



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:14 PM UTC

PDB ID : 3LZF / pdb_00003lzf
Title : Crystal Structure of Fab 2D1 in Complex with the 1918 Influenza Virus Hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2010-03-01
Resolution : 2.80 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:

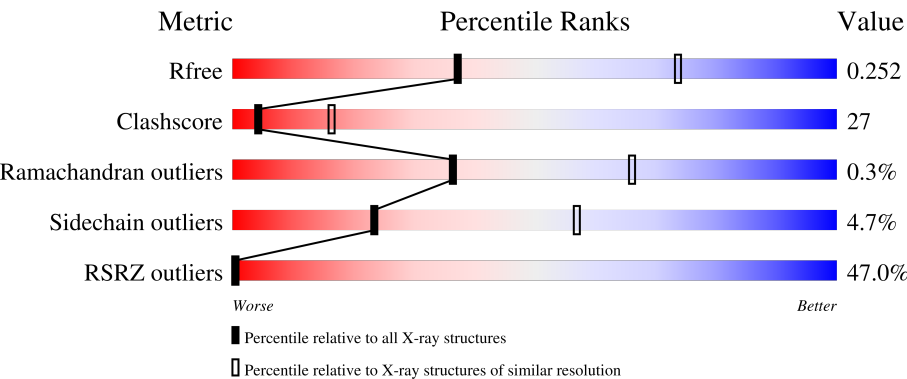
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.80 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.



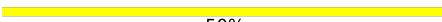
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	331	9% 64% 31% ..
2	B	179	56% 62% 32% ...
3	H	230	61% 52% 38% 6%
4	L	217	76% 64% 31% ..
5	C	2	100%

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Mol	Chain	Length	Quality of chain
5	E	2	 100%
6	D	4	 50%  50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7207 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 Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2506	1580	430	485	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9WFX3
A	8	ASP	-	expression tag	UNP Q9WFX3
A	9	PRO	-	expression tag	UNP Q9WFX3
A	10	GLY	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin, HA2 Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1391	868	239	278	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP Q9WFX3
B	178	GLY	-	expression tag	UNP Q9WFX3
B	179	ARG	-	expression tag	UNP Q9WFX3

- Molecule 3 is a protein called 2D1 Fab, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1623	1030	264	322	7			

- Molecule 4 is a protein called 2D1 Fab, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1567	982	260	321	4			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O		0	0	0
			28	16	2	10				
5	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O		0	0	0
			50	28	2	20				

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

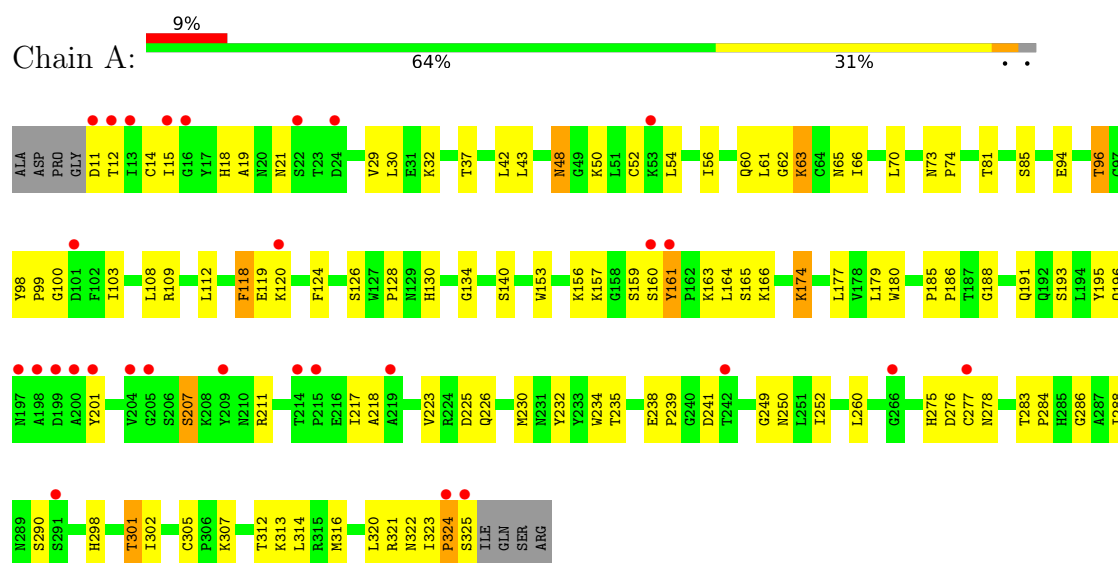


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0

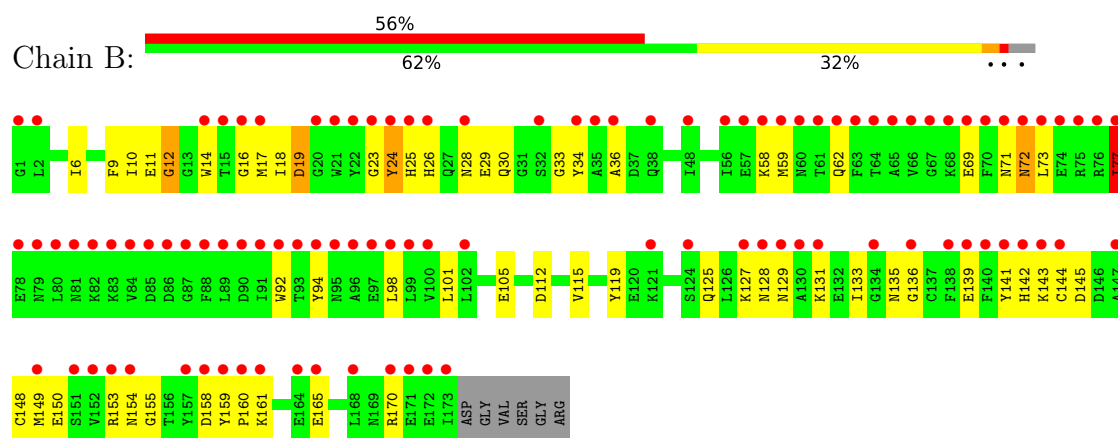
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hemagglutinin, HA1 Subunit

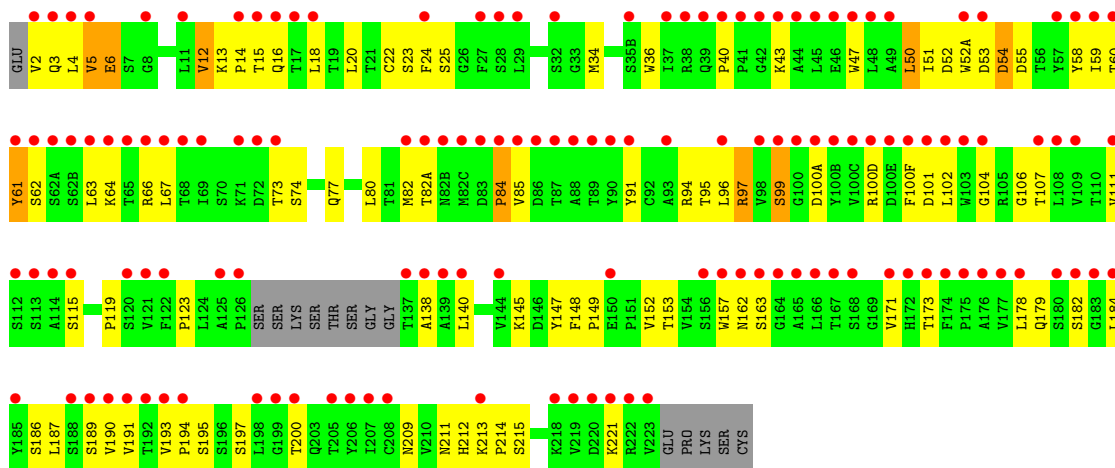


• Molecule 2: Hemagglutinin, HA2 Subunit

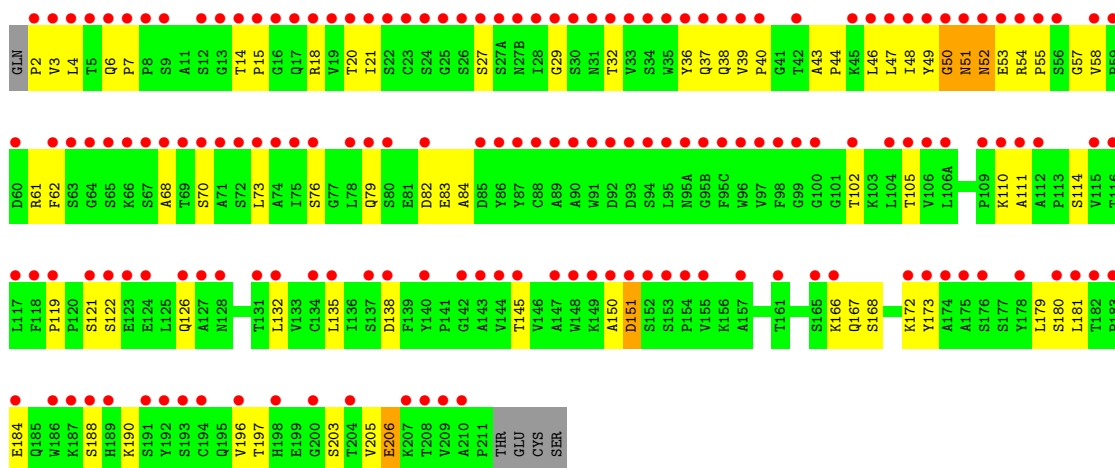
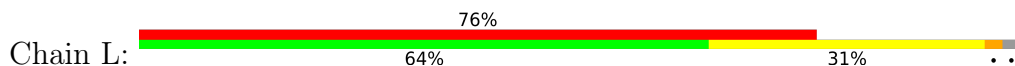


