



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:28 AM UTC

PDB ID : 4DAG / pdb_00004dag
Title : Structure of the Human Metapneumovirus Fusion Protein with Neutralizing Antibody Identifies a Pneumovirus Antigenic Site
Authors : Jardetzky, T.S.; Wen, X.
Deposited on : 2012-01-12
Resolution : 3.39 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

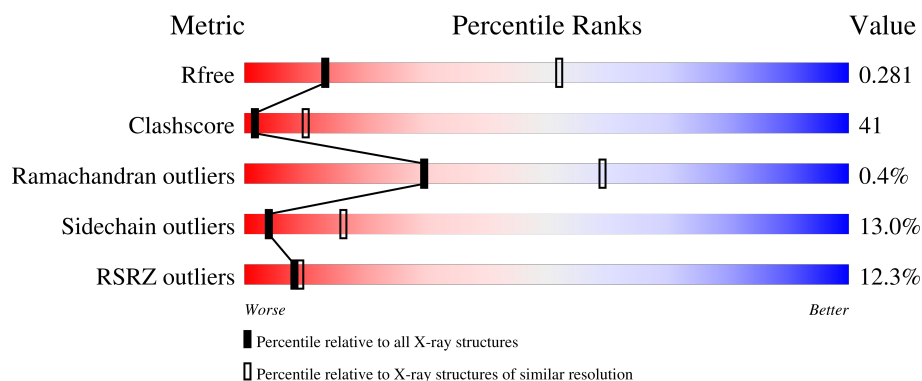
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	415	20% 38% 44% 9% 8%
2	H	220	5% 42% 49% 9%
3	L	213	4% 39% 54% 7%
4	B	5	60% 40%
4	C	5	20% 80%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6064 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2740	1707	473	540	20			

- Molecule 2 is a protein called Neutralizing Antibody DS7 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1621	1021	272	319	9			

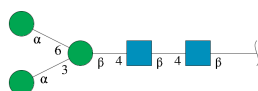
- Molecule 3 is a protein called Neutralizing Antibody DS7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1581	985	259	330	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	233	MET	-	expression tag	UNP Q8N5F4

- Molecule 4 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
4	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

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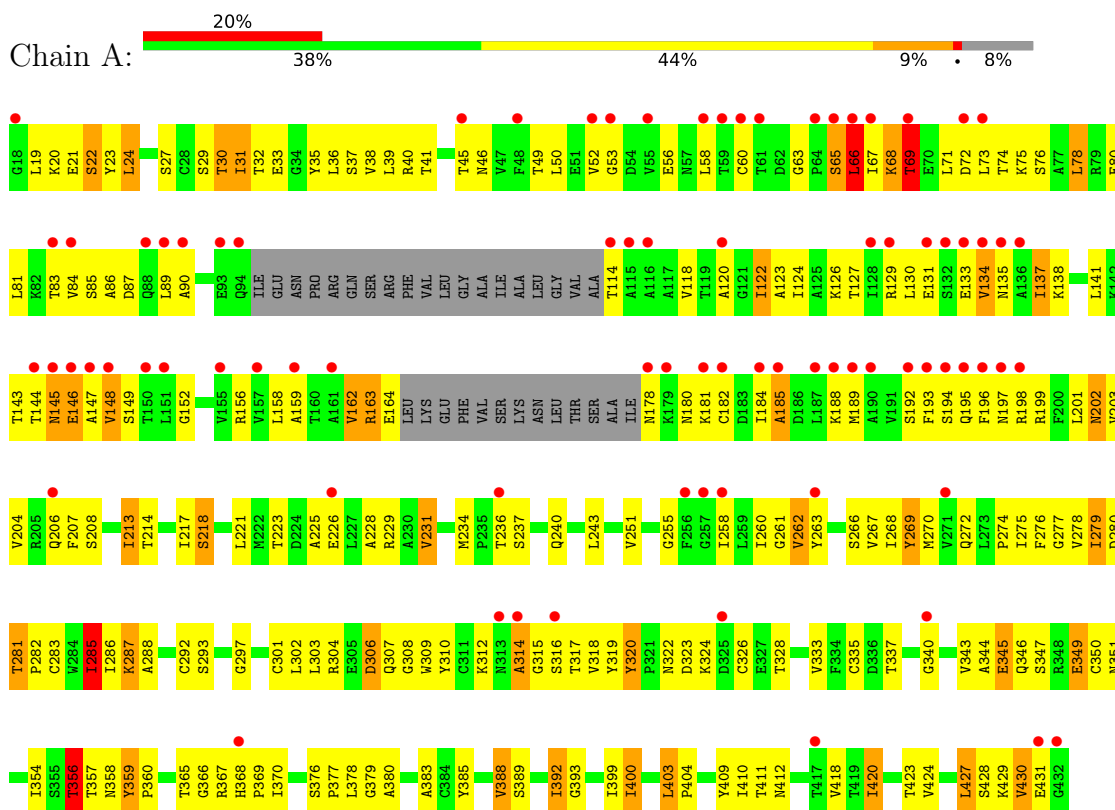
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

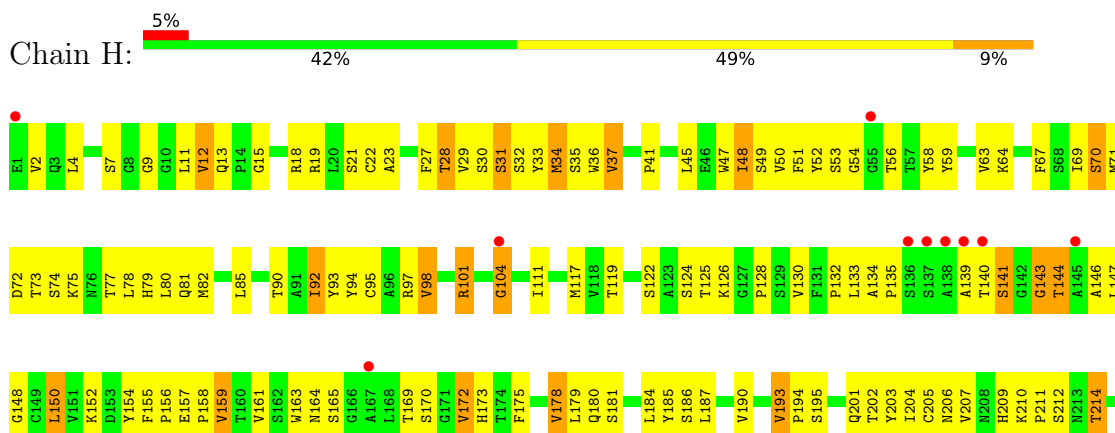
3 Residue-property plots

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

• Molecule 1: Fusion glycoprotein F0

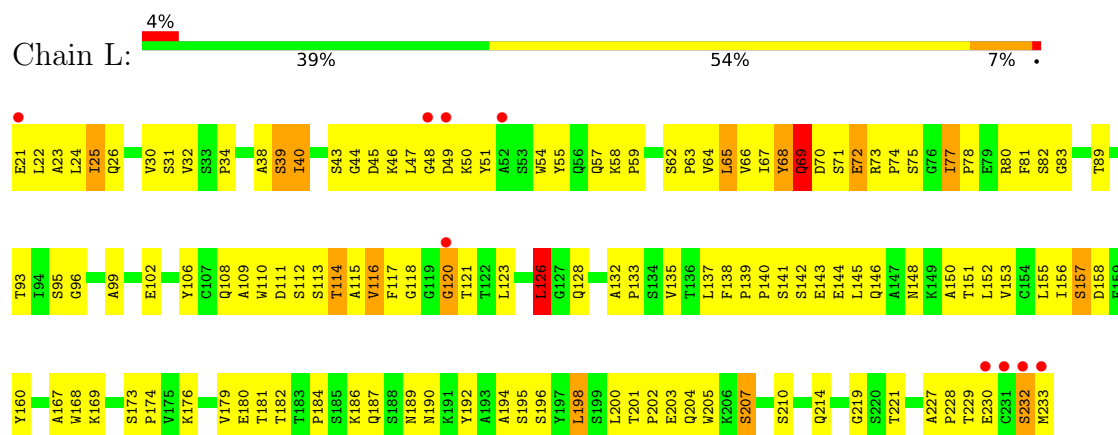


• Molecule 2: Neutralizing Antibody DS7 heavy chain





- Molecule 3: Neutralizing Antibody DS7 light chain



- Molecule 4: 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



- Molecule 4: 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 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	258.96Å 258.96Å 167.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.85 – 3.39 44.85 – 3.39	Depositor EDS
% Data completeness (in resolution range)	78.8 (44.85-3.39) 78.4 (44.85-3.39)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.260 , 0.289 0.245 , 0.281	Depositor DCC
R_{free} test set	1855 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/2776	1.21	23/3785 (0.6%)
2	H	0.76	0/1659	1.25	15/2260 (0.7%)
3	L	0.64	0/1618	1.14	10/2211 (0.5%)
All	All	0.67	0/6053	1.20	48/8256 (0.6%)

