



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:39 AM UTC

PDB ID : 7WG3 / pdb_00007wg3
Title : Structural basis of interleukin-17B receptor in complex with a neutralizing antibody D9 for guiding humanization and affinity maturation for cancer therapy
Authors : Lee, W.H.; Chen, X.R.; Liu, I.J.; Lee, J.H.; Hu, C.M.; Wu, H.C.; Wang, S.K.; Lee, W.H.; Ma, C.
Deposited on : 2021-12-28
Resolution : 2.19 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

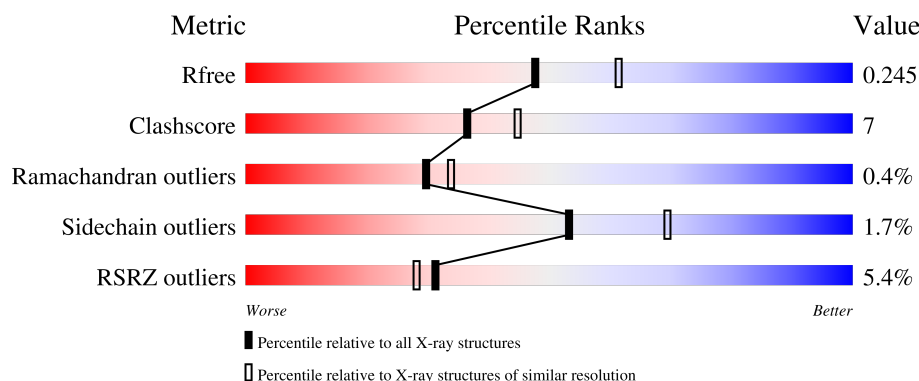
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	213	
1	B	213	
1	C	213	
1	D	213	
2	E	220	

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Mol	Chain	Length	Quality of chain
2	F	220	% 91% 8% .
2	G	220	4% 92% 8%
2	H	220	2% 83% 17%
3	I	255	13% 77% 20% .
3	J	255	13% 69% 25% . .
3	K	255	8% 81% 15% . .
3	L	255	13% 65% 26% . 7%
4	M	6	33% 50% 17%
5	N	5	80% 20%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21987 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 Light chain of D9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	1	0
			1638	1024	270	336	8			
1	B	213	Total	C	N	O	S	0	1	0
			1622	1016	268	330	8			
1	C	213	Total	C	N	O	S	0	0	0
			1624	1016	268	333	7			
1	D	213	Total	C	N	O	S	0	0	0
			1624	1017	269	331	7			

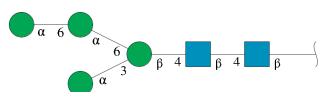
- Molecule 2 is a protein called Heavy chain of D9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	220	Total	C	N	O	S	0	1	0
			1633	1029	270	328	6			
2	F	220	Total	C	N	O	S	0	0	0
			1644	1036	269	334	5			
2	G	220	Total	C	N	O	S	0	0	0
			1628	1028	265	330	5			
2	H	220	Total	C	N	O	S	0	0	0
			1635	1031	266	332	6			

- Molecule 3 is a protein called IL17RB protein.

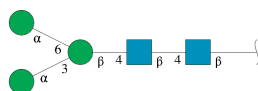
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	248	Total	C	N	O	S	0	0	0
			1905	1198	329	362	16			
3	J	245	Total	C	N	O	S	0	0	0
			1883	1188	322	357	16			
3	K	251	Total	C	N	O	S	0	0	0
			1927	1210	333	368	16			
3	L	236	Total	C	N	O	S	0	1	0
			1800	1140	305	339	16			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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.



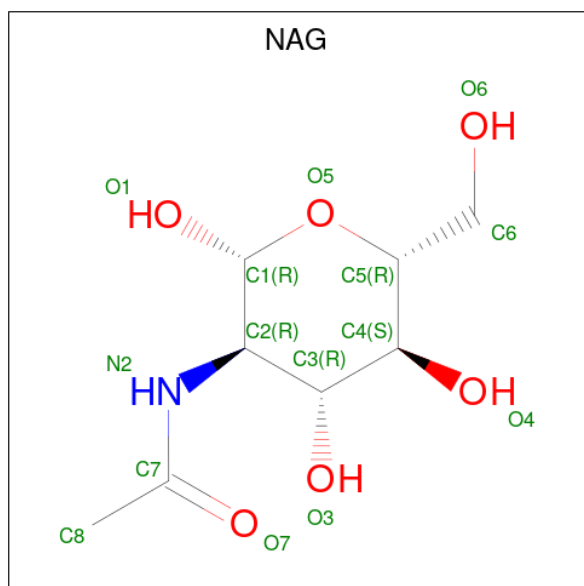
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total	O	0	0
			139	139		
7	B	83	Total	O	0	0
			83	83		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	145	Total 145	O 145	0	0
7	D	118	Total 118	O 118	0	0
7	E	90	Total 90	O 90	0	0
7	F	98	Total 98	O 98	0	0
7	G	111	Total 111	O 111	0	0
7	H	66	Total 66	O 66	0	0
7	I	62	Total 62	O 62	0	0
7	J	30	Total 30	O 30	0	0
7	K	62	Total 62	O 62	0	0
7	L	35	Total 35	O 35	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: Light chain of D9 Fab

Chain A:  91% 9%



- Molecule 1: Light chain of D9 Fab

Chain B:  87% 12%



- Molecule 1: Light chain of D9 Fab

Chain C:  95% 5%



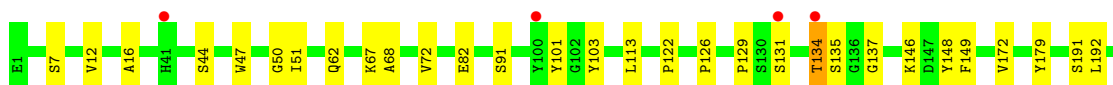
- Molecule 1: Light chain of D9 Fab

Chain D:  88% 12%



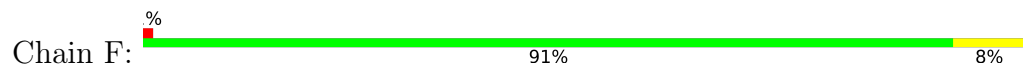
- Molecule 2: Heavy chain of D9 Fab

Chain E:  84% 15%

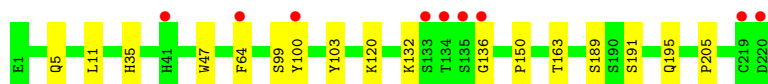




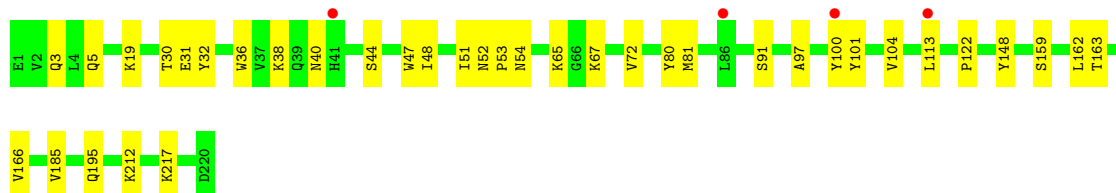
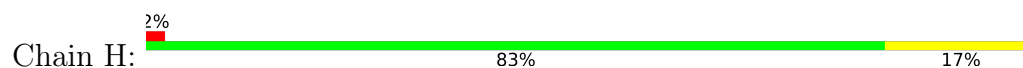
- Molecule 2: Heavy chain of D9 Fab



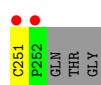
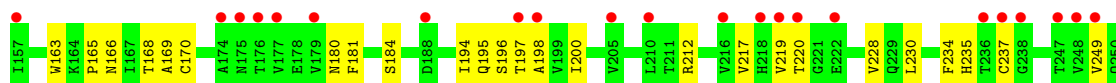
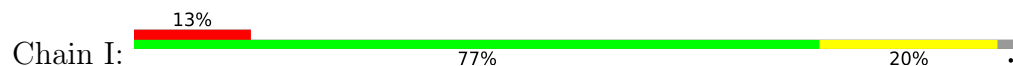
- Molecule 2: Heavy chain of D9 Fab