• Molecule 3: 2D1 Fab, Heavy Chain





• Molecule 4: 2D1 Fab, Light Chain



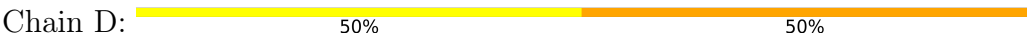
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BGLA3
MAIN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.75Å 161.75Å 143.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.69 – 2.80 49.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.69-2.80) 98.1 (49.69-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.230 , 0.259 0.226 , 0.252	Depositor DCC
R_{free} test set	2596 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7207	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	3/2570 (0.1%)	1.24	10/3501 (0.3%)
2	B	0.86	1/1418 (0.1%)	1.04	6/1909 (0.3%)
3	H	0.93	1/1660 (0.1%)	1.22	9/2274 (0.4%)
4	L	0.77	1/1608 (0.1%)	1.07	6/2199 (0.3%)
All	All	0.95	6/7256 (0.1%)	1.16	31/9883 (0.3%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	57	GLY	C-N	10.21	1.42	1.33
3	H	99	SER	C-O	5.90	1.30	1.23
1	A	11	ASP	CG-OD2	5.36	1.35	1.25
1	A	120	LYS	CE-NZ	5.20	1.65	1.49
2	B	77	ILE	CA-CB	-5.11	1.47	1.54
1	A	288	ILE	CA-CB	-5.05	1.48	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	PHE	CA-C-N	-8.76	110.71	119.90
1	A	124	PHE	C-N-CA	-8.76	110.71	119.90
4	L	150	ALA	N-CA-C	-8.50	99.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	61	TYR	N-CA-C	-8.28	103.07	113.01
2	B	127	LYS	CB-CA-C	-7.63	107.76	116.54
2	B	33	GLY	N-CA-C	6.67	119.63	110.56
1	A	211	ARG	N-CA-C	6.58	119.53	108.02
1	A	12	THR	N-CA-C	6.31	118.66	109.07
1	A	29	VAL	CB-CA-C	-6.17	103.98	111.88
4	L	51	ASN	CB-CA-C	-5.90	101.95	112.27
3	H	200	THR	N-CA-C	-5.79	106.00	114.39
1	A	207	SER	N-CA-C	-5.68	103.86	112.04
4	L	50	GLY	CA-C-N	-5.66	114.38	122.93
4	L	50	GLY	C-N-CA	-5.66	114.38	122.93
2	B	62	GLN	N-CA-C	5.66	118.53	110.10
2	B	77	ILE	CB-CG1-CD1	-5.56	102.13	113.80
2	B	12	GLY	N-CA-C	5.54	119.23	111.14
2	B	11	GLU	N-CA-C	5.50	117.99	111.33
1	A	174	LYS	CB-CA-C	-5.50	100.39	111.17
3	H	54	ASP	N-CA-C	5.46	120.44	113.18
3	H	100(A)	ASP	N-CA-C	-5.45	102.46	110.52
3	H	12	VAL	CB-CA-C	-5.44	101.23	111.30
4	L	57	GLY	O-C-N	5.26	128.44	122.55
1	A	278	ASN	N-CA-C	5.17	117.33	108.90
1	A	252	ILE	CB-CA-C	-5.17	107.44	113.22
1	A	120	LYS	CD-CE-NZ	5.14	128.34	111.90
3	H	97	ARG	CA-C-N	-5.13	116.83	123.19
3	H	97	ARG	C-N-CA	-5.13	116.83	123.19
4	L	68	ALA	CB-CA-C	-5.13	110.68	116.63
3	H	22	CYS	CA-C-N	-5.08	115.57	122.93
3	H	22	CYS	C-N-CA	-5.08	115.57	122.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2427	94	0
2	B	1391	0	1302	96	0
3	H	1623	0	1601	129	0
4	L	1567	0	1511	73	0
5	C	28	0	25	0	0
5	E	28	0	25	0	0
6	D	50	0	43	1	0
7	A	14	0	13	1	0
All	All	7207	0	6947	382	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 27.

