



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:27 PM EDT

PDB ID : 5HDH / pdb_00005hdh
Title : Crystal structure of human TLR8 with an uncleaved Z-loop
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2016-01-05
Resolution : 2.60 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

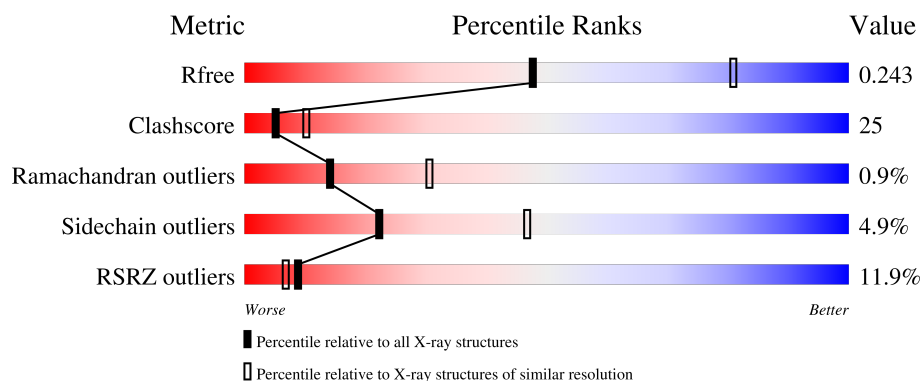
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	801	11% 58% 30% 5% 6%
2	B	4	25% 50% 25%
3	C	2	50% 50%
4	D	5	20% 80%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6371 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	751	6042	3865	1029	1128	20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ASN	ARG	engineered mutation	UNP Q9NR97
A	453	GLN	LYS	engineered mutation	UNP Q9NR97
A	454	SER	ARG	engineered mutation	UNP Q9NR97
A	455	ASN	ARG	engineered mutation	UNP Q9NR97

- Molecule 2 is an oligosaccharide called 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.



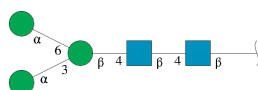
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

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



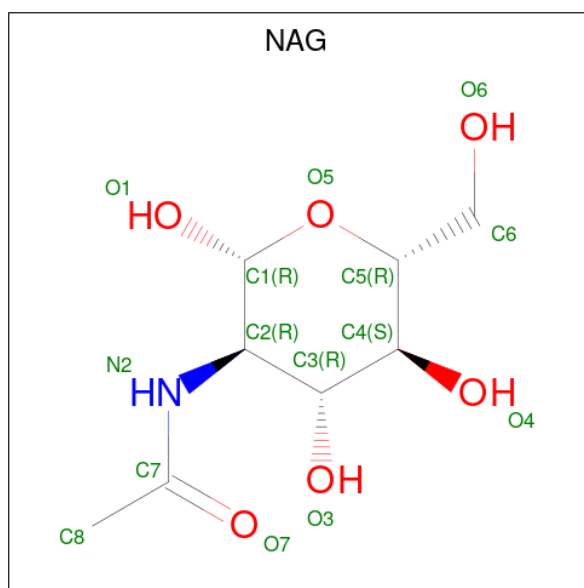
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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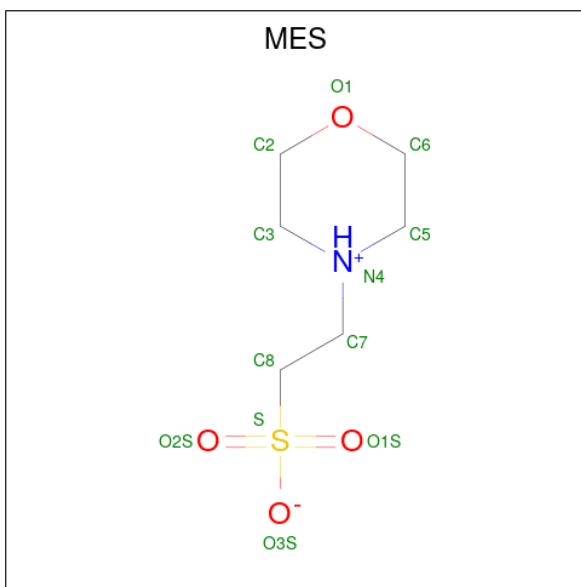
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

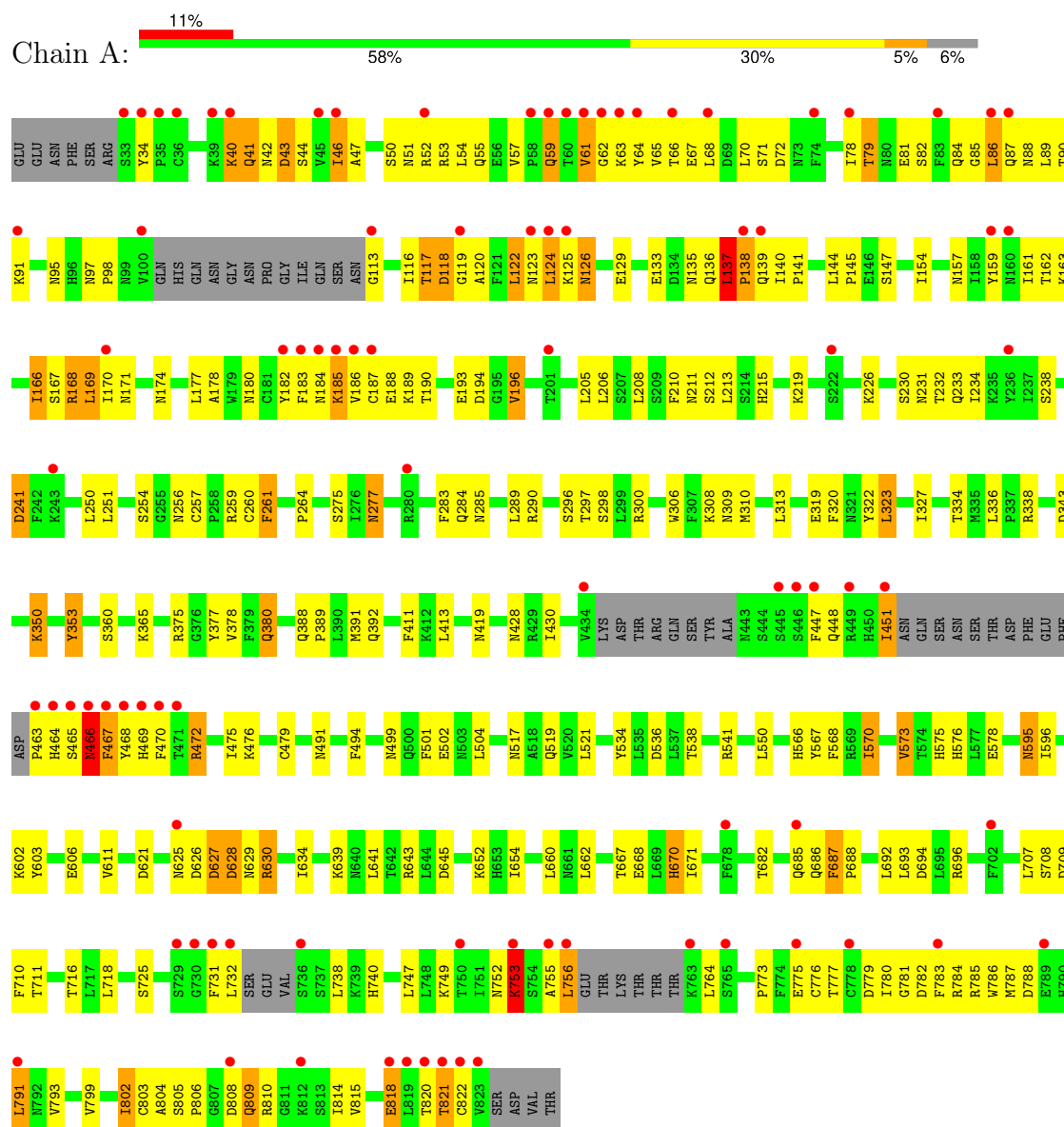
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total	O	0	0
			79	79		

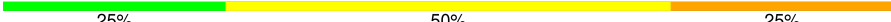
3 Residue-property plots [i](#)

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: Toll-like receptor 8



- Molecule 2: 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

Chain B:  25% 50% 25%

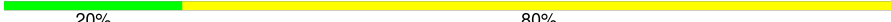


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%



- 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

Chain D:  20% 80%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	171.52Å 171.52Å 301.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.02 – 2.60 45.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.02-2.60) 100.0 (45.02-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.239 0.212 , 0.243	Depositor DCC
R_{free} test set	2610 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: SO4, NAG, MES, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	7/6164 (0.1%)	1.16	44/8355 (0.5%)