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	8
3	L	0	4
All	All	0	12

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	118	GLY	N-CA-C	-9.11	96.96	110.90
1	A	420	ILE	N-CA-C	8.74	120.51	112.29
1	A	66	LEU	N-CA-C	8.22	122.65	108.02
1	A	316	SER	N-CA-C	-8.17	96.56	109.23
2	H	143	GLY	N-CA-C	-8.12	104.56	115.36
3	L	219	GLY	N-CA-C	-8.08	105.08	114.69
2	H	48	ILE	N-CA-C	7.95	120.70	112.83
1	A	197	ASN	N-CA-C	-7.79	103.35	113.17
1	A	356	THR	CB-CA-C	-7.69	99.08	110.16
2	H	15	GLY	N-CA-C	-7.51	103.51	115.08
1	A	143	THR	CB-CA-C	-7.06	108.42	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	LEU	CA-C-N	7.03	126.99	120.03
1	A	403	LEU	C-N-CA	7.03	126.99	120.03
1	A	69	THR	CB-CA-C	-6.80	107.98	117.23
1	A	314	ALA	N-CA-C	6.68	119.57	111.82
3	L	117	PHE	N-CA-C	-6.52	99.54	109.85
1	A	285	ILE	N-CA-C	6.49	117.47	108.12
1	A	367	ARG	N-CA-C	-6.08	105.52	113.17
3	L	48	GLY	N-CA-C	6.06	120.42	110.97
1	A	297	GLY	N-CA-C	-6.05	106.61	115.63
2	H	12	VAL	CB-CA-C	-6.05	102.25	110.42
2	H	146	ALA	N-CA-C	6.04	118.25	108.34
3	L	39	SER	N-CA-C	5.97	117.62	108.42
2	H	134	ALA	CA-C-N	5.89	125.82	119.76
2	H	134	ALA	C-N-CA	5.89	125.82	119.76
2	H	92	ILE	N-CA-C	-5.75	103.71	110.21
1	A	368	HIS	CA-C-N	5.69	126.14	119.99
1	A	368	HIS	C-N-CA	5.69	126.14	119.99
2	H	48	ILE	CB-CA-C	-5.65	101.88	111.37
3	L	157	SER	N-CA-C	5.61	116.98	108.07
2	H	172	VAL	CB-CA-C	-5.57	103.13	110.98
1	A	340	GLY	N-CA-C	-5.49	102.24	110.42
2	H	130	VAL	CB-CA-C	-5.46	103.66	111.31
3	L	69	GLN	N-CA-C	-5.37	105.12	110.97
2	H	154	TYR	N-CA-C	5.35	118.16	109.06
1	A	320	TYR	CA-C-N	5.24	124.85	119.56
1	A	320	TYR	C-N-CA	5.24	124.85	119.56
2	H	104	GLY	N-CA-C	5.18	120.42	114.16
2	H	2	VAL	N-CA-C	5.17	115.53	107.99
2	H	101	ARG	CB-CA-C	-5.16	110.21	117.23
3	L	117	PHE	CA-C-N	-5.16	116.55	121.46
3	L	117	PHE	C-N-CA	-5.16	116.55	121.46
3	L	135	VAL	N-CA-C	5.16	115.73	108.36
1	A	63	GLY	CA-C-N	-5.09	115.03	121.91
1	A	63	GLY	C-N-CA	-5.09	115.03	121.91
1	A	429	LYS	N-CA-C	-5.07	107.15	113.38
1	A	163	ARG	N-CA-C	5.06	115.02	107.88
1	A	345	GLU	N-CA-C	-5.06	106.89	113.16

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ILE	Peptide
1	A	145	ASN	Peptide
1	A	185	ALA	Peptide
1	A	195	GLN	Peptide
1	A	293	SER	Peptide
1	A	420	ILE	Peptide
1	A	66	LEU	Peptide
1	A	68	LYS	Peptide
3	L	120	GLY	Peptide
3	L	126	LEU	Peptide
3	L	229	THR	Peptide
3	L	69	GLN	Peptide

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	2740	0	2604	239	0
2	H	1621	0	1596	127	0
3	L	1581	0	1519	134	0
4	B	61	0	50	1	0
4	C	61	0	52	5	0
All	All	6064	0	5821	483	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 41.