All (382) 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)
2:B:26:HIS:HB2	2:B:149:MET:CE	1.66	1.24
3:H:6:GLU:OE1	3:H:106:GLY:HA2	1.41	1.17
2:B:133:ILE:HD12	2:B:139:GLU:HB2	1.18	1.15
2:B:26:HIS:CB	2:B:149:MET:HE2	1.78	1.12
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.07	1.11
2:B:26:HIS:CB	2:B:149:MET:CE	2.29	1.10
3:H:96:LEU:HB3	3:H:100(D):ARG:HG3	1.32	1.10
3:H:123:PRO:HG3	3:H:221:LYS:HE3	1.30	1.09
4:L:151:ASP:CB	4:L:190:LYS:HE3	1.82	1.08
4:L:151:ASP:HB3	4:L:190:LYS:CE	1.84	1.08
4:L:39:VAL:HG13	4:L:40:PRO:HD2	1.31	1.07
2:B:24:TYR:CE1	2:B:153:ARG:HG2	1.89	1.07
3:H:96:LEU:HB3	3:H:100(D):ARG:CG	1.85	1.07
3:H:96:LEU:HB3	3:H:100(D):ARG:CB	1.88	1.04
2:B:26:HIS:HB2	2:B:149:MET:HE2	1.04	1.00
2:B:141:TYR:HE1	2:B:170:ARG:CD	1.74	1.00
2:B:141:TYR:HE1	2:B:170:ARG:HD3	1.20	0.99
2:B:142:HIS:HD2	2:B:143:LYS:O	1.46	0.99
2:B:141:TYR:CE1	2:B:170:ARG:CG	2.47	0.98
4:L:51:ASN:O	4:L:52:ASN:CG	2.06	0.98
3:H:34:MET:O	3:H:52(A):TRP:HB2	1.64	0.97
3:H:54:ASP:O	3:H:55:ASP:HB2	1.65	0.97
4:L:151:ASP:OD1	4:L:190:LYS:HG2	1.64	0.97
2:B:141:TYR:CE1	2:B:170:ARG:HG3	2.00	0.95
2:B:25:HIS:HD2	2:B:34:TYR:CE2	1.84	0.95
2:B:158:ASP:OD1	2:B:160:PRO:HD2	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG23	1:A:305:CYS:SG	2.07	0.94
2:B:133:ILE:HD12	2:B:139:GLU:CB	1.95	0.94
3:H:4:LEU:HD21	3:H:24:PHE:CE1	2.02	0.94
1:A:50:LYS:HD3	1:A:275:HIS:ND1	1.83	0.94
1:A:128:PRO:O	1:A:157:LYS:NZ	2.01	0.92
1:A:323:ILE:HG22	1:A:323:ILE:O	1.70	0.92
1:A:50:LYS:CD	1:A:275:HIS:ND1	2.33	0.91
2:B:141:TYR:CE1	2:B:170:ARG:HD3	2.05	0.91
3:H:52(A):TRP:HE3	3:H:52(A):TRP:O	1.54	0.91
1:A:157:LYS:HE2	3:H:54:ASP:OD2	1.70	0.90
4:L:6:GLN:HE21	4:L:102:THR:HG23	1.38	0.89
2:B:141:TYR:CD1	2:B:170:ARG:HB2	2.07	0.89
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.55	0.89
2:B:30:GLN:NE2	2:B:145:ASP:HB2	1.87	0.89
4:L:39:VAL:CG1	4:L:40:PRO:HD2	2.03	0.88
3:H:4:LEU:CD2	3:H:24:PHE:CE1	2.57	0.87
3:H:171:VAL:HG22	3:H:191:VAL:HG22	1.55	0.87
3:H:96:LEU:HB3	3:H:100(D):ARG:HB2	1.55	0.86
4:L:151:ASP:HB3	4:L:190:LYS:HE3	0.91	0.86
4:L:50:GLY:O	4:L:51:ASN:HB2	1.74	0.85
4:L:6:GLN:NE2	4:L:102:THR:HG23	1.91	0.84
3:H:52(A):TRP:HH2	3:H:73:THR:HA	1.43	0.84
2:B:133:ILE:CG2	2:B:133:ILE:O	2.25	0.83
3:H:14:PRO:O	3:H:15:THR:OG1	1.96	0.82
2:B:158:ASP:OD2	2:B:161:LYS:HB2	1.79	0.82
3:H:6:GLU:OE1	3:H:106:GLY:CA	2.27	0.82
3:H:123:PRO:HG3	3:H:221:LYS:CE	2.09	0.82
2:B:28:ASN:ND2	2:B:149:MET:CG	2.44	0.81
4:L:48:ILE:HG23	4:L:52:ASN:HA	1.62	0.81
2:B:142:HIS:CD2	2:B:143:LYS:O	2.34	0.81
1:A:320:LEU:HD12	1:A:320:LEU:C	2.07	0.80
1:A:283:THR:CG2	1:A:284:PRO:HD2	2.12	0.79
4:L:14:THR:HG23	4:L:15:PRO:HD2	1.62	0.79
2:B:24:TYR:CD1	2:B:153:ARG:HG2	2.16	0.79
3:H:60:THR:HG21	3:H:63:LEU:HD11	1.62	0.79
4:L:37:GLN:HB2	4:L:47:LEU:CD1	2.11	0.79
4:L:7:PRO:O	4:L:102:THR:HG22	1.83	0.79
2:B:25:HIS:CD2	2:B:34:TYR:CE2	2.71	0.78
1:A:156:LYS:HD3	1:A:196:GLN:HG2	1.64	0.77
3:H:3:GLN:HG2	3:H:4:LEU:N	1.99	0.77
3:H:96:LEU:CB	3:H:100(D):ARG:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ILE:O	2:B:133:ILE:HG22	1.86	0.75
3:H:96:LEU:CB	3:H:100(D):ARG:HG3	2.16	0.75
2:B:28:ASN:HD21	2:B:149:MET:CG	1.98	0.75
3:H:67:LEU:HD21	3:H:82:MET:HE2	1.68	0.75
4:L:52:ASN:OD1	4:L:52:ASN:C	2.28	0.75
3:H:59:ILE:HG22	3:H:64:LYS:HD2	1.68	0.74
3:H:6:GLU:OE1	3:H:91:TYR:HA	1.87	0.74
2:B:141:TYR:CE1	2:B:170:ARG:CD	2.62	0.73
3:H:63:LEU:HD13	3:H:67:LEU:HD11	1.70	0.73
3:H:3:GLN:HB3	3:H:25:SER:OG	1.89	0.73
2:B:150:GLU:O	2:B:154:ASN:HB2	1.90	0.72
3:H:4:LEU:CD2	3:H:24:PHE:CZ	2.73	0.72
2:B:26:HIS:HB3	2:B:149:MET:CE	2.18	0.71
2:B:128:ASN:HB3	2:B:170:ARG:NH1	2.05	0.71
2:B:141:TYR:CE1	2:B:170:ARG:HB2	2.25	0.71
3:H:52(A):TRP:CH2	3:H:73:THR:HA	2.25	0.71
4:L:48:ILE:CG2	4:L:52:ASN:H	2.03	0.71
2:B:19:ASP:HB2	2:B:36:ALA:CB	2.20	0.70
1:A:283:THR:HG22	1:A:284:PRO:HD2	1.73	0.70
1:A:50:LYS:HD3	1:A:275:HIS:CE1	2.27	0.69
2:B:131:LYS:HE3	2:B:133:ILE:CG1	2.23	0.69
2:B:28:ASN:HD21	2:B:149:MET:HG2	1.56	0.69
2:B:24:TYR:CE1	2:B:153:ARG:CG	2.71	0.69
4:L:14:THR:CG2	4:L:15:PRO:HD2	2.21	0.69
1:A:50:LYS:HD2	1:A:275:HIS:ND1	2.09	0.68
2:B:141:TYR:CZ	2:B:170:ARG:HG3	2.29	0.67
2:B:28:ASN:ND2	2:B:149:MET:HG2	2.08	0.67
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.74	0.67
3:H:52:ASP:HB3	3:H:54:ASP:HB3	1.76	0.67
3:H:94:ARG:O	3:H:101:ASP:N	2.26	0.66
1:A:52:CYS:HG	1:A:277:CYS:CB	2.09	0.66
2:B:9:PHE:O	2:B:135:ASN:HA	1.95	0.66
2:B:59:MET:HE3	2:B:59:MET:HA	1.78	0.66
1:A:48:ASN:HB3	1:A:50:LYS:H	1.62	0.65
4:L:38:GLN:O	4:L:84:ALA:HB1	1.96	0.65
1:A:283:THR:HG22	1:A:284:PRO:CD	2.26	0.65
2:B:30:GLN:HE22	2:B:145:ASP:CB	1.98	0.64
3:H:123:PRO:CG	3:H:221:LYS:HE3	2.16	0.64
2:B:141:TYR:CE1	2:B:170:ARG:CB	2.79	0.64
4:L:51:ASN:O	4:L:52:ASN:CB	2.45	0.64
2:B:26:HIS:HB2	2:B:149:MET:HE1	1.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD21	1:A:302:ILE:HG22	1.78	0.64
3:H:213:LYS:N	3:H:214:PRO:CD	2.60	0.64
3:H:3:GLN:HG2	3:H:4:LEU:H	1.62	0.63
2:B:131:LYS:HE3	2:B:133:ILE:HD11	1.81	0.63
1:A:164:LEU:C	1:A:164:LEU:HD12	2.22	0.63
4:L:51:ASN:O	4:L:52:ASN:ND2	2.31	0.63
3:H:187:LEU:C	3:H:187:LEU:HD12	2.24	0.63
1:A:48:ASN:ND2	1:A:50:LYS:HB2	2.13	0.63
4:L:3:VAL:HG12	4:L:4:LEU:N	2.12	0.63
1:A:42:LEU:HD11	1:A:316:MET:HE3	1.81	0.62
1:A:60:GLN:HE21	1:A:62:GLY:H	1.46	0.62
3:H:4:LEU:HD21	3:H:24:PHE:CZ	2.34	0.62
4:L:55:PRO:HD2	4:L:58:VAL:HG21	1.82	0.62
3:H:47:TRP:HZ2	3:H:50:LEU:HB3	1.65	0.61
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.81	0.61
3:H:194:PRO:HG2	3:H:197:SER:OG	1.99	0.61
3:H:3:GLN:NE2	3:H:5:VAL:HG22	2.14	0.61
4:L:21:ILE:CG2	4:L:102:THR:HG21	2.30	0.61
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.36	0.61
3:H:96:LEU:CA	3:H:100(D):ARG:HB2	2.31	0.60
3:H:190:VAL:HG12	3:H:191:VAL:N	2.16	0.60
3:H:193:VAL:HB	3:H:194:PRO:HD2	1.84	0.60
2:B:133:ILE:HD11	2:B:139:GLU:OE1	2.01	0.60
2:B:26:HIS:CG	2:B:149:MET:HE2	2.35	0.60
3:H:4:LEU:HD22	3:H:24:PHE:CZ	2.35	0.59
4:L:48:ILE:HG23	4:L:52:ASN:CA	2.31	0.59
4:L:48:ILE:CG2	4:L:52:ASN:HA	2.31	0.59
3:H:13:LYS:O	3:H:16:GLN:HG3	2.02	0.59
2:B:159:TYR:N	2:B:160:PRO:CD	2.66	0.59
2:B:129:ASN:ND2	2:B:159:TYR:CD2	2.72	0.58
2:B:24:TYR:CZ	2:B:153:ARG:HG2	2.36	0.58
3:H:54:ASP:O	3:H:55:ASP:CB	2.43	0.58
3:H:59:ILE:CG2	3:H:64:LYS:HD2	2.34	0.58
3:H:67:LEU:HD21	3:H:82:MET:CE	2.33	0.58
1:A:96:THR:HG23	1:A:232:TYR:CE1	2.39	0.58
1:A:283:THR:CG2	1:A:298:HIS:HB3	2.34	0.57
1:A:65:ASN:C	1:A:65:ASN:OD1	2.47	0.57
2:B:72:ASN:C	2:B:72:ASN:HD22	2.11	0.57
6:D:1:NAG:H62	6:D:2:NAG:C1	2.35	0.57
1:A:283:THR:HG22	1:A:284:PRO:N	2.19	0.57
2:B:131:LYS:CE	2:B:133:ILE:HD11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HG	1:A:277:CYS:HB3	1.69	0.57
1:A:98:TYR:CD2	1:A:230:MET:HB2	2.40	0.57
2:B:142:HIS:HB2	2:B:165:GLU:CD	2.30	0.57
4:L:196:VAL:HG22	4:L:205:VAL:HG13	1.87	0.57
4:L:46:LEU:HG	4:L:55:PRO:HG3	1.86	0.56
3:H:34:MET:O	3:H:52(A):TRP:CB	2.48	0.56
3:H:18:LEU:HD21	3:H:20:LEU:CG	2.35	0.56
3:H:52:ASP:OD2	3:H:54:ASP:HB2	2.06	0.56
4:L:48:ILE:CG2	4:L:52:ASN:N	2.68	0.56
3:H:18:LEU:HD21	3:H:20:LEU:HG	1.87	0.56
1:A:156:LYS:HD3	1:A:196:GLN:CG	2.34	0.56
1:A:283:THR:HG23	1:A:298:HIS:HB3	1.88	0.56
3:H:3:GLN:HE22	3:H:5:VAL:HG22	1.70	0.56
3:H:36:TRP:CG	3:H:80:LEU:HD22	2.41	0.56
1:A:157:LYS:CE	3:H:54:ASP:OD2	2.50	0.55
1:A:61:LEU:HD11	1:A:66:ILE:HD13	1.88	0.55
3:H:163:SER:HA	3:H:209:ASN:OD1	2.06	0.55
4:L:48:ILE:HD12	4:L:52:ASN:HA	1.88	0.55
4:L:138:ASP:HA	4:L:172:LYS:HB3	1.87	0.55
3:H:60:THR:HG23	3:H:60:THR:O	2.06	0.55
3:H:18:LEU:HD21	3:H:20:LEU:HD11	1.89	0.55
1:A:48:ASN:ND2	1:A:52:CYS:SG	2.79	0.55
3:H:147:TYR:CE1	3:H:152:VAL:HG23	2.42	0.55
1:A:320:LEU:CD1	1:A:321:ARG:O	2.54	0.55
2:B:158:ASP:CG	2:B:161:LYS:HB2	2.31	0.55
2:B:94:TYR:CZ	2:B:98:LEU:HD22	2.42	0.55
4:L:184:GLU:O	4:L:188:SER:HB2	2.07	0.55
1:A:324:PRO:O	1:A:325:SER:C	2.50	0.54
3:H:60:THR:O	3:H:64:LYS:HD3	2.06	0.54
1:A:323:ILE:O	1:A:323:ILE:CG2	2.44	0.54
1:A:195:TYR:CE2	1:A:250:ASN:N	2.65	0.54
2:B:133:ILE:O	2:B:133:ILE:HG23	2.07	0.54
4:L:3:VAL:CG1	4:L:4:LEU:N	2.71	0.54
4:L:126:GLN:O	4:L:126:GLN:NE2	2.40	0.54
1:A:43:LEU:HB2	1:A:314:LEU:HB2	1.88	0.54
2:B:131:LYS:HE3	2:B:133:ILE:CD1	2.37	0.54
4:L:20:THR:HA	4:L:73:LEU:O	2.07	0.54
4:L:83:GLU:HG3	4:L:105:THR:HA	1.89	0.54
1:A:188:GLY:HA2	1:A:217:ILE:HD13	1.90	0.53
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.90	0.53
3:H:140:LEU:HD12	3:H:140:LEU:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:VAL:HG11	3:H:94:ARG:NH1	2.23	0.53
3:H:96:LEU:H	3:H:100(D):ARG:HB2	1.74	0.52
