



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:53 AM UTC

PDB ID : 2B4X / pdb_00002b4x
Title : Crystal Structure of Antithrombin-III
Authors : Adams, T.E.; Huntington, J.A.; Johnson, D.J.D.; Bock, S.C.
Deposited on : 2005-09-27
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

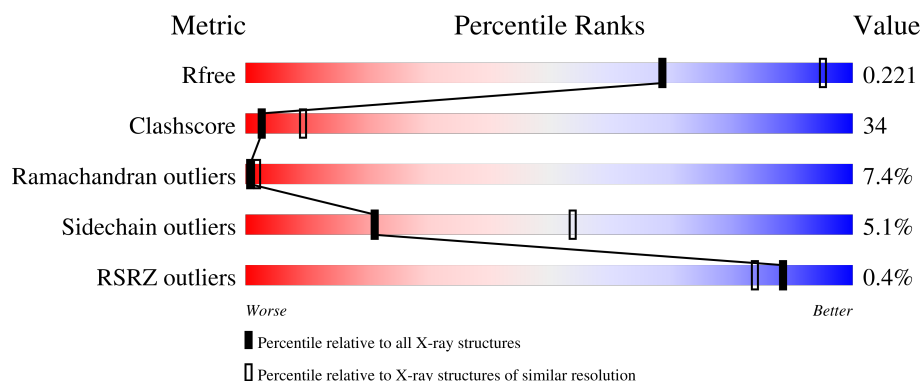
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

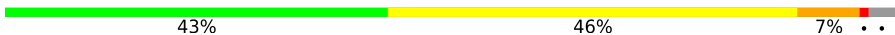
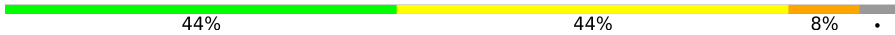
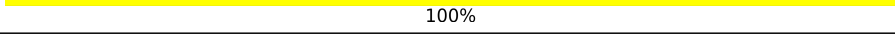
The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	I	427	
2	L	427	
3	A	2	
3	B	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1	X	-	-	-
4	NAG	I	861	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6560 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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	413	Total	C	N	O	S	0	0	0
			3203	2044	528	615	16			

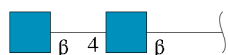
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	135	ALA	ASN	engineered mutation	UNP P01008
I	220	LEU	TYR	engineered mutation	UNP P01008

- Molecule 2 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	410	Total	C	N	O	S	0	0	0
			3078	1969	497	595	17			

- 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	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	B	2	Total	C	N	O	0	0	0
			27	16	2	9			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

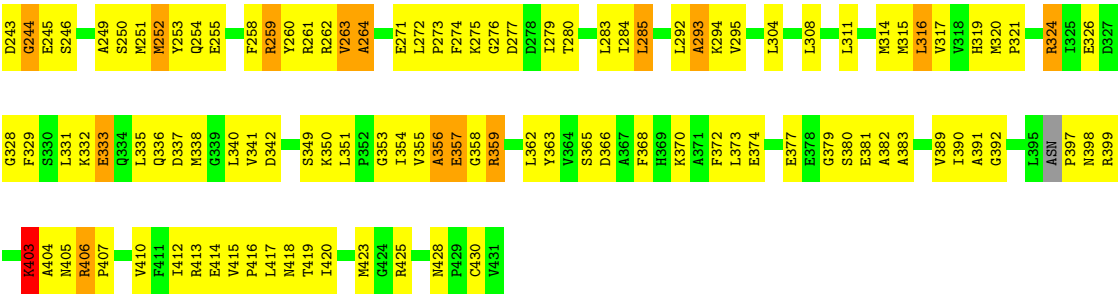
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	84	Total	O	0	0
			84	84		
5	L	56	Total	O	0	0
			56	56		