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	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	VAL	C-N	5.97	1.40	1.33
1	A	309	ASN	CA-C	-5.92	1.45	1.53
1	A	472	ARG	C-N	5.80	1.40	1.33
1	A	144	LEU	C-N	5.69	1.40	1.33
1	A	566	HIS	CG-ND1	-5.66	1.32	1.38
1	A	670	HIS	CG-ND1	-5.25	1.32	1.38
1	A	145	PRO	N-CD	5.06	1.54	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ASN	N-CA-C	9.36	124.57	112.41
1	A	377	TYR	N-CA-C	-8.38	100.81	112.45
1	A	570	ILE	N-CA-C	8.20	119.67	108.84
1	A	323	LEU	N-CA-C	8.12	121.97	112.72
1	A	166	ILE	N-CA-C	7.81	119.09	111.67
1	A	55	GLN	N-CA-C	-7.70	104.03	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	THR	N-CA-C	6.76	120.17	109.50
1	A	472	ARG	CA-C-N	-6.61	113.49	120.03
1	A	472	ARG	C-N-CA	-6.61	113.49	120.03
1	A	777	THR	N-CA-C	-6.57	100.25	110.17
1	A	57	VAL	CA-C-N	-6.53	112.78	119.83
1	A	57	VAL	C-N-CA	-6.53	112.78	119.83
1	A	802	ILE	N-CA-C	6.42	119.54	108.95
1	A	144	LEU	CA-C-N	-6.38	113.71	120.03
1	A	144	LEU	C-N-CA	-6.38	113.71	120.03
1	A	196	VAL	CB-CA-C	-6.14	103.99	112.04
1	A	634	ILE	N-CA-C	6.04	116.78	110.62
1	A	57	VAL	CB-CA-C	-5.96	104.34	110.71
1	A	308	LYS	CB-CA-C	-5.66	101.07	110.68
1	A	138	PRO	CA-N-CD	-5.61	104.15	112.00
1	A	709	ASP	N-CA-C	-5.59	106.44	113.20
1	A	174	ASN	N-CA-C	5.57	117.49	108.41
1	A	667	THR	N-CA-C	-5.55	107.14	114.31
1	A	662	LEU	N-CA-C	-5.55	102.42	110.08
1	A	687	PHE	CA-C-N	5.50	125.34	119.28
1	A	687	PHE	C-N-CA	5.50	125.34	119.28
1	A	791	LEU	N-CA-C	-5.49	106.55	113.20
1	A	654	ILE	CA-C-N	-5.47	114.12	119.76
1	A	654	ILE	C-N-CA	-5.47	114.12	119.76
1	A	652	LYS	N-CA-C	-5.43	107.02	113.97
1	A	126	ASN	N-CA-C	-5.38	105.42	112.41
1	A	360	SER	N-CA-C	5.27	117.09	110.24
1	A	753	LYS	N-CA-C	5.26	116.69	111.07
1	A	241	ASP	N-CA-C	5.24	116.99	111.28
1	A	380	GLN	N-CA-C	5.12	119.66	113.41
1	A	336	LEU	N-CA-C	5.08	118.61	110.73
1	A	639	LYS	N-CA-C	5.08	118.94	112.34
1	A	300	ARG	N-CA-C	-5.07	107.64	113.88
1	A	137	LEU	CA-C-N	-5.06	113.52	119.84
1	A	137	LEU	C-N-CA	-5.06	113.52	119.84
1	A	776	CYS	N-CA-C	5.04	118.51	110.70
1	A	79	THR	N-CA-C	5.01	116.43	108.96
1	A	257	CYS	CA-C-N	-5.00	115.41	120.21
1	A	257	CYS	C-N-CA	-5.00	115.41	120.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	TYR	Sidechain
1	A	466	ASN	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	6042	0	6035	308	0
2	B	50	0	43	5	0
3	C	28	0	25	0	0
4	D	61	0	52	0	0
5	A	84	0	78	2	0
6	A	15	0	0	0	0
7	A	12	0	13	0	0
8	A	79	0	0	5	0
All	All	6371	0	6246	308	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 25.