All (483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:272:GLN:HG2	1.38	1.06
2:H:34:MET:HE3	2:H:78:LEU:HD22	1.44	0.99
3:L:47:LEU:O	3:L:50:LYS:N	1.97	0.97
1:A:314:ALA:N	1:A:315:GLY:HA2	1.80	0.97
1:A:39:LEU:HB2	1:A:278:VAL:HG23	1.46	0.96
1:A:307:GLN:HB2	1:A:308:GLY:HA2	1.46	0.96
2:H:157:GLU:HG3	2:H:158:PRO:HA	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HG2	2:H:97:ARG:HA	1.49	0.94
3:L:22:LEU:HD12	3:L:23:ALA:N	1.84	0.92
3:L:32:VAL:HG22	3:L:38:ALA:HB3	1.53	0.91
3:L:32:VAL:HG22	3:L:38:ALA:CB	2.01	0.90
1:A:288:ALA:HB3	1:A:307:GLN:NE2	1.88	0.89
1:A:49:THR:O	1:A:162:VAL:HG23	1.72	0.89
2:H:132:PRO:O	3:L:141:SER:OG	1.91	0.89
3:L:71:SER:OG	3:L:83:GLY:O	1.92	0.87
3:L:34:PRO:HD3	3:L:126:LEU:O	1.74	0.87
2:H:220:VAL:O	3:L:233:MET:HE1	1.76	0.86
1:A:127:THR:HG22	1:A:270:MET:HE1	1.59	0.85
1:A:393:GLY:HA2	1:A:400:ILE:HG22	1.58	0.85
1:A:33:GLU:OE2	2:H:101:ARG:NH2	2.11	0.84
3:L:32:VAL:CG2	3:L:38:ALA:HB3	2.08	0.84
3:L:167:ALA:HB3	3:L:214:GLN:HB3	1.60	0.84
2:H:148:GLY:HA2	2:H:163:TRP:CH2	2.13	0.83
1:A:127:THR:HG22	1:A:270:MET:CE	2.08	0.83
1:A:376:SER:HB2	1:A:379:GLY:O	1.78	0.83
2:H:28:THR:HB	2:H:31:SER:HB3	1.57	0.83
1:A:288:ALA:HB3	1:A:307:GLN:HE22	1.43	0.82
1:A:20:LYS:HB2	3:L:49:ASP:O	1.79	0.82
1:A:20:LYS:HD3	3:L:50:LYS:HA	1.61	0.82
2:H:45:LEU:HD12	3:L:106:TYR:CD1	2.15	0.81
1:A:240:GLN:HG3	1:A:279:ILE:HB	1.60	0.81
2:H:34:MET:CE	2:H:78:LEU:HD22	2.09	0.81
1:A:45:THR:HG22	1:A:272:GLN:CG	2.10	0.81
2:H:148:GLY:HA2	2:H:163:TRP:HH2	1.44	0.81
1:A:123:ALA:HB1	1:A:272:GLN:HE22	1.48	0.79
2:H:143:GLY:O	2:H:195:SER:N	2.14	0.79
1:A:234:MET:SD	1:A:275:ILE:HG22	2.22	0.78
2:H:147:LEU:HD21	2:H:203:TYR:CD2	2.19	0.78
2:H:12:VAL:HG22	2:H:18:ARG:HE	1.49	0.77
3:L:182:THR:CG2	3:L:195:SER:H	1.98	0.77
1:A:343:VAL:HG22	1:A:344:ALA:H	1.49	0.77
2:H:135:PRO:HG3	2:H:147:LEU:HB3	1.65	0.77
3:L:69:GLN:O	3:L:70:ASP:HB2	1.84	0.77
1:A:310:TYR:CD1	1:A:319:TYR:HB2	2.19	0.77
3:L:55:TYR:HE1	3:L:65:LEU:HD12	1.48	0.77
2:H:23:ALA:HB2	2:H:77:THR:HG22	1.66	0.77
1:A:118:VAL:O	1:A:122:ILE:N	2.19	0.76
1:A:370:ILE:HG13	1:A:370:ILE:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:VAL:HG22	1:A:320:TYR:HE1	1.52	0.75
2:H:141:SER:HB3	2:H:144:THR:O	1.85	0.75
3:L:108:GLN:HG2	3:L:109:ALA:N	2.01	0.75
3:L:156:ILE:HG22	3:L:157:SER:H	1.51	0.75
3:L:132:ALA:HB1	3:L:133:PRO:HD2	1.69	0.74
1:A:27:SER:OG	1:A:29:SER:OG	2.04	0.74
1:A:240:GLN:NE2	1:A:277:GLY:O	2.20	0.74
1:A:281:THR:HG23	1:A:282:PRO:HD2	1.69	0.73
1:A:399:ILE:O	1:A:399:ILE:HG23	1.88	0.73
1:A:347:SER:HA	1:A:359:TYR:CE2	2.25	0.72
3:L:153:VAL:CG1	3:L:155:LEU:HD13	2.20	0.72
3:L:182:THR:HG21	3:L:195:SER:H	1.55	0.71
3:L:22:LEU:HD12	3:L:23:ALA:H	1.55	0.71
3:L:65:LEU:HD23	3:L:74:PRO:HG3	1.72	0.71
3:L:71:SER:HA	3:L:83:GLY:H	1.55	0.70
1:A:37:SER:HB3	1:A:283:CYS:SG	2.31	0.70
3:L:22:LEU:HD11	3:L:24:LEU:HD12	1.73	0.70
1:A:20:LYS:HE2	3:L:50:LYS:HG2	1.73	0.69
1:A:346:GLN:O	1:A:359:TYR:HD2	1.74	0.69
3:L:182:THR:HG22	3:L:195:SER:O	1.92	0.69
1:A:137:ILE:HD12	1:A:138:LYS:HA	1.74	0.69
1:A:163:ARG:HG3	1:A:164:GLU:H	1.57	0.69
1:A:307:GLN:HB2	1:A:308:GLY:CA	2.22	0.69
1:A:347:SER:HA	1:A:359:TYR:HE2	1.57	0.69
1:A:388:VAL:HG13	1:A:389:SER:N	2.07	0.69
1:A:127:THR:CG2	1:A:270:MET:HE1	2.21	0.69
2:H:9:GLY:O	2:H:18:ARG:NH1	2.25	0.69
2:H:58:TYR:CE2	3:L:113:SER:HB2	2.27	0.69
2:H:209:HIS:CE1	2:H:211:PRO:HG2	2.27	0.69
2:H:45:LEU:HD12	3:L:106:TYR:CE1	2.27	0.69
3:L:156:ILE:HG22	3:L:157:SER:N	2.08	0.69
1:A:349:GLU:CD	1:A:356:THR:HG21	2.18	0.69
1:A:392:ILE:HG22	1:A:418:VAL:HG22	1.75	0.68
4:B:3:BMA:O2	4:B:4:MAN:O5	2.12	0.68
1:A:237:SER:OG	1:A:240:GLN:OE1	2.11	0.68
1:A:127:THR:HG21	1:A:258:ILE:HD12	1.76	0.67
1:A:359:TYR:CD1	1:A:359:TYR:C	2.71	0.67
2:H:157:GLU:HG3	2:H:158:PRO:CA	2.22	0.67
1:A:193:PHE:HD1	1:A:196:PHE:CZ	2.11	0.67
2:H:147:LEU:HD21	2:H:203:TYR:HD2	1.58	0.67
2:H:150:LEU:HD21	2:H:152:LYS:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG22	2:H:18:ARG:NE	2.10	0.66
3:L:201:THR:HG22	3:L:204:GLN:CD	2.20	0.66
2:H:82:MET:HE3	2:H:85:LEU:HD11	1.78	0.66
1:A:20:LYS:HE2	3:L:50:LYS:CG	2.26	0.66
2:H:52:TYR:HB2	2:H:56:THR:HG23	1.77	0.66
1:A:269:TYR:C	1:A:269:TYR:HD1	2.03	0.65
1:A:163:ARG:HG3	1:A:164:GLU:N	2.12	0.65
1:A:269:TYR:HD1	1:A:269:TYR:O	1.80	0.65
1:A:24:LEU:HD11	1:A:31:ILE:HG22	1.78	0.65
3:L:137:LEU:HD12	3:L:153:VAL:O	1.96	0.65
1:A:411:THR:HG21	3:L:46:LYS:HE2	1.77	0.65
2:H:35:SER:HB2	2:H:49:SER:O	1.97	0.65
3:L:143:GLU:OE1	3:L:143:GLU:N	2.20	0.65
3:L:68:TYR:H	3:L:68:TYR:HD2	1.45	0.65
1:A:78:LEU:HB3	1:A:204:VAL:HG13	1.79	0.64
1:A:269:TYR:C	1:A:269:TYR:CD1	2.76	0.64
1:A:39:LEU:HB2	1:A:278:VAL:CG2	2.24	0.64
1:A:262:VAL:HG13	1:A:263:TYR:H	1.63	0.64
3:L:44:GLY:O	3:L:45:ASP:C	2.40	0.64
1:A:236:THR:HG21	1:A:277:GLY:HA2	1.81	0.63
3:L:168:TRP:CE3	3:L:198:LEU:HD12	2.33	0.63
1:A:225:ALA:O	1:A:229:ARG:HG3	1.99	0.63
1:A:411:THR:HG21	3:L:46:LYS:CE	2.28	0.63
2:H:133:LEU:HD12	2:H:148:GLY:O	1.99	0.63
1:A:193:PHE:CD1	1:A:196:PHE:CZ	2.87	0.63
1:A:23:TYR:CD1	1:A:409:TYR:HB2	2.33	0.63
1:A:260:ILE:H	1:A:269:TYR:HA	1.64	0.63
1:A:163:ARG:CG	1:A:164:GLU:H	2.11	0.62
2:H:72:ASP:O	2:H:73:THR:HG22	2.00	0.62
1:A:133:GLU:OE2	1:A:134:VAL:N	2.23	0.62
1:A:201:LEU:HD12	1:A:201:LEU:H	1.65	0.62
1:A:137:ILE:O	1:A:141:LEU:N	2.33	0.62
3:L:39:SER:HB3	3:L:93:THR:HA	1.82	0.62
1:A:279:ILE:HG23	1:A:280:ASP:H	1.65	0.61
1:A:181:LYS:HA	1:A:182:CYS:C	2.25	0.61
1:A:19:LEU:HD21	1:A:35:TYR:HE1	1.65	0.61
1:A:383:ALA:HB1	1:A:385:TYR:CE2	2.35	0.61
1:A:162:VAL:HG22	1:A:163:ARG:N	2.16	0.60
2:H:33:TYR:CD1	2:H:52:TYR:HD1	2.19	0.60
1:A:258:ILE:HD11	1:A:270:MET:CE	2.31	0.60
1:A:213:ILE:HG22	1:A:258:ILE:CG2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HD13	1:A:255:GLY:HA3	1.83	0.60
1:A:58:LEU:O	1:A:58:LEU:HD12	2.02	0.60
2:H:36:TRP:NE1	2:H:80:LEU:HB2	2.16	0.60
3:L:153:VAL:HG13	3:L:155:LEU:HD13	1.82	0.60
2:H:152:LYS:HE3	3:L:151:THR:OG1	2.01	0.60
3:L:158:ASP:OD1	3:L:187:GLN:NE2	2.34	0.59
1:A:127:THR:O	1:A:131:GLU:N	2.35	0.59
1:A:73:LEU:HD13	1:A:73:LEU:O	2.02	0.59
2:H:29:VAL:HG22	2:H:71:MET:SD	2.43	0.59
2:H:19:ARG:NH1	2:H:79:HIS:NE2	2.51	0.58
2:H:28:THR:HG22	2:H:29:VAL:H	1.68	0.58
2:H:29:VAL:HG22	2:H:71:MET:CE	2.33	0.58
1:A:240:GLN:OE1	1:A:240:GLN:N	2.36	0.58
3:L:145:LEU:HD23	3:L:150:ALA:HB2	1.86	0.57
1:A:19:LEU:HD21	1:A:35:TYR:CE1	2.39	0.57
1:A:258:ILE:HG13	1:A:270:MET:HE2	1.86	0.57
1:A:41:THR:HA	1:A:337:THR:HG21	1.87	0.57
1:A:133:GLU:CD	1:A:134:VAL:H	2.10	0.57
1:A:285:ILE:HG12	1:A:285:ILE:O	2.04	0.57
2:H:34:MET:HA	2:H:98:VAL:HG23	1.87	0.57
3:L:168:TRP:CD1	3:L:179:VAL:HG21	2.39	0.57
3:L:168:TRP:CD2	3:L:198:LEU:HD12	2.39	0.57
1:A:20:LYS:NZ	1:A:22:SER:OG	2.31	0.57
2:H:51:PHE:CD2	2:H:71:MET:HE3	2.39	0.57
2:H:126:LYS:HD3	2:H:184:LEU:HD21	1.87	0.57
3:L:169:LYS:HG2	3:L:174:PRO:HG3	1.87	0.57
1:A:193:PHE:O	1:A:194:SER:HB2	2.04	0.57
3:L:71:SER:OG	3:L:83:GLY:C	2.48	0.57
2:H:147:LEU:HD12	2:H:147:LEU:O	2.05	0.57
2:H:193:VAL:HG22	2:H:194:PRO:HD2	1.85	0.56
2:H:11:LEU:HB2	2:H:156:PRO:HG3	1.87	0.56
2:H:19:ARG:NH1	2:H:79:HIS:CD2	2.73	0.56