- Molecule 1: Antithrombin-III

V388	M315	E232	I161	G93	V5
V389	L316	E232	S162	A94	K11
V390			E163	G95	P12
A391	M319	L238	L164	N96	R13
	M320	F239	V165	D97	D14
N396	P321	V240	Y166	T98	I15
V397	R322	K241	G167	L99	P16
N398	F323	A242	A168		
V399		D243	K169	L102	M17
V400	E326	G244	L170		N18
T401	D327	E245	Q171	V105	P19
F402		S246	P172		M20
K403	L331	C247	L173	F108	C21
	K332		D174	D109	I22
R406	E333	M252	F175	T110	Y23
	Q334	Y253	K176	I111	
L409	L335	Q254	E177	S112	
V410	Q336	E255	N178	E113	K29
F411	D337		A179	K114	ALA
L412	M338	R259	E180	T115	THR
R413	G339	Y260	Q181	GLU	GLU
E414	L340	R261	S182	ASP	ASP
V415	V341	R262	R183	D117	GLU
P416	D342		A184	Q118	GLY
L417	L343	L272	A185	T119	GLY
N418	F344		I186	H120	SER
T419	S345	G276		A186	E37
I420	P346	D277	W189	Q38	Q38
I421	E347	D278	V190	F122	K39
F422	K348	L279	S191	F123	I40
	S349	T280	N192	K125	P41
	K350	M281	K193	L126	E42
N428	L351	V282	T194	L130	A43
P429	P352	L283	E195	Y131	R47
C430	G353	L284	G196	R132	V48
V431	I354	L285	R197	K133	
	V4L	P286	I198	ALA	L51
	ALA	K287	T199	ALA	
	GLU	P288	K136	K136	S56
	GLY	E289	V201	S137	
	ARG		L202	S138	N71
		A293	P203		D72
	D360	K294	S204	S142	N73
	D361	V295		A143	D74
	L362			N144	N75
	V363	E298	N207	R145	I76
	V364	L299	E209	L146	F77
	A367			F147	L78
		E302	L213	G148	
	K370		V214	D149	L81
	V375	Q305	L215	K150	S82
		E306	V216	S151	I83
		V307	N217	L152	S84
	E381	L308	T218	T153	T85
A382	D309		I219	F154	A86
A383	S310		L220	N155	F87
A384	L311		F221	A88	
	S385	E312	K222	Y158	M89
T386	E313			Q159	T90
A387	V214		F209	L160	K91
					L92

- Molecule 2: Antithrombin-III

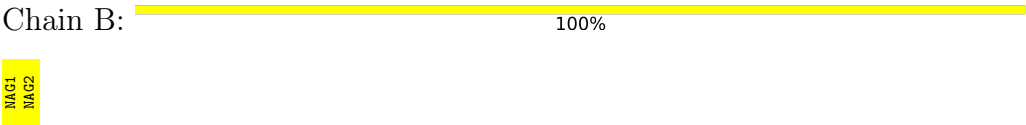
Y158	Y18	SF79	V5
S162	D6	P80	I7
L164		L81	
V165		S84	P16
		A88	M17
Q171		K91	N18
P172			P19
L173			M20
D174		A94	C21
F175		C95	Y23
		N96	R24
A179		P97	S25
			P26
S182		Q100	GLU
R183		Q101	LVS
A184		L102	LVS
A185		M103	ALA
		E104	THR
V190		V105	GLU
S191		F106	ASP
		K107	GLU
I198			GLY
T199		S112	SER
D200		E113	GLU
V201		K114	GLN
I202		T115	LVS
P203		S116	I1E
S204		D117	P80
		I118	GLU
T207		I119	A43
N208		H120	T44
E209		F121	N45
L210		F122	R46
T211		F123	
G212		A124	
L213		K125	
L214			L51
L215		R129	S52
V216		L130	K53
N217		Y131	A54
T218			
F221		K136	A59
K222		S137	T61
		S138	F62
			Y63
			Q64
A225		V141	A67
K226		S142	D68
S227		A143	S69
K228		N144	K70
F229		R145	N71
		L146	D72
T234		F147	N73
		G148	D74
			N75
E237		F154	I76
L238		N155	F177
F239			T78
Y240		F156	
		T157	