- Molecule 2: Heavy chain of D9 Fab

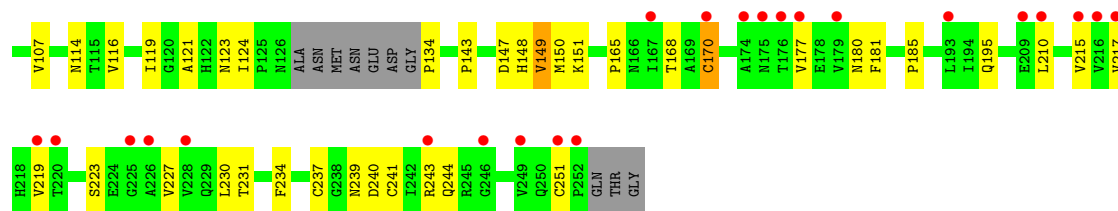


- Molecule 3: IL17RB protein

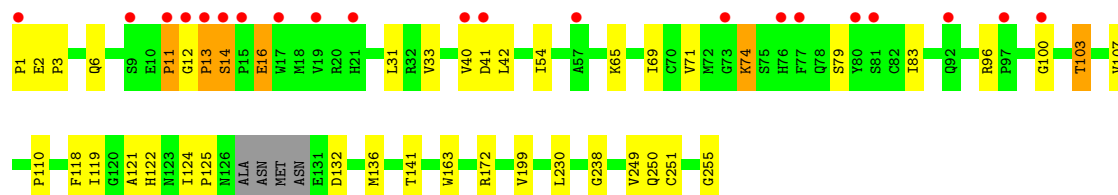
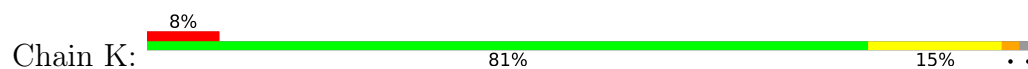


- Molecule 3: IL17RB protein

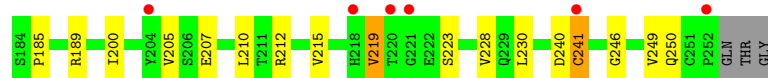
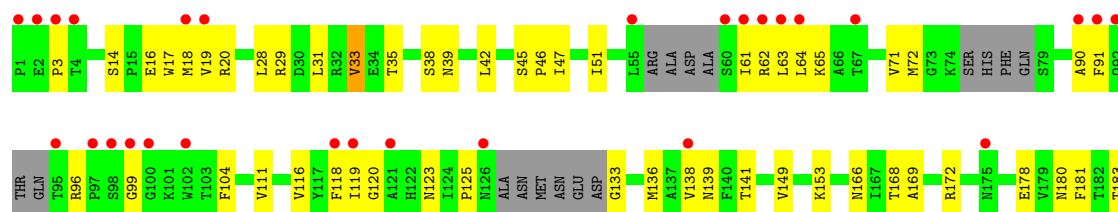




• Molecule 3: IL17RB protein



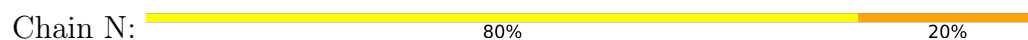
• Molecule 3: IL17RB protein



• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.02Å 195.03Å 98.84Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	38.03 – 2.19 38.03 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.03-2.19) 100.0 (38.03-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.238 (Not available) , 0.245	Depositor DCC
R_{free} test set	6858 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21987	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/1676	0.62	0/2276
1	B	0.36	0/1660	0.60	0/2256
1	C	0.42	0/1662	0.65	0/2259
1	D	0.38	0/1662	0.62	0/2258
2	E	0.35	0/1674	0.61	0/2285
2	F	0.37	0/1686	0.62	0/2301
2	G	0.36	0/1670	0.61	0/2282
2	H	0.35	0/1677	0.61	0/2290
3	I	0.34	0/1949	0.61	0/2654
3	J	0.36	1/1927 (0.1%)	0.60	0/2623
3	K	0.35	0/1970	0.70	0/2679
3	L	0.33	0/1838	0.63	0/2497
All	All	0.36	1/21051 (0.0%)	0.63	0/28660