2:B:142:HIS:HB2	2:B:165:GLU:OE2	2.08	0.52
3:H:100(F):PHE:HB2	4:L:36:TYR:CE1	2.44	0.52
2:B:17:MET:SD	2:B:23:GLY:HA3	2.50	0.52
3:H:171:VAL:HG22	3:H:191:VAL:CG2	2.34	0.52
1:A:283:THR:CG2	1:A:298:HIS:CB	2.87	0.52
2:B:14:TRP:CH2	2:B:25:HIS:HB2	2.45	0.51
2:B:19:ASP:HB2	2:B:36:ALA:HB2	1.91	0.51
1:A:14:CYS:O	2:B:24:TYR:HA	2.09	0.51
3:H:34:MET:SD	3:H:94:ARG:CD	2.99	0.51
3:H:60:THR:C	3:H:62:SER:H	2.19	0.51
4:L:6:GLN:HB3	4:L:7:PRO:HD2	1.92	0.51
4:L:166:LYS:HE2	4:L:173:TYR:OH	2.10	0.51
1:A:283:THR:CG2	1:A:284:PRO:CD	2.84	0.51
1:A:283:THR:HG21	1:A:298:HIS:CB	2.40	0.51
1:A:238:GLU:O	1:A:239:PRO:C	2.54	0.51
3:H:6:GLU:OE2	3:H:104:GLY:HA3	2.11	0.51
3:H:14:PRO:C	3:H:15:THR:HG1	2.05	0.51
4:L:197:THR:HA	4:L:203:SER:O	2.10	0.51
2:B:24:TYR:CD1	2:B:153:ARG:CG	2.90	0.51
2:B:133:ILE:CD1	2:B:139:GLU:CD	2.84	0.51
3:H:63:LEU:HD12	3:H:63:LEU:C	2.36	0.51
1:A:159:SER:O	1:A:159:SER:OG	2.22	0.51
3:H:50:LEU:C	3:H:50:LEU:HD23	2.36	0.51
3:H:152:VAL:HG12	3:H:153:THR:N	2.24	0.51
3:H:96:LEU:N	3:H:100(D):ARG:HB2	2.26	0.50
4:L:54:ARG:HD3	4:L:62:PHE:O	2.11	0.50
1:A:99:PRO:HG3	1:A:223:VAL:O	2.12	0.50
1:A:109:ARG:HE	2:B:69:GLU:CD	2.19	0.50
3:H:60:THR:CG2	3:H:63:LEU:HD11	2.37	0.50
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.94	0.50
1:A:160:SER:HA	3:H:99:SER:OG	2.12	0.50
2:B:125:GLN:HE22	2:B:155:GLY:C	2.19	0.50
2:B:25:HIS:HD2	2:B:34:TYR:HE2	1.48	0.50
3:H:2:VAL:HG12	3:H:102:LEU:HD21	1.94	0.50
1:A:320:LEU:HD12	1:A:321:ARG:O	2.11	0.50
2:B:16:GLY:O	2:B:18:ILE:HG23	2.11	0.50
4:L:49:TYR:CE1	4:L:53:GLU:HB2	2.47	0.49
1:A:30:LEU:HD12	2:B:105:GLU:OE2	2.11	0.49
3:H:190:VAL:CG1	3:H:191:VAL:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:HD1	1:A:118:PHE:C	2.20	0.49
1:A:56:ILE:HD12	1:A:56:ILE:N	2.28	0.49
2:B:24:TYR:CD1	2:B:153:ARG:CD	2.95	0.49
3:H:60:THR:HG21	3:H:63:LEU:CD1	2.38	0.49
3:H:149:PRO:O	3:H:212:HIS:HE1	1.95	0.49
2:B:28:ASN:ND2	2:B:149:MET:HG3	2.26	0.49
1:A:118:PHE:C	1:A:118:PHE:CD1	2.91	0.49
1:A:18:HIS:CG	1:A:19:ALA:N	2.81	0.49
4:L:32:THR:HG22	4:L:51:ASN:ND2	2.27	0.49
1:A:126:SER:HB3	1:A:166:LYS:HE3	1.94	0.49
2:B:145:ASP:O	2:B:148:CYS:HB3	2.13	0.49
3:H:94:ARG:NH2	3:H:101:ASP:OD2	2.42	0.49
4:L:6:GLN:HE21	4:L:102:THR:CG2	2.19	0.49
1:A:60:GLN:NE2	1:A:62:GLY:H	2.09	0.48
3:H:18:LEU:CD2	3:H:20:LEU:HG	2.43	0.48
3:H:12:VAL:CG1	3:H:16:GLN:HB2	2.43	0.48
1:A:307:LYS:HE3	2:B:92:TRP:CD1	2.48	0.48
2:B:72:ASN:HD22	2:B:73:LEU:N	2.12	0.48
1:A:130:HIS:NE2	1:A:164:LEU:HB3	2.29	0.48
3:H:179:GLN:C	3:H:182:SER:N	2.71	0.48
4:L:6:GLN:HB3	4:L:102:THR:CG2	2.44	0.48
1:A:283:THR:HG21	1:A:298:HIS:HB2	1.95	0.48
1:A:180:TRP:HZ3	1:A:235:THR:HG22	1.78	0.47
3:H:40:PRO:HB2	3:H:43:LYS:CG	2.44	0.47
1:A:323:ILE:HG21	2:B:12:GLY:HA2	1.96	0.47
3:H:18:LEU:HD21	3:H:20:LEU:CD1	2.43	0.47
3:H:61:TYR:CE2	4:L:2:PRO:HG2	2.50	0.47
4:L:49:TYR:CD1	4:L:53:GLU:O	2.67	0.47
3:H:95:THR:HA	3:H:100(D):ARG:O	2.14	0.47
1:A:103:ILE:N	1:A:103:ILE:HD12	2.29	0.47
1:A:15:ILE:N	1:A:15:ILE:HD12	2.30	0.47
1:A:179:LEU:N	1:A:179:LEU:HD12	2.30	0.47
3:H:34:MET:HA	3:H:95:THR:O	2.14	0.47
4:L:18:ARG:HG2	4:L:76:SER:HA	1.96	0.47
3:H:73:THR:HG23	3:H:74:SER:N	2.29	0.47
3:H:145:LYS:HA	3:H:186:SER:OG	2.15	0.47
4:L:184:GLU:OE1	4:L:184:GLU:N	2.45	0.47
1:A:156:LYS:HE2	1:A:193:SER:O	2.15	0.47
1:A:322:ASN:O	1:A:324:PRO:HD3	2.15	0.46
3:H:212:HIS:HD2	3:H:215:SER:OG	1.97	0.46
4:L:119:PRO:HA	4:L:132:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:23:SER:OG	3:H:77:GLN:HG2	2.15	0.46
1:A:161:TYR:HD2	1:A:161:TYR:O	1.99	0.46
3:H:13:LYS:HB2	3:H:16:GLN:HG3	1.98	0.46
4:L:54:ARG:HB3	4:L:58:VAL:HB	1.97	0.46
1:A:301:THR:CG2	1:A:305:CYS:SG	2.94	0.46
4:L:167:GLN:HG2	4:L:168:SER:N	2.30	0.46
1:A:320:LEU:HD12	1:A:321:ARG:N	2.30	0.46
3:H:34:MET:CG	3:H:52(A):TRP:HD1	2.28	0.46
4:L:52:ASN:OD1	4:L:53:GLU:N	2.49	0.46
2:B:141:TYR:HE1	2:B:170:ARG:CG	1.98	0.46
3:H:50:LEU:HD22	3:H:58:TYR:HD2	1.81	0.45
4:L:179:LEU:HD21	4:L:181:LEU:HD21	1.98	0.45
2:B:73:LEU:HD23	2:B:73:LEU:HA	1.75	0.45
1:A:320:LEU:HD12	1:A:321:ARG:C	2.41	0.45
2:B:6:ILE:HG13	2:B:112:ASP:HA	1.98	0.45
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.51	0.45
3:H:52(A):TRP:HH2	3:H:73:THR:CA	2.21	0.45
3:H:60:THR:C	3:H:62:SER:N	2.74	0.45
3:H:148:PHE:HB2	3:H:184:LEU:HD23	1.99	0.45
1:A:126:SER:O	1:A:166:LYS:NZ	2.46	0.45
4:L:61:ARG:HD2	4:L:76:SER:O	2.17	0.45
2:B:133:ILE:CD1	2:B:139:GLU:OE1	2.63	0.44
3:H:13:LYS:H	3:H:16:GLN:HE21	1.65	0.44
3:H:60:THR:CG2	3:H:63:LEU:CD1	2.94	0.44
3:H:157:TRP:O	3:H:162:ASN:C	2.59	0.44
2:B:131:LYS:HE3	2:B:133:ILE:HG13	1.98	0.44
3:H:6:GLU:H	3:H:6:GLU:HG2	1.30	0.44
1:A:37:THR:HG23	1:A:320:LEU:O	2.17	0.44
2:B:145:ASP:H	2:B:148:CYS:HB3	1.83	0.44
3:H:52(A):TRP:HE3	3:H:52(A):TRP:C	2.20	0.44
1:A:207:SER:HB2	1:A:241:ASP:OD1	2.17	0.44
2:B:28:ASN:O	2:B:29:GLU:C	2.61	0.44
3:H:52:ASP:CG	3:H:97:ARG:HH22	2.26	0.44
1:A:108:LEU:HB2	1:A:234:TRP:CE2	2.53	0.44
4:L:39:VAL:CG1	4:L:40:PRO:CD	2.86	0.44
3:H:6:GLU:CD	3:H:106:GLY:H	2.26	0.44
1:A:21:ASN:OD1	1:A:21:ASN:C	2.60	0.43
1:A:195:TYR:CD2	1:A:250:ASN:N	2.68	0.43
3:H:34:MET:HB2	3:H:95:THR:O	2.17	0.43
4:L:50:GLY:O	4:L:51:ASN:C	2.53	0.43
4:L:55:PRO:HD2	4:L:58:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD12	1:A:164:LEU:O	2.16	0.43
3:H:152:VAL:CG1	3:H:153:THR:N	2.80	0.43
3:H:190:VAL:HG21	4:L:135:LEU:HD12	1.99	0.43
1:A:225:ASP:O	1:A:226:GLN:NE2	2.50	0.43
1:A:283:THR:HB	1:A:286:GLY:O	2.18	0.43
2:B:131:LYS:HG3	2:B:133:ILE:HG13	2.00	0.43
1:A:163:LYS:HE3	1:A:201:TYR:OH	2.17	0.43
3:H:173:THR:HA	3:H:189:SER:HA	2.01	0.43
3:H:63:LEU:HD13	3:H:67:LEU:CD1	2.45	0.43
3:H:179:GLN:C	3:H:182:SER:H	2.24	0.43
4:L:39:VAL:O	4:L:40:PRO:C	2.61	0.43
1:A:100:GLY:HA3	1:A:230:MET:O	2.19	0.43
1:A:320:LEU:C	1:A:320:LEU:CD1	2.80	0.43
4:L:18:ARG:CG	4:L:76:SER:HA	2.49	0.42
4:L:48:ILE:HG22	4:L:52:ASN:H	1.80	0.42
1:A:177:LEU:HG	1:A:179:LEU:HD11	2.01	0.42
4:L:14:THR:CG2	4:L:15:PRO:CD	2.95	0.42
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.35	0.42
4:L:43:ALA:HA	4:L:44:PRO:HD3	1.93	0.42
3:H:34:MET:SD	3:H:94:ARG:HD3	2.59	0.42
1:A:18:HIS:CG	1:A:19:ALA:H	2.37	0.42
4:L:166:LYS:HE2	4:L:173:TYR:CZ	2.54	0.42
1:A:177:LEU:HB2	1:A:260:LEU:HD11	2.01	0.42
3:H:148:PHE:HB2	3:H:184:LEU:CD2	2.49	0.42
4:L:48:ILE:HG23	4:L:52:ASN:N	2.34	0.42
1:A:186:PRO:HA	1:A:218:ALA:O	2.20	0.42
2:B:26:HIS:HB3	2:B:149:MET:HE3	1.97	0.42
2:B:59:MET:HE3	2:B:59:MET:CA	2.42	0.42
3:H:96:LEU:CB	3:H:100(D):ARG:CB	2.72	0.42
3:H:193:VAL:CB	3:H:194:PRO:HD2	2.47	0.42
1:A:70:LEU:HD12	1:A:108:LEU:HD21	2.02	0.42
3:H:138:ALA:N	3:H:193:VAL:O	2.51	0.42
1:A:301:THR:HG21	1:A:305:CYS:HB2	2.02	0.41
3:H:61:TYR:CD1	3:H:61:TYR:N	2.88	0.41
1:A:119:GLU:OE1	1:A:174:LYS:NZ	2.51	0.41
3:H:66:ARG:HD2	3:H:82(A):THR:O	2.20	0.41
4:L:37:GLN:HB2	4:L:47:LEU:HD12	1.97	0.41
4:L:121:SER:O	4:L:122:SER:C	2.63	0.41
2:B:159:TYR:CD1	2:B:159:TYR:C	2.99	0.41
2:B:71:ASN:OD1	2:B:71:ASN:C	2.62	0.41
4:L:79:GLN:O	4:L:82:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:152:VAL:HG13	3:H:211:ASN:O	2.19	0.41
2:B:28:ASN:OD1	2:B:144:CYS:O	2.39	0.41
3:H:84:PRO:HA	3:H:111:VAL:HB	2.02	0.41
2:B:14:TRP:C	2:B:16:GLY:N	2.78	0.41
3:H:6:GLU:CD	3:H:106:GLY:HA2	2.34	0.41
4:L:52:ASN:OD1	4:L:53:GLU:OE2	2.37	0.41
4:L:110:LYS:HG2	4:L:111:ALA:N	2.35	0.41
2:B:26:HIS:CB	2:B:149:MET:HE1	2.36	0.41
2:B:26:HIS:CB	2:B:149:MET:HE3	2.39	0.41
2:B:77:ILE:HG21	2:B:77:ILE:HD13	1.63	0.41
2:B:142:HIS:NE2	2:B:144:CYS:HB2	2.36	0.41
3:H:13:LYS:H	3:H:16:GLN:NE2	2.18	0.41
3:H:40:PRO:HB2	3:H:43:LYS:HB2	2.03	0.41
4:L:27:SER:HA	4:L:29:GLY:HA3	2.03	0.41
3:H:50:LEU:HD23	3:H:51:ILE:N	2.36	0.40
3:H:145:LYS:HG3	3:H:186:SER:OG	2.21	0.40
3:H:187:LEU:C	3:H:187:LEU:CD1	2.92	0.40
2:B:58:LYS:HA	2:B:58:LYS:HD3	1.82	0.40
1:A:63:LYS:O	1:A:63:LYS:HG2	2.21	0.40
3:H:60:THR:O	3:H:60:THR:CG2	2.69	0.40
3:H:60:THR:CG2	3:H:62:SER:HB3	2.51	0.40
1:A:21:ASN:ND2	7:A:401:NAG:C7	2.83	0.40
2:B:72:ASN:C	2:B:72:ASN:ND2	2.80	0.40
3:H:12:VAL:O	3:H:111:VAL:HA	2.22	0.40
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.93	0.40
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.57	0.40
3:H:52(A):TRP:O	3:H:52(A):TRP:CE3	2.47	0.40
4:L:205:VAL:HG22	4:L:206:GLU:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/331 (97%)	292 (91%)	27 (8%)	2 (1%)	21	51
2	B	171/179 (96%)	159 (93%)	12 (7%)	0	100	100
3	H	212/230 (92%)	199 (94%)	13 (6%)	0	100	100
4	L	210/217 (97%)	193 (92%)	16 (8%)	1 (0%)	24	55
All	All	914/957 (96%)	843 (92%)	68 (7%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
4	L	52	ASN
1	A	324	PRO