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



● Molecule 3: 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	68.47Å 98.67Å 89.24Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.80) 99.6 (19.98-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.283 0.231 , 0.221	Depositor DCC
R_{free} test set	1438 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: 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	I	0.49	0/3265	1.04	19/4423 (0.4%)
2	L	0.50	0/3141	1.00	14/4277 (0.3%)
All	All	0.50	0/6406	1.02	33/8700 (0.4%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	185	ALA	N-CA-C	-7.54	102.73	112.23
2	L	18	ASN	CA-C-N	6.73	128.25	119.84
2	L	18	ASN	C-N-CA	6.73	128.25	119.84
2	L	88	ALA	N-CA-C	-6.50	104.27	111.36
1	I	272	LEU	CA-C-N	-6.50	113.83	120.85
1	I	272	LEU	C-N-CA	-6.50	113.83	120.85
2	L	403	LYS	N-CA-C	6.16	123.93	110.80
1	I	322	ARG	N-CA-C	-6.14	101.39	110.48
1	I	320	MET	CA-C-N	6.13	126.05	119.85
1	I	320	MET	C-N-CA	6.13	126.05	119.85
1	I	165	VAL	N-CA-C	6.10	116.29	110.74
1	I	96	ASN	CB-CA-C	-6.03	108.61	115.79
2	L	354	ILE	N-CA-C	6.01	117.38	111.67
2	L	226	LYS	N-CA-C	-5.94	104.72	111.07
1	I	229	PHE	N-CA-C	-5.90	102.92	110.53
1	I	182	SER	N-CA-C	-5.86	102.59	111.56
2	L	252	MET	N-CA-C	-5.80	101.88	110.46
1	I	162	SER	N-CA-C	-5.65	105.58	113.37
1	I	332	LYS	N-CA-C	5.53	117.77	111.02
1	I	11	LYS	N-CA-C	-5.48	101.71	110.10
2	L	412	ILE	N-CA-C	-5.43	99.33	107.37
2	L	81	LEU	N-CA-C	-5.36	105.35	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	88	ALA	N-CA-C	-5.34	104.89	111.40
2	L	272	LEU	CA-C-N	5.32	125.22	119.85
2	L	272	LEU	C-N-CA	5.32	125.22	119.85
1	I	152	LEU	N-CA-C	5.30	122.08	110.80
1	I	414	GLU	N-CA-C	-5.25	99.23	108.20
2	L	240	TYR	N-CA-C	5.12	116.95	108.20
2	L	183	ARG	N-CA-C	-5.09	104.81	111.02
2	L	259	ARG	N-CA-C	-5.07	101.70	109.76
1	I	154	PHE	N-CA-C	-5.03	100.20	108.49
1	I	345	SER	CA-C-N	5.02	124.32	118.85
1	I	345	SER	C-N-CA	5.02	124.32	118.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3203	0	3086	213	0
2	L	3078	0	2857	210	0
3	A	28	0	25	1	0
3	B	27	0	25	0	0
4	I	42	0	39	9	0
4	L	42	0	39	5	0
5	I	84	0	0	7	0
5	L	56	0	0	3	0
All	All	6560	0	6071	421	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 34.