All (308) 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:79:THR:HA	1:A:117:THR:CG2	1.49	1.42
1:A:79:THR:HA	1:A:117:THR:HG21	1.28	1.14
1:A:79:THR:HA	1:A:117:THR:HG22	1.30	1.12
1:A:755:ALA:HA	1:A:786:TRP:HZ3	1.07	1.11
1:A:755:ALA:HA	1:A:786:TRP:CZ3	1.89	1.07
1:A:59:GLN:N	1:A:59:GLN:OE1	1.88	1.06
1:A:388:GLN:HA	1:A:391:MET:CE	1.88	1.03
1:A:91:LYS:HG3	1:A:129:GLU:HB3	1.43	1.00
1:A:261:PHE:HE2	1:A:350:LYS:HG2	1.27	0.98
1:A:708:SER:HB2	1:A:732:LEU:CD1	1.96	0.96
1:A:261:PHE:HE2	1:A:350:LYS:CG	1.80	0.95
1:A:79:THR:CA	1:A:117:THR:CG2	2.44	0.95
1:A:626:ASP:O	1:A:627:ASP:HB2	1.67	0.94
1:A:193:GLU:O	1:A:196:VAL:HG23	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:CA	1:A:117:THR:HG21	2.02	0.90
1:A:694:ASP:OD2	1:A:696:ARG:NH1	2.02	0.90
1:A:185:LYS:H	1:A:186:VAL:HA	1.35	0.89
1:A:375:ARG:NH2	1:A:470:PHE:CE2	2.40	0.88
1:A:388:GLN:HA	1:A:391:MET:HE2	1.53	0.88
1:A:621:ASP:O	1:A:625:ASN:HB2	1.73	0.88
1:A:467:PHE:CE1	2:B:1:NAG:O6	2.27	0.87
1:A:708:SER:CB	1:A:732:LEU:HD13	2.04	0.87
1:A:319:GLU:OE2	1:A:468:TYR:HB3	1.74	0.86
1:A:46:ILE:HD13	1:A:47:ALA:N	1.92	0.84
1:A:627:ASP:OD1	1:A:630:ARG:HB2	1.79	0.83
1:A:708:SER:HB2	1:A:732:LEU:HD13	1.59	0.83
1:A:692:LEU:HD23	1:A:693:LEU:N	1.94	0.83
1:A:392:GLN:HB3	8:A:1013:HOH:O	1.79	0.82
1:A:338:ARG:O	1:A:338:ARG:HD3	1.80	0.82
1:A:626:ASP:O	1:A:627:ASP:CB	2.28	0.81
1:A:261:PHE:CE2	1:A:350:LYS:HG2	2.15	0.81
1:A:753:LYS:H	1:A:753:LYS:CD	1.94	0.80
1:A:753:LYS:H	1:A:753:LYS:HD3	1.44	0.80
1:A:463:PRO:HA	1:A:464:HIS:CB	2.10	0.80
1:A:694:ASP:OD1	1:A:696:ARG:HD3	1.81	0.79
1:A:95:ASN:OD1	1:A:133:GLU:N	2.16	0.78
1:A:193:GLU:O	1:A:196:VAL:CG2	2.31	0.78
1:A:350:LYS:H	1:A:350:LYS:HD2	1.49	0.77
1:A:185:LYS:N	1:A:186:VAL:HA	2.00	0.76
1:A:157:ASN:O	1:A:159:TYR:CE2	2.39	0.75
1:A:731:PHE:HB3	1:A:732:LEU:HG	1.69	0.75
1:A:183:PHE:HB2	1:A:184:ASN:HD22	1.52	0.75
1:A:67:GLU:CB	1:A:91:LYS:HB2	2.17	0.74
1:A:78:ILE:O	1:A:117:THR:HG22	1.86	0.74
1:A:40:LYS:O	1:A:41:GLN:HB2	1.85	0.74
1:A:44:SER:HB2	1:A:66:THR:OG1	1.88	0.74
1:A:752:ASN:HB3	1:A:753:LYS:HE2	1.68	0.73
1:A:463:PRO:HA	1:A:464:HIS:HB3	1.70	0.72
1:A:86:LEU:O	1:A:88:ASN:N	2.21	0.71
1:A:261:PHE:CZ	1:A:350:LYS:HE2	2.26	0.71
1:A:350:LYS:HD2	1:A:350:LYS:N	2.05	0.70
1:A:168:ARG:O	1:A:170:ILE:HG12	1.91	0.70
1:A:467:PHE:O	1:A:468:TYR:HB2	1.91	0.70
1:A:159:TYR:CD1	1:A:187:CYS:SG	2.86	0.69
1:A:756:LEU:O	1:A:756:LEU:HD13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:O	1:A:137:LEU:HD23	1.92	0.69
1:A:809:GLN:HA	1:A:809:GLN:OE1	1.91	0.69
1:A:465:SER:O	1:A:466:ASN:HB2	1.93	0.69
1:A:185:LYS:H	1:A:186:VAL:CA	2.06	0.69
1:A:168:ARG:NH1	1:A:168:ARG:HG2	2.08	0.68
1:A:350:LYS:H	1:A:350:LYS:CD	2.01	0.68
1:A:67:GLU:HB3	1:A:91:LYS:HB2	1.73	0.68
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.57	0.67
1:A:86:LEU:N	1:A:86:LEU:HD22	2.08	0.67
1:A:388:GLN:HB3	1:A:389:PRO:HD3	1.77	0.67
1:A:793:VAL:HG23	1:A:793:VAL:O	1.95	0.67
1:A:261:PHE:CE2	1:A:350:LYS:CG	2.70	0.67
1:A:388:GLN:HA	1:A:391:MET:HE3	1.77	0.67
1:A:627:ASP:CG	1:A:628:ASP:H	2.03	0.67
1:A:451:ILE:C	1:A:451:ILE:HD12	2.20	0.66
1:A:470:PHE:O	1:A:472:ARG:HG2	1.96	0.66
1:A:467:PHE:HE1	2:B:1:NAG:O6	1.78	0.66
1:A:205:LEU:HD23	1:A:205:LEU:C	2.21	0.65
1:A:694:ASP:CG	1:A:696:ARG:HH11	2.05	0.65
1:A:466:ASN:HB3	2:B:1:NAG:O7	1.97	0.65
1:A:250:LEU:C	1:A:250:LEU:HD23	2.21	0.64
1:A:183:PHE:HB2	1:A:184:ASN:ND2	2.13	0.64
1:A:90:THR:HA	1:A:126:ASN:O	1.97	0.64
1:A:40:LYS:H	1:A:40:LYS:HD3	1.60	0.64
1:A:375:ARG:NH2	1:A:470:PHE:CD2	2.62	0.64
1:A:188:GLU:C	1:A:189:LYS:HD2	2.23	0.64
1:A:65:VAL:O	1:A:89:LEU:HD23	1.98	0.63
1:A:79:THR:HG23	1:A:81:GLU:HB3	1.80	0.63
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.12	0.63
1:A:34:TYR:CE1	1:A:815:VAL:HG21	2.34	0.63
1:A:137:LEU:HD23	1:A:137:LEU:N	2.13	0.63
1:A:125:LYS:HD2	1:A:147:SER:HB3	1.81	0.63
1:A:277:ASN:C	1:A:277:ASN:HD22	2.08	0.62
1:A:818:GLU:OE1	1:A:818:GLU:N	2.33	0.62
1:A:117:THR:HG23	1:A:120:ALA:HB2	1.82	0.62
1:A:205:LEU:HD23	1:A:206:LEU:N	2.15	0.61
1:A:708:SER:HB2	1:A:732:LEU:HD12	1.79	0.61
1:A:46:ILE:HD13	1:A:47:ALA:C	2.25	0.61
1:A:696:ARG:HD2	1:A:718:LEU:HB3	1.82	0.61
1:A:84:GLN:O	1:A:86:LEU:HD22	2.01	0.61
1:A:117:THR:O	1:A:120:ALA:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LEU:H	1:A:786:TRP:HH2	1.48	0.61
1:A:84:GLN:C	1:A:86:LEU:HD22	2.26	0.61
1:A:708:SER:CB	1:A:732:LEU:CD1	2.68	0.61
1:A:166:ILE:HA	1:A:169:LEU:HD23	1.83	0.60
1:A:284:GLN:OE1	5:A:901:NAG:H61	2.02	0.60
1:A:40:LYS:HD3	1:A:40:LYS:N	2.16	0.60
1:A:86:LEU:C	1:A:87:GLN:HG3	2.25	0.60
1:A:259:ARG:HD2	1:A:322:TYR:CZ	2.36	0.60
1:A:467:PHE:CD1	2:B:1:NAG:O6	2.54	0.60
1:A:707:LEU:CD2	1:A:711:THR:HG22	2.31	0.60
1:A:41:GLN:OE1	1:A:42:ASN:HB3	2.01	0.60
1:A:334:THR:HG22	1:A:365:LYS:HD2	1.83	0.60
1:A:91:LYS:HG3	1:A:129:GLU:CB	2.23	0.60
1:A:51:ASN:HA	1:A:72:ASP:O	2.02	0.59
1:A:212:SER:HB3	1:A:233:GLN:NE2	2.17	0.59
1:A:388:GLN:CA	1:A:391:MET:HE2	2.30	0.59
1:A:62:GLY:O	1:A:65:VAL:HG23	2.02	0.59
1:A:692:LEU:HD23	1:A:692:LEU:C	2.27	0.59
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.03	0.59
1:A:671:ILE:O	1:A:671:ILE:HG22	2.02	0.59
1:A:238:SER:N	1:A:241:ASP:OD2	2.25	0.58
1:A:125:LYS:HG3	1:A:125:LYS:O	2.03	0.58
1:A:682:THR:HA	1:A:710:PHE:CD1	2.37	0.58
1:A:805:SER:HB2	1:A:806:PRO:HA	1.85	0.58
1:A:113:GLY:HA2	1:A:136:GLN:HB3	1.85	0.58
1:A:53:ARG:NH2	1:A:799:VAL:HG12	2.19	0.58
1:A:118:ASP:OD1	1:A:118:ASP:N	2.37	0.58
1:A:756:LEU:C	1:A:756:LEU:HD22	2.30	0.57
1:A:79:THR:CA	1:A:117:THR:HG22	2.18	0.57
1:A:725:SER:HA	1:A:747:LEU:O	2.05	0.57
1:A:79:THR:O	1:A:82:SER:HB2	2.05	0.56
1:A:219:LYS:HE2	1:A:219:LYS:HA	1.87	0.56
1:A:137:LEU:O	1:A:157:ASN:HB2	2.04	0.56
1:A:782:ASP:O	1:A:785:ARG:HB3	2.05	0.56
1:A:68:LEU:HD21	1:A:70:LEU:HD11	1.87	0.56
1:A:184:ASN:O	1:A:185:LYS:HD2	2.06	0.56
1:A:708:SER:HB3	1:A:732:LEU:HD13	1.85	0.56
1:A:123:ASN:ND2	1:A:123:ASN:O	2.39	0.56
1:A:628:ASP:O	1:A:629:ASN:HB2	2.06	0.56
1:A:64:TYR:HA	1:A:88:ASN:OD1	2.06	0.55
1:A:289:LEU:HD23	1:A:310:MET:SD	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:O	1:A:159:TYR:CD2	2.60	0.55
1:A:707:LEU:CD2	1:A:711:THR:CG2	2.84	0.55
1:A:53:ARG:HH21	1:A:799:VAL:HG12	1.72	0.54
1:A:749:LYS:O	1:A:775:GLU:N	2.24	0.54
1:A:212:SER:CB	1:A:233:GLN:HE21	2.20	0.54
1:A:140:ILE:O	1:A:141:PRO:C	2.50	0.54
1:A:261:PHE:HE2	1:A:350:LYS:HG3	1.69	0.54
1:A:50:SER:HB2	1:A:71:SER:O	2.08	0.54
1:A:138:PRO:HD2	1:A:139:GLN:H	1.72	0.54
1:A:277:ASN:C	1:A:277:ASN:ND2	2.66	0.54
1:A:413:LEU:C	1:A:413:LEU:HD12	2.33	0.54
1:A:85:GLY:C	1:A:87:GLN:HG3	2.33	0.54
1:A:784:ARG:NH2	1:A:814:ILE:O	2.41	0.54
1:A:319:GLU:OE2	1:A:468:TYR:CB	2.52	0.53
1:A:820:THR:C	1:A:822:CYS:H	2.14	0.53
1:A:140:ILE:HD13	1:A:166:ILE:HG12	1.91	0.53
1:A:125:LYS:O	1:A:125:LYS:CG	2.56	0.53
1:A:185:LYS:N	1:A:186:VAL:CA	2.70	0.53
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.91	0.53
1:A:707:LEU:HD23	1:A:711:THR:HG22	1.89	0.53
1:A:78:ILE:HB	1:A:116:ILE:HG12	1.91	0.52
1:A:67:GLU:HB2	1:A:91:LYS:HB2	1.91	0.52
1:A:259:ARG:NH1	1:A:322:TYR:CD1	2.77	0.52
1:A:567:TYR:O	1:A:575:HIS:HE1	1.92	0.52
1:A:250:LEU:HD23	1:A:251:LEU:N	2.24	0.52
1:A:802:ILE:CG2	1:A:803:CYS:N	2.72	0.52
1:A:52:ARG:O	1:A:54:LEU:HD23	2.09	0.52
1:A:212:SER:CB	1:A:233:GLN:NE2	2.74	0.52
1:A:806:PRO:O	1:A:809:GLN:N	2.43	0.52
1:A:188:GLU:HG3	1:A:189:LYS:H	1.75	0.51
1:A:189:LYS:HA	1:A:212:SER:OG	2.10	0.51
1:A:323:LEU:O	1:A:327:ILE:HG13	2.10	0.51
1:A:275:SER:HB3	1:A:298:SER:O	2.10	0.51
1:A:731:PHE:CB	1:A:732:LEU:HG	2.40	0.51
1:A:448:GLN:HA	1:A:448:GLN:HE21	1.74	0.51
1:A:54:LEU:HD23	1:A:54:LEU:N	2.26	0.51
1:A:86:LEU:N	1:A:86:LEU:CD2	2.73	0.51
1:A:731:PHE:HB3	1:A:732:LEU:CG	2.40	0.51
1:A:212:SER:HB3	1:A:233:GLN:HE21	1.74	0.51
1:A:319:GLU:HG2	1:A:343:ASP:CG	2.36	0.51
1:A:169:LEU:O	1:A:171:ASN:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:N	1:A:350:LYS:CD	2.70	0.51
1:A:205:LEU:C	1:A:205:LEU:CD2	2.84	0.50
1:A:65:VAL:HB	1:A:89:LEU:HD21	1.92	0.50
1:A:756:LEU:N	1:A:786:TRP:HH2	2.10	0.50
1:A:138:PRO:HD2	1:A:139:GLN:N	2.27	0.50
1:A:183:PHE:CB	1:A:184:ASN:HD22	2.24	0.50
1:A:499:ASN:HA	1:A:502:GLU:HG2	1.93	0.50
1:A:285:ASN:OD1	5:A:901:NAG:O5	2.23	0.50
1:A:388:GLN:NE2	1:A:391:MET:HE1	2.27	0.49
1:A:211:ASN:O	1:A:232:THR:HA	2.13	0.49
1:A:595:ASN:HD22	1:A:595:ASN:N	2.10	0.49
1:A:260:CYS:O	1:A:261:PHE:C	2.55	0.49
1:A:411:PHE:CD1	1:A:504:LEU:HD21	2.47	0.49
1:A:43:ASP:N	1:A:43:ASP:OD2	2.45	0.49
1:A:338:ARG:O	1:A:338:ARG:CD	2.56	0.49
1:A:773:PRO:HA	1:A:804:ALA:HB2	1.95	0.49
1:A:122:LEU:CD1	1:A:122:LEU:N	2.76	0.49
1:A:463:PRO:CA	1:A:464:HIS:CB	2.88	0.49
1:A:63:LYS:H	1:A:63:LYS:HD3	1.78	0.49
1:A:86:LEU:HD22	1:A:86:LEU:H	1.76	0.48
1:A:136:GLN:HG3	1:A:157:ASN:ND2	2.28	0.48
1:A:466:ASN:O	1:A:467:PHE:HB2	2.13	0.48
1:A:161:ILE:HG22	1:A:196:VAL:HG11	1.94	0.48
1:A:180:ASN:HD22	1:A:180:ASN:N	2.12	0.48
1:A:177:LEU:HB2	1:A:208:LEU:HD23	1.95	0.48
1:A:475:ILE:O	1:A:476:LYS:C	2.52	0.48
1:A:501:PHE:HB3	1:A:504:LEU:HD12	1.95	0.48
1:A:494:PHE:O	1:A:517:ASN:HA	2.14	0.48
1:A:46:ILE:HD13	1:A:46:ILE:C	2.39	0.48
1:A:643:ARG:HG3	1:A:668:GLU:HB3	1.96	0.48
1:A:136:GLN:HG3	1:A:157:ASN:HD21	1.77	0.48
1:A:469:HIS:HD2	8:A:1012:HOH:O	1.96	0.47
1:A:764:LEU:HD12	1:A:764:LEU:O	2.13	0.47
1:A:79:THR:O	1:A:82:SER:CB	2.62	0.47
1:A:182:TYR:O	1:A:183:PHE:C	2.58	0.47
1:A:627:ASP:CG	1:A:628:ASP:N	2.73	0.47
1:A:788:ASP:O	1:A:791:LEU:CD1	2.63	0.47
1:A:466:ASN:HD22	1:A:466:ASN:HA	1.45	0.47
1:A:86:LEU:CD2	1:A:86:LEU:H	2.27	0.47
1:A:50:SER:O	1:A:52:ARG:HD2	2.15	0.47
1:A:163:LYS:HA	1:A:167:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:LYS:HD3	1:A:753:LYS:N	2.21	0.47
1:A:731:PHE:HA	1:A:732:LEU:HD23	1.96	0.47
1:A:447:PHE:O	1:A:447:PHE:CD2	2.69	0.47
1:A:731:PHE:HB3	1:A:732:LEU:CD2	2.45	0.47
1:A:793:VAL:O	1:A:793:VAL:CG2	2.60	0.46
1:A:692:LEU:C	1:A:692:LEU:CD2	2.88	0.46
1:A:84:GLN:N	1:A:86:LEU:CD2	2.78	0.46
1:A:536:ASP:OD1	1:A:538:THR:HG23	2.16	0.46
1:A:820:THR:C	1:A:822:CYS:N	2.73	0.46
1:A:388:GLN:N	1:A:389:PRO:CD	2.78	0.46
1:A:602:LYS:HZ1	1:A:606:GLU:CD	2.24	0.46
1:A:124:LEU:N	1:A:124:LEU:HD23	2.30	0.46
1:A:139:GLN:O	1:A:141:PRO:HD3	2.16	0.46
1:A:183:PHE:HA	1:A:184:ASN:HA	1.49	0.45
1:A:283:PHE:HD2	1:A:306:TRP:HB3	1.81	0.45
1:A:779:ASP:C	1:A:781:GLY:H	2.23	0.45
1:A:392:GLN:CB	8:A:1013:HOH:O	2.52	0.45
1:A:451:ILE:C	1:A:451:ILE:CD1	2.89	0.45
1:A:296:SER:HA	1:A:320:PHE:O	2.17	0.45
1:A:79:THR:N	1:A:82:SER:OG	2.38	0.45
1:A:716:THR:HG23	1:A:740:HIS:HB3	1.98	0.45
1:A:802:ILE:HG22	1:A:803:CYS:N	2.32	0.45
1:A:61:VAL:O	1:A:62:GLY:C	2.60	0.44
1:A:85:GLY:O	1:A:87:GLN:HG3	2.17	0.44
1:A:570:ILE:HB	1:A:573:VAL:CG1	2.48	0.44
1:A:696:ARG:HD2	1:A:718:LEU:CB	2.47	0.44
1:A:780:ILE:O	1:A:780:ILE:HG23	2.17	0.44
1:A:806:PRO:HD2	1:A:809:GLN:HB2	1.99	0.44
1:A:466:ASN:O	1:A:467:PHE:CD2	2.70	0.44
1:A:41:GLN:CD	1:A:42:ASN:HA	2.43	0.44
1:A:755:ALA:O	1:A:756:LEU:C	2.61	0.44
1:A:138:PRO:CD	1:A:139:GLN:N	2.80	0.44
1:A:353:TYR:CZ	1:A:380:GLN:HG2	2.52	0.44
1:A:708:SER:N	1:A:732:LEU:HD11	2.31	0.44
1:A:621:ASP:O	1:A:625:ASN:CB	2.57	0.44
1:A:97:ASN:HA	1:A:98:PRO:HA	1.68	0.44
1:A:818:GLU:CD	1:A:818:GLU:H	2.24	0.43
1:A:166:ILE:HA	1:A:169:LEU:CD2	2.48	0.43
1:A:230:SER:HA	1:A:254:SER:O	2.18	0.43
1:A:821:THR:HG22	1:A:821:THR:O	2.18	0.43
1:A:67:GLU:OE1	1:A:91:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ILE:O	1:A:784:ARG:HB2	2.17	0.43
1:A:783:PHE:O	1:A:786:TRP:HB3	2.18	0.43
1:A:570:ILE:HB	1:A:573:VAL:HG11	2.00	0.43
1:A:219:LYS:HE2	1:A:219:LYS:CA	2.49	0.43
1:A:154:ILE:HG23	1:A:178:ALA:O	2.18	0.43
1:A:430:ILE:HD12	1:A:430:ILE:N	2.34	0.43
1:A:476:LYS:HD2	8:A:1075:HOH:O	2.17	0.42
1:A:79:THR:O	1:A:82:SER:N	2.52	0.42
1:A:319:GLU:H	1:A:319:GLU:HG3	1.51	0.42
1:A:122:LEU:CD1	1:A:122:LEU:H	2.32	0.42
1:A:783:PHE:O	1:A:784:ARG:C	2.63	0.42
1:A:79:THR:HG23	1:A:82:SER:H	1.83	0.42
1:A:234:ILE:O	1:A:256:ASN:HB3	2.20	0.42
1:A:611:VAL:C	1:A:641:LEU:HD12	2.45	0.42
1:A:568:PHE:CD1	1:A:596:ILE:HG12	2.55	0.42
1:A:466:ASN:HB3	1:A:467:PHE:H	1.64	0.42
1:A:79:THR:CG2	1:A:81:GLU:HB3	2.47	0.42
1:A:125:LYS:CD	1:A:147:SER:HB3	2.49	0.42
1:A:213:LEU:C	1:A:215:HIS:H	2.28	0.42
1:A:290:ARG:C	1:A:313:LEU:HD12	2.45	0.42
1:A:226:LYS:HG2	1:A:250:LEU:HB3	2.02	0.41
1:A:261:PHE:CE2	1:A:350:LYS:HG3	2.48	0.41
1:A:521:LEU:HD13	1:A:550:LEU:HD21	2.02	0.41
1:A:119:GLY:HA2	1:A:122:LEU:HD13	2.02	0.41
1:A:137:LEU:O	1:A:157:ASN:N	2.47	0.41
1:A:163:LYS:HG3	8:A:1035:HOH:O	2.20	0.41
1:A:250:LEU:C	1:A:250:LEU:CD2	2.88	0.41
1:A:42:ASN:O	1:A:43:ASP:HB2	2.19	0.41
1:A:670:HIS:HA	1:A:694:ASP:HB3	2.03	0.41
1:A:428:ASN:O	1:A:491:ASN:HA	2.20	0.41
1:A:517:ASN:OD1	1:A:519:GLN:HG2	2.21	0.41
1:A:773:PRO:CA	1:A:804:ALA:HB2	2.51	0.41
1:A:467:PHE:HA	2:B:1:NAG:H2	2.02	0.41
1:A:749:LYS:HA	1:A:773:PRO:O	2.20	0.41
1:A:193:GLU:O	1:A:196:VAL:HG22	2.18	0.41
1:A:256:ASN:O	1:A:297:THR:HA	2.21	0.41
1:A:517:ASN:OD1	1:A:517:ASN:C	2.64	0.41
1:A:685:GLN:HG2	1:A:710:PHE:HA	2.02	0.41
1:A:40:LYS:O	1:A:41:GLN:CB	2.58	0.41
1:A:479:CYS:SG	1:A:534:TYR:CD1	3.14	0.41
1:A:603:TYR:CZ	1:A:630:ARG:NH1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ASN:N	1:A:625:ASN:HD22	2.18	0.41
1:A:687:PHE:HA	1:A:688:PRO:HD2	1.93	0.41
1:A:135:ASN:C	1:A:137:LEU:HD23	2.46	0.41
1:A:210:PHE:CE2	1:A:231:ASN:OD1	2.74	0.41
1:A:645:ASP:C	1:A:645:ASP:OD1	2.64	0.40
1:A:375:ARG:NH2	1:A:470:PHE:HE2	2.10	0.40
1:A:470:PHE:CD1	1:A:470:PHE:N	2.88	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	739/801 (92%)	675 (91%)	57 (8%)	7 (1%)	14	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PHE
1	A	466	ASN
1	A	627	ASP
1	A	467	PHE
1	A	378	VAL
1	A	821	THR
1	A	264	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	698/745 (94%)	664 (95%)	34 (5%)	22	47