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	170	CYS	CB-SG	-5.55	1.62	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1569	18	0
1	B	1622	0	1549	21	0
1	C	1624	0	1550	8	0
1	D	1624	0	1557	18	0
2	E	1633	0	1567	30	0
2	F	1644	0	1575	18	0
2	G	1628	0	1543	14	0
2	H	1635	0	1563	29	0
3	I	1905	0	1853	35	0
3	J	1883	0	1843	51	0
3	K	1927	0	1888	23	0
3	L	1800	0	1762	47	1
4	M	72	0	61	3	0
5	N	61	0	52	2	0
6	I	56	0	52	2	1
6	J	56	0	52	1	0
6	K	70	0	65	0	0
6	L	70	0	65	3	0
7	A	139	0	0	8	0
7	B	83	0	0	5	1
7	C	145	0	0	3	0
7	D	118	0	0	3	1
7	E	90	0	0	7	1
7	F	98	0	0	8	1
7	G	111	0	0	4	0
7	H	66	0	0	10	0
7	I	62	0	0	3	0
7	J	30	0	0	4	0
7	K	62	0	0	4	0
7	L	35	0	0	3	0
All	All	21987	0	20166	294	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (294) 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:H:54:ASN:HD21	3:L:116:VAL:HG11	1.29	0.96
2:H:195:GLN:O	7:H:301:HOH:O	1.85	0.95
1:A:141:ARG:HD3	7:A:307:HOH:O	1.65	0.94
2:H:212:LYS:NZ	7:H:304:HOH:O	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:ASP:OD2	7:F:301:HOH:O	1.90	0.89
2:F:220:ASP:OD2	7:F:302:HOH:O	1.90	0.88
1:A:107:ARG:NH1	1:A:108:THR:O	2.08	0.87
3:K:110:PRO:O	7:K:401:HOH:O	1.92	0.87
2:H:65:LYS:O	7:H:302:HOH:O	1.93	0.86
7:A:317:HOH:O	2:E:44:SER:HB2	1.74	0.86
3:I:1:PRO:HG3	4:M:5:MAN:H3	1.58	0.84
3:J:241:CYS:O	3:J:243:ARG:NH1	2.14	0.81
2:G:191:SER:HB2	2:G:195:GLN:HG3	1.63	0.80
1:D:160:GLU:OE2	7:D:303:HOH:O	2.00	0.80
3:L:65:LYS:HG2	3:L:125:PRO:HD3	1.63	0.79
3:J:54:ILE:HG12	3:J:103:THR:HG22	1.62	0.79
2:H:54:ASN:ND2	3:L:116:VAL:HG11	1.98	0.78
3:K:1:PRO:HB3	3:K:96:ARG:HD3	1.66	0.77
3:I:148:HIS:HA	3:I:151:LYS:HD3	1.66	0.76
1:D:107:ARG:NH1	1:D:108:THR:O	2.19	0.76
3:I:24:THR:HG1	6:I:302:NAG:HO3	1.30	0.75
1:A:213:CYS:SG	7:A:393:HOH:O	2.45	0.75
3:K:74:LYS:HD2	3:K:118:PHE:HB2	1.67	0.75
2:G:132:LYS:O	7:G:302:HOH:O	2.04	0.75
2:G:64:PHE:O	7:G:301:HOH:O	2.04	0.75
1:D:104:GLU:OE2	1:D:141:ARG:NH2	2.20	0.74
2:G:11:LEU:HD21	2:G:150:PRO:HG3	1.68	0.74
3:J:10:GLU:OE1	3:J:84:ARG:HB2	1.87	0.74
3:K:255:GLY:O	7:K:402:HOH:O	2.05	0.74
2:F:84:ARG:NH2	7:F:304:HOH:O	2.19	0.73
1:B:107:ARG:NH1	1:B:108:THR:O	2.22	0.73
3:L:118:PHE:HA	3:L:139:ASN:OD1	1.89	0.71
1:C:207:SER:O	7:C:301:HOH:O	2.07	0.71
1:B:108:THR:OG1	7:B:301:HOH:O	2.08	0.71
3:J:219:VAL:HG21	3:J:223:SER:HB3	1.72	0.71
1:B:198:GLN:NE2	7:B:305:HOH:O	2.22	0.71
3:K:11:PRO:C	3:K:13:PRO:HD3	2.15	0.71
3:J:99:GLY:O	7:J:401:HOH:O	2.09	0.70
2:E:191:SER:HB2	2:E:195:GLN:HG3	1.72	0.70
7:F:304:HOH:O	2:G:5:GLN:HG3	1.92	0.69
3:J:68:LYS:HE3	3:J:82:CYS:HB3	1.72	0.69
2:H:91:SER:O	7:H:305:HOH:O	2.10	0.69
3:L:71:VAL:HG22	3:L:119:ILE:HG12	1.76	0.68
3:J:84:ARG:NH1	3:J:86:ASN:OD1	2.27	0.67
1:B:79:ALA:HA	1:B:105:ILE:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:HB3	2:F:47:TRP:CD2	2.30	0.66
2:H:52:ASN:ND2	6:L:303:NAG:O6	2.28	0.66
3:J:114:ASN:OD1	7:J:402:HOH:O	2.13	0.66
3:K:54:ILE:HG22	3:K:103:THR:HG23	1.79	0.65
3:L:189:ARG:HG3	3:L:189:ARG:HH11	1.62	0.65
3:J:165:PRO:HG3	3:J:244:GLN:HG3	1.79	0.64
3:J:231:THR:HG23	3:J:243:ARG:HE	1.61	0.64
2:G:100:TYR:HD2	2:G:103:TYR:HH	1.45	0.64
3:L:64:LEU:HD11	3:L:123:ASN:HB3	1.79	0.64
2:F:100:TYR:CE1	6:J:302:NAG:H5	2.33	0.64
1:A:52:LYS:NZ	7:A:302:HOH:O	2.15	0.64
1:A:95:PHE:HB3	2:E:47:TRP:CD2	2.33	0.64
1:A:160:GLU:OE1	7:A:301:HOH:O	2.14	0.63
4:M:3:BMA:H61	4:M:5:MAN:H2	1.79	0.63
1:B:144:LYS:HB3	1:B:196:THR:HB	1.79	0.63
2:H:3:GLN:OE1	2:H:5:GLN:NE2	2.24	0.63
3:K:12:GLY:N	3:K:13:PRO:HD3	2.14	0.62
3:J:231:THR:HA	3:J:243:ARG:HG3	1.81	0.62
3:L:166:ASN:O	3:L:212:ARG:NH2	2.31	0.62
1:B:11:MET:HE1	1:B:21:MET:HB3	1.82	0.62
2:F:11:LEU:HD22	2:F:119:THR:HG23	1.81	0.62
3:I:163:TRP:CZ2	3:I:165:PRO:HB3	2.35	0.62
3:J:55:LEU:HB2	3:J:102:TRP:HB2	1.81	0.62
1:D:95:PHE:HB3	2:H:47:TRP:CD2	2.35	0.61
1:C:95:PHE:HB3	2:G:47:TRP:CD2	2.36	0.61
3:L:111:VAL:O	3:L:153:LYS:NZ	2.30	0.61
2:H:100:TYR:HA	7:H:303:HOH:O	2.00	0.61
1:A:60:ARG:NH1	1:A:81:ASP:OD1	2.34	0.61
3:L:219:VAL:HG11	3:L:223:SER:HB3	1.83	0.61
3:K:238:GLY:O	7:K:403:HOH:O	2.16	0.60
3:J:13:PRO:O	3:J:80:TYR:OH	2.12	0.60
3:K:33:VAL:HG21	3:K:119:ILE:HD12	1.84	0.59
3:L:19:VAL:HG13	6:L:303:NAG:H62	1.85	0.59
3:J:65:LYS:HE3	3:J:124:ILE:HG22	1.84	0.59
1:C:78:GLU:OE2	7:C:302:HOH:O	2.17	0.58
3:I:39:ASN:HB3	3:I:42:LEU:HD13	1.85	0.58
3:J:2:GLU:HG2	3:J:96:ARG:HH11	1.68	0.58
2:E:135:SER:C	2:E:137:GLY:H	2.12	0.58
2:G:35:HIS:CD2	2:G:99:SER:HB3	2.40	0.57
3:I:1:PRO:HB3	3:I:96:ARG:HH22	1.68	0.57
3:K:31:LEU:HB2	3:K:136:MET:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:VAL:CG1	2:E:16:ALA:HB3	2.34	0.57
3:L:20:ARG:HD3	3:L:133:GLY:N	2.19	0.57
1:A:160:GLU:OE2	7:A:303:HOH:O	2.17	0.57
2:H:166:VAL:HG22	2:H:185:VAL:HG12	1.86	0.57
1:B:42:SER:O	7:B:303:HOH:O	2.17	0.57
2:F:76:SER:N	7:F:301:HOH:O	2.02	0.57
3:L:64:LEU:HD12	3:L:125:PRO:HD2	1.87	0.57
1:D:1:GLN:HB2	1:D:94:PRO:HD2	1.86	0.56
3:I:170:CYS:HB2	6:I:304:NAG:H83	1.87	0.56
3:I:166:ASN:O	3:I:212:ARG:NH2	2.22	0.56
3:J:18:MET:HA	3:J:134:PRO:HG3	1.86	0.56
3:J:74:LYS:O	3:J:116:VAL:HG12	2.05	0.56
3:J:143:PRO:HG2	3:J:150:MET:HG3	1.88	0.56
1:D:16:GLY:N	1:D:77:MET:O	2.31	0.56
3:K:14:SER:C	3:K:16:GLU:H	2.14	0.56
2:E:91:SER:HA	2:E:113:LEU:O	2.05	0.55
3:I:196:SER:C	3:I:198:ALA:H	2.14	0.55
3:J:231:THR:HG23	3:J:243:ARG:NE	2.21	0.55
2:F:73:ASP:OD2	2:F:76:SER:OG	2.23	0.55
3:J:143:PRO:HB2	3:J:147:ASP:HB2	1.89	0.55
3:J:68:LYS:HE2	3:J:70:CYS:SG	2.47	0.55
3:L:35:THR:HG22	3:L:149:VAL:HG11	1.89	0.54
3:L:39:ASN:HB2	3:L:45:SER:HB2	1.89	0.54
1:B:166:ASP:OD2	7:B:304:HOH:O	2.19	0.54
2:E:195:GLN:OE1	7:E:305:HOH:O	2.18	0.54
2:E:7:SER:O	7:E:306:HOH:O	2.19	0.54
2:G:11:LEU:HD11	2:G:205:PRO:HB3	1.90	0.53
3:K:6:GLN:NE2	7:K:406:HOH:O	2.32	0.53
1:D:77:MET:SD	1:D:103:LEU:HD21	2.49	0.53
2:E:12:VAL:HG13	2:E:16:ALA:HB3	1.90	0.53
3:L:38:SER:OG	3:L:46:PRO:HG2	2.09	0.52
1:B:11:MET:HE3	1:B:21:MET:HE2	1.91	0.52
1:B:148:LYS:HG3	1:B:153:LEU:HA	1.91	0.52
3:J:195:GLN:NE2	7:J:404:HOH:O	2.42	0.52
3:K:2:GLU:HB2	3:K:3:PRO:HD3	1.91	0.52
3:L:61:ILE:HA	7:L:420:HOH:O	2.09	0.52
1:B:212:GLU:O	1:B:213:CYS:HB3	2.10	0.51
2:G:120:LYS:NZ	7:G:309:HOH:O	2.42	0.51
3:L:33:VAL:HG23	3:L:51:ILE:HG12	1.91	0.51
1:A:95:PHE:HB3	2:E:47:TRP:CE2	2.45	0.51
1:B:122:GLU:HA	1:B:125[B]:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:64:LEU:CD1	3:L:123:ASN:HB3	2.40	0.51
2:H:30:THR:HA	2:H:53:PRO:HG2	1.93	0.51
2:E:131:SER:HA	2:E:134:THR:HG23	1.94	0.50
3:L:168:THR:OG1	3:L:180:ASN:HB2	2.12	0.50
2:E:131:SER:HB3	2:E:216:PRO:HB3	1.94	0.50
3:L:205:VAL:HG21	3:L:215:VAL:HG21	1.93	0.50
3:L:241:CYS:HB2	7:L:406:HOH:O	2.11	0.50
3:I:169:ALA:CB	3:I:228:VAL:HG21	2.41	0.50
2:E:82:GLU:OE1	7:E:304:HOH:O	2.18	0.50
3:I:18:MET:HE2	3:I:72:MET:HE3	1.94	0.49
2:F:67:LYS:HE3	2:F:90:ASP:OD1	2.13	0.49
3:L:18:MET:HE3	3:L:120:GLY:N	2.27	0.49
3:L:181:PHE:CG	3:L:230:LEU:HD21	2.47	0.49
2:H:97:ALA:HB1	2:H:104:VAL:CG1	2.42	0.49
3:K:65:LYS:HE2	3:K:125:PRO:HD3	1.93	0.49
3:J:219:VAL:HG21	3:J:223:SER:CB	2.40	0.49
2:H:44:SER:HB2	7:H:345:HOH:O	2.12	0.49
3:I:30:ASP:OD2	3:I:56:ARG:HD3	2.12	0.49
1:B:15:PRO:HG3	1:B:105:ILE:HD11	1.94	0.49
2:H:159:SER:OG	7:H:306:HOH:O	2.20	0.49
2:H:32:TYR:CE2	2:H:100:TYR:HB2	2.48	0.48
2:H:162:LEU:O	7:H:307:HOH:O	2.20	0.48
3:J:71:VAL:HG22	3:J:119:ILE:HG12	1.95	0.48
2:H:97:ALA:HB1	2:H:104:VAL:HG11	1.94	0.48
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.95	0.48
3:I:234:PHE:HB2	3:I:237:CYS:SG	2.54	0.48
3:J:14:SER:OG	3:J:16:GLU:OE1	2.17	0.48
3:J:68:LYS:O	3:J:121:ALA:HA	2.13	0.48
2:F:146:LYS:HB2	2:F:146:LYS:HE3	1.60	0.48
2:G:132:LYS:C	7:G:302:HOH:O	2.51	0.48
3:K:33:VAL:HG21	3:K:119:ILE:CD1	2.43	0.48
3:L:39:ASN:HB2	3:L:45:SER:CB	2.44	0.48
1:A:33:HIS:CG	2:E:103:TYR:HB3	2.49	0.47
2:E:101:TYR:N	7:E:303:HOH:O	2.46	0.47
3:L:168:THR:HB	6:L:305:NAG:H81	1.96	0.47
3:J:73:GLY:O	3:J:78:GLN:HA	2.14	0.47
3:J:148:HIS:NE2	3:J:149:VAL:HG23	2.29	0.47
2:H:36:TRP:CE3	2:H:81:MET:HE2	2.49	0.47
1:D:107:ARG:HD2	1:D:170:SER:HB2	1.96	0.47
2:F:122:PRO:HD2	2:F:208:THR:HG21	1.96	0.47
3:I:1:PRO:HG3	4:M:5:MAN:C3	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ASP:OD1	3:I:149:VAL:HG12	2.15	0.47
3:L:249:VAL:HG12	3:L:250:GLN:N	2.30	0.47
1:C:11:MET:HB2	3:L:99:GLY:HA2	1.96	0.47
3:J:12:GLY:HA2	3:J:68:LYS:HZ1	1.80	0.46
3:J:168:THR:OG1	3:J:180:ASN:HB2	2.15	0.46
3:J:2:GLU:HG2	3:J:96:ARG:NH1	2.30	0.46
2:H:51:ILE:HD13	2:H:72:VAL:HG13	1.97	0.46
2:H:31:GLU:HG2	3:L:141:THR:H	1.81	0.46
2:F:101:TYR:N	7:F:306:HOH:O	2.36	0.46
3:J:74:LYS:NZ	3:J:74:LYS:HB3	2.31	0.46
2:E:67[B]:LYS:HB2	2:E:67[B]:LYS:HE3	1.78	0.46
3:I:17:TRP:CZ3	3:I:134:PRO:HB3	2.50	0.46
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.98	0.46
3:I:15:PRO:HB2	3:I:72:MET:HE2	1.96	0.46
3:I:200:ILE:O	3:I:220:THR:HG23	2.16	0.46
3:J:95:THR:HB	3:J:100:GLY:O	2.16	0.46
3:K:69:ILE:HD12	3:K:83:ILE:HD11	1.98	0.45
1:A:141:ARG:NH1	7:A:307:HOH:O	2.30	0.45
1:A:77:MET:SD	1:A:103:LEU:HD21	2.57	0.45
2:G:100:TYR:HD2	2:G:103:TYR:OH	1.97	0.45
2:H:91:SER:HA	2:H:113:LEU:O	2.16	0.45
3:I:200:ILE:O	3:I:219:VAL:HA	2.16	0.45
3:K:41:ASP:OD1	3:K:42:LEU:HG	2.16	0.45
3:L:47:ILE:HG22	3:L:111:VAL:HB	1.98	0.45
1:A:107:ARG:HD2	1:A:170:SER:HB2	1.99	0.45
1:A:122:GLU:OE2	2:E:212:LYS:NZ	2.41	0.45
3:J:107:VAL:HG21	5:N:1:NAG:H82	1.98	0.45
1:B:125[A]:LYS:HB3	1:B:125[A]:LYS:HE2	1.86	0.45
1:C:162:VAL:HG22	1:C:174:LEU:HD12	1.99	0.45
3:I:61:ILE:HG21	3:I:94:GLN:HA	1.99	0.45
3:I:163:TRP:CD1	3:I:184:SER:HB2	2.51	0.45
3:J:96:ARG:HG2	3:J:98:SER:H	1.82	0.45
2:E:68:ALA:HA	2:E:82:GLU:O	2.17	0.45
2:E:149:PHE:CG	2:H:163:THR:HG21	2.52	0.45
2:H:101:TYR:N	7:H:303:HOH:O	1.94	0.45
1:D:144:LYS:HB3	1:D:196:THR:HB	1.99	0.44
2:E:51:ILE:HD13	2:E:72:VAL:HG13	1.98	0.44
3:I:10:GLU:HG2	3:I:68:LYS:HE2	1.99	0.44
1:A:210:ARG:NH1	7:A:304:HOH:O	2.19	0.44
1:D:16:GLY:HA2	1:D:76:SER:OG	2.17	0.44
2:E:196:THR:HG23	2:E:213:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ASP:HB2	7:I:429:HOH:O	2.17	0.44
3:L:249:VAL:HG12	3:L:250:GLN:H	1.82	0.44
2:F:73:ASP:CG	7:F:301:HOH:O	2.51	0.44
2:F:88:SER:HB2	2:G:163:THR:HG21	2.00	0.44
3:L:185:PRO:HB3	3:L:210:LEU:HD11	1.98	0.44
1:C:123:GLN:HG2	1:C:128:THR:O	2.18	0.44
3:J:240:ASP:HA	3:J:243:ARG:HH12	1.81	0.44
3:K:121:ALA:HB3	3:K:136:MET:HE3	1.99	0.44
3:I:195:GLN:HG3	3:I:198:ALA:C	2.42	0.44
3:K:163:TRP:CH2	3:K:230:LEU:HD13	2.52	0.44
1:D:56:GLY:CA	2:E:62:GLN:HG3	2.48	0.43
1:D:144:LYS:HE3	1:D:146:GLN:HG3	1.99	0.43
1:B:141:ARG:NH1	7:B:317:HOH:O	2.51	0.43
2:E:172:VAL:HG23	7:E:336:HOH:O	2.17	0.43
3:J:96:ARG:NH2	3:J:98:SER:OG	2.51	0.43
1:C:1:GLN:N	1:C:93:ASN:O	2.50	0.43
1:D:198:GLN:NE2	7:D:306:HOH:O	2.26	0.43
3:J:243:ARG:NH2	7:J:409:HOH:O	2.51	0.43
1:A:104:GLU:OE2	1:A:141:ARG:NH2	2.52	0.43
3:L:228:VAL:HG12	3:L:246:GLY:C	2.44	0.43
3:J:74:LYS:HG2	3:J:78:GLN:HG2	1.99	0.43
1:D:49:ASP:OD1	3:L:29:ARG:NH2	2.48	0.43
3:J:239:ASN:C	3:J:243:ARG:HH22	2.26	0.43
3:K:132:ASP:OD1	3:K:132:ASP:N	2.51	0.43
3:I:168:THR:OG1	3:I:180:ASN:HB2	2.19	0.42
3:J:181:PHE:CD1	3:J:230:LEU:HD21	2.54	0.42
3:K:172:ARG:HH12	3:K:251:CYS:HB2	1.83	0.42
1:D:123:GLN:HG2	1:D:128:THR:O	2.18	0.42
3:I:114:ASN:OD1	7:I:402:HOH:O	2.21	0.42
2:H:40:ASN:ND2	7:H:315:HOH:O	2.52	0.42
3:I:196:SER:O	3:I:198:ALA:N	2.49	0.42
2:E:126:PRO:HD3	2:E:212:LYS:HE3	2.00	0.42
2:H:19:LYS:HE2	2:H:80:TYR:CB	2.50	0.42
3:L:31:LEU:HB2	3:L:136:MET:HB3	2.02	0.42
3:L:63:LEU:HD22	3:L:90:ALA:HB1	2.01	0.42
3:J:18:MET:HA	3:J:134:PRO:CG	2.48	0.42
2:F:29:PHE:CE2	2:F:53:PRO:HB3	2.54	0.42
2:G:136:GLY:O	2:G:189:SER:OG	2.24	0.42
3:I:163:TRP:CE2	3:I:165:PRO:HB3	2.55	0.42
3:J:64:LEU:HD13	3:J:123:ASN:HB3	2.01	0.42
3:L:16:GLU:N	3:L:16:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:2:NAG:O3	5:N:5:MAN:H5	2.20	0.42
3:J:148:HIS:HA	3:J:151:LYS:HD3	2.01	0.42
3:L:3:PRO:O	3:L:104:PHE:HE2	2.02	0.42
3:L:200:ILE:O	3:L:219:VAL:HA	2.20	0.42
1:A:106:LYS:HA	1:A:139:TYR:OH	2.20	0.41
1:C:160:GLU:OE1	7:C:303:HOH:O	2.21	0.41
3:I:2:GLU:OE1	7:I:403:HOH:O	2.22	0.41
3:L:17:TRP:CE2	3:L:18:MET:HG3	2.55	0.41
3:L:63:LEU:HD21	3:L:91:PHE:O	2.20	0.41
1:A:80[B]:GLU:CD	1:A:80[B]:GLU:H	2.27	0.41
2:E:122:PRO:HB3	2:E:148:TYR:HB3	2.03	0.41
3:J:231:THR:CG2	3:J:243:ARG:HE	2.32	0.41
3:K:249:VAL:HG12	3:K:250:GLN:N	2.35	0.41
3:L:42:LEU:HD13	3:L:42:LEU:HA	1.82	0.41
1:B:11:MET:CE	1:B:21:MET:HB3	2.50	0.41
1:B:185:TYR:HA	1:B:191:TYR:OH	2.21	0.41
3:J:30:ASP:O	3:J:53:TRP:HA	2.21	0.41
1:D:30:TYR:HE2	3:L:28:LEU:HD23	1.85	0.41
2:E:179:TYR:OH	7:E:302:HOH:O	2.11	0.41
2:E:129:PRO:HG3	2:E:192:LEU:HD22	2.03	0.41
3:L:169:ALA:HA	3:L:178:GLU:O	2.21	0.41
1:D:57:VAL:O	7:D:305:HOH:O	2.22	0.41
3:I:230:LEU:HD12	3:I:230:LEU:HA	1.93	0.41
3:K:14:SER:HB3	3:K:16:GLU:HG2	2.03	0.41
2:E:149:PHE:CD1	2:H:163:THR:HG21	2.56	0.41
3:I:194:ILE:CG1	3:I:217:VAL:HG11	2.51	0.41
3:L:96:ARG:HG2	7:L:424:HOH:O	2.20	0.41
3:I:1:PRO:HB3	3:I:96:ARG:HH12	1.85	0.41
3:J:185:PRO:HD3	3:J:210:LEU:HD23	2.03	0.41
3:J:234:PHE:HB2	3:J:237:CYS:SG	2.61	0.41
2:E:146:LYS:NZ	7:E:307:HOH:O	2.36	0.40
2:F:179:TYR:OH	7:F:303:HOH:O	2.11	0.40
1:B:95:PHE:HB3	2:F:47:TRP:CE2	2.56	0.40
3:I:181:PHE:CG	3:I:230:LEU:HD21	2.56	0.40
3:I:30:ASP:O	3:I:53:TRP:HA	2.22	0.40
3:J:64:LEU:CD1	3:J:123:ASN:HB3	2.50	0.40
3:J:72:MET:HA	3:J:79:SER:O	2.22	0.40
3:J:177:VAL:HB	3:J:217:VAL:HG13	2.04	0.40
3:L:172:ARG:HD3	3:L:172:ARG:HA	1.87	0.40
1:B:33:HIS:CG	2:F:103:TYR:HB3	2.57	0.40
1:D:144:LYS:HE3	1:D:146:GLN:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:GLY:C	3:I:23:LEU:HD11	2.47	0.40
1:B:12:SER:HA	1:B:104:GLU:O	2.21	0.40
3:L:183:THR:HG21	3:L:207:GLU:HG2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:371:HOH:O	7:E:385:HOH:O[2_656]	1.85	0.35
3:L:240:ASP:OD1	6:I:304:NAG:O6[1_455]	2.03	0.17
7:D:370:HOH:O	7:F:396:HOH:O[2_545]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	212/213 (100%)	208 (98%)	4 (2%)	0	100	100
1	B	212/213 (100%)	208 (98%)	4 (2%)	0	100	100
1	C	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
1	D	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
2	E	219/220 (100%)	207 (94%)	12 (6%)	0	100	100
2	F	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
2	G	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
2	H	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
3	I	244/255 (96%)	229 (94%)	12 (5%)	3 (1%)	10	8
3	J	241/255 (94%)	230 (95%)	11 (5%)	0	100	100
3	K	247/255 (97%)	226 (92%)	16 (6%)	5 (2%)	6	4
3	L	227/255 (89%)	210 (92%)	15 (7%)	2 (1%)	14	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2678/2752 (97%)	2564 (96%)	104 (4%)	10 (0%)	30 34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	197	THR
3	K	11	PRO
3	K	13	PRO
3	L	62	ARG
3	I	235	HIS
3	K	79	SER
3	I	251	CYS
3	K	74	LYS
3	K	100	GLY
3	L	14	SER