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	A	279/285 (98%)	264 (95%)	15 (5%)	20	51
2	B	147/152 (97%)	141 (96%)	6 (4%)	27	62
3	H	188/204 (92%)	178 (95%)	10 (5%)	20	52
4	L	176/181 (97%)	170 (97%)	6 (3%)	32	68
All	All	790/822 (96%)	753 (95%)	37 (5%)	23	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	63	LYS
1	A	81	THR
1	A	85	SER
1	A	94	GLU
1	A	96	THR
1	A	112	LEU
1	A	118	PHE

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Mol	Chain	Res	Type
1	A	140	SER
1	A	161	TYR
1	A	165	SER
1	A	290	SER
1	A	301	THR
1	A	312	THR
1	A	313	LYS
2	B	19	ASP
2	B	24	TYR
2	B	72	ASN
2	B	77	ILE
2	B	101	LEU
2	B	115	VAL
3	H	5	VAL
3	H	6	GLU
3	H	50	LEU
3	H	53	ASP
3	H	84	PRO
3	H	85	VAL
3	H	107	THR
3	H	115	SER
3	H	178	LEU
3	H	195	SER
4	L	70	SER
4	L	114	SER
4	L	145	THR
4	L	151	ASP
4	L	180	SER
4	L	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	60	GLN
1	A	92	ASN
1	A	192	GLN
1	A	226	GLN
2	B	25	HIS
2	B	28	ASN
2	B	30	GLN
2	B	42	GLN

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Mol	Chain	Res	Type
2	B	62	GLN
2	B	72	ASN
2	B	125	GLN
2	B	135	ASN
2	B	142	HIS
3	H	3	GLN
3	H	16	GLN
3	H	212	HIS

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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	1	1,5	14,14,15	0.51	0	17,19,21	1.33	4 (23%)
5	NAG	C	2	5	14,14,15	0.67	0	17,19,21	1.83	4 (23%)
6	NAG	D	1	1,6	14,14,15	0.91	1 (7%)	17,19,21	1.55	3 (17%)
6	NAG	D	2	6	14,14,15	0.62	0	17,19,21	2.13	5 (29%)
6	BMA	D	3	6	11,11,12	0.69	0	15,15,17	1.60	1 (6%)
6	MAN	D	4	6	11,11,12	0.57	0	15,15,17	1.24	2 (13%)
5	NAG	E	1	1,5	14,14,15	0.63	0	17,19,21	1.94	3 (17%)
5	NAG	E	2	5	14,14,15	0.76	1 (7%)	17,19,21	1.37	3 (17%)

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	NAG	C	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	0/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	NAG	C1-C2	2.33	1.55	1.52
6	D	1	NAG	O5-C1	-2.21	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	NAG	C1-O5-C5	5.97	120.19	112.19
5	E	1	NAG	O5-C1-C2	-5.51	102.76	111.29
6	D	3	BMA	O5-C5-C6	4.50	116.42	107.66
5	E	1	NAG	C3-C4-C5	3.75	117.03	110.23
5	C	2	NAG	O5-C5-C6	3.60	114.66	107.66
5	C	2	NAG	O5-C1-C2	3.29	116.38	111.29
5	E	2	NAG	C1-O5-C5	-3.09	108.05	112.19
5	C	1	NAG	C4-C3-C2	3.05	115.48	111.02
5	C	2	NAG	C1-C2-N2	-3.03	105.67	110.43
6	D	1	NAG	O6-C6-C5	-2.99	101.16	111.33
6	D	2	NAG	O5-C1-C2	2.78	115.59	111.29
5	C	1	NAG	C3-C4-C5	2.66	115.06	110.23
6	D	1	NAG	C1-O5-C5	2.65	115.73	112.19
5	E	2	NAG	C1-C2-N2	2.52	114.41	110.43
6	D	2	NAG	C2-N2-C7	-2.52	119.52	122.90
6	D	1	NAG	O3-C3-C4	-2.51	104.46	110.38
5	E	2	NAG	O5-C5-C6	2.38	112.30	107.66
5	C	2	NAG	O5-C5-C4	-2.37	105.07	110.83
5	C	1	NAG	C2-N2-C7	-2.26	119.87	122.90
5	C	1	NAG	O5-C5-C6	2.19	111.93	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	NAG	C1-C2-N2	-2.19	106.98	110.43
5	E	1	NAG	C6-C5-C4	-2.13	107.79	113.02
6	D	4	MAN	C1-C2-C3	-2.12	106.56	109.64
6	D	4	MAN	O5-C5-C6	2.05	111.66	107.66
6	D	2	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

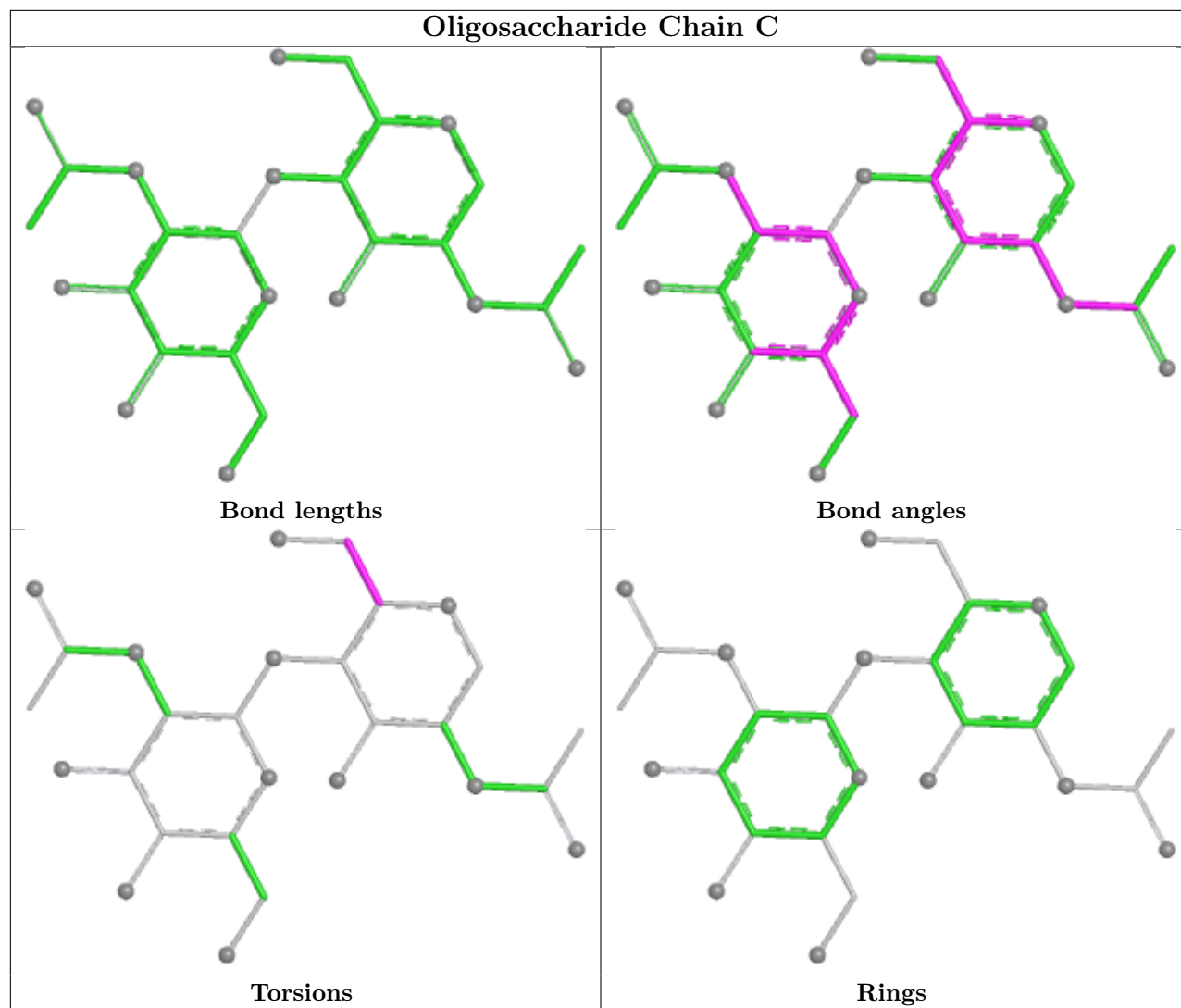
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6