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	41	GLN
1	A	43	ASP
1	A	46	ILE
1	A	59	GLN
1	A	61	VAL
1	A	86	LEU
1	A	117	THR
1	A	118	ASP
1	A	122	LEU
1	A	124	LEU
1	A	137	LEU
1	A	168	ARG
1	A	169	LEU
1	A	185	LYS
1	A	190	THR
1	A	194	ASP
1	A	277	ASN
1	A	350	LYS
1	A	451	ILE
1	A	466	ASN
1	A	541	ARG
1	A	573	VAL
1	A	595	ASN
1	A	628	ASP
1	A	630	ARG
1	A	738	LEU
1	A	753	LYS
1	A	756	LEU
1	A	787	MET
1	A	808	ASP
1	A	809	GLN
1	A	810	ARG
1	A	818	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	77	HIS
1	A	84	GLN
1	A	99	ASN
1	A	157	ASN
1	A	184	ASN
1	A	233	GLN
1	A	277	ASN
1	A	312	HIS
1	A	388	GLN
1	A	448	GLN
1	A	450	HIS
1	A	466	ASN
1	A	575	HIS
1	A	595	ASN
1	A	604	ASN
1	A	625	ASN
1	A	629	ASN
1	A	752	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
2	NAG	B	1	2,1	14,14,15	1.01	2 (14%)	17,19,21	1.83	2 (11%)
2	NAG	B	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.15	2 (11%)
2	BMA	B	3	2	11,11,12	0.35	0	15,15,17	0.81	0
2	MAN	B	4	2	11,11,12	0.63	0	15,15,17	0.81	1 (6%)
3	NAG	C	1	3,1	14,14,15	0.61	0	17,19,21	1.43	5 (29%)
3	NAG	C	2	3	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	D	1	4,1	14,14,15	0.68	0	17,19,21	1.33	3 (17%)
4	NAG	D	2	4	14,14,15	0.81	1 (7%)	17,19,21	1.75	3 (17%)
4	BMA	D	3	4	11,11,12	0.62	0	15,15,17	1.51	1 (6%)
4	MAN	D	4	4	11,11,12	0.41	0	15,15,17	0.89	1 (6%)
4	MAN	D	5	4	11,11,12	0.75	0	15,15,17	1.02	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
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.55	1.39	1.43
2	B	1	NAG	O5-C5	-2.17	1.39	1.43
4	D	2	NAG	O5-C1	-2.09	1.40	1.43
2	B	1	NAG	O5-C1	-2.02	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-5.25	103.17	111.29
4	D	3	BMA	O3-C3-C2	4.59	119.43	110.05
4	D	2	NAG	O5-C1-C2	-4.14	104.89	111.29
4	D	2	NAG	C2-N2-C7	-3.69	117.95	122.90
2	B	1	NAG	C1-O5-C5	-3.31	107.74	112.19
2	B	2	NAG	O5-C1-C2	-2.93	106.75	111.29
3	C	1	NAG	C1-O5-C5	-2.84	108.38	112.19
4	D	1	NAG	O5-C1-C2	-2.74	107.05	111.29
3	C	1	NAG	O7-C7-C8	-2.43	117.73	122.05
3	C	1	NAG	O7-C7-N2	2.41	126.24	121.98
4	D	1	NAG	O5-C5-C6	2.36	112.26	107.66
2	B	2	NAG	O4-C4-C3	-2.30	104.95	110.38
4	D	2	NAG	C1-C2-N2	2.25	113.99	110.43
2	B	4	MAN	C1-C2-C3	2.25	112.92	109.64
4	D	4	MAN	C1-O5-C5	2.20	115.14	112.19
3	C	1	NAG	O4-C4-C3	-2.17	105.26	110.38
4	D	1	NAG	O3-C3-C4	2.10	115.32	110.38
3	C	1	NAG	O5-C1-C2	-2.06	108.11	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