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	186/186 (100%)	184 (99%)	2 (1%)	65 79
1	B	182/186 (98%)	178 (98%)	4 (2%)	45 61
1	C	183/186 (98%)	183 (100%)	0	100 100
1	D	183/186 (98%)	180 (98%)	3 (2%)	55 71
2	E	180/186 (97%)	179 (99%)	1 (1%)	78 89
2	F	183/186 (98%)	180 (98%)	3 (2%)	55 71
2	G	178/186 (96%)	178 (100%)	0	100 100
2	H	182/186 (98%)	180 (99%)	2 (1%)	65 79
3	I	215/224 (96%)	213 (99%)	2 (1%)	70 84
3	J	214/224 (96%)	206 (96%)	8 (4%)	30 41
3	K	219/224 (98%)	209 (95%)	10 (5%)	24 32
3	L	203/224 (91%)	198 (98%)	5 (2%)	42 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2308/2384 (97%)	2268 (98%)	40 (2%)	53 69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	60	ARG
1	B	44	LYS
1	B	105	ILE
1	B	134	LEU
1	B	213	CYS
1	D	3	VAL
1	D	92	SER
1	D	136	ASN
2	E	134	THR
2	F	72	VAL
2	F	208	THR
2	F	220	ASP
2	H	67	LYS
2	H	217	LYS
3	I	111	VAL
3	I	249	VAL
3	J	2	GLU
3	J	74	LYS
3	J	79	SER
3	J	149	VAL
3	J	170	CYS
3	J	215	VAL
3	J	227	VAL
3	J	251	CYS
3	K	14	SER
3	K	16	GLU
3	K	40	VAL
3	K	71	VAL
3	K	103	THR
3	K	107	VAL
3	K	122	HIS
3	K	124	ILE
3	K	141	THR
3	K	199	VAL
3	L	33	VAL
3	L	72	MET