3:L:184:PRO:HA	3:L:194:ALA:HB2	1.87	0.56
3:L:22:LEU:HD11	3:L:24:LEU:CD1	2.33	0.56
2:H:133:LEU:HD11	2:H:150:LEU:HB2	1.87	0.56
1:A:393:GLY:HA2	1:A:400:ILE:CG2	2.34	0.56
2:H:163:TRP:O	2:H:165:SER:O	2.24	0.56
2:H:169:THR:O	2:H:172:VAL:HG23	2.06	0.56
3:L:66:VAL:HG21	3:L:81:PHE:CD1	2.41	0.56
2:H:139:ALA:HB1	2:H:140:THR:HG22	1.88	0.56
2:H:111:ILE:HD12	2:H:111:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:73:ARG:NH1	3:L:81:PHE:O	2.40	0.55
1:A:68:LYS:HG3	1:A:69:THR:N	2.21	0.55
1:A:146:GLU:HB2	1:A:148:VAL:HG22	1.87	0.55
3:L:112:SER:OG	3:L:113:SER:N	2.40	0.55
2:H:159:VAL:HG12	2:H:159:VAL:O	2.06	0.55
1:A:21:GLU:OE1	1:A:378:LEU:HB2	2.07	0.55
1:A:40:ARG:O	1:A:337:THR:HB	2.07	0.55
1:A:304:ARG:NE	1:A:306:ASP:OD2	2.39	0.55
1:A:349:GLU:OE2	2:H:54:GLY:HA3	2.07	0.55
2:H:147:LEU:CD2	2:H:203:TYR:HD2	2.20	0.55
3:L:169:LYS:HA	3:L:174:PRO:HA	1.88	0.55
1:A:261:GLY:N	1:A:268:ILE:O	2.31	0.55
1:A:213:ILE:HG22	1:A:258:ILE:HG22	1.90	0.54
1:A:309:TRP:O	1:A:319:TYR:HD1	1.90	0.54
1:A:356:THR:CG2	1:A:358:ASN:HB2	2.38	0.54
1:A:380:ALA:CB	1:A:427:LEU:HD11	2.38	0.54
1:A:310:TYR:HD1	1:A:319:TYR:HB2	1.72	0.54
1:A:286:ILE:CD1	1:A:304:ARG:NH2	2.70	0.54
2:H:94:TYR:HE1	3:L:62:SER:HA	1.73	0.54
1:A:127:THR:HG22	1:A:270:MET:HE2	1.88	0.54
1:A:292:CYS:HB2	1:A:385:TYR:CE1	2.43	0.54
1:A:356:THR:HG22	1:A:358:ASN:HB2	1.89	0.54
1:A:81:LEU:HA	1:A:84:VAL:HB	1.90	0.53
3:L:70:ASP:OD1	3:L:71:SER:N	2.41	0.53
1:A:152:GLY:N	1:A:158:LEU:O	2.33	0.53
1:A:343:VAL:HG22	1:A:344:ALA:N	2.21	0.53
2:H:178:VAL:HG12	2:H:178:VAL:O	2.07	0.53
3:L:181:THR:HG23	3:L:196:SER:HB2	1.90	0.53
3:L:169:LYS:HZ1	3:L:214:GLN:CD	2.15	0.53
1:A:292:CYS:HA	1:A:301:CYS:HA	1.90	0.53
1:A:217:ILE:CD1	1:A:255:GLY:HA3	2.38	0.53
3:L:108:GLN:CG	3:L:109:ALA:N	2.70	0.53
1:A:198:ARG:HA	1:A:201:LEU:HD13	1.90	0.53
2:H:36:TRP:CD1	2:H:80:LEU:HB2	2.44	0.53
2:H:159:VAL:HG22	2:H:209:HIS:HB2	1.90	0.53
3:L:55:TYR:CE1	3:L:65:LEU:HD12	2.37	0.53
1:A:307:GLN:CB	1:A:308:GLY:HA2	2.14	0.53
1:A:163:ARG:CG	1:A:164:GLU:N	2.70	0.53
2:H:7:SER:HB3	2:H:21:SER:HB2	1.90	0.53
1:A:258:ILE:HG13	1:A:270:MET:CE	2.40	0.52
3:L:115:ALA:O	3:L:116:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:HA	1:A:159:ALA:HB3	1.92	0.52
1:A:218:SER:OG	1:A:221:LEU:N	2.40	0.52
2:H:4:LEU:HD11	2:H:27:PHE:HZ	1.75	0.52
2:H:59:TYR:HE1	2:H:69:ILE:HG22	1.74	0.52
3:L:128:GLN:HG3	3:L:160:TYR:CZ	2.45	0.52
3:L:144:GLU:OE1	3:L:151:THR:HB	2.10	0.52
1:A:20:LYS:CD	3:L:50:LYS:HA	2.38	0.52
1:A:127:THR:CG2	1:A:258:ILE:HD12	2.40	0.51
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.92	0.51
2:H:70:SER:O	2:H:78:LEU:HD12	2.10	0.51
1:A:133:GLU:OE2	1:A:134:VAL:HG23	2.11	0.51
2:H:203:TYR:O	2:H:220:VAL:HG12	2.11	0.51
3:L:40:ILE:HD11	3:L:54:TRP:CH2	2.45	0.51
1:A:322:ASN:HB2	1:A:324:LYS:O	2.10	0.51
1:A:399:ILE:O	1:A:399:ILE:CG2	2.56	0.51
1:A:258:ILE:HD11	1:A:270:MET:HE3	1.92	0.51
1:A:320:TYR:HD2	1:A:326:CYS:SG	2.34	0.51
2:H:74:SER:OG	2:H:75:LYS:N	2.44	0.51
3:L:214:GLN:HE21	3:L:221:THR:HG21	1.74	0.51
1:A:383:ALA:HB1	1:A:385:TYR:HE2	1.74	0.51
1:A:365:THR:HG22	1:A:366:GLY:N	2.26	0.51
3:L:25:ILE:O	3:L:25:ILE:HG22	2.10	0.51
1:A:309:TRP:CZ3	1:A:333:VAL:HG21	2.45	0.51
1:A:428:SER:HB2	1:A:430:VAL:H	1.76	0.51
3:L:32:VAL:HG21	3:L:38:ALA:HB3	1.90	0.51
3:L:186:LYS:HE3	3:L:190:ASN:HA	1.93	0.51
2:H:161:VAL:HG22	2:H:207:VAL:HG22	1.92	0.50
1:A:388:VAL:CG1	1:A:389:SER:N	2.75	0.50
1:A:261:GLY:O	1:A:268:ILE:N	2.39	0.50
2:H:33:TYR:HB2	2:H:98:VAL:O	2.11	0.50
1:A:214:THR:HG21	1:A:221:LEU:HD11	1.93	0.50
2:H:147:LEU:HD12	2:H:147:LEU:C	2.37	0.50
1:A:223:THR:HB	1:A:226:GLU:HB2	1.93	0.50
3:L:66:VAL:HA	3:L:77:ILE:HD12	1.94	0.50
1:A:184:ILE:O	1:A:185:ALA:HB2	2.10	0.50
1:A:359:TYR:O	1:A:360:PRO:C	2.54	0.50
1:A:199:ARG:O	1:A:203:VAL:HG23	2.11	0.49
1:A:307:GLN:CB	1:A:308:GLY:CA	2.88	0.49
1:A:392:ILE:HG21	1:A:410:ILE:HD13	1.94	0.49
2:H:33:TYR:OH	2:H:104:GLY:O	2.19	0.49
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HD2	1:A:21:GLU:O	2.12	0.49
1:A:40:ARG:O	1:A:337:THR:CG2	2.60	0.49
1:A:428:SER:CB	1:A:430:VAL:H	2.25	0.49
2:H:67:PHE:N	2:H:67:PHE:CD1	2.80	0.49
2:H:101:ARG:NH2	3:L:51:TYR:HD2	2.09	0.49
3:L:128:GLN:HG3	3:L:160:TYR:OH	2.12	0.49
3:L:201:THR:HG23	3:L:204:GLN:H	1.77	0.49
1:A:304:ARG:HB3	1:A:306:ASP:OD2	2.13	0.49
1:A:318:VAL:HG22	1:A:320:TYR:CE1	2.40	0.49
1:A:380:ALA:HB3	1:A:427:LEU:HD11	1.93	0.49
3:L:58:LYS:HB3	3:L:59:PRO:HD2	1.95	0.49
1:A:193:PHE:HD1	1:A:196:PHE:CE2	2.30	0.49
1:A:310:TYR:CE1	1:A:319:TYR:HB2	2.47	0.49
3:L:40:ILE:O	3:L:40:ILE:HG13	2.12	0.49
3:L:68:TYR:N	3:L:68:TYR:CD2	2.80	0.49
1:A:258:ILE:CD1	1:A:270:MET:CE	2.91	0.49
1:A:262:VAL:HG13	1:A:263:TYR:N	2.27	0.49
1:A:328:THR:HG21	1:A:431:GLU:OE2	2.13	0.49
1:A:221:LEU:O	1:A:269:TYR:OH	2.23	0.49
1:A:66:LEU:O	1:A:67:ILE:HG23	2.13	0.49
3:L:114:THR:HG23	3:L:115:ALA:N	2.28	0.49
1:A:83:THR:O	1:A:87:ASP:N	2.46	0.48
1:A:320:TYR:CE2	1:A:335:CYS:HB3	2.47	0.48
2:H:63:VAL:HG23	2:H:63:VAL:O	2.12	0.48
3:L:146:GLN:O	3:L:146:GLN:NE2	2.46	0.48
1:A:217:ILE:HD12	1:A:217:ILE:N	2.27	0.48
2:H:4:LEU:HD23	2:H:95:CYS:SG	2.52	0.48
3:L:54:TRP:O	3:L:66:VAL:HG12	2.14	0.48
3:L:182:THR:HG22	3:L:195:SER:H	1.76	0.48
1:A:65:SER:C	1:A:66:LEU:HD12	2.39	0.48
1:A:65:SER:HB3	1:A:188:LYS:HE3	1.96	0.48
2:H:41:PRO:HG3	2:H:117:MET:HE1	1.95	0.48
2:H:204:ILE:HG23	2:H:218:LYS:O	2.13	0.48
3:L:57:GLN:HB2	3:L:63:PRO:HB3	1.94	0.48
1:A:202:ASN:O	1:A:206:GLN:HG3	2.13	0.48
2:H:4:LEU:HD13	2:H:111:ILE:HD13	1.95	0.48
1:A:346:GLN:O	1:A:359:TYR:CD2	2.61	0.48
2:H:181:SER:N	3:L:180:GLU:OE2	2.41	0.48
4:C:2:NAG:H5	4:C:3:BMA:C2	2.44	0.48
1:A:19:LEU:CD2	1:A:35:TYR:CE1	2.96	0.48
1:A:286:ILE:O	1:A:307:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:VAL:HG13	1:A:389:SER:H	1.79	0.48
2:H:133:LEU:HB2	2:H:148:GLY:O	2.14	0.48
1:A:71:LEU:O	1:A:74:THR:OG1	2.21	0.48
1:A:312:LYS:HB3	1:A:317:THR:HA	1.96	0.47
2:H:193:VAL:HG11	2:H:203:TYR:HE2	1.78	0.47
3:L:181:THR:OG1	3:L:196:SER:OG	2.20	0.47
1:A:81:LEU:HD21	1:A:208:SER:HB3	1.96	0.47
1:A:350:CYS:O	1:A:354:ILE:HD12	2.14	0.47
3:L:152:LEU:N	3:L:198:LEU:O	2.41	0.47
2:H:178:VAL:HG23	3:L:182:THR:HB	1.96	0.47
3:L:40:ILE:HD11	3:L:54:TRP:CZ3	2.49	0.47
1:A:39:LEU:CD2	1:A:335:CYS:HB2	2.44	0.47
1:A:196:PHE:CG	1:A:196:PHE:O	2.68	0.47
1:A:304:ARG:HH21	1:A:306:ASP:HB2	1.80	0.47
2:H:37:VAL:O	2:H:37:VAL:HG12	2.13	0.47
3:L:80:ARG:HB2	3:L:96:GLY:H	1.80	0.47
1:A:85:SER:HA	1:A:89:LEU:HD13	1.95	0.47
1:A:24:LEU:N	1:A:24:LEU:HD12	2.30	0.47
3:L:201:THR:HG22	3:L:204:GLN:NE2	2.29	0.47
3:L:203:GLU:O	3:L:207:SER:HB3	2.14	0.47
1:A:20:LYS:HG3	1:A:21:GLU:N	2.30	0.46
1:A:198:ARG:O	1:A:202:ASN:ND2	2.47	0.46
1:A:129:ARG:HH12	1:A:156:ARG:HB2	1.81	0.46
2:H:4:LEU:HD23	2:H:22:CYS:SG	2.56	0.46
2:H:49:SER:OG	2:H:50:VAL:N	2.49	0.46
2:H:193:VAL:HG11	2:H:203:TYR:CE2	2.51	0.46
3:L:156:ILE:CG2	3:L:157:SER:N	2.78	0.46
1:A:306:ASP:O	1:A:310:TYR:OH	2.30	0.46
3:L:232:SER:HA	3:L:233:MET:HA	1.72	0.46
3:L:148:ASN:CG	3:L:148:ASN:O	2.58	0.46
1:A:37:SER:OG	1:A:281:THR:HB	2.16	0.46
1:A:39:LEU:HD21	1:A:335:CYS:HB2	1.97	0.46