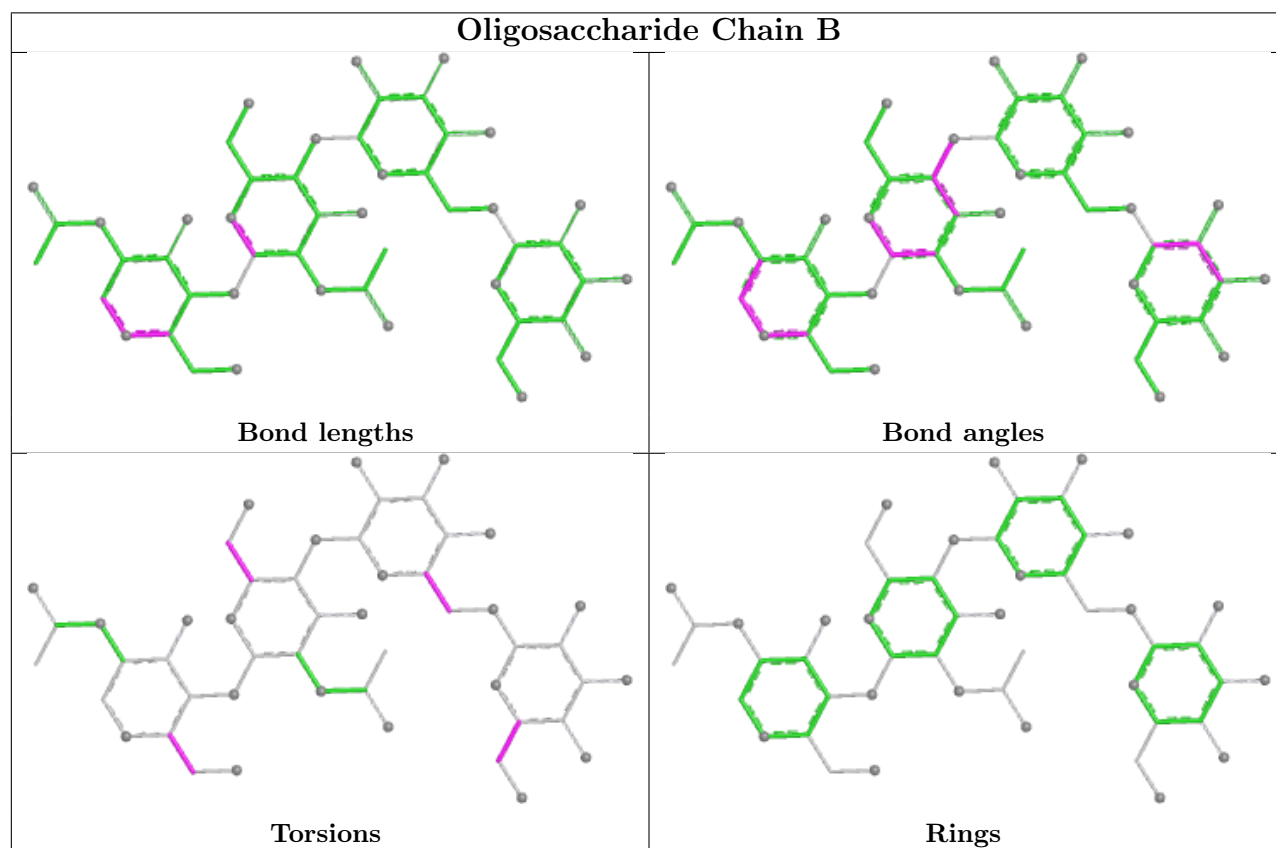
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