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Mol	Chain	Res	Type
3	L	138	VAL
3	L	219	VAL
3	L	241	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	146	GLN
1	B	137	ASN
1	D	159	GLN
2	E	39	GLN
2	G	40	ASN
2	H	54	ASN
3	I	89	GLN
3	I	218	HIS
3	J	89	GLN
3	J	229	GLN
3	K	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 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
4	NAG	M	1	3,4	14,14,15	0.41	0	17,19,21	0.73	0
4	NAG	M	2	4	14,14,15	0.35	0	17,19,21	0.53	0
4	BMA	M	3	4	11,11,12	0.72	0	15,15,17	0.92	0
4	MAN	M	4	4	11,11,12	1.22	1 (9%)	15,15,17	0.92	1 (6%)
4	MAN	M	5	4	11,11,12	1.15	1 (9%)	15,15,17	1.18	1 (6%)
4	MAN	M	6	4	11,11,12	1.18	2 (18%)	15,15,17	0.80	0
5	NAG	N	1	3,5	14,14,15	0.55	0	17,19,21	0.41	0
5	NAG	N	2	5	14,14,15	0.24	0	17,19,21	0.48	0
5	BMA	N	3	5	11,11,12	0.90	0	15,15,17	1.61	3 (20%)
5	MAN	N	4	5	11,11,12	0.83	0	15,15,17	1.41	1 (6%)
5	MAN	N	5	5	11,11,12	1.20	1 (9%)	15,15,17	1.39	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	1/2/19/22	0/1/1/1
4	MAN	M	4	4	-	0/2/19/22	0/1/1/1
4	MAN	M	5	4	-	2/2/19/22	0/1/1/1
4	MAN	M	6	4	-	0/2/19/22	0/1/1/1
5	NAG	N	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	3/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
5	MAN	N	4	5	-	1/2/19/22	0/1/1/1
5	MAN	N	5	5	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	4	MAN	O5-C1	-2.68	1.39	1.43
5	N	5	MAN	O5-C5	2.36	1.48	1.43
4	M	5	MAN	O5-C1	-2.33	1.39	1.43
4	M	6	MAN	O5-C1	-2.33	1.39	1.43
4	M	6	MAN	C2-C3	2.08	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	4	MAN	C1-O5-C5	4.88	118.73	112.19
5	N	5	MAN	C1-O5-C5	4.04	117.59	112.19
5	N	3	BMA	C1-C2-C3	-3.73	104.21	109.64
5	N	5	MAN	O2-C2-C3	-2.92	104.10	110.15
4	M	5	MAN	C2-C3-C4	2.68	115.58	110.86
5	N	3	BMA	C3-C4-C5	-2.44	105.81	110.23
4	M	4	MAN	O2-C2-C3	-2.15	105.71	110.15
5	N	3	BMA	O2-C2-C3	-2.01	105.98	110.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	5	MAN	O5-C5-C6-O6
4	M	5	MAN	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
5	N	2	NAG	C1-C2-N2-C7
5	N	2	NAG	C4-C5-C6-O6
5	N	5	MAN	C4-C5-C6-O6

