1:L:6:THR:O	2:M:649:MET:HE1	2.19	0.42
1:L:117:LYS:CE	6:L:843:HOH:O	2.66	0.42
1:L:130:HIS:HD2	6:L:852:HOH:O	2.02	0.42
1:J:6:THR:O	2:K:526:HIS:HA	2.19	0.42
1:J:37:LEU:HB2	1:J:315:LEU:HB2	2.00	0.42
1:J:48:ARG:HG2	1:J:278:CYS:O	2.20	0.42
1:J:180:TRP:HB3	1:J:254:PRO:HG3	2.01	0.42
1:L:42:ASN:ND2	1:L:42:ASN:C	2.78	0.42
1:L:115:PHE:C	1:L:116:GLU:HG3	2.41	0.42
2:M:627:ARG:HD2	2:M:660:PRO:HA	2.01	0.42
1:H:38:GLU:O	1:H:296:GLN:HA	2.20	0.42
2:I:567:GLY:HA2	6:I:688:HOH:O	2.19	0.42
2:I:659:TYR:HD2	2:I:659:TYR:HA	1.75	0.42
1:J:161:TYR:CZ	1:J:249:GLY:HA2	2.55	0.42
1:L:300:PRO:HD3	1:L:309:TYR:CZ	2.54	0.42
1:H:195:TYR:O	1:H:197:ASN:N	2.50	0.42
1:J:60:ASN:O	1:J:61:ILE:C	2.61	0.42
1:L:195:TYR:O	1:L:196:GLN:HB2	2.18	0.42
2:I:607:THR:O	2:I:610:PHE:HB3	2.19	0.42
1:J:186:PRO:HA	1:J:218:ALA:O	2.20	0.42
1:L:85:GLU:O	1:L:270:THR:HA	2.19	0.42
1:L:67:GLY:O	1:L:149:ARG:HG2	2.20	0.42
2:M:504:GLY:O	2:M:508:GLY:HA3	2.19	0.42
2:M:650:GLU:OE2	2:M:653:ARG:HD2	2.20	0.42
1:J:195:TYR:O	1:J:197:ASN:N	2.53	0.42
1:H:42:ASN:HD22	1:H:45:LYS:H	1.65	0.42
1:L:44:GLY:HA2	1:L:286:HIS:O	2.19	0.42
1:H:180:TRP:CE2	1:H:233:TYR:HB2	2.55	0.41
2:M:509:PHE:O	2:M:635:ASN:HA	2.20	0.41
1:L:9:ILE:HD12	2:M:619:TYR:HA	2.01	0.41
1:L:130:HIS:CE1	1:L:162:PRO:HD2	2.55	0.41
2:I:551:LYS:HG3	1:L:23:VAL:CG1	2.49	0.41
2:I:552:VAL:O	2:I:556:ILE:HG13	2.21	0.41
1:L:48:ARG:HH11	1:L:279:ASP:CG	2.27	0.41
1:H:152:LEU:HD23	1:H:152:LEU:HA	1.91	0.41
2:I:625:GLN:HE22	2:I:655:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:HIS:HB2	2:I:520:GLY:O	2.20	0.41
1:H:48:ARG:HG2	1:H:278:CYS:O	2.19	0.41
2:K:561:THR:CG2	2:K:562:GLN:H	2.34	0.41
1:H:220:ARG:O	1:H:221:PRO:C	2.63	0.41
1:L:7:LEU:HA	2:M:526:HIS:HA	2.03	0.41
1:L:163:LYS:HE2	1:L:201:TYR:OH	2.20	0.41
1:L:178:VAL:O	1:L:234:TRP:HA	2.21	0.41
1:L:126:SER:HB3	1:L:166:LYS:HE2	2.02	0.41
1:L:304:GLY:O	2:M:563:PHE:HA	2.20	0.41
2:M:526:HIS:HD2	2:M:649:MET:HG3	1.85	0.41
2:I:642:HIS:O	2:I:643:LYS:O	2.38	0.41
2:K:633:ILE:O	2:K:633:ILE:HG22	2.20	0.41
2:I:528:ASN:ND2	2:I:645:ASP:HA	2.36	0.41
2:I:650:GLU:O	2:I:654:ASN:ND2	2.54	0.41
1:J:7:LEU:CD2	2:K:652:VAL:HG11	2.51	0.41
1:H:185:PRO:HG2	1:H:191:GLN:NE2	2.34	0.40
2:I:527:GLN:HG3	2:I:532:SER:OG	2.21	0.40
1:H:178:VAL:O	1:H:234:TRP:HA	2.21	0.40
1:J:191:GLN:HA	1:J:191:GLN:NE2	2.36	0.40
2:K:656:THR:O	2:K:657:TYR:C	2.63	0.40
2:M:628:ASN:O	2:M:641:TYR:CE1	2.74	0.40
2:I:555:VAL:O	2:I:559:MET:HG2	2.21	0.40
1:L:35:ASN:HD22	1:L:35:ASN:C	2.29	0.40
1:H:282:CYS:HB2	1:H:305:GLU:O	2.22	0.40
1:H:76:THR:HG23	6:H:916:HOH:O	2.21	0.40
1:J:7:LEU:HA	2:K:526:HIS:HA	2.04	0.40
1:J:48:ARG:HB2	1:J:51:ILE:C	2.46	0.40
1:J:72:ASP:HA	1:J:75:LEU:HG	2.04	0.40
1:J:220:ARG:HE	1:L:210:ASP:CG	2.29	0.40
1:L:9:ILE:HD11	2:M:622:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	322/328 (98%)	299 (93%)	22 (7%)	1 (0%)	36	55
1	J	322/328 (98%)	304 (94%)	17 (5%)	1 (0%)	36	55
1	L	322/328 (98%)	301 (94%)	20 (6%)	1 (0%)	36	55
2	I	158/160 (99%)	134 (85%)	16 (10%)	8 (5%)	1	2
2	K	158/160 (99%)	139 (88%)	12 (8%)	7 (4%)	2	2
2	M	158/160 (99%)	139 (88%)	13 (8%)	6 (4%)	2	3
All	All	1440/1464 (98%)	1316 (91%)	100 (7%)	24 (2%)	7	13