All (421) 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:I:150:LYS:HA	1:I:172:PRO:HB2	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:404:ALA:HB2	2:L:428:ASN:ND2	1.78	0.98
2:L:7:ILE:HD12	2:L:7:ILE:H	1.30	0.96
2:L:404:ALA:HB2	2:L:428:ASN:HD22	1.32	0.94
1:I:190:VAL:HB	1:I:201:VAL:HG21	1.51	0.91
2:L:94:ALA:HA	2:L:351:LEU:HD23	1.52	0.91
2:L:292:LEU:HD23	2:L:407:PRO:HG2	1.54	0.89
1:I:143:ALA:HB3	1:I:218:THR:HG23	1.51	0.89
2:L:124:ALA:HB2	2:L:165:VAL:HG13	1.58	0.84
2:L:211:THR:HA	2:L:391:ALA:O	1.78	0.83
2:L:365:SER:HB3	2:L:392:GLY:H	1.46	0.81
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.64	0.79
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.64	0.79
2:L:215:LEU:HD12	2:L:215:LEU:H	1.48	0.79
1:I:281:MET:HE3	1:I:283:LEU:HD21	1.65	0.78
2:L:285:LEU:N	2:L:285:LEU:HD23	1.99	0.78
1:I:161:ILE:C	1:I:163:GLU:H	1.92	0.78
1:I:232:GLU:OE1	2:L:262:ARG:HD2	1.84	0.78
2:L:73:ASN:HB3	2:L:404:ALA:O	1.84	0.77
2:L:71:ASN:HB2	5:L:652:HOH:O	1.82	0.77
2:L:239:PHE:HE1	2:L:404:ALA:HB1	1.50	0.77
1:I:192:ASN:HD21	4:I:861:NAG:H2	1.49	0.77
1:I:183:ARG:HB2	1:I:207:ILE:HD12	1.66	0.76
2:L:145:ARG:HG2	2:L:147:PHE:CE1	2.22	0.74
1:I:176:LYS:HA	1:I:209:GLU:HG3	1.69	0.74
2:L:215:LEU:HD12	2:L:215:LEU:N	2.04	0.73
2:L:213:LEU:HB3	2:L:390:ILE:HD12	1.71	0.73
2:L:62:PHE:CD1	2:L:338:MET:HE1	2.23	0.72
2:L:405:ASN:CG	2:L:406:ARG:H	1.97	0.72
2:L:244:GLY:HA2	5:L:537:HOH:O	1.90	0.71
2:L:91:LYS:NZ	2:L:120:HIS:NE2	2.37	0.71
1:I:261:ARG:NH1	1:I:261:ARG:HA	2.05	0.71
1:I:192:ASN:HD21	4:I:861:NAG:C2	2.03	0.71
1:I:154:PHE:HA	1:I:354:ILE:HG23	1.74	0.70
1:I:213:LEU:HD23	1:I:364:VAL:HG22	1.74	0.70
1:I:354:ILE:N	1:I:354:ILE:HD12	2.08	0.69
2:L:252:MET:HE2	2:L:320:MET:HG2	1.73	0.69
2:L:190:VAL:HG21	2:L:201:VAL:HG21	1.73	0.69
1:I:192:ASN:HD21	4:I:861:NAG:C1	2.06	0.68
2:L:59:ALA:HB1	2:L:423:MET:CE	2.23	0.68
2:L:91:LYS:HE2	2:L:120:HIS:NE2	2.07	0.68
1:I:183:ARG:HE	1:I:204:SER:HA	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:336:GLN:HA	1:I:340:LEU:O	1.93	0.68
1:I:262:ARG:HG3	1:I:262:ARG:HH11	1.59	0.67
1:I:332:LYS:O	1:I:336:GLN:HG3	1.95	0.66
2:L:7:ILE:HG12	2:L:164:LEU:O	1.96	0.66
2:L:77:PHE:CZ	2:L:373:LEU:HB2	2.30	0.66
1:I:281:MET:CE	1:I:320:MET:HE1	2.26	0.66