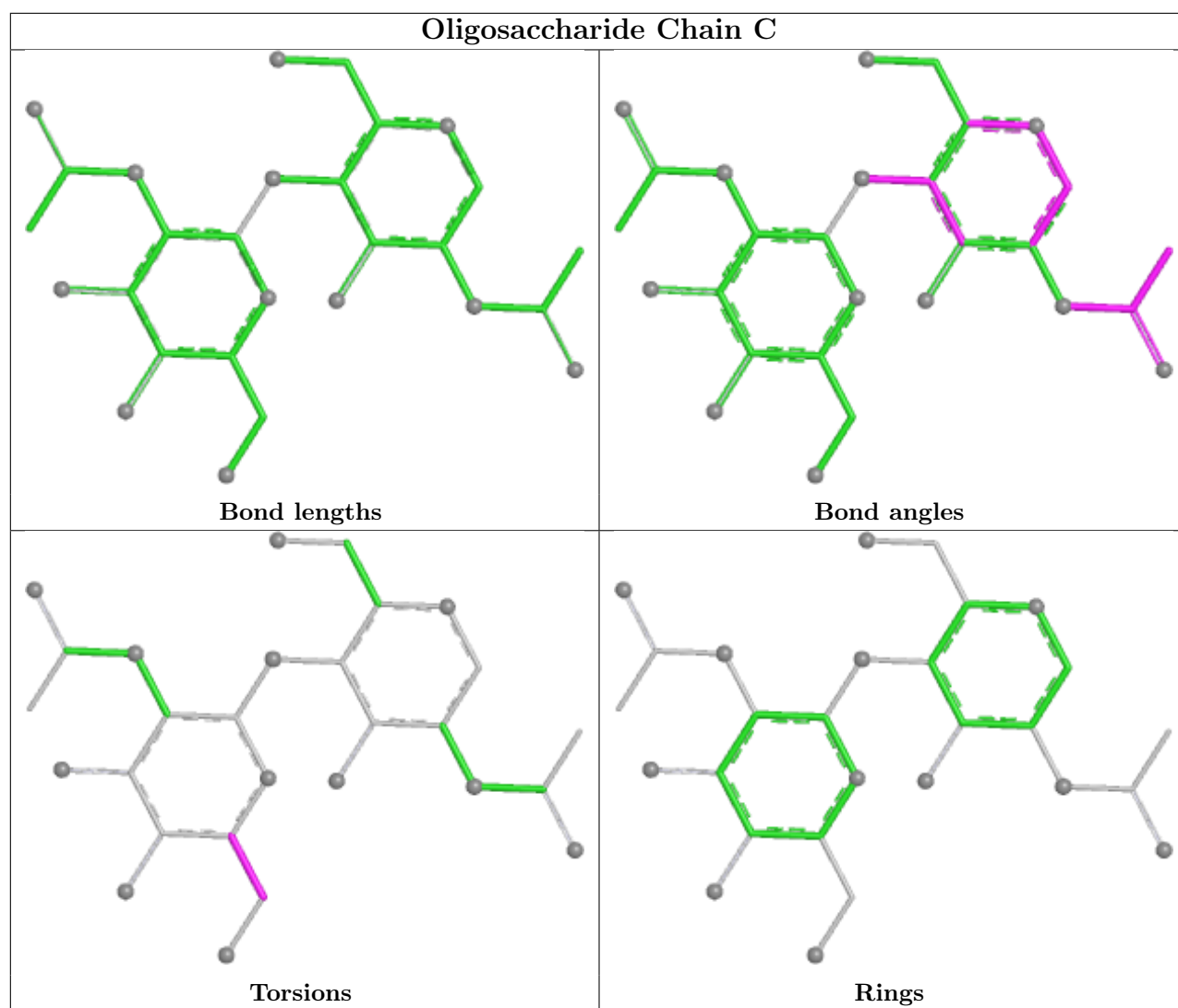
There are no ring outliers.