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	635	ASN
2	K	657	TYR
2	K	658	ASP
2	K	659	TYR
2	M	635	ASN
2	M	657	TYR
2	I	511	GLU
2	I	643	LYS
2	I	657	TYR
2	K	526	HIS
2	M	643	LYS
2	I	526	HIS
2	I	658	ASP
2	I	659	TYR
2	K	511	GLU
2	K	643	LYS
2	M	658	ASP
2	M	659	TYR
2	I	629	ASN
1	J	196	GLN
1	L	263	GLY
2	M	526	HIS
1	H	196	GLN
2	K	635	ASN

5.3.2 Protein sidechains ⓘ

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	279/281 (99%)	267 (96%)	12 (4%)	26	51
1	J	279/281 (99%)	266 (95%)	13 (5%)	23	47
1	L	279/281 (99%)	265 (95%)	14 (5%)	22	44
2	I	134/134 (100%)	128 (96%)	6 (4%)	24	49
2	K	134/134 (100%)	127 (95%)	7 (5%)	21	42
2	M	134/134 (100%)	128 (96%)	6 (4%)	24	49
All	All	1239/1245 (100%)	1181 (95%)	58 (5%)	23	47

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	42	ASN
1	H	55	GLN
1	H	58	LYS
1	H	109	LEU
1	H	115	PHE
1	H	152	LEU
1	H	246	GLU
1	H	281	LYS
1	H	308	LYS
1	H	310	VAL
1	H	321	LEU
1	H	327	ARG
2	I	518	ILE
2	I	526	HIS
2	I	580	LEU
2	I	598	LEU
2	I	629	ASN
2	I	659	TYR
1	J	42	ASN
1	J	55	GLN
1	J	58	LYS
1	J	109	LEU

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Mol	Chain	Res	Type
1	J	115	PHE
1	J	152	LEU
1	J	278	CYS
1	J	281	LYS
1	J	308	LYS
1	J	310	VAL
1	J	313	THR
1	J	321	LEU
1	J	327	ARG
2	K	518	ILE
2	K	526	HIS
2	K	580	LEU
2	K	598	LEU
2	K	602	LEU
2	K	629	ASN
2	K	659	TYR
1	L	42	ASN
1	L	55	GLN
1	L	58	LYS
1	L	115	PHE
1	L	136	THR
1	L	152	LEU
1	L	224	ARG
1	L	246	GLU
1	L	281	LYS
1	L	308	LYS
1	L	310	VAL
1	L	313	THR
1	L	321	LEU
1	L	327	ARG
2	M	518	ILE
2	M	526	HIS
2	M	580	LEU
2	M	598	LEU
2	M	629	ASN
2	M	659	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	35	ASN
1	H	42	ASN