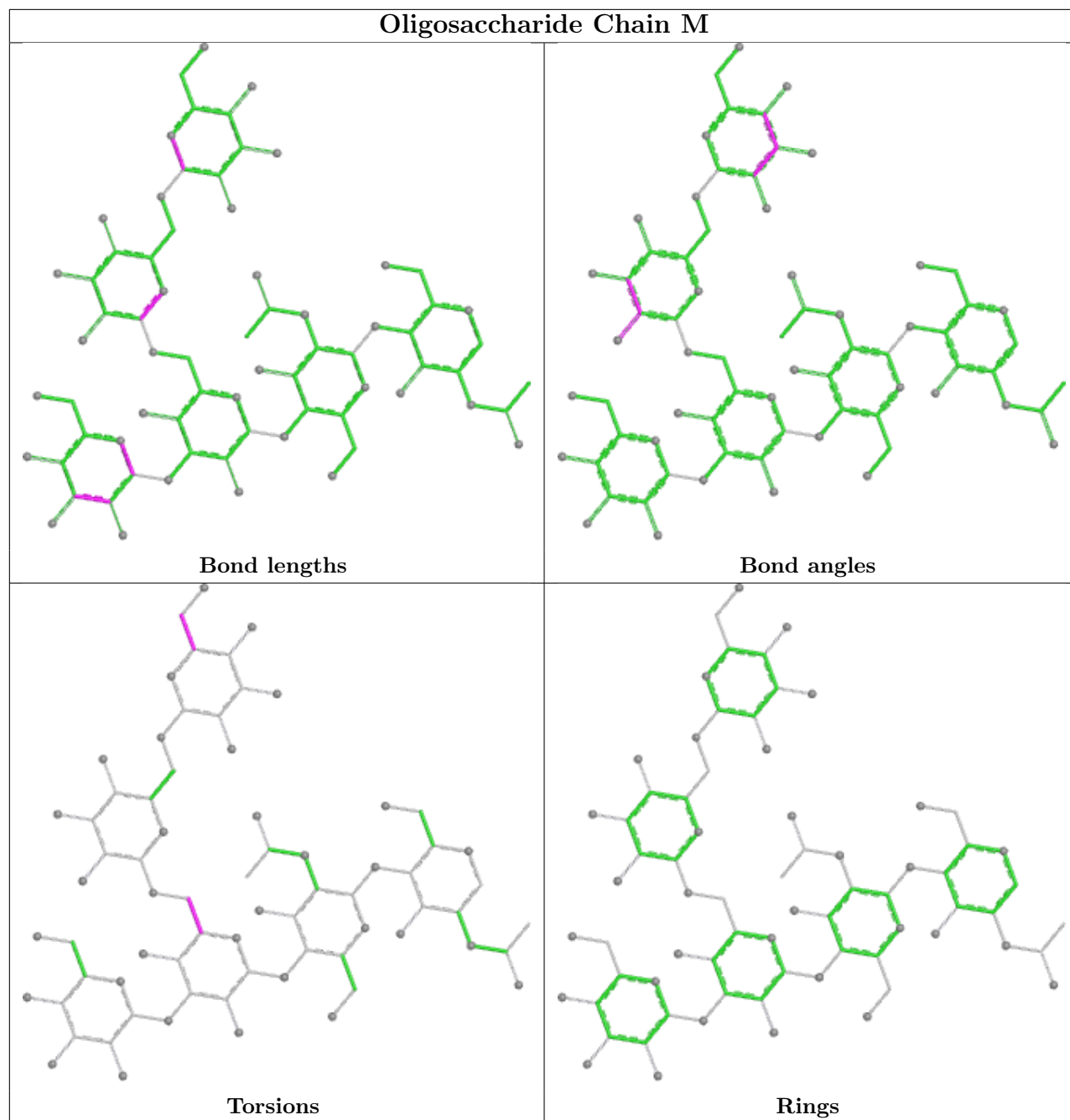
There are no ring outliers.

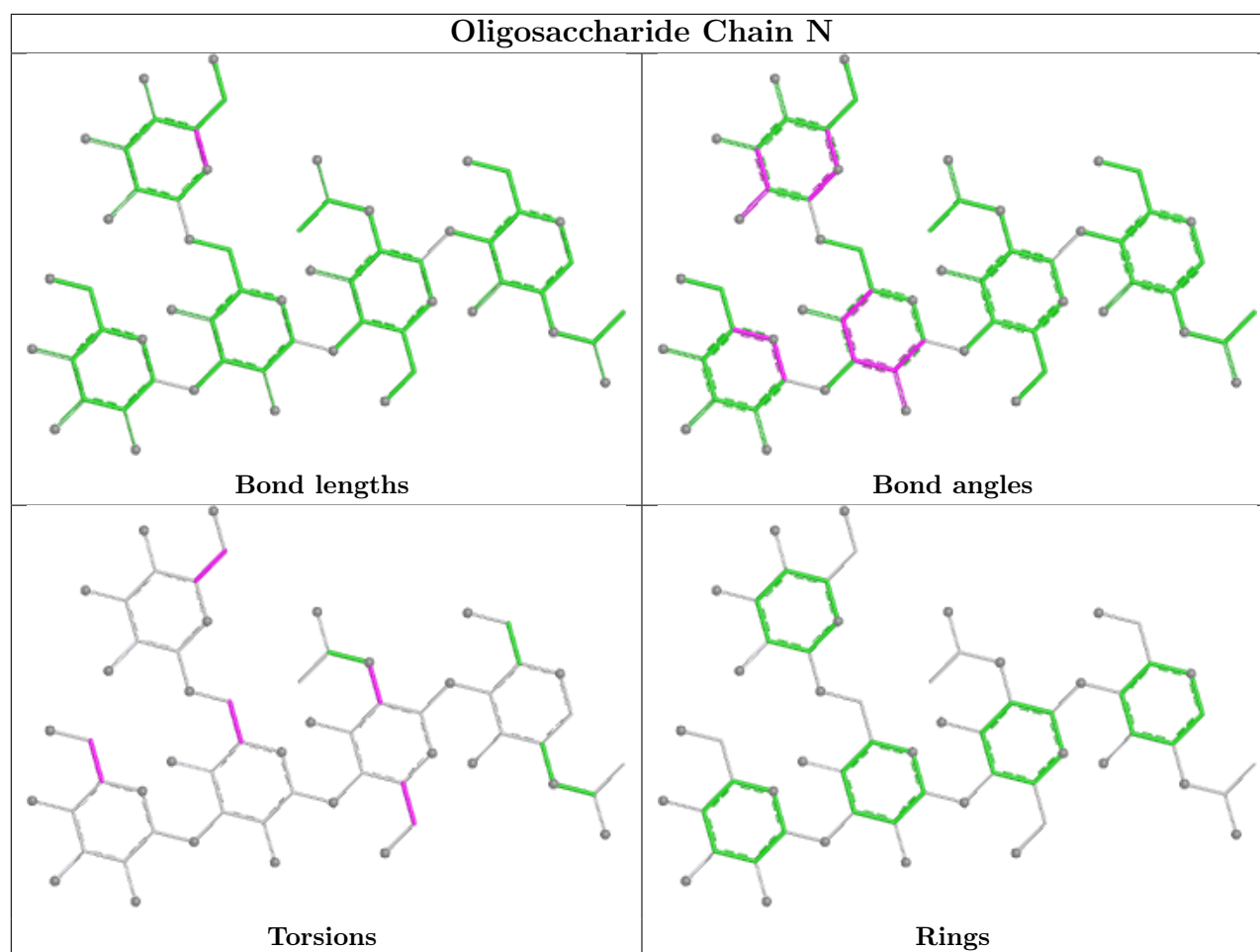
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	2	NAG	1	0
5	N	5	MAN	1	0
5	N	1	NAG	1	0
4	M	5	MAN	3	0
4	M	3	BMA	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.