2:H:214:THR:O	2:H:214:THR:HG22	2.15	0.46
3:L:67:ILE:HD11	3:L:82:SER:HA	1.98	0.46
1:A:68:LYS:CG	1:A:69:THR:N	2.79	0.45
2:H:13:GLN:O	2:H:13:GLN:HG3	2.17	0.45
2:H:27:PHE:CD1	2:H:28:THR:O	2.68	0.45
1:A:129:ARG:NH1	1:A:156:ARG:HB2	2.31	0.45
2:H:169:THR:O	2:H:172:VAL:CG2	2.65	0.45
2:H:35:SER:HB3	2:H:50:VAL:HG23	1.98	0.45
1:A:137:ILE:O	1:A:138:LYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HG22	1:A:358:ASN:H	1.80	0.45
2:H:11:LEU:CD1	2:H:155:PHE:CE2	3.00	0.45
1:A:126:LYS:O	1:A:130:LEU:HD12	2.17	0.45
1:A:133:GLU:HG3	1:A:134:VAL:O	2.17	0.45
1:A:269:TYR:O	1:A:269:TYR:CD1	2.66	0.45
3:L:111:ASP:O	3:L:112:SER:C	2.57	0.45
1:A:124:ILE:O	1:A:127:THR:N	2.48	0.45
1:A:156:ARG:HA	1:A:156:ARG:HD3	1.67	0.45
2:H:9:GLY:HA2	2:H:18:ARG:HD3	1.99	0.45
1:A:38:VAL:HG21	1:A:243:LEU:HD21	1.98	0.45
1:A:83:THR:HA	1:A:86:ALA:HB3	1.99	0.45
1:A:279:ILE:HG23	1:A:280:ASP:N	2.29	0.45
3:L:227:ALA:HB1	3:L:228:PRO:CD	2.46	0.45
1:A:30:THR:O	1:A:30:THR:HG22	2.13	0.45
1:A:56:GLU:OE1	1:A:56:GLU:HA	2.16	0.45
1:A:260:ILE:N	1:A:268:ILE:O	2.49	0.45
3:L:198:LEU:HD22	3:L:200:LEU:HD21	1.99	0.45
2:H:35:SER:HB2	2:H:50:VAL:HA	1.99	0.45
2:H:33:TYR:HD1	2:H:52:TYR:HA	1.82	0.45
2:H:180:GLN:OE1	2:H:186:SER:OG	2.32	0.45
2:H:209:HIS:CE1	2:H:212:SER:HG	2.24	0.45
1:A:53:GLY:O	1:A:164:GLU:C	2.60	0.44
3:L:167:ALA:N	3:L:214:GLN:O	2.35	0.44
1:A:50:LEU:O	1:A:267:VAL:HG12	2.17	0.44
1:A:135:ASN:HB2	1:A:138:LYS:CB	2.46	0.44
1:A:147:ALA:O	1:A:162:VAL:HG12	2.16	0.44
1:A:286:ILE:CD1	1:A:304:ARG:HH22	2.30	0.44
1:A:213:ILE:HD12	1:A:213:ILE:O	2.18	0.44
3:L:176:LYS:O	3:L:179:VAL:HG12	2.17	0.44
4:C:3:BMA:H61	4:C:5:MAN:H2	1.62	0.44
1:A:23:TYR:CE1	1:A:409:TYR:HB2	2.52	0.44
1:A:74:THR:OG1	1:A:75:LYS:N	2.50	0.44
1:A:127:THR:HA	1:A:130:LEU:HB2	2.00	0.44
1:A:148:VAL:HG23	1:A:149:SER:N	2.33	0.44
1:A:144:THR:HA	1:A:145:ASN:HA	1.38	0.44
2:H:33:TYR:CE1	2:H:52:TYR:HD1	2.36	0.44
2:H:150:LEU:O	2:H:150:LEU:HD23	2.16	0.44
3:L:102:GLU:OE1	3:L:128:GLN:NE2	2.50	0.44
1:A:76:SER:O	1:A:80:GLU:N	2.46	0.44
2:H:11:LEU:CD1	2:H:155:PHE:HE2	2.30	0.44
3:L:43:SER:HB3	3:L:89:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:ASN:N	2:H:204:ILE:O	2.45	0.44
1:A:163:ARG:CD	1:A:164:GLU:H	2.31	0.43
3:L:47:LEU:O	3:L:49:ASP:HA	2.18	0.43
2:H:164:ASN:O	2:H:206:ASN:ND2	2.47	0.43
2:H:193:VAL:HG21	2:H:203:TYR:CZ	2.53	0.43
1:A:33:GLU:CD	2:H:101:ARG:HH21	2.25	0.43
2:H:82:MET:CE	2:H:85:LEU:HD11	2.48	0.43
2:H:85:LEU:HA	2:H:85:LEU:HD23	1.71	0.43
2:H:126:LYS:HD3	2:H:184:LEU:CD2	2.47	0.43
3:L:156:ILE:CG2	3:L:157:SER:H	2.25	0.43
1:A:163:ARG:HA	1:A:163:ARG:HD3	1.93	0.43
1:A:319:TYR:C	1:A:320:TYR:CD1	2.97	0.43
1:A:378:LEU:O	1:A:412:ASN:ND2	2.52	0.43
2:H:29:VAL:HG13	2:H:30:SER:H	1.83	0.43
3:L:44:GLY:O	3:L:45:ASP:O	2.36	0.43
2:H:128:PRO:HD2	2:H:214:THR:HG21	2.00	0.43
1:A:411:THR:OG1	1:A:412:ASN:N	2.51	0.43
3:L:30:VAL:HG21	3:L:40:ILE:HG22	2.01	0.43
4:C:1:NAG:H4	4:C:2:NAG:H2	1.61	0.43
1:A:302:LEU:HG	1:A:303:LEU:N	2.34	0.43
3:L:68:TYR:O	3:L:69:GLN:C	2.62	0.43
2:H:139:ALA:HB1	2:H:140:THR:CG2	2.48	0.43
1:A:137:ILE:HD12	1:A:138:LYS:CA	2.46	0.43
1:A:287:LYS:HA	1:A:287:LYS:HD2	1.51	0.43
1:A:392:ILE:CG2	1:A:410:ILE:HD13	2.49	0.43
1:A:424:VAL:HG23	1:A:424:VAL:O	2.19	0.43
2:H:41:PRO:CG	2:H:117:MET:HE1	2.49	0.43
1:A:72:ASP:OD1	1:A:73:LEU:N	2.52	0.43
1:A:309:TRP:CH2	1:A:333:VAL:HG21	2.54	0.43
2:H:101:ARG:NH2	3:L:51:TYR:CD2	2.86	0.43
3:L:201:THR:O	3:L:202:PRO:C	2.58	0.43
1:A:251:VAL:HG13	1:A:274:PRO:HG2	2.01	0.42
3:L:230:GLU:CD	3:L:230:GLU:C	2.87	0.42
1:A:317:THR:HG23	1:A:345:GLU:HG2	2.01	0.42
1:A:320:TYR:CD1	1:A:320:TYR:N	2.86	0.42
3:L:152:LEU:HB2	3:L:198:LEU:HB3	2.00	0.42
3:L:201:THR:OG1	3:L:203:GLU:OE1	2.28	0.42
3:L:65:LEU:CD2	3:L:74:PRO:HG3	2.47	0.42
1:A:120:ALA:HA	1:A:123:ALA:HB3	2.01	0.42
3:L:30:VAL:HG12	3:L:31:SER:N	2.32	0.42
1:A:319:TYR:C	1:A:320:TYR:HD1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:77:ILE:HG23	3:L:78:PRO:HD2	2.01	0.42
1:A:39:LEU:O	1:A:276:PHE:HA	2.20	0.42
2:H:50:VAL:O	2:H:50:VAL:HG13	2.20	0.42
3:L:187:GLN:HG3	3:L:189:ASN:H	1.84	0.42
1:A:286:ILE:HD12	1:A:304:ARG:NH2	2.34	0.42
1:A:347:SER:HA	1:A:359:TYR:CD2	2.55	0.42
2:H:18:ARG:CG	2:H:19:ARG:N	2.82	0.42
2:H:73:THR:O	2:H:73:THR:HG23	2.19	0.42
2:H:210:LYS:N	2:H:211:PRO:HD2	2.35	0.42
3:L:152:LEU:HD23	3:L:152:LEU:HA	1.86	0.42
1:A:32:THR:HG21	1:A:377:PRO:HG2	2.00	0.42
3:L:70:ASP:C	3:L:72:GLU:N	2.76	0.42
3:L:186:LYS:HD2	3:L:192:TYR:CE2	2.55	0.42
1:A:24:LEU:HD23	1:A:351:ASN:O	2.20	0.42
1:A:178:ASN:ND2	1:A:180:ASN:HD22	2.18	0.42
1:A:349:GLU:CG	1:A:356:THR:HG21	2.49	0.42
1:A:20:LYS:CG	1:A:21:GLU:N	2.83	0.42
1:A:162:VAL:CG2	1:A:163:ARG:N	2.83	0.42
2:H:147:LEU:HD21	2:H:203:TYR:CE2	2.55	0.42
3:L:108:GLN:HE22	3:L:110:TRP:NE1	2.17	0.42
1:A:114:THR:O	1:A:114:THR:OG1	2.36	0.41
1:A:258:ILE:CG1	1:A:270:MET:CE	2.97	0.41
2:H:69:ILE:HG23	2:H:69:ILE:O	2.19	0.41
2:H:148:GLY:HA2	2:H:163:TRP:CZ2	2.53	0.41
2:H:181:SER:OG	3:L:180:GLU:OE2	2.30	0.41
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.73	0.41
3:L:156:ILE:H	3:L:156:ILE:HD12	1.85	0.41
1:A:228:ALA:O	1:A:231:VAL:HB	2.20	0.41
3:L:102:GLU:OE2	3:L:186:LYS:NZ	2.38	0.41
3:L:145:LEU:CD2	3:L:150:ALA:HB2	2.50	0.41
2:H:209:HIS:CE1	2:H:212:SER:HB3	2.55	0.41
3:L:45:ASP:CG	3:L:46:LYS:H	2.29	0.41
3:L:108:GLN:HG2	3:L:109:ALA:H	1.82	0.41
3:L:140:PRO:HD2	3:L:205:TRP:CZ2	2.55	0.41
4:C:1:NAG:O7	4:C:1:NAG:O3	2.33	0.41
2:H:34:MET:HE3	2:H:34:MET:HB3	1.58	0.41
3:L:68:TYR:CG	3:L:69:GLN:N	2.88	0.41
1:A:20:LYS:HE2	3:L:50:LYS:HG3	2.01	0.41
1:A:127:THR:CG2	1:A:270:MET:CE	2.87	0.41
2:H:185:TYR:CD1	2:H:185:TYR:N	2.89	0.41
2:H:201:GLN:OE1	2:H:202:THR:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:68:TYR:HD2	3:L:68:TYR:N	2.13	0.41
3:L:73:ARG:NH1	3:L:73:ARG:HB3	2.36	0.41
3:L:138:PHE:HA	3:L:139:PRO:HD2	1.96	0.41
1:A:204:VAL:O	1:A:207:PHE:N	2.53	0.41
1:A:262:VAL:O	1:A:266:SER:O	2.39	0.41
1:A:323:ASP:OD1	1:A:323:ASP:N	2.54	0.41
1:A:403:LEU:HA	1:A:404:PRO:HD3	1.85	0.41
3:L:99:ALA:O	3:L:190:ASN:ND2	2.54	0.41
1:A:301:CYS:SG	1:A:369:PRO:HB3	2.61	0.40
1:A:180:ASN:O	1:A:182:CYS:HB2	2.20	0.40
3:L:26:GLN:HE21	3:L:120:GLY:N	2.18	0.40
1:A:262:VAL:HG22	1:A:263:TYR:O	2.21	0.40
1:A:359:TYR:O	1:A:359:TYR:CG	2.73	0.40
2:H:47:TRP:HZ2	2:H:50:VAL:HB	1.86	0.40
2:H:170:SER:O	2:H:172:VAL:HG23	2.21	0.40
3:L:66:VAL:HG21	3:L:81:PHE:CE1	2.56	0.40
4:C:2:NAG:H5	4:C:3:BMA:O2	2.21	0.40
1:A:86:ALA:HA	1:A:90:ALA:HB3	2.02	0.40
1:A:403:LEU:HD11	1:A:410:ILE:HD11	2.02	0.40
2:H:92:ILE:O	2:H:93:TYR:CD1	2.75	0.40
2:H:173:HIS:CG	2:H:175:PHE:HE2	2.39	0.40
3:L:153:VAL:HG13	3:L:155:LEU:CD1	2.49	0.40
1:A:37:SER:CB	1:A:283:CYS:SG	3.08	0.40
2:H:52:TYR:HB2	2:H:56:THR:O	2.22	0.40
2:H:80:LEU:C	2:H:80:LEU:HD12	2.46	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	377/415 (91%)	327 (87%)	48 (13%)	2 (0%)	24 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	24	54
3	L	211/213 (99%)	197 (93%)	14 (7%)	0	100	100
All	All	806/848 (95%)	728 (90%)	75 (9%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	MET
2	H	141	SER
1	A	162	VAL