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Mol	Chain	Res	Type
1	H	91	ASN
1	H	159	ASN
1	H	191	GLN
1	H	196	GLN
1	H	250	ASN
2	I	530	GLN
2	I	550	ASN
2	I	625	GLN
2	I	629	ASN
1	J	35	ASN
1	J	42	ASN
1	J	91	ASN
1	J	159	ASN
1	J	191	GLN
1	J	196	GLN
1	J	250	ASN
1	J	276	HIS
2	K	530	GLN
2	K	625	GLN
2	K	629	ASN
1	L	27	ASN
1	L	35	ASN
1	L	42	ASN
1	L	91	ASN
1	L	150	ASN
1	L	171	ASN
1	L	191	GLN
1	L	196	GLN
1	L	250	ASN
1	L	286	HIS
2	M	530	GLN
2	M	550	ASN
2	M	625	GLN
2	M	629	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	11,11,12	3.02	6 (54%)	15,15,17	1.44	2 (13%)
3	SIA	A	2	3	20,20,21	3.92	7 (35%)	21,28,31	2.35	9 (42%)
4	BGC	B	1	4	12,12,12	2.55	6 (50%)	17,17,17	0.61	0
4	GAL	B	2	4	11,11,12	2.33	2 (18%)	15,15,17	0.94	1 (6%)
4	NAG	B	3	4	14,14,15	1.94	6 (42%)	17,19,21	0.90	0
4	GAL	B	4	4	11,11,12	2.71	6 (54%)	15,15,17	1.38	1 (6%)
4	SIA	B	5	4	20,20,21	3.77	6 (30%)	21,28,31	2.43	8 (38%)
3	GAL	C	1	3	11,11,12	2.84	6 (54%)	15,15,17	1.06	1 (6%)
3	SIA	C	2	3	20,20,21	3.92	8 (40%)	21,28,31	2.35	8 (38%)