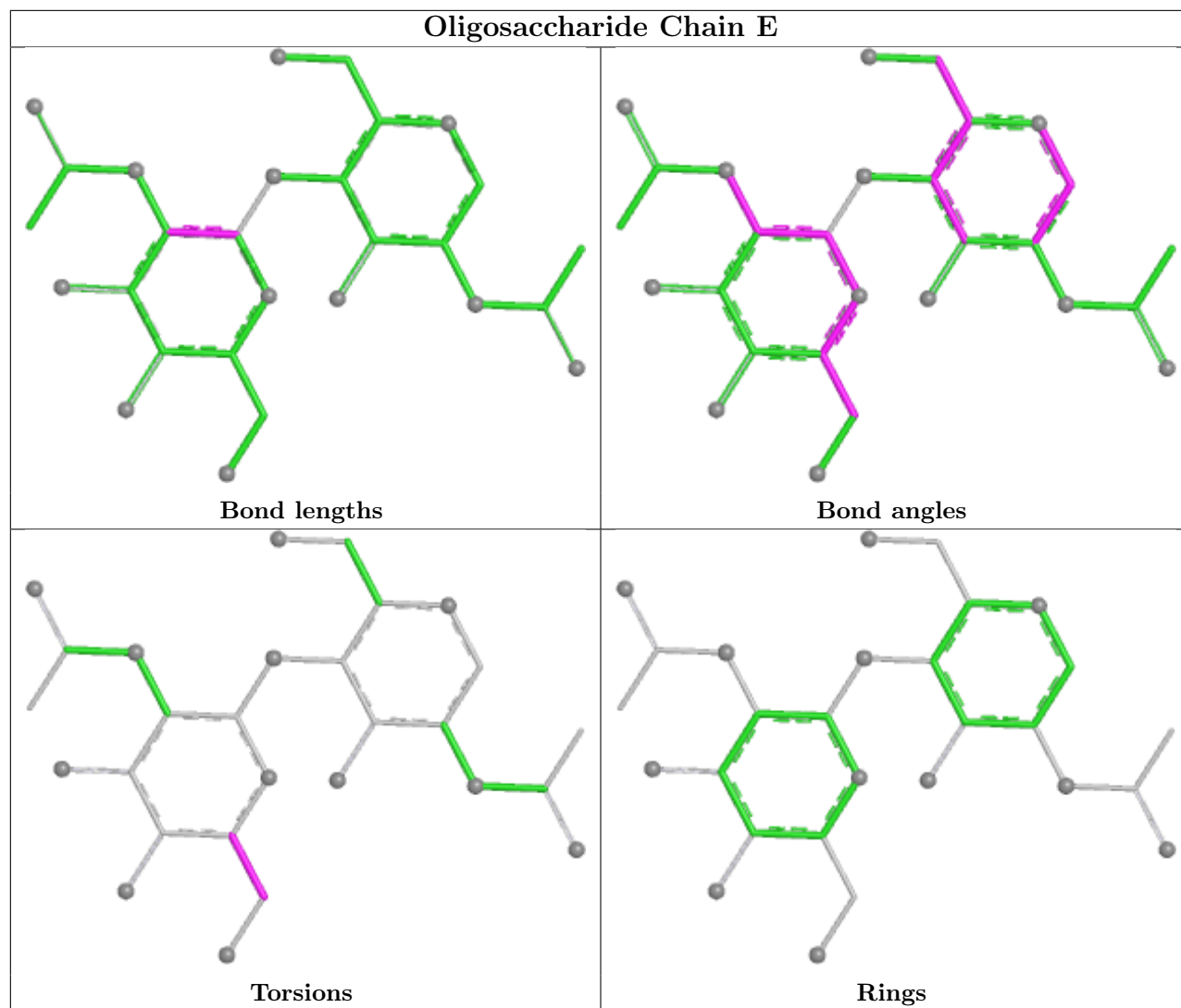
There are no ring outliers.

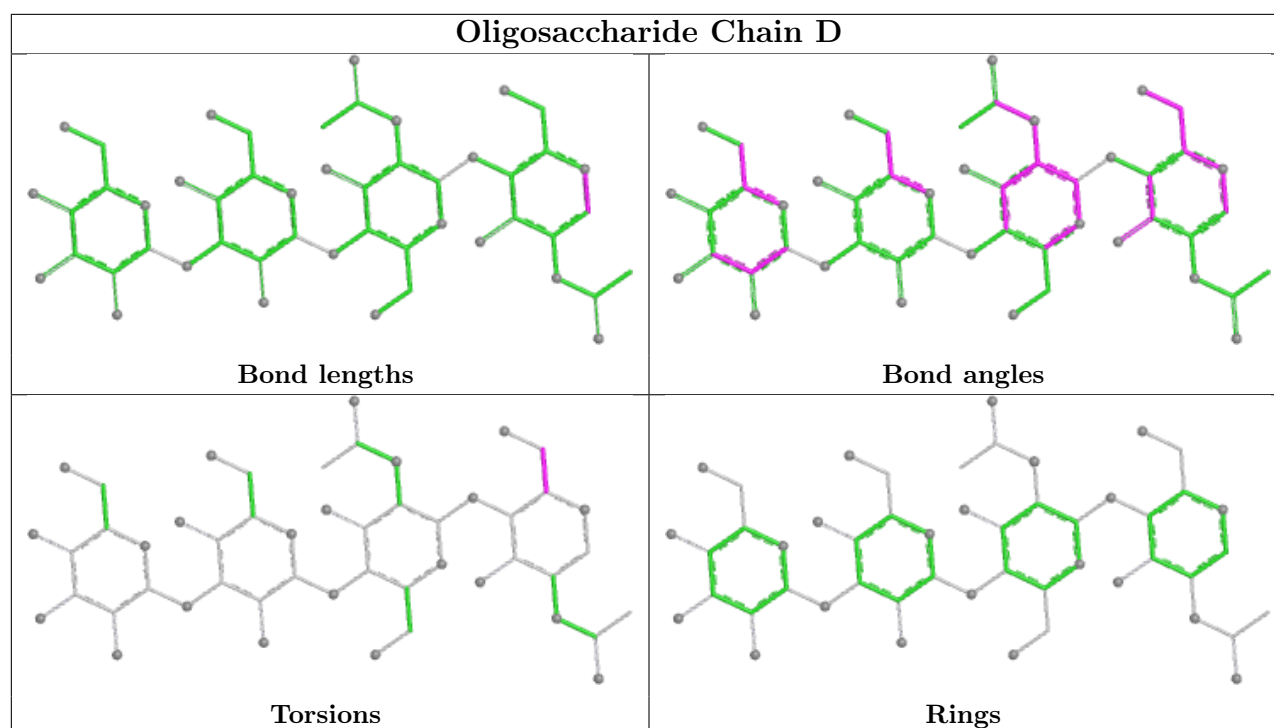
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2	NAG	1	0
6	D	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
7	NAG	A	401	1	14,14,15	0.65	0	17,19,21	1.50	2 (11%)

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
7	NAG	A	401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	NAG	C4-C3-C2	-3.54	105.83	111.02
7	A	401	NAG	C1-O5-C5	2.96	116.16	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	NAG	1	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	A	323/331 (97%)	0.87	29 (8%) 15 11	68, 80, 91, 101	0
2	B	173/179 (96%)	2.82	100 (57%) 0 0	68, 82, 92, 105	0
3	H	216/230 (93%)	2.62	140 (64%) 0 0	58, 82, 95, 108	1 (0%)
4	L	212/217 (97%)	3.61	165 (77%) 0 0	71, 83, 90, 97	0
All	All	924/957 (96%)	2.27	434 (46%) 0 0	58, 81, 92, 108	1 (0%)

All (434) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	2	PRO	13.6
4	L	95(B)	GLY	9.7
4	L	93	ASP	9.3
2	B	72	ASN	9.2
2	B	70	PHE	8.9
4	L	91	TRP	8.8
4	L	68	ALA	8.7
1	A	11	ASP	8.5
2	B	68	LYS	8.5
4	L	33	VAL	8.1
4	L	95(C)	PHE	8.0
2	B	73	LEU	7.8
4	L	27	SER	7.7
2	B	69	GLU	7.7
4	L	96	TRP	7.7
2	B	65	ALA	7.7
2	B	67	GLY	7.7
2	B	140	PHE	7.4
3	H	139	ALA	7.4
3	H	138	ALA	7.4
4	L	90	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
4	L	3	VAL	7.3
3	H	100(B)	TYR	7.3
4	L	32	THR	7.3
3	H	44	ALA	7.3
3	H	64	LYS	7.3
2	B	77	ILE	7.3
2	B	76	ARG	7.2
2	B	66	VAL	7.2
4	L	89	ALA	7.1
4	L	97	VAL	7.0
4	L	30	SER	7.0
4	L	34	SER	6.9
4	L	65	SER	6.9
4	L	193	SER	6.9
4	L	66	LYS	6.9
2	B	81	ASN	6.8
2	B	62	GLN	6.7
2	B	71	ASN	6.7
4	L	4	LEU	6.6
2	B	80	LEU	6.5
4	L	150	ALA	6.5
2	B	75	ARG	6.5
1	A	12	THR	6.4
4	L	71	ALA	6.4
2	B	86	ASP	6.2
4	L	31	ASN	6.2
2	B	78	GLU	6.1
4	L	99	GLY	6.1
4	L	95(A)	ASN	6.1
4	L	50	GLY	6.1
4	L	73	LEU	6.1
4	L	35	TRP	6.1
2	B	74	GLU	6.0
4	L	98	PHE	5.9
4	L	92	ASP	5.9
2	B	63	PHE	5.8
4	L	95	LEU	5.7
2	B	83	LYS	5.7
4	L	153	SER	5.7
4	L	194	CYS	5.7
4	L	28	ILE	5.7
4	L	88	CYS	5.7