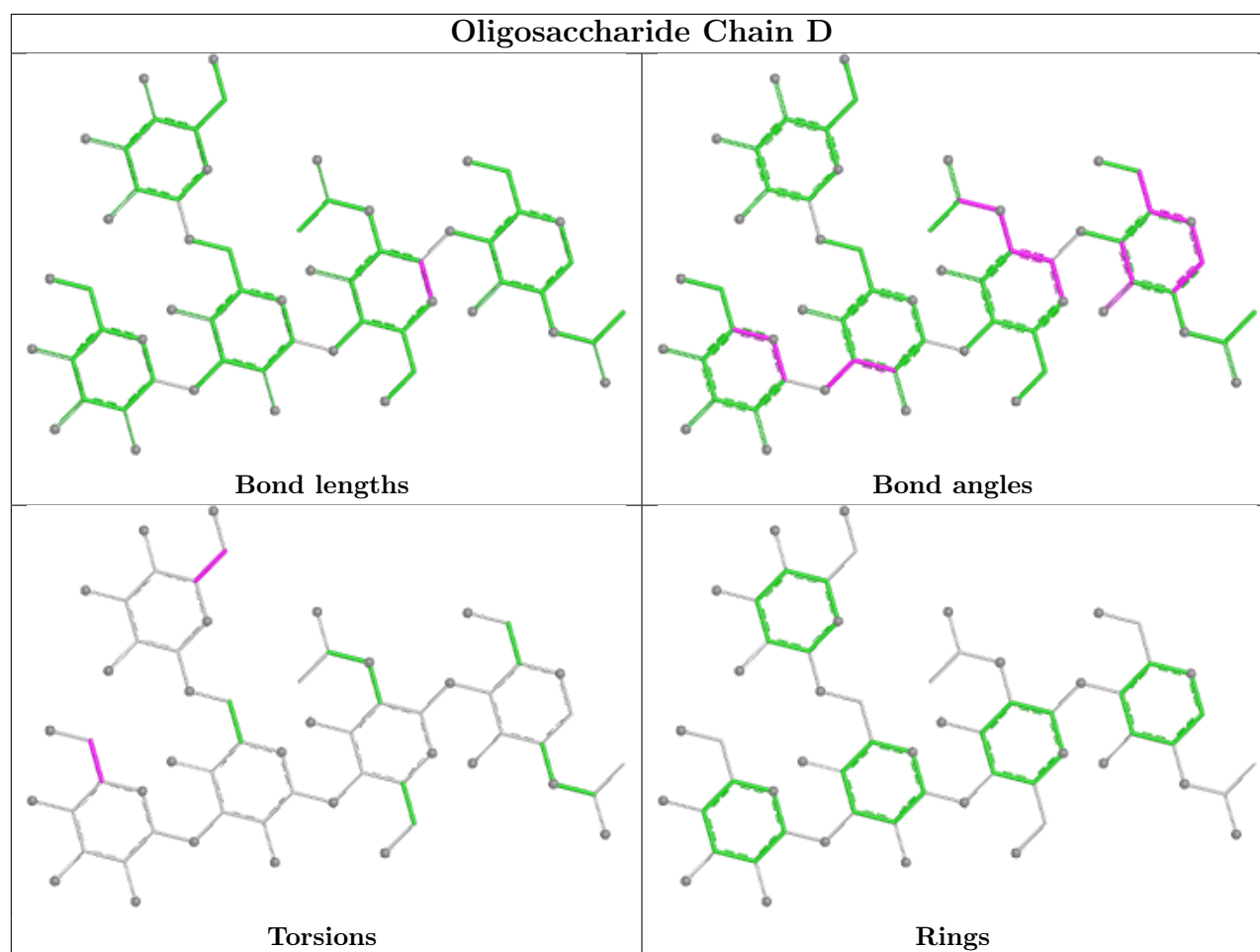
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	5	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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	910	1	14,14,15	0.88	1 (7%)	17,19,21	1.50	2 (11%)
6	SO4	A	918	-	4,4,4	0.40	0	6,6,6	0.28	0
5	NAG	A	906	1	14,14,15	0.61	0	17,19,21	0.79	0
6	SO4	A	919	-	4,4,4	0.42	0	6,6,6	0.26	0
5	NAG	A	907	1	14,14,15	0.59	0	17,19,21	1.10	1 (5%)
5	NAG	A	917	1	14,14,15	0.62	0	17,19,21	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	901	1	14,14,15	0.30	0	17,19,21	0.56	0
6	SO4	A	920	-	4,4,4	0.49	0	6,6,6	0.26	0
7	MES	A	921	-	12,12,12	2.37	1 (8%)	15,16,16	1.41	3 (20%)
5	NAG	A	911	1	14,14,15	0.57	0	17,19,21	1.01	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	910	1	-	1/6/23/26	0/1/1/1
5	NAG	A	906	1	-	0/6/23/26	0/1/1/1
5	NAG	A	907	1	-	0/6/23/26	0/1/1/1
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
5	NAG	A	901	1	-	1/6/23/26	0/1/1/1
7	MES	A	921	-	-	5/6/14/14	0/1/1/1
5	NAG	A	911	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	921	MES	C8-S	-7.74	1.66	1.77
5	A	910	NAG	O5-C1	-2.18	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	917	NAG	C4-C3-C2	-3.00	106.61	111.02
5	A	907	NAG	C1-O5-C5	2.93	116.12	112.19
7	A	921	MES	O1S-S-C8	2.63	110.70	106.73
5	A	910	NAG	C6-C5-C4	-2.59	106.66	113.02
7	A	921	MES	C2-C3-N4	2.37	113.72	110.12
7	A	921	MES	O2S-S-C8	2.24	110.12	106.73
5	A	911	NAG	C1-C2-N2	2.15	113.82	110.43
5	A	917	NAG	C1-C2-N2	-2.14	107.06	110.43
5	A	910	NAG	O3-C3-C4	-2.01	105.64	110.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	910	NAG	C1-C2-N2-C7
7	A	921	MES	C8-C7-N4-C3
5	A	901	NAG	O5-C5-C6-O6
7	A	921	MES	C7-C8-S-O3S
7	A	921	MES	C7-C8-S-O1S
7	A	921	MES	C7-C8-S-O2S
7	A	921	MES	N4-C7-C8-S
5	A	911	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	NAG	2	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	751/801 (93%)	0.63	89 (11%) 9 7	37, 73, 136, 171	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	VAL	9.7
1	A	756	LEU	7.8
1	A	451	ILE	7.4
1	A	467	PHE	7.1
1	A	100	VAL	6.7
1	A	732	LEU	6.3
1	A	434	VAL	6.1
1	A	447	PHE	5.9
1	A	736	SER	5.1
1	A	463	PRO	5.0
1	A	731	PHE	4.8
1	A	186	VAL	4.6
1	A	45	VAL	4.4
1	A	35	PRO	4.3
1	A	791	LEU	4.3
1	A	113	GLY	4.2
1	A	625	ASN	4.1
1	A	464	HIS	4.0
1	A	470	PHE	4.0
1	A	468	TYR	4.0
1	A	819	LEU	3.8
1	A	755	ALA	3.6
1	A	119	GLY	3.5
1	A	812	LYS	3.5
1	A	64	TYR	3.4
1	A	182	TYR	3.4
1	A	74	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	702	PHE	3.4
1	A	33	SER	3.3
1	A	36	CYS	3.2
1	A	183	PHE	3.1
1	A	185	LYS	3.1
1	A	753	LYS	3.0
1	A	124	LEU	3.0
1	A	40	LYS	3.0
1	A	763	LYS	2.9
1	A	449	ARG	2.9
1	A	820	THR	2.9
1	A	778	CYS	2.9
1	A	822	CYS	2.9
1	A	471	THR	2.9
1	A	86	LEU	2.9
1	A	678	PHE	2.8
1	A	139	GLN	2.8
1	A	783	PHE	2.7
1	A	236	TYR	2.7
1	A	469	HIS	2.7
1	A	63	LYS	2.7
1	A	62	GLY	2.7
1	A	765	SER	2.7
1	A	39	LYS	2.7
1	A	68	LEU	2.7
1	A	789	GLU	2.6
1	A	125	LYS	2.6
1	A	66	THR	2.6
1	A	465	SER	2.6
1	A	243	LYS	2.5
1	A	818	GLU	2.5
1	A	159	TYR	2.5
1	A	170	ILE	2.4
1	A	58	PRO	2.4
1	A	83	PHE	2.4
1	A	46	ILE	2.4
1	A	201	THR	2.4
1	A	750	THR	2.3
1	A	808	ASP	2.3
1	A	445	SER	2.3
1	A	60	THR	2.3
1	A	466	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	2.3
1	A	91	LYS	2.2
1	A	61	VAL	2.2
1	A	87	GLN	2.1
1	A	123	ASN	2.1
1	A	730	GLY	2.1
1	A	138	PRO	2.1
1	A	821	THR	2.1
1	A	59	GLN	2.1
1	A	446	SER	2.1
1	A	160	ASN	2.1
1	A	187	CYS	2.1
1	A	34	TYR	2.1
1	A	78	ILE	2.1
1	A	52	ARG	2.0
1	A	775	GLU	2.0
1	A	222	SER	2.0
1	A	729	SER	2.0
1	A	685	GLN	2.0
1	A	184	ASN	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.

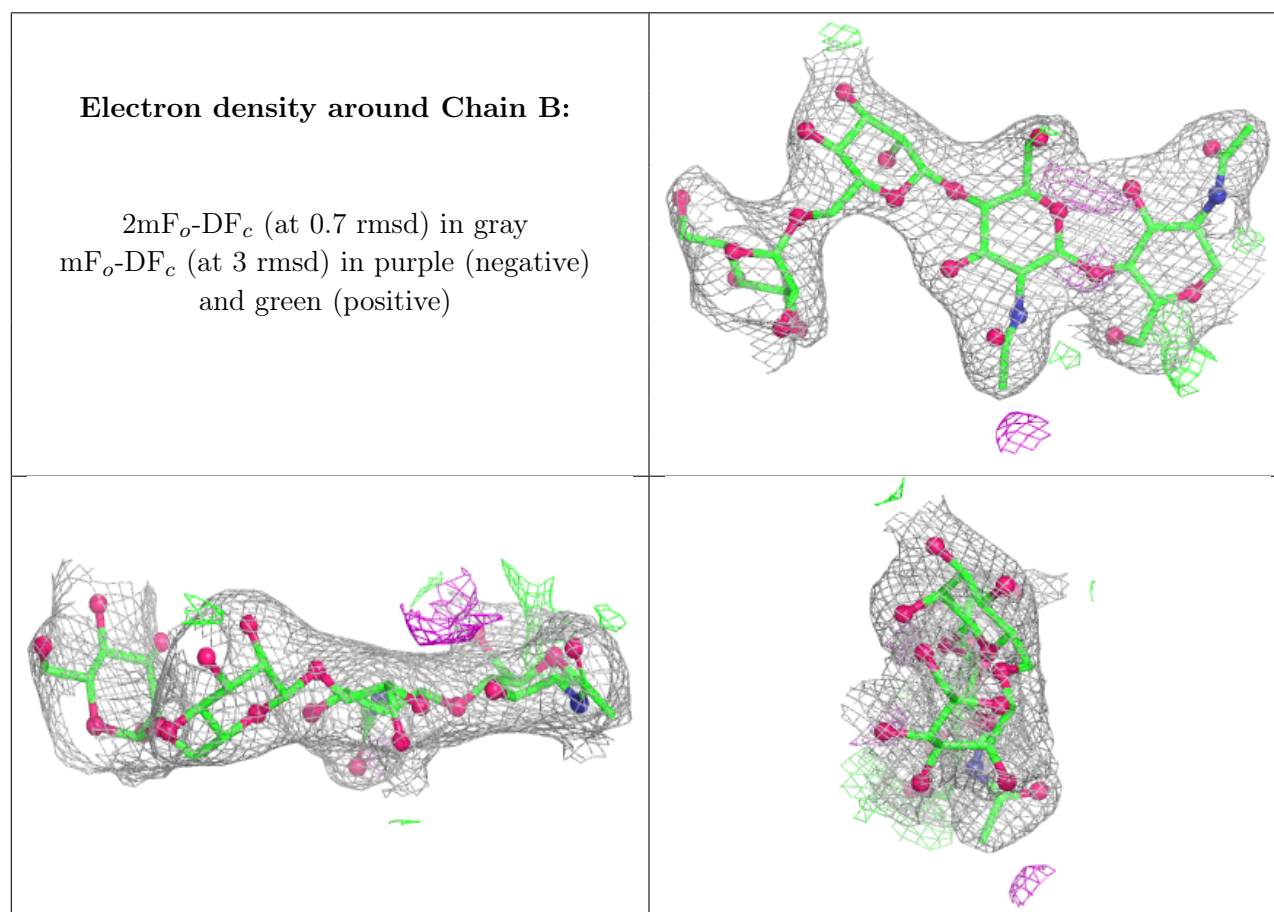
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	4	11/12	0.71	0.12	109,119,129,131	0
2	MAN	B	4	11/12	0.74	0.13	100,122,138,138	0
4	MAN	D	5	11/12	0.74	0.13	88,103,119,128	0
3	NAG	C	2	14/15	0.79	0.16	58,94,121,129	0
2	BMA	B	3	11/12	0.89	0.11	68,98,115,130	0
4	BMA	D	3	11/12	0.89	0.11	68,97,107,125	0
2	NAG	B	1	14/15	0.96	0.07	44,52,62,73	0
4	NAG	D	1	14/15	0.96	0.06	43,46,51,54	0