1:I:91:LYS:NZ	1:I:120:HIS:NE2	2.38	0.66
4:L:841:NAG:O4	4:L:842:NAG:C1	2.44	0.66
1:I:146:LEU:HD13	1:I:215:LEU:HD13	1.78	0.66
2:L:77:PHE:CE2	2:L:373:LEU:HB2	2.32	0.65
2:L:324:ARG:HG3	2:L:324:ARG:O	1.96	0.65
1:I:259:ARG:NH2	1:I:311:LEU:HB2	2.11	0.65
2:L:292:LEU:CD2	2:L:407:PRO:HG2	2.26	0.65
2:L:355:VAL:HG23	2:L:362:LEU:HD11	1.77	0.65
1:I:143:ALA:HB3	1:I:218:THR:CG2	2.23	0.64
2:L:91:LYS:CE	2:L:120:HIS:NE2	2.60	0.64
2:L:341:VAL:HG23	2:L:342:ASP:H	1.61	0.64
1:I:71:ASN:HD22	1:I:72:ASP:H	1.45	0.64
2:L:413:ARG:NH2	2:L:415:VAL:HG13	2.12	0.64
2:L:182:SER:O	2:L:185:ALA:HB3	1.97	0.64
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.79	0.64
1:I:294:LYS:O	1:I:298:GLU:HG3	1.96	0.64
2:L:237:GLU:HB2	5:L:656:HOH:O	1.97	0.64
2:L:365:SER:CB	2:L:392:GLY:H	2.12	0.63
2:L:239:PHE:CE1	2:L:404:ALA:HB1	2.32	0.63
2:L:261:ARG:HG3	2:L:263:VAL:CG1	2.29	0.63
1:I:182:SER:O	1:I:184:ALA:N	2.25	0.63
1:I:174:ASP:HB3	1:I:178:ASN:HB2	1.79	0.63
1:I:312:GLU:HB2	5:I:588:HOH:O	1.99	0.63
2:L:283:LEU:HD11	2:L:320:MET:HE1	1.80	0.63
1:I:289:GLU:H	1:I:289:GLU:CD	2.08	0.62
2:L:71:ASN:ND2	2:L:73:ASN:HB2	2.14	0.62
1:I:183:ARG:O	1:I:183:ARG:HG2	2.00	0.62
1:I:78:LEU:N	1:I:78:LEU:HD23	2.15	0.62
1:I:190:VAL:HG21	1:I:201:VAL:HG11	1.80	0.62
2:L:208:ASN:C	2:L:208:ASN:HD22	2.08	0.61
1:I:343:LEU:HD11	1:I:364:VAL:HG23	1.83	0.61
2:L:341:VAL:HG23	2:L:342:ASP:N	2.14	0.61
1:I:144:ASN:HB2	5:I:519:HOH:O	1.99	0.61
2:L:125:LYS:O	2:L:129:ARG:HG2	2.00	0.61
2:L:229:PHE:HB2	2:L:377:GLU:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:331:LEU:O	2:L:335:LEU:HB2	1.99	0.61
1:I:331:LEU:HB2	1:I:367:ALA:HB3	1.82	0.61
2:L:175:PHE:O	2:L:209:GLU:HA	2.01	0.61
2:L:191:SER:OG	2:L:199:THR:HG22	2.01	0.61
1:I:326:GLU:HG2	1:I:370:LYS:HE3	1.82	0.60
1:I:190:VAL:CB	1:I:201:VAL:HG21	2.27	0.60
2:L:222:LYS:HG2	2:L:381:GLU:HG3	1.82	0.60
1:I:51:LEU:HA	1:I:111:ILE:HD11	1.83	0.60
2:L:261:ARG:O	2:L:263:VAL:HG13	2.02	0.60
1:I:194:THR:O	1:I:197:ARG:HG2	2.02	0.60
2:L:91:LYS:HZ3	2:L:120:HIS:CD2	2.19	0.59
2:L:274:PHE:HD2	2:L:279:ILE:O	1.84	0.59
1:I:18:ASN:O	1:I:21:CYS:HB2	2.03	0.59
1:I:161:ILE:C	1:I:163:GLU:N	2.59	0.59
5:I:609:HOH:O	2:L:249:ALA:HB2	2.02	0.59
1:I:159:GLN:CB	1:I:170:LEU:HD21	2.32	0.59