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	279/347 (80%)	243 (87%)	36 (13%)	4	16
2	H	182/182 (100%)	156 (86%)	26 (14%)	3	13
3	L	178/178 (100%)	157 (88%)	21 (12%)	5	20
All	All	639/707 (90%)	556 (87%)	83 (13%)	4	16

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	24	LEU
1	A	30	THR
1	A	31	ILE
1	A	36	LEU
1	A	52	VAL
1	A	60	CYS
1	A	65	SER
1	A	69	THR
1	A	78	LEU
1	A	122	ILE

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Mol	Chain	Res	Type
1	A	134	VAL
1	A	146	GLU
1	A	148	VAL
1	A	192	SER
1	A	202	ASN
1	A	213	ILE
1	A	218	SER
1	A	231	VAL
1	A	262	VAL
1	A	269	TYR
1	A	279	ILE
1	A	281	THR
1	A	285	ILE
1	A	287	LYS
1	A	306	ASP
1	A	349	GLU
1	A	356	THR
1	A	357	THR
1	A	359	TYR
1	A	388	VAL
1	A	392	ILE
1	A	400	ILE
1	A	423	THR
1	A	427	LEU
1	A	430	VAL
2	H	28	THR
2	H	31	SER
2	H	32	SER
2	H	34	MET
2	H	37	VAL
2	H	48	ILE
2	H	53	SER
2	H	64	LYS
2	H	70	SER
2	H	81	GLN
2	H	90	THR
2	H	98	VAL
2	H	119	THR
2	H	122	SER
2	H	124	SER
2	H	125	THR
2	H	144	THR

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Mol	Chain	Res	Type
2	H	150	LEU
2	H	159	VAL
2	H	178	VAL
2	H	179	LEU
2	H	187	LEU
2	H	190	VAL
2	H	193	VAL
2	H	205	CYS
2	H	214	THR
3	L	21	GLU
3	L	25	ILE
3	L	40	ILE
3	L	64	VAL
3	L	65	LEU
3	L	68	TYR
3	L	72	GLU
3	L	75	SER
3	L	77	ILE
3	L	95	SER
3	L	114	THR
3	L	116	VAL
3	L	121	THR
3	L	123	LEU
3	L	126	LEU
3	L	142	SER
3	L	173	SER
3	L	198	LEU
3	L	207	SER
3	L	210	SER
3	L	232	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	247	ASN
1	A	272	GLN
1	A	342	ASN
1	A	412	ASN
3	L	26	GLN
3	L	146	GLN
3	L	204	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 ⓘ

10 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	B	1	4,1	14,14,15	2.33	6 (42%)	17,19,21	1.31	3 (17%)
4	NAG	B	2	4	14,14,15	2.34	6 (42%)	17,19,21	1.26	3 (17%)
4	BMA	B	3	4	11,11,12	2.44	4 (36%)	15,15,17	1.39	3 (20%)
4	MAN	B	4	4	11,11,12	2.51	4 (36%)	15,15,17	1.15	1 (6%)
4	MAN	B	5	4	11,11,12	2.58	5 (45%)	15,15,17	1.13	0
4	NAG	C	1	4,1	14,14,15	2.22	5 (35%)	17,19,21	1.69	4 (23%)
4	NAG	C	2	4	14,14,15	2.42	6 (42%)	17,19,21	1.61	3 (17%)
4	BMA	C	3	4	11,11,12	2.56	6 (54%)	15,15,17	1.98	4 (26%)
4	MAN	C	4	4	11,11,12	2.29	4 (36%)	15,15,17	1.13	1 (6%)
4	MAN	C	5	4	11,11,12	2.40	3 (27%)	15,15,17	2.17	7 (46%)

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	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1

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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5	MAN	O5-C5	6.63	1.56	1.43
4	C	4	MAN	O5-C5	6.12	1.55	1.43
4	B	4	MAN	O5-C5	4.93	1.53	1.43
4	C	3	BMA	C4-C3	-4.89	1.39	1.52
4	C	2	NAG	C7-N2	4.84	1.50	1.34
4	B	3	BMA	C4-C3	-4.74	1.40	1.52
4	C	3	BMA	C2-C3	-4.46	1.45	1.52
4	B	2	NAG	C1-C2	-4.41	1.46	1.52
4	B	5	MAN	O5-C5	4.38	1.52	1.43
4	B	1	NAG	C7-N2	4.33	1.48	1.34
4	B	2	NAG	C7-N2	4.32	1.48	1.34
4	C	1	NAG	C1-C2	-4.12	1.46	1.52
4	B	1	NAG	C1-C2	-4.06	1.46	1.52
4	C	1	NAG	C7-N2	3.95	1.47	1.34
4	C	1	NAG	O5-C1	3.90	1.50	1.43
4	B	5	MAN	O2-C2	-3.78	1.35	1.43
4	B	5	MAN	C4-C3	-3.75	1.42	1.52
4	B	1	NAG	O5-C1	3.70	1.49	1.43
4	B	4	MAN	C4-C3	-3.67	1.42	1.52
4	B	4	MAN	O2-C2	-3.59	1.35	1.43
4	B	3	BMA	C2-C3	-3.47	1.47	1.52
4	B	2	NAG	O5-C1	3.47	1.49	1.43
4	B	3	BMA	O5-C1	-3.47	1.37	1.43
4	C	2	NAG	C1-C2	-3.23	1.48	1.52
4	C	2	NAG	C2-N2	3.20	1.51	1.46
4	C	2	NAG	O5-C1	3.16	1.49	1.43
4	B	5	MAN	O5-C1	-3.14	1.38	1.43
4	C	2	NAG	C4-C3	-2.96	1.44	1.52
4	C	2	NAG	C3-C2	-2.85	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3	BMA	O2-C2	-2.79	1.37	1.43
4	B	2	NAG	C3-C2	-2.76	1.46	1.52
4	B	1	NAG	C3-C2	-2.63	1.47	1.52
4	C	3	BMA	O5-C1	-2.62	1.39	1.43
4	C	3	BMA	O2-C2	-2.59	1.37	1.43
4	C	5	MAN	C1-C2	2.59	1.58	1.52
4	C	4	MAN	C1-C2	2.50	1.58	1.52
4	B	1	NAG	C4-C3	-2.46	1.45	1.52
4	C	1	NAG	C3-C2	-2.43	1.47	1.52
4	B	2	NAG	C4-C3	-2.40	1.46	1.52
4	B	1	NAG	C2-N2	2.39	1.50	1.46
4	C	3	BMA	O5-C5	2.38	1.48	1.43
4	C	1	NAG	C4-C3	-2.35	1.46	1.52
4	B	4	MAN	O5-C1	-2.34	1.39	1.43
4	B	2	NAG	C2-N2	2.33	1.50	1.46
4	B	5	MAN	C2-C3	-2.28	1.49	1.52
4	C	4	MAN	C4-C3	-2.19	1.46	1.52
4	C	4	MAN	O2-C2	-2.19	1.38	1.43
4	C	3	BMA	O4-C4	-2.05	1.37	1.43
4	C	5	MAN	C4-C3	-2.03	1.47	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BMA	C1-C2-C3	-5.29	101.95	109.64
4	C	5	MAN	C1-O5-C5	4.15	117.75	112.19
4	C	1	NAG	C2-N2-C7	-4.02	117.51	122.90
4	C	5	MAN	O2-C2-C3	3.37	117.13	110.15
4	C	5	MAN	O6-C6-C5	3.31	122.61	111.33
4	C	2	NAG	C8-C7-N2	3.11	121.27	116.12
4	C	3	BMA	O4-C4-C3	-3.02	103.25	110.38
4	C	2	NAG	O7-C7-C8	-3.01	116.70	122.05
4	C	3	BMA	O6-C6-C5	2.99	121.50	111.33
4	C	1	NAG	C3-C4-C5	2.84	115.39	110.23
4	C	5	MAN	C6-C5-C4	2.78	119.84	113.02
4	B	3	BMA	O3-C3-C2	2.68	115.53	110.05
4	B	3	BMA	O4-C4-C3	-2.68	104.07	110.38
4	B	2	NAG	C8-C7-N2	2.63	120.48	116.12
4	B	2	NAG	O6-C6-C5	2.60	120.18	111.33
4	C	2	NAG	O5-C1-C2	2.54	115.22	111.29
4	C	1	NAG	C8-C7-N2	2.48	120.22	116.12
4	B	1	NAG	C8-C7-N2	2.47	120.21	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	MAN	O5-C1-C2	2.47	116.67	110.79
4	B	1	NAG	O6-C6-C5	2.35	119.32	111.33
4	B	1	NAG	C3-C4-C5	2.34	114.47	110.23
4	C	4	MAN	O5-C5-C6	2.22	111.99	107.66
4	C	5	MAN	C2-C3-C4	2.21	114.76	110.86
4	B	4	MAN	O6-C6-C5	2.15	118.66	111.33
4	C	5	MAN	C3-C4-C5	-2.05	106.51	110.23
4	C	3	BMA	C6-C5-C4	2.03	118.01	113.02
4	B	3	BMA	O6-C6-C5	2.02	118.20	111.33
4	C	1	NAG	C4-C3-C2	2.01	113.97	111.02
4	B	2	NAG	O7-C7-C8	-2.01	118.48	122.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	B	4	MAN	O5-C5-C6-O6
4	B	4	MAN	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	B	5	MAN	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	5	MAN	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C3-C2-N2-C7
4	B	1	NAG	O5-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6