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

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	SIA	C2-C1	11.22	1.65	1.52
3	A	2	SIA	C2-C1	10.63	1.65	1.52
4	B	5	SIA	C2-C1	9.98	1.64	1.52
3	C	2	SIA	O4-C4	-7.91	1.26	1.43
4	B	5	SIA	O4-C4	-7.52	1.27	1.43
3	A	2	SIA	O4-C4	-7.24	1.28	1.43
3	A	2	SIA	C4-C5	7.08	1.59	1.53
4	B	5	SIA	C6-C5	6.73	1.63	1.53
3	A	2	SIA	C6-C5	6.57	1.63	1.53
4	B	2	GAL	O5-C5	6.08	1.55	1.43
3	C	2	SIA	C6-C5	5.99	1.62	1.53
3	C	1	GAL	O5-C5	5.74	1.54	1.43
4	B	5	SIA	C4-C5	5.61	1.58	1.53
3	C	2	SIA	C3-C4	5.44	1.63	1.52
3	A	1	GAL	O5-C5	5.37	1.53	1.43
3	C	2	SIA	C4-C5	5.34	1.58	1.53
4	B	5	SIA	C3-C4	5.12	1.62	1.52
3	A	2	SIA	C3-C4	4.98	1.62	1.52
3	A	1	GAL	C1-C2	4.62	1.63	1.52
4	B	1	BGC	O4-C4	4.60	1.54	1.43
4	B	4	GAL	O5-C5	4.52	1.52	1.43
3	C	1	GAL	O5-C1	4.09	1.50	1.43
4	B	1	BGC	C4-C5	4.07	1.61	1.53
3	A	1	GAL	C4-C5	3.60	1.60	1.53
3	A	1	GAL	O5-C1	3.59	1.49	1.43
4	B	4	GAL	C1-C2	3.59	1.60	1.52
4	B	4	GAL	C4-C5	3.47	1.60	1.53
3	C	1	GAL	C1-C2	3.31	1.60	1.52
4	B	1	BGC	O5-C1	3.25	1.50	1.42
4	B	4	GAL	C2-C3	3.22	1.57	1.52
4	B	1	BGC	C3-C2	3.19	1.60	1.52
4	B	3	NAG	O5-C1	3.17	1.49	1.43
4	B	5	SIA	O6-C6	-3.16	1.39	1.44
3	C	1	GAL	C4-C5	3.14	1.59	1.53
3	A	2	SIA	O6-C6	-3.06	1.39	1.44
3	A	1	GAL	C2-C3	3.04	1.57	1.52
3	A	1	GAL	C4-C3	2.99	1.60	1.52
4	B	4	GAL	O5-C1	2.97	1.48	1.43
4	B	4	GAL	C4-C3	2.87	1.59	1.52
4	B	3	NAG	C2-N2	2.83	1.50	1.46
4	B	2	GAL	O5-C1	2.77	1.48	1.43
3	C	2	SIA	O6-C6	-2.73	1.39	1.44
3	C	1	GAL	C4-C3	2.66	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	BGC	C1-C2	2.58	1.58	1.52
4	B	3	NAG	O4-C4	2.48	1.49	1.43
3	C	1	GAL	C2-C3	2.42	1.56	1.52
4	B	3	NAG	O5-C5	2.42	1.48	1.43
4	B	3	NAG	C4-C5	2.20	1.57	1.53
3	C	2	SIA	C7-C6	-2.11	1.50	1.52
4	B	1	BGC	O5-C5	2.10	1.49	1.44
4	B	3	NAG	C4-C3	2.06	1.57	1.52
3	A	2	SIA	C3-C2	-2.05	1.49	1.52
3	C	2	SIA	O1B-C1	-2.02	1.24	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	SIA	O6-C2-C3	-4.88	103.99	110.56
3	C	2	SIA	O6-C2-C3	-4.81	104.09	110.56
4	B	5	SIA	C11-C10-N5	4.66	123.85	116.12
3	A	2	SIA	O1B-C1-C2	4.57	124.59	112.71
3	C	2	SIA	O1B-C1-C2	4.57	124.59	112.71
3	A	2	SIA	C11-C10-N5	4.48	123.55	116.12
4	B	5	SIA	O1B-C1-C2	4.48	124.36	112.71
3	C	2	SIA	C11-C10-N5	4.37	123.37	116.12
3	A	2	SIA	O6-C2-C3	-4.34	104.73	110.56
4	B	5	SIA	C5-N5-C10	3.95	132.36	123.11
4	B	5	SIA	O1A-C1-C2	-3.76	114.74	122.85
3	A	2	SIA	O1A-C1-C2	-3.69	114.89	122.85
3	A	2	SIA	C5-N5-C10	3.67	131.71	123.11
4	B	4	GAL	C1-O5-C5	3.64	117.07	112.19
3	A	1	GAL	C1-O5-C5	3.63	117.05	112.19
3	C	2	SIA	C5-N5-C10	3.54	131.39	123.11
3	C	2	SIA	O1A-C1-C2	-3.42	115.46	122.85
3	C	2	SIA	C6-C5-N5	-2.81	106.43	110.91
3	A	2	SIA	C6-C5-N5	-2.66	106.66	110.91
4	B	5	SIA	C6-C5-N5	-2.42	107.04	110.91
4	B	5	SIA	O10-C10-N5	-2.36	117.81	121.98
3	A	2	SIA	O4-C4-C3	-2.22	104.32	109.86
3	A	2	SIA	O10-C10-C11	-2.19	118.15	122.05
4	B	2	GAL	O5-C5-C6	2.17	111.89	107.66
3	C	2	SIA	O10-C10-N5	-2.09	118.28	121.98
4	B	5	SIA	O10-C10-C11	-2.08	118.34	122.05
3	A	2	SIA	O10-C10-N5	-2.08	118.30	121.98
3	C	2	SIA	O10-C10-C11	-2.08	118.35	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	GAL	C1-O5-C5	2.07	114.96	112.19
3	A	1	GAL	C2-C3-C4	-2.01	107.33	110.86

There are no chirality outliers.