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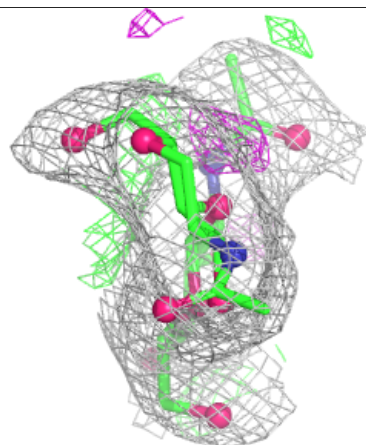
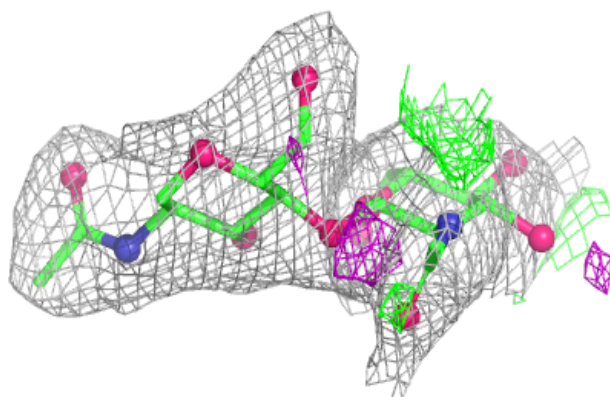
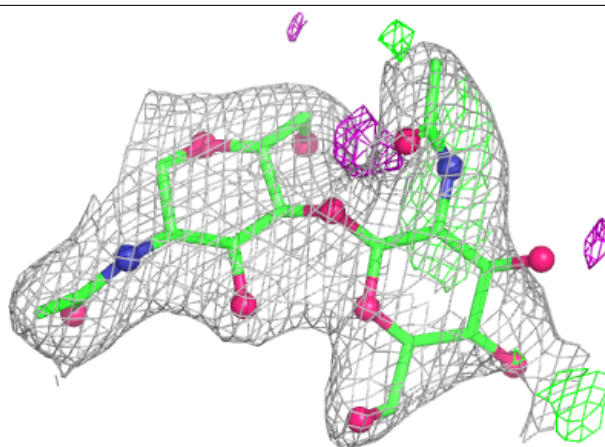
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	2	14/15	0.96	0.07	42,53,68,75	0
2	NAG	B	2	14/15	0.97	0.07	52,60,72,74	0
3	NAG	C	1	14/15	0.97	0.07	42,47,57,64	0

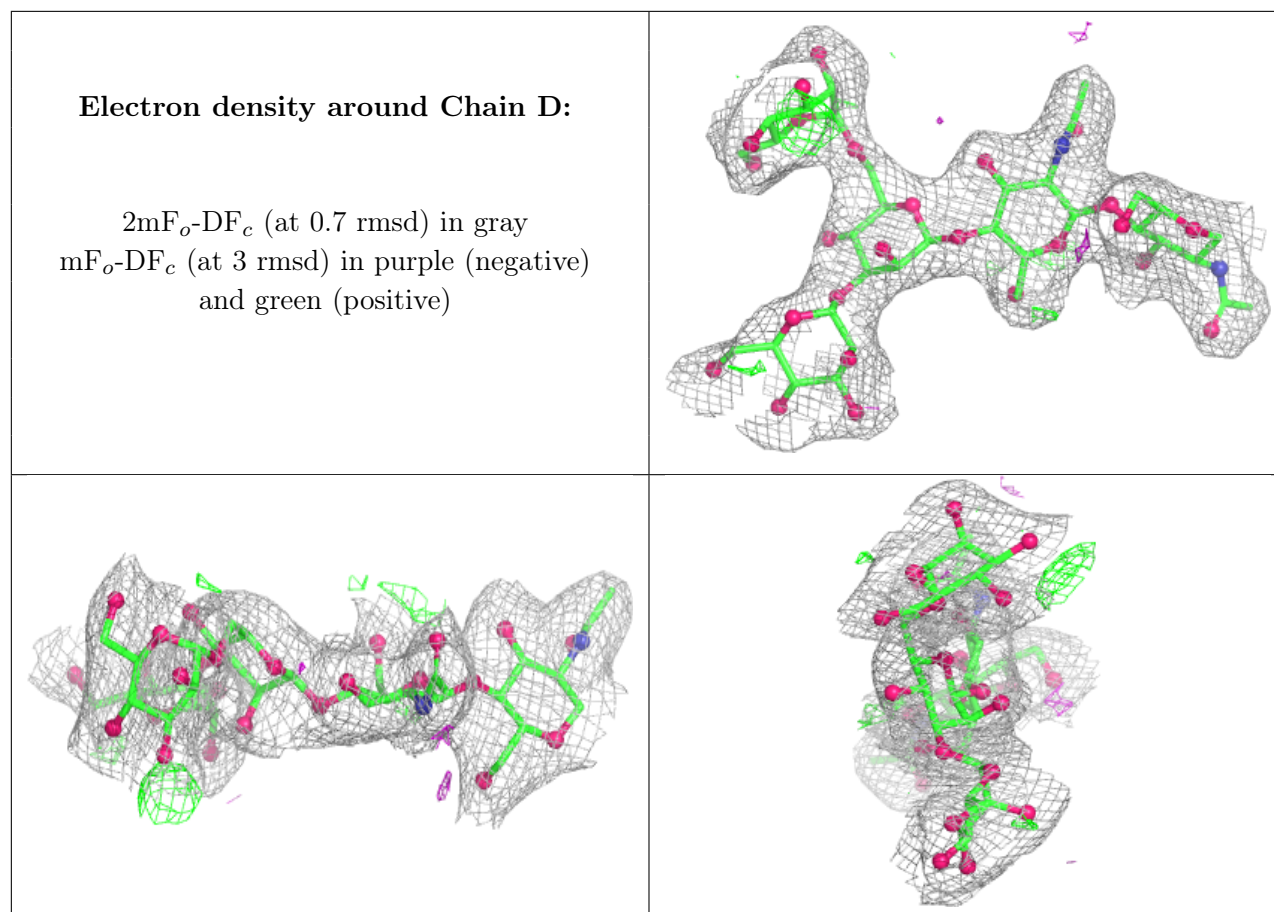
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	911	14/15	0.67	0.16	101,115,142,145	0
5	NAG	A	901	14/15	0.68	0.16	83,106,122,122	0
6	SO4	A	920	5/5	0.83	0.08	97,98,109,112	0
6	SO4	A	919	5/5	0.85	0.12	94,108,132,136	0
5	NAG	A	910	14/15	0.85	0.14	77,91,103,104	0
7	MES	A	921	12/12	0.85	0.22	58,78,82,86	12
5	NAG	A	907	14/15	0.86	0.12	81,95,108,116	0
5	NAG	A	906	14/15	0.93	0.09	64,73,81,82	0
5	NAG	A	917	14/15	0.93	0.09	64,72,85,87	0
6	SO4	A	918	5/5	0.93	0.11	71,85,90,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.