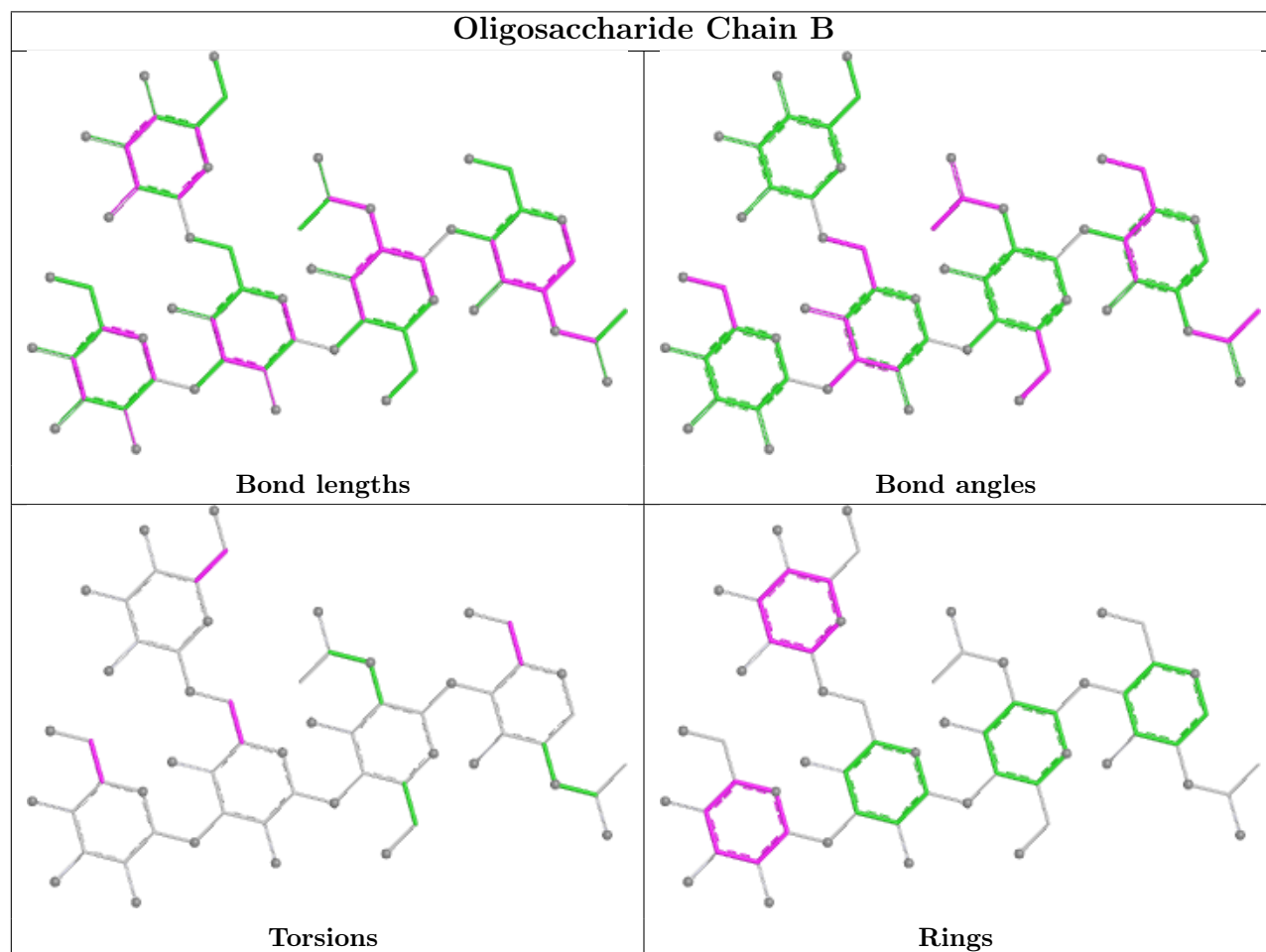
All (3) ring outliers are listed below:

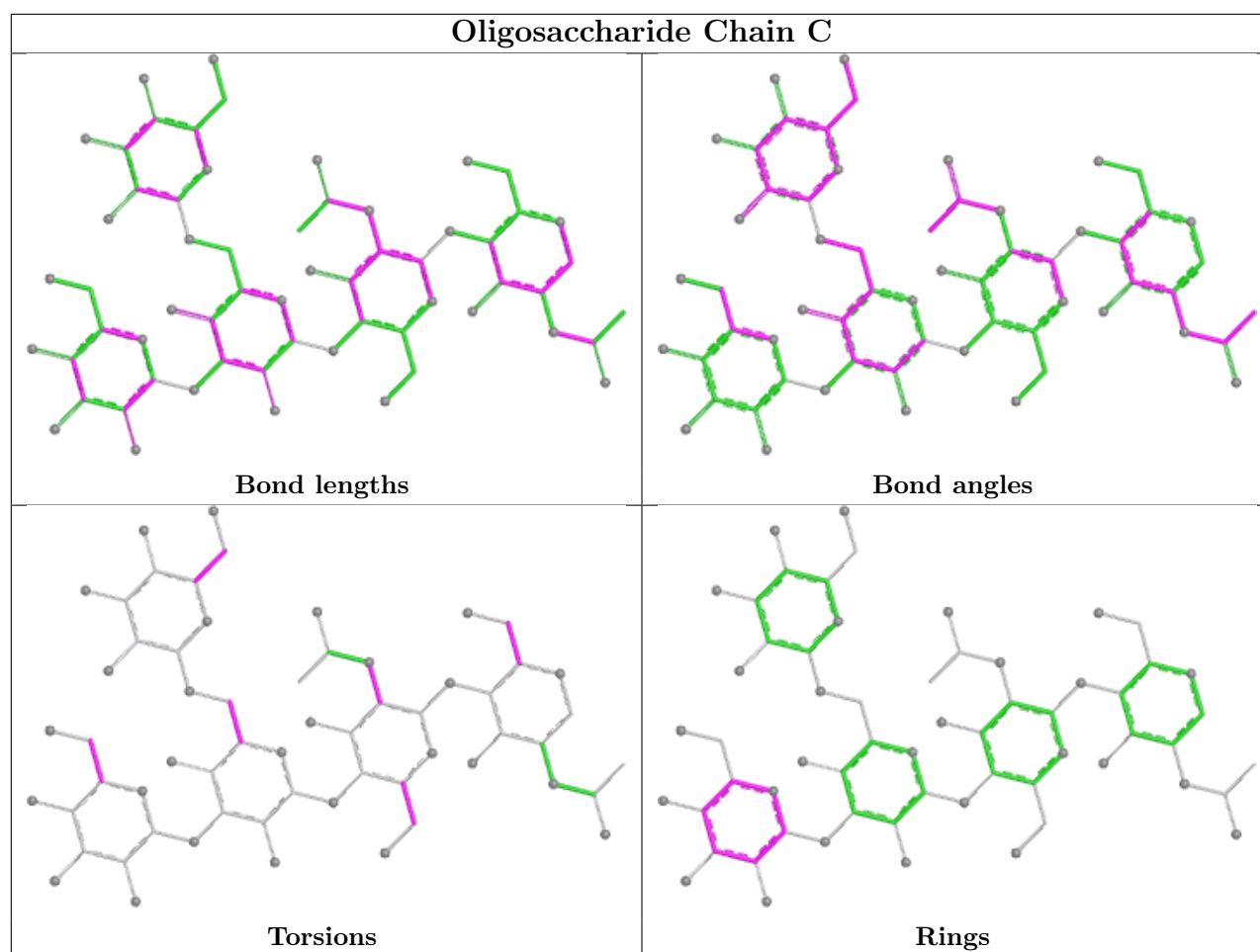
Mol	Chain	Res	Type	Atoms
4	C	4	MAN	C1-C2-C3-C4-C5-O5
4	B	5	MAN	C1-C2-C3-C4-C5-O5
4	B	4	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	BMA	3	0
4	C	5	MAN	1	0
4	B	3	BMA	1	0
4	B	4	MAN	1	0
4	C	2	NAG	3	0
4	C	1	NAG	2	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](#)

There are no ligands in this entry.