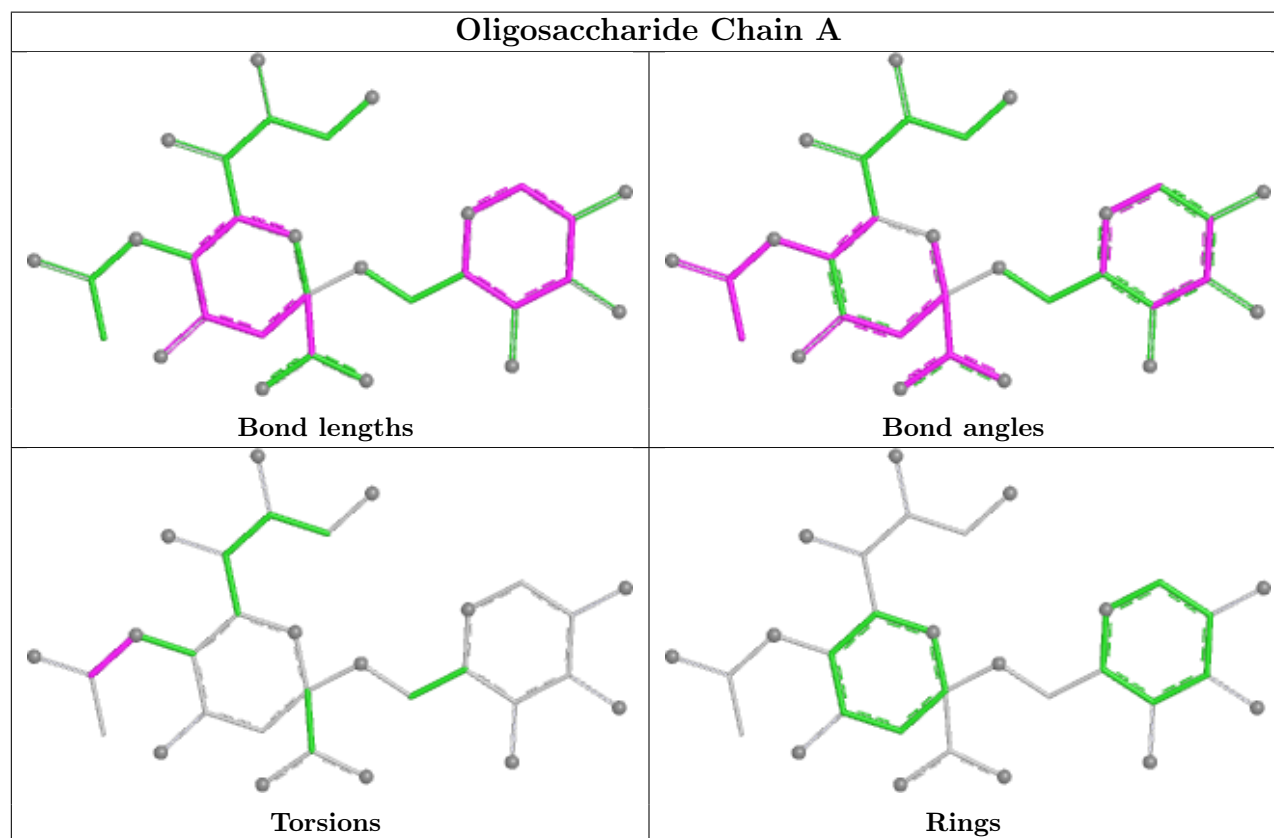
All (6) torsion outliers are listed below:

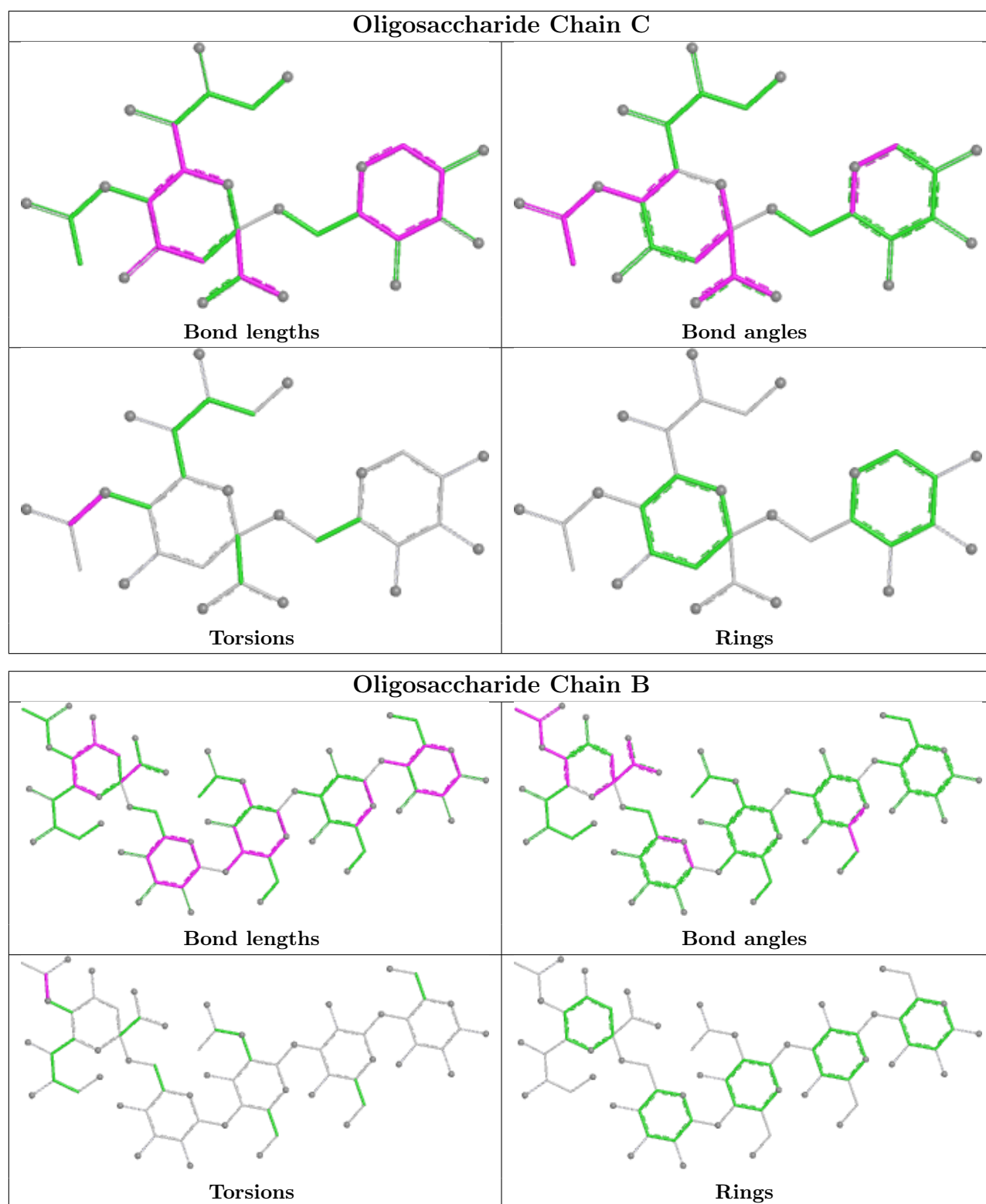
Mol	Chain	Res	Type	Atoms
3	A	2	SIA	C11-C10-N5-C5
3	A	2	SIA	O10-C10-N5-C5
3	C	2	SIA	C11-C10-N5-C5
3	C	2	SIA	O10-C10-N5-C5
4	B	5	SIA	C11-C10-N5-C5
4	B	5	SIA	O10-C10-N5-C5

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

3 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	$\# Z > 2$
5	NDG	J	740	-	15,15,15	0.45	0	21,21,21	0.72	0
5	NDG	H	742	-	15,15,15	0.44	0	21,21,21	0.81	0
5	NDG	L	744	-	15,15,15	0.50	0	21,21,21	0.80	0

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
5	NDG	J	740	-	-	6/6/26/26	0/1/1/1
5	NDG	H	742	-	-	4/6/26/26	0/1/1/1
5	NDG	L	744	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	742	NDG	C3-C2-N2-C7
5	J	740	NDG	C3-C2-N2-C7
5	L	744	NDG	C3-C2-N2-C7
5	H	742	NDG	C8-C7-N2-C2
5	J	740	NDG	C8-C7-N2-C2
5	H	742	NDG	C1-C2-N2-C7
5	J	740	NDG	O5-C5-C6-O6
5	J	740	NDG	O7-C7-N2-C2
5	H	742	NDG	O7-C7-N2-C2
5	L	744	NDG	C1-C2-N2-C7
5	J	740	NDG	C4-C5-C6-O6
5	J	740	NDG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	740	NDG	7	0
5	H	742	NDG	11	0
5	L	744	NDG	8	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.