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Mol	Chain	Res	Type	RSRZ
2	B	79	ASN	5.6
4	L	18	ARG	5.6
4	L	51	ASN	5.6
2	B	85	ASP	5.5
3	H	192	THR	5.5
2	B	93	THR	5.4
4	L	94	SER	5.4
2	B	141	TYR	5.4
4	L	46	LEU	5.4
3	H	61	TYR	5.3
4	L	100	GLY	5.3
4	L	186	TRP	5.3
4	L	21	ILE	5.2
4	L	47	LEU	5.2
2	B	84	VAL	5.2
4	L	180	SER	5.2
3	H	100	GLY	5.2
4	L	8	PRO	5.2
2	B	82	LYS	5.1
4	L	72	SER	5.1
4	L	209	VAL	5.1
2	B	61	THR	5.1
2	B	138	PHE	5.1
4	L	48	ILE	5.1
3	H	37	ILE	5.0
4	L	87	TYR	5.0
2	B	92	TRP	5.0
2	B	143	LYS	5.0
2	B	91	ILE	4.9
4	L	13	GLY	4.9
4	L	152	SER	4.9
4	L	148	TRP	4.9
4	L	69	THR	4.8
2	B	88	PHE	4.8
2	B	164	GLU	4.8
4	L	191	SER	4.8
4	L	70	SER	4.8
3	H	191	VAL	4.7
4	L	12	SER	4.7
4	L	26	SER	4.7
2	B	87	GLY	4.7
4	L	144	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
3	H	62(A)	SER	4.7
3	H	100(D)	ARG	4.7
4	L	149	LYS	4.6
4	L	122	SER	4.6
2	B	89	LEU	4.5
1	A	16	GLY	4.5
4	L	53	GLU	4.5
3	H	63	LEU	4.5
4	L	27(A)	SER	4.5
4	L	27(B)	ASN	4.5
4	L	67	SER	4.5
4	L	6	GLN	4.5
3	H	43	LYS	4.4
4	L	36	TYR	4.4
4	L	192	TYR	4.4
2	B	94	TYR	4.4
2	B	64	THR	4.4
3	H	165	ALA	4.4
4	L	154	PRO	4.4
2	B	157	TYR	4.4
4	L	62	PHE	4.4
3	H	60	THR	4.4
4	L	24	SER	4.3
2	B	90	ASP	4.3
2	B	35	ALA	4.2
3	H	100(F)	PHE	4.2
4	L	52	ASN	4.2
3	H	58	TYR	4.2
2	B	97	GLU	4.1
3	H	47	TRP	4.1
3	H	126	PRO	4.1
3	H	3	GLN	4.1
4	L	82	ASP	4.0
4	L	49	TYR	4.0
4	L	29	GLY	4.0
4	L	178	TYR	4.0
4	L	126	GLN	4.0
4	L	132	LEU	3.9
4	L	75	ILE	3.9
4	L	134	CYS	3.9
4	L	64	GLY	3.9
3	H	28	SER	3.9

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Mol	Chain	Res	Type	RSRZ
4	L	5	THR	3.9
3	H	40	PRO	3.9
3	H	100(A)	ASP	3.8
3	H	62	SER	3.8
3	H	46	GLU	3.8
4	L	23	CYS	3.8
3	H	41	PRO	3.8
1	A	199	ASP	3.8
3	H	111	VAL	3.8
4	L	60	ASP	3.8
3	H	59	ILE	3.8
2	B	60	ASN	3.8
3	H	183	GLY	3.8
4	L	118	PHE	3.8
3	H	102	LEU	3.7
4	L	128	ASN	3.7
3	H	38	ARG	3.7
3	H	193	VAL	3.7
3	H	90	TYR	3.7
3	H	91	TYR	3.7
4	L	7	PRO	3.7
3	H	82(B)	ASN	3.7
3	H	65	THR	3.7
4	L	110	LYS	3.7
3	H	207	ILE	3.7
4	L	15	PRO	3.7
2	B	96	ALA	3.7
3	H	100(E)	ASP	3.7
2	B	95	ASN	3.6
3	H	96	LEU	3.6
4	L	181	LEU	3.6
4	L	166	LYS	3.6
3	H	100(C)	VAL	3.6
4	L	116	THR	3.6
2	B	173	ILE	3.6
3	H	62(B)	SER	3.6
2	B	59	MET	3.5
3	H	221	LYS	3.5
3	H	137	THR	3.5
2	B	165	GLU	3.5
3	H	48	LEU	3.5
3	H	166	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
4	L	105	THR	3.5
4	L	157	ALA	3.5
1	A	15	ILE	3.5
2	B	136	GLY	3.5
3	H	168	SER	3.5
4	L	188	SER	3.5
3	H	29	LEU	3.4
2	B	153	ARG	3.4
4	L	22	SER	3.4
4	L	55	PRO	3.4
2	B	142	HIS	3.4
2	B	22	TYR	3.4
3	H	82(A)	THR	3.4
2	B	98	LEU	3.4
3	H	84	PRO	3.4
3	H	17	THR	3.4
4	L	25	GLY	3.4
3	H	87	THR	3.4
3	H	219	VAL	3.4
4	L	155	VAL	3.4
4	L	123	GLU	3.4
3	H	52(A)	TRP	3.4
3	H	103	TRP	3.3
3	H	205	THR	3.3
4	L	63	SER	3.3
3	H	198	LEU	3.3
4	L	106(A)	LEU	3.3
3	H	39	GLN	3.3
4	L	207	LYS	3.3
3	H	176	ALA	3.3
4	L	59	PRO	3.2
3	H	162	ASN	3.2
3	H	190	VAL	3.2
3	H	223	VAL	3.2
4	L	131	THR	3.2
4	L	76	SER	3.2
3	H	99	SER	3.2
3	H	180	SER	3.2
2	B	144	CYS	3.1
3	H	86	ASP	3.1
3	H	125	ALA	3.1
3	H	15	THR	3.1

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Mol	Chain	Res	Type	RSRZ
4	L	182	THR	3.1
3	H	45	LEU	3.1
3	H	220	ASP	3.1
4	L	142	GLY	3.1
3	H	27	PHE	3.1
4	L	42	THR	3.1
2	B	124	SER	3.1
3	H	164	GLY	3.1
4	L	45	LYS	3.1
4	L	210	ALA	3.0
4	L	37	GLN	3.0
3	H	14	PRO	3.0
2	B	168	LEU	3.0
3	H	67	LEU	3.0
3	H	173	THR	3.0
3	H	88	ALA	3.0
3	H	5	VAL	3.0
3	H	42	GLY	3.0
3	H	189	SER	3.0
2	B	172	GLU	3.0
3	H	85	VAL	3.0
4	L	121	SER	3.0
4	L	143	ALA	3.0
3	H	49	ALA	2.9
3	H	177	VAL	2.9
3	H	140	LEU	2.9
4	L	79	GLN	2.9
4	L	119	PRO	2.9
2	B	28	ASN	2.9
2	B	158	ASP	2.9
3	H	218	LYS	2.9
3	H	206	TYR	2.9
3	H	112	SER	2.9
3	H	115	SER	2.9
3	H	178	LEU	2.9
3	H	2	VAL	2.9
4	L	78	LEU	2.9
3	H	101	ASP	2.8
3	H	156	SER	2.8
3	H	163	SER	2.8
3	H	188	SER	2.8
4	L	16	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	147	ALA	2.8
2	B	171	GLU	2.8
2	B	102	LEU	2.8
4	L	208	THR	2.8
3	H	16	GLN	2.7
3	H	122	PHE	2.7
3	H	174	PHE	2.7
3	H	184	LEU	2.7
2	B	160	PRO	2.7
3	H	98	VAL	2.7
4	L	115	VAL	2.7
4	L	112	ALA	2.7
3	H	57	TYR	2.7
4	L	187	LYS	2.7
3	H	200	THR	2.7
3	H	68	THR	2.7
4	L	109	PRO	2.7
3	H	72	ASP	2.7
4	L	124	GLU	2.7
1	A	160	SER	2.7
4	L	117	LEU	2.7
2	B	16	GLY	2.6
4	L	20	THR	2.6
3	H	108	LEU	2.6
4	L	127	ALA	2.6
3	H	222	ARG	2.6
2	B	99	LEU	2.6
3	H	144	VAL	2.6
4	L	106	VAL	2.6
2	B	56	ILE	2.6
3	H	93	ALA	2.6
4	L	86	TYR	2.6
2	B	127	LYS	2.6
4	L	58	VAL	2.6
4	L	17	GLN	2.6
3	H	24	PHE	2.6
1	A	22	SER	2.6
4	L	196	VAL	2.6
4	L	176	SER	2.5
4	L	14	THR	2.5
1	A	277	CYS	2.5
1	A	219	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	L	198	HIS	2.5
2	B	161	LYS	2.5
2	B	23	GLY	2.5
1	A	325	SER	2.5
3	H	113	SER	2.5
3	H	18	LEU	2.5
3	H	194	PRO	2.5
1	A	13	ILE	2.5
1	A	209	TYR	2.5
2	B	139	GLU	2.5
2	B	26	HIS	2.5
4	L	54	ARG	2.5
3	H	175	PRO	2.4
3	H	66	ARG	2.4
2	B	58	LYS	2.4
3	H	185	TYR	2.4
4	L	140	TYR	2.4
3	H	89	THR	2.4
4	L	102	THR	2.4
4	L	189	HIS	2.4
4	L	165	SER	2.4
2	B	121	LYS	2.4
1	A	161	TYR	2.4
3	H	107	THR	2.4
2	B	57	GLU	2.4
4	L	56	SER	2.4
4	L	137	SER	2.4
2	B	130	ALA	2.4
2	B	24	TYR	2.4
2	B	154	ASN	2.4
4	L	40	PRO	2.4
3	H	182	SER	2.4
3	H	172	HIS	2.4
1	A	215	PRO	2.4
1	A	197	ASN	2.3
2	B	20	GLY	2.3
1	A	24	ASP	2.3
3	H	157	TRP	2.3
4	L	183	PRO	2.3
3	H	8	GLY	2.3
2	B	2	LEU	2.3
2	B	15	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	H	73	THR	2.3
2	B	170	ARG	2.3
2	B	129	ASN	2.3
3	H	82	MET	2.3
2	B	21	TRP	2.3
2	B	100	VAL	2.3
2	B	152	VAL	2.3
3	H	171	VAL	2.3
1	A	198	ALA	2.3
2	B	38	GLN	2.3
1	A	53	LYS	2.3
2	B	14	TRP	2.3
1	A	324	PRO	2.3
1	A	266	GLY	2.3
2	B	131	LYS	2.2
4	L	172	LYS	2.2
4	L	85	ASP	2.2
4	L	151	ASP	2.2
3	H	208	CYS	2.2
3	H	109	VAL	2.2
4	L	19	VAL	2.2
2	B	34	TYR	2.2
3	H	199	GLY	2.2
4	L	184	GLU	2.2
1	A	120	LYS	2.2
4	L	138	ASP	2.2
4	L	161	THR	2.2
1	A	201	TYR	2.2
2	B	32	SER	2.2
2	B	159	TYR	2.2
3	H	213	LYS	2.2
3	H	53	ASP	2.2
3	H	121	VAL	2.2
3	H	32	SER	2.2
3	H	82(C)	MET	2.2
4	L	9	SER	2.2
4	L	104	LEU	2.2
3	H	150	GLU	2.2
4	L	174	ALA	2.2
1	A	204	VAL	2.1
1	A	242	THR	2.1
4	L	200	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	291	SER	2.1
3	H	114	ALA	2.1
4	L	80	SER	2.1
4	L	147	ALA	2.1
3	H	83	ASP	2.1
3	H	104	GLY	2.1
4	L	135	LEU	2.1
4	L	74	ALA	2.1
2	B	151	SER	2.1
3	H	35(B)	SER	2.1
3	H	69	ILE	2.1
2	B	25	HIS	2.1
4	L	39	VAL	2.1
4	L	145	THR	2.1
4	L	38	GLN	2.1
2	B	1	GLY	2.1
2	B	48	ILE	2.1
2	B	17	MET	2.0
3	H	4	LEU	2.0
3	H	11	LEU	2.0
1	A	205	GLY	2.0
1	A	214	THR	2.0
3	H	167	THR	2.0
4	L	204	THR	2.0
1	A	101	ASP	2.0
2	B	36	ALA	2.0
4	L	173	TYR	2.0
2	B	149	MET	2.0
3	H	120	SER	2.0
2	B	128	ASN	2.0
2	B	134	GLY	2.0
1	A	200	ALA	2.0
4	L	111	ALA	2.0
4	L	175	ALA	2.0
3	H	71	LYS	2.0