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	383/415 (92%)	1.15	81 (21%) 2 4	55, 111, 158, 178	0
2	H	220/220 (100%)	0.24	10 (4%) 38 28	44, 69, 135, 193	0
3	L	213/213 (100%)	0.40	9 (4%) 40 29	45, 86, 125, 181	0
All	All	816/848 (96%)	0.71	100 (12%) 8 9	44, 91, 152, 193	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	SER	8.4
1	A	181	LYS	7.3
1	A	66	LEU	7.2
1	A	195	GLN	6.6
1	A	67	ILE	5.9
1	A	114	THR	5.6
1	A	18	GLY	5.5
1	A	89	LEU	5.2
1	A	151	LEU	5.1
1	A	144	THR	4.9
1	A	145	ASN	4.8
1	A	432	GLY	4.7
1	A	128	ILE	4.7
1	A	197	ASN	4.5
1	A	157	VAL	4.5
1	A	52	VAL	4.4
1	A	257	GLY	4.3
1	A	314	ALA	4.3
1	A	184	ILE	4.2
1	A	155	VAL	4.2
1	A	69	THR	4.1
3	L	49	ASP	4.1
1	A	187	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	4.0
1	A	90	ALA	4.0
1	A	340	GLY	3.9
1	A	150	THR	3.7
1	A	116	ALA	3.7
1	A	263	TYR	3.7
1	A	159	ALA	3.6
2	H	139	ALA	3.6
1	A	58	LEU	3.6
1	A	193	PHE	3.5
3	L	231	CYS	3.5
1	A	256	PHE	3.5
3	L	233	MET	3.5
1	A	72	ASP	3.4
2	H	140	THR	3.4
1	A	194	SER	3.3
2	H	138	ALA	3.3
1	A	192	SER	3.2
1	A	73	LEU	3.2
1	A	84	VAL	3.2
1	A	65	SER	3.1
1	A	148	VAL	3.1
1	A	93	GLU	3.1
1	A	196	PHE	3.0
1	A	313	ASN	3.0
1	A	182	CYS	3.0
1	A	120	ALA	2.9
1	A	134	VAL	2.9
1	A	53	GLY	2.9
1	A	161	ALA	2.9
2	H	136	SER	2.8
1	A	48	PHE	2.8
2	H	104	GLY	2.8
1	A	60	CYS	2.8
1	A	129	ARG	2.8
1	A	147	ALA	2.8
1	A	271	VAL	2.7
2	H	167	ALA	2.7
1	A	179	LYS	2.7
3	L	21	GLU	2.6
3	L	232	SER	2.6
1	A	131	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	83	THR	2.6
1	A	185	ALA	2.5
1	A	61	THR	2.5
3	L	120	GLY	2.5
1	A	88	GLN	2.5
1	A	178	ASN	2.5
1	A	136	ALA	2.5
1	A	115	ALA	2.4
1	A	64	PRO	2.4
1	A	189	MET	2.4
1	A	45	THR	2.3
1	A	325	ASP	2.3
1	A	198	ARG	2.3
1	A	417	THR	2.3
3	L	48	GLY	2.3
3	L	230	GLU	2.3
1	A	206	GLN	2.3
1	A	236	THR	2.3
1	A	133	GLU	2.2
1	A	258	ILE	2.2
3	L	52	ALA	2.2
2	H	137	SER	2.2
2	H	145	ALA	2.2
1	A	316	SER	2.1
1	A	431	GLU	2.1
1	A	226	GLU	2.1
2	H	55	GLY	2.1
1	A	188	LYS	2.1
2	H	1	GLU	2.1
1	A	368	HIS	2.1
1	A	146	GLU	2.1
1	A	55	VAL	2.0
1	A	135	ASN	2.0
1	A	94	GLN	2.0
1	A	59	THR	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 ⓘ

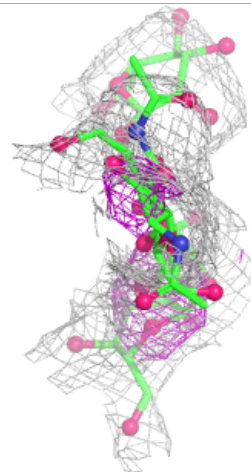
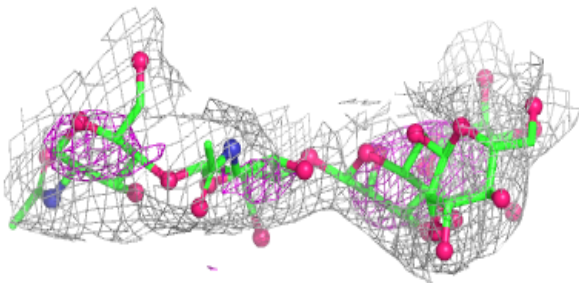
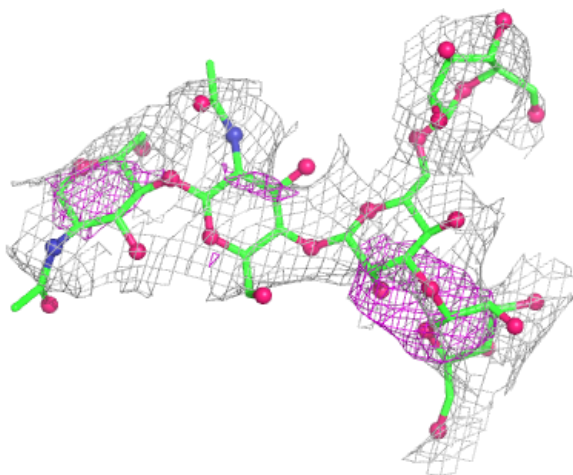
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

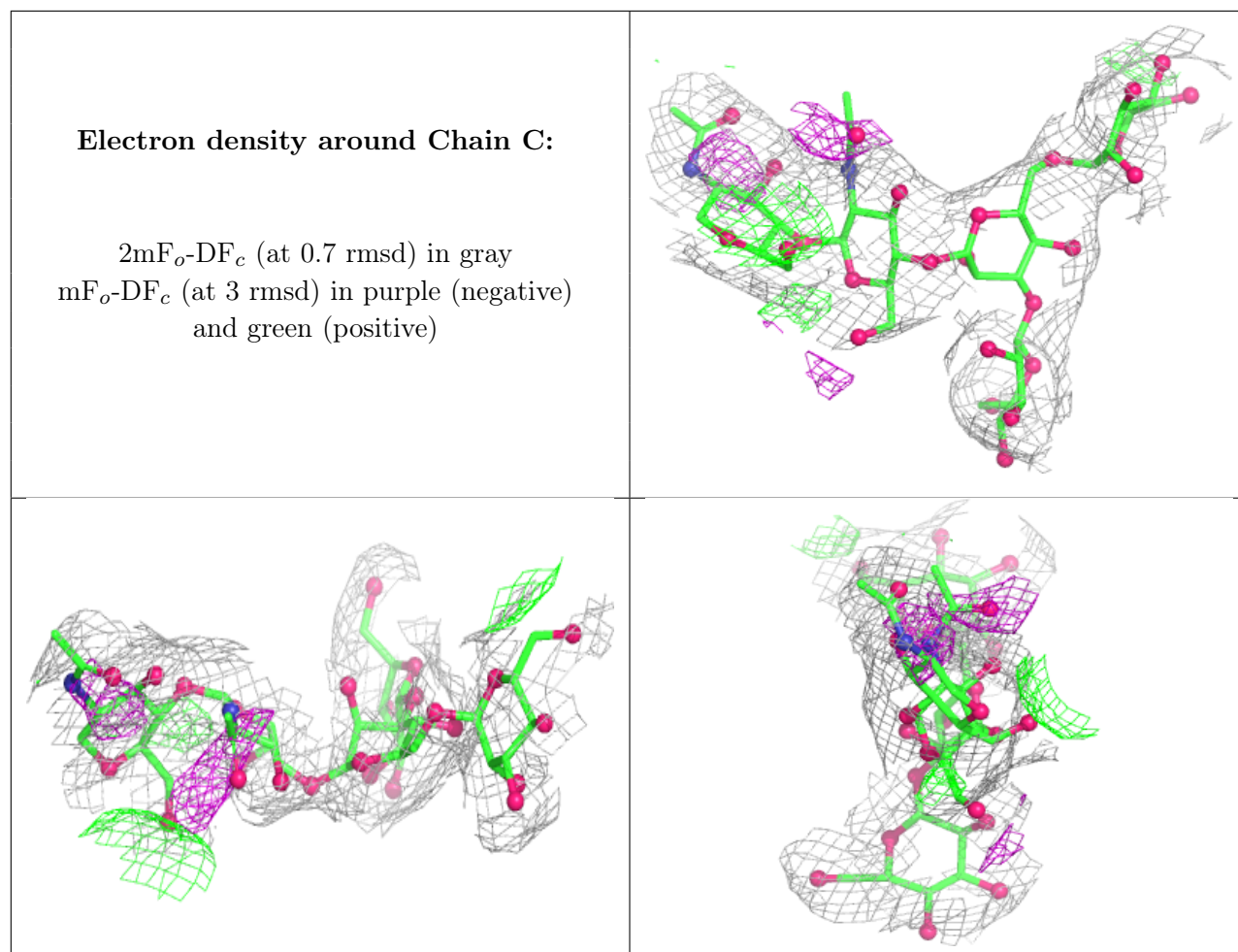
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1	14/15	-	-	127,144,158,169	0
4	NAG	B	2	14/15	-	-	138,164,173,178	0
4	BMA	B	3	11/12	-	-	175,182,187,190	0
4	MAN	B	4	11/12	-	-	138,167,189,189	0
4	MAN	B	5	11/12	-	-	144,162,175,175	0
4	NAG	C	1	14/15	-	-	40,48,70,91	0
4	NAG	C	2	14/15	-	-	97,123,150,163	0
4	BMA	C	3	11/12	-	-	143,148,164,185	0
4	MAN	C	4	11/12	-	-	105,158,187,207	0
4	MAN	C	5	11/12	-	-	124,151,190,240	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 B:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.