Oligosaccharide Chain M





5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
6	NAG	K	302	3	14,14,15	0.38	0	17,19,21	0.39	0
6	NAG	L	301	3	14,14,15	0.63	1 (7%)	17,19,21	0.82	1 (5%)
6	NAG	K	305	3	14,14,15	0.32	0	17,19,21	0.63	0
6	NAG	L	303	3	14,14,15	0.74	1 (7%)	17,19,21	0.82	1 (5%)
6	NAG	L	305	3	14,14,15	0.56	0	17,19,21	0.42	0
6	NAG	I	301	3	14,14,15	0.49	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	L	302	3	14,14,15	0.40	0	17,19,21	0.47	0
6	NAG	J	302	3	14,14,15	0.50	0	17,19,21	0.43	0
6	NAG	J	303	3	14,14,15	0.54	0	17,19,21	0.55	0
6	NAG	K	304	3	14,14,15	0.49	0	17,19,21	0.47	0
6	NAG	I	304	3	14,14,15	0.57	0	17,19,21	0.53	0
6	NAG	J	301	3	14,14,15	0.60	0	17,19,21	0.52	0
6	NAG	J	304	3	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	L	304	3	14,14,15	0.43	0	17,19,21	0.59	0
6	NAG	K	303	3	14,14,15	0.56	0	17,19,21	0.52	0
6	NAG	I	302	3	14,14,15	0.31	0	17,19,21	0.59	0
6	NAG	K	301	3	14,14,15	0.58	0	17,19,21	0.58	0
6	NAG	I	303	3	14,14,15	0.39	0	17,19,21	0.50	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
6	NAG	K	302	3	-	2/6/23/26	0/1/1/1
6	NAG	L	301	3	-	0/6/23/26	0/1/1/1
6	NAG	K	305	3	-	0/6/23/26	0/1/1/1
6	NAG	L	303	3	-	0/6/23/26	0/1/1/1
6	NAG	L	305	3	-	0/6/23/26	0/1/1/1
6	NAG	I	301	3	-	0/6/23/26	0/1/1/1
6	NAG	L	302	3	-	2/6/23/26	0/1/1/1
6	NAG	J	302	3	-	0/6/23/26	0/1/1/1
6	NAG	J	303	3	-	2/6/23/26	0/1/1/1
6	NAG	K	304	3	-	0/6/23/26	0/1/1/1
6	NAG	I	304	3	-	2/6/23/26	0/1/1/1
6	NAG	J	301	3	-	0/6/23/26	0/1/1/1
6	NAG	J	304	3	-	0/6/23/26	0/1/1/1
6	NAG	L	304	3	-	0/6/23/26	0/1/1/1
6	NAG	K	303	3	-	0/6/23/26	0/1/1/1
6	NAG	I	302	3	-	0/6/23/26	0/1/1/1
6	NAG	K	301	3	-	2/6/23/26	0/1/1/1
6	NAG	I	303	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	303	NAG	O5-C1	-2.37	1.39	1.43
6	L	301	NAG	O5-C1	2.18	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	NAG	C1-O5-C5	2.66	115.75	112.19
6	L	303	NAG	C1-O5-C5	-2.27	109.14	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	301	NAG	C8-C7-N2-C2
6	K	301	NAG	O7-C7-N2-C2
6	K	302	NAG	O5-C5-C6-O6
6	K	302	NAG	C4-C5-C6-O6
6	L	302	NAG	O5-C5-C6-O6
6	L	302	NAG	C4-C5-C6-O6
6	I	304	NAG	O5-C5-C6-O6
6	I	304	NAG	C4-C5-C6-O6
6	J	303	NAG	C4-C5-C6-O6
6	J	303	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	303	NAG	2	0
6	L	305	NAG	1	0
6	J	302	NAG	1	0
6	I	304	NAG	1	1
6	I	302	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	213/213 (100%)	-0.34	1 (0%) 87 85	19, 30, 48, 67	1 (0%)
1	B	213/213 (100%)	0.13	2 (0%) 81 79	21, 42, 66, 77	1 (0%)
1	C	213/213 (100%)	-0.35	2 (0%) 81 79	21, 31, 45, 73	0
1	D	213/213 (100%)	-0.13	1 (0%) 87 85	26, 36, 50, 64	0
2	E	220/220 (100%)	0.09	5 (2%) 61 58	21, 38, 68, 96	1 (0%)
2	F	220/220 (100%)	-0.02	2 (0%) 81 79	23, 38, 54, 77	0
2	G	220/220 (100%)	0.04	9 (4%) 41 38	25, 37, 67, 95	0
2	H	220/220 (100%)	0.22	4 (1%) 67 64	26, 41, 62, 80	0
3	I	248/255 (97%)	0.70	33 (13%) 7 5	22, 57, 95, 116	0
3	J	245/255 (96%)	0.87	32 (13%) 7 5	31, 61, 96, 117	0
3	K	251/255 (98%)	0.63	21 (8%) 17 14	25, 51, 86, 110	0
3	L	236/255 (92%)	0.93	34 (14%) 6 4	31, 60, 93, 111	1 (0%)
All	All	2712/2752 (98%)	0.25	146 (5%) 31 28	19, 42, 84, 117	4 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1	PRO	4.6
2	G	136	GLY	4.5
3	L	91	PHE	4.4
3	L	97	PRO	4.4
3	K	81	SER	4.4
3	L	63	LEU	4.3
3	I	1	PRO	4.2
3	L	98	SER	4.1
3	K	12	GLY	4.1
1	D	213	CYS	4.0
3	L	204[A]	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
3	L	90	ALA	3.9
3	L	55	LEU	3.9
3	K	77	PHE	3.8
2	G	219	CYS	3.6
2	G	220	ASP	3.6
3	K	19	VAL	3.5
2	G	100	TYR	3.5
2	G	41	HIS	3.5
3	L	64	LEU	3.4
3	I	252	PRO	3.3
3	I	220	THR	3.2
3	L	102	TRP	3.2
3	J	167	ILE	3.2
3	I	251	CYS	3.2
3	J	216	VAL	3.2
3	L	92	GLN	3.2
3	K	80	TYR	3.2
3	L	99	GLY	3.2
2	E	219	CYS	3.2
3	J	219	VAL	3.1
3	I	197	THR	3.1
3	I	40	VAL	3.1
3	J	174	ALA	3.1
3	I	19	VAL	3.1
3	L	100	GLY	3.0
3	J	1	PRO	3.0
1	B	212	GLU	3.0
3	J	226	ALA	3.0
3	I	157	ILE	3.0
3	I	174	ALA	3.0
3	I	219	VAL	2.9
3	K	100	GLY	2.9
3	L	126	ASN	2.9
3	L	19	VAL	2.8
3	L	221	GLY	2.8
3	L	2	GLU	2.8
3	I	236	THR	2.8
3	J	19	VAL	2.8
3	K	13	PRO	2.8
3	L	62	ARG	2.8
3	J	176	THR	2.8
2	H	41	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	61	ILE	2.7
3	J	21	HIS	2.7
3	K	17	TRP	2.7
3	I	247	THR	2.7
3	I	248	VAL	2.7
3	J	215	VAL	2.7
1	C	1	GLN	2.7
3	L	118	PHE	2.7
3	I	222	GLU	2.7
3	I	21	HIS	2.7
3	J	177	VAL	2.7
3	J	217	VAL	2.7
3	J	170	CYS	2.7
3	I	205	VAL	2.6
3	I	216	VAL	2.6
3	K	1	PRO	2.6
3	K	97	PRO	2.6
2	F	218	SER	2.6
3	L	241	CYS	2.6
1	A	1	GLN	2.6
2	H	100	TYR	2.6
3	K	76	HIS	2.6
3	L	3	PRO	2.6
3	I	218	HIS	2.5
3	J	243	ARG	2.5
2	E	134	THR	2.5
3	L	95	THR	2.5
3	J	252	PRO	2.5
3	L	121	ALA	2.5
3	J	98	SER	2.5
3	I	238	GLY	2.5
3	J	179	VAL	2.5
3	I	152	TYR	2.5
3	I	41	ASP	2.4
2	H	113	LEU	2.4
3	I	148	HIS	2.4
3	J	251	CYS	2.4
2	G	133	SER	2.4
3	L	252	PRO	2.4
3	I	249	VAL	2.4
3	K	40	VAL	2.4
3	I	176	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	K	15	PRO	2.4
3	K	41	ASP	2.4
3	K	11	PRO	2.3
1	B	213	CYS	2.3
1	C	213	CYS	2.3
2	F	219	CYS	2.3
3	J	57	ALA	2.3
3	K	57	ALA	2.3
2	E	131	SER	2.3
3	J	209	GLU	2.3
3	K	21	HIS	2.3
3	L	119	ILE	2.3
3	J	13	PRO	2.3
3	L	67	THR	2.3
3	I	133	GLY	2.3
2	G	135	SER	2.2
3	J	249	VAL	2.2
3	I	175	ASN	2.2
3	I	198	ALA	2.2
3	K	73	GLY	2.2
2	E	41	HIS	2.2
3	L	18	MET	2.2
3	J	225	GLY	2.2
3	J	59	ALA	2.2
3	J	46	PRO	2.2
3	L	138	VAL	2.2
3	K	14	SER	2.2
3	L	175	ASN	2.2
3	J	220	THR	2.2
3	L	4	THR	2.2
3	J	210	LEU	2.1
3	K	9	SER	2.1
3	L	60	SER	2.1
2	G	64	PHE	2.1
3	I	77	PHE	2.1
3	I	177	VAL	2.1
3	I	188	ASP	2.1
2	G	134	THR	2.1
3	K	92	GLN	2.1
3	I	179	VAL	2.1
3	I	237	CYS	2.1
3	J	175	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	246	GLY	2.1
3	J	193	LEU	2.0
3	L	220	THR	2.0
3	J	228	VAL	2.0
2	H	86	LEU	2.0
3	I	210	LEU	2.0
3	J	76	HIS	2.0
3	L	218	HIS	2.0
2	E	100	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