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

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

6.3 Carbohydrates

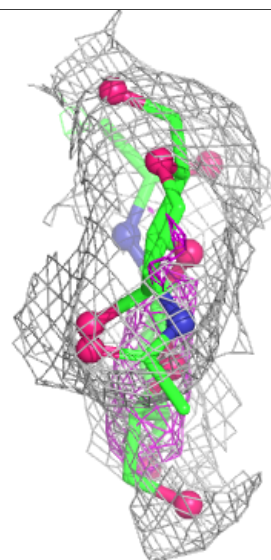
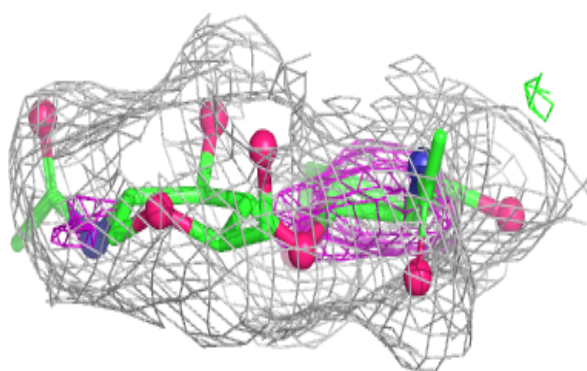
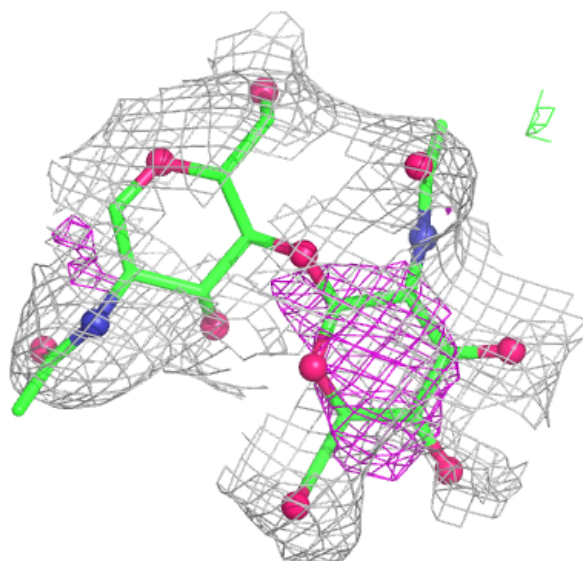
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	122,129,134,140	0
5	NAG	C	2	14/15	-	-	145,147,148,149	0
5	NAG	E	2	14/15	0.22	0.25	138,140,141,141	0
5	NAG	E	1	14/15	0.69	0.20	119,128,130,135	0
6	NAG	D	1	14/15	-	-	70,79,83,89	0
6	NAG	D	2	14/15	-	-	93,96,102,109	0
6	BMA	D	3	11/12	-	-	114,116,120,123	0
6	MAN	D	4	11/12	-	-	128,129,131,131	0

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

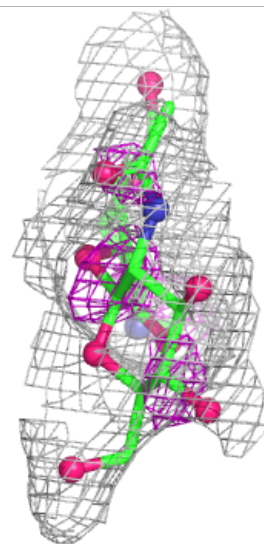
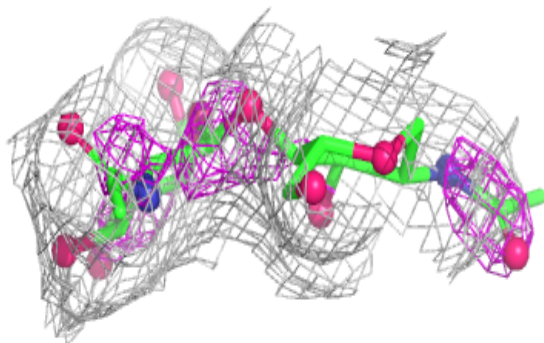
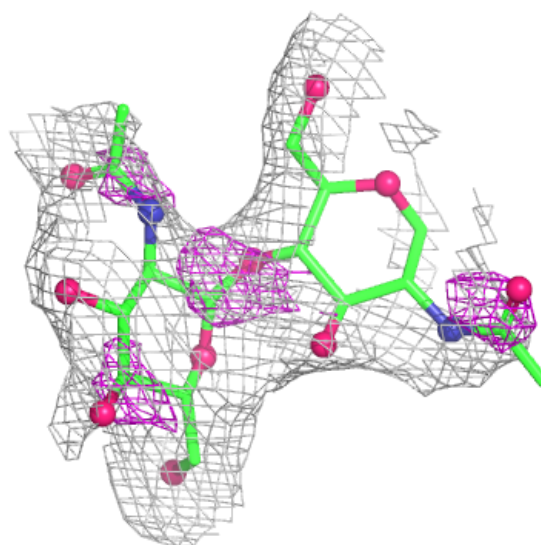
Electron density around Chain C:

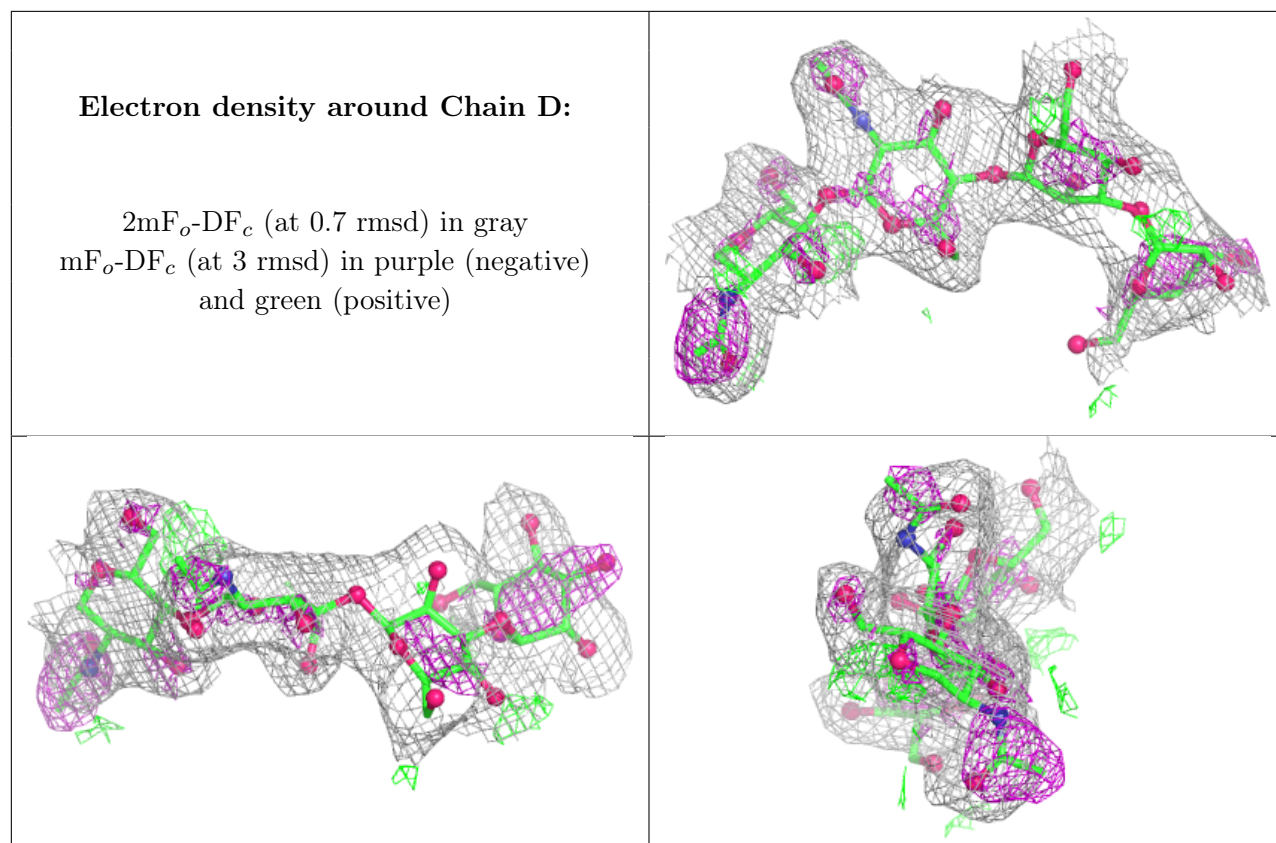
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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
7	NAG	A	401	14/15	0.34	0.26	119,127,132,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.