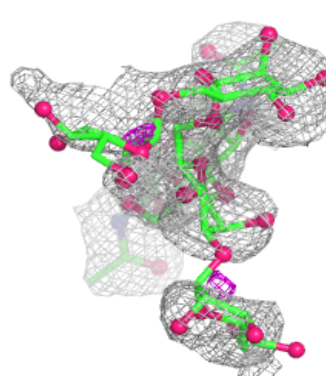
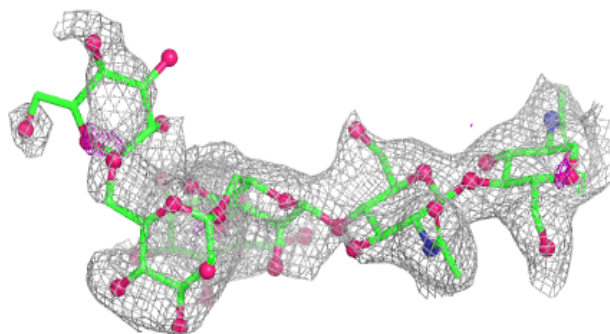
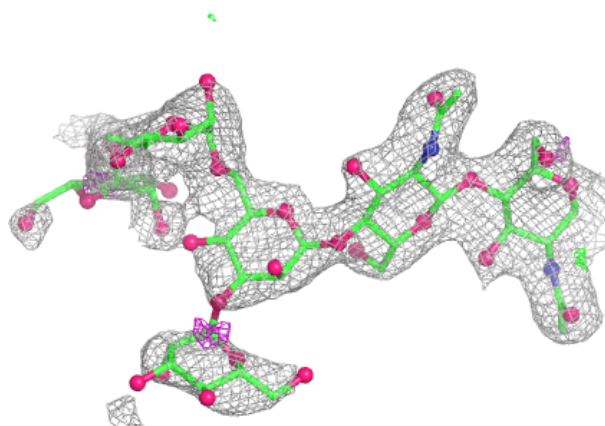
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

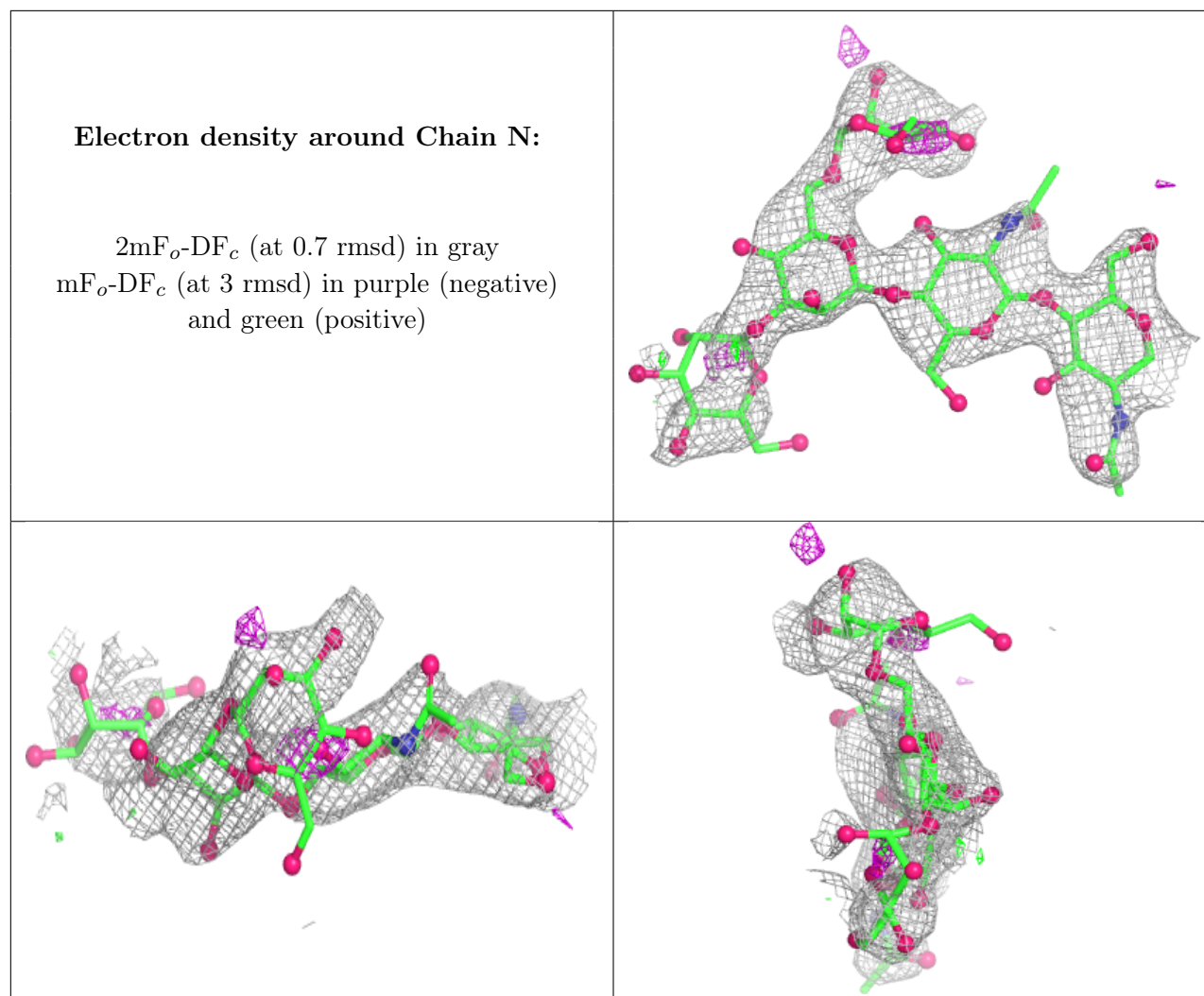
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	N	4	11/12	0.34	0.16	98,105,111,114	0
4	MAN	M	5	11/12	0.45	0.15	85,101,105,109	0
4	MAN	M	6	11/12	0.48	0.14	102,107,109,109	0
5	MAN	N	5	11/12	0.48	0.18	82,89,97,99	0
4	BMA	M	3	11/12	0.66	0.10	89,93,101,106	0
5	BMA	N	3	11/12	0.67	0.11	84,86,95,101	0
4	MAN	M	4	11/12	0.68	0.12	77,81,91,94	0
5	NAG	N	2	14/15	0.78	0.12	76,83,90,90	0
4	NAG	M	2	14/15	0.80	0.10	55,67,79,89	0
5	NAG	N	1	14/15	0.86	0.10	62,69,78,81	0
4	NAG	M	1	14/15	0.89	0.08	38,44,51,57	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 M:

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





6.4 Ligands ⓘ

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
6	NAG	I	302	14/15	0.49	0.17	52,70,74,74	0
6	NAG	L	304	14/15	0.51	0.16	69,89,94,94	0
6	NAG	J	303	14/15	0.58	0.15	92,98,100,102	0
6	NAG	J	304	14/15	0.61	0.14	81,93,96,96	0
6	NAG	K	304	14/15	0.64	0.15	63,71,77,77	0
6	NAG	L	305	14/15	0.64	0.13	65,71,82,87	0
6	NAG	K	303	14/15	0.65	0.16	44,67,73,73	0
6	NAG	I	304	14/15	0.66	0.13	80,85,93,94	0
6	NAG	L	303	14/15	0.69	0.16	64,76,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	L	302	14/15	0.72	0.12	74,83,88,95	0
6	NAG	I	303	14/15	0.75	0.13	66,74,81,89	0
6	NAG	L	301	14/15	0.79	0.11	61,72,76,79	0
6	NAG	K	302	14/15	0.82	0.10	58,62,67,77	0
6	NAG	J	302	14/15	0.82	0.10	47,50,54,54	0
6	NAG	K	301	14/15	0.85	0.10	50,63,70,70	0
6	NAG	K	305	14/15	0.88	0.10	40,44,53,54	0
6	NAG	J	301	14/15	0.91	0.08	48,53,58,58	0
6	NAG	I	301	14/15	0.96	0.05	30,33,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.