1:I:170:LEU:O	1:I:171:GLN:HB3	2.02	0.59
1:I:177:GLU:C	1:I:178:ASN:HD22	2.11	0.59
2:L:102:LEU:HD23	2:L:340:LEU:HD11	1.84	0.59
1:I:111:ILE:O	1:I:114:LYS:HB2	2.03	0.58
1:I:182:SER:O	1:I:185:ALA:N	2.36	0.58
1:I:108:PHE:HB3	1:I:119:ILE:HG12	1.85	0.58
2:L:119:ILE:HG22	2:L:120:HIS:N	2.16	0.58
1:I:183:ARG:HG2	1:I:183:ARG:HH11	1.67	0.58
2:L:144:ASN:HD22	2:L:217:ASN:HA	1.68	0.58
2:L:221:PHE:CE1	2:L:279:ILE:HG21	2.39	0.58
2:L:252:MET:CE	2:L:320:MET:HG2	2.34	0.58
1:I:183:ARG:CB	1:I:207:ILE:HD12	2.34	0.58
2:L:428:ASN:OD1	2:L:430:CYS:HB2	2.03	0.58
1:I:391:ALA:O	2:L:321:PRO:HD3	2.02	0.58
2:L:7:ILE:H	2:L:7:ILE:CD1	2.07	0.58
2:L:24:ARG:HA	2:L:114:LYS:O	2.04	0.58
2:L:54:ALA:HB1	2:L:107:LYS:O	2.03	0.58
2:L:292:LEU:HD21	2:L:407:PRO:O	2.05	0.57
1:I:47:ARG:HB3	1:I:122:PHE:CD1	2.39	0.57
1:I:232:GLU:CD	2:L:262:ARG:HD2	2.30	0.57
1:I:115:THR:H	1:I:118:GLN:NE2	2.03	0.57
1:I:182:SER:C	1:I:184:ALA:H	2.12	0.57
2:L:254:GLN:NE2	2:L:258:PHE:HZ	2.02	0.57
1:I:19:PRO:C	1:I:21:CYS:H	2.13	0.57
1:I:286:PRO:HB3	1:I:295:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:71:ASN:C	2:L:73:ASN:H	2.13	0.57
2:L:207:ILE:HG23	2:L:211:THR:HG21	1.85	0.56
1:I:115:THR:H	1:I:118:GLN:HE21	1.51	0.56
1:I:331:LEU:HB3	1:I:335:LEU:HD11	1.87	0.56
2:L:52:SER:HB2	2:L:419:THR:HG22	1.87	0.56
1:I:260:TYR:CD2	1:I:261:ARG:N	2.73	0.56
2:L:131:TYR:CE1	2:L:142:SER:HB2	2.39	0.56
2:L:261:ARG:HG3	2:L:263:VAL:HG13	1.87	0.56
1:I:396:ASN:OD1	1:I:398:ASN:N	2.36	0.56
1:I:71:ASN:HD22	1:I:72:ASP:N	2.03	0.56
1:I:387:ALA:O	2:L:316:LEU:HB2	2.06	0.56
1:I:284:ILE:HD13	1:I:307:TRP:HZ3	1.70	0.56
1:I:302:GLU:CD	1:I:302:GLU:H	2.13	0.56
1:I:183:ARG:HG2	1:I:183:ARG:NH1	2.21	0.56
2:L:255:GLU:OE2	2:L:315:MET:HE1	2.07	0.55
1:I:153:THR:HG22	1:I:354:ILE:C	2.32	0.55
2:L:116:SER:O	2:L:118:GLN:N	2.40	0.55
1:I:285:LEU:HD11	1:I:406:ARG:HG3	1.87	0.55
1:I:51:LEU:HD22	1:I:122:PHE:CB	2.36	0.55
2:L:7:ILE:HD12	2:L:7:ILE:N	2.11	0.55
2:L:222:LYS:CG	2:L:381:GLU:HG3	2.37	0.55
2:L:96:ASN:ND2	4:L:801:NAG:C1	2.70	0.55
2:L:366:ASP:OD2	2:L:368:PHE:CZ	2.60	0.55
2:L:405:ASN:CG	2:L:406:ARG:N	2.65	0.55
1:I:192:ASN:ND2	4:I:861:NAG:H2	2.18	0.55
2:L:332:LYS:O	2:L:336:GLN:HG3	2.07	0.55
1:I:191:SER:HA	1:I:198:ILE:O	2.07	0.54
1:I:342:ASP:O	1:I:349:SER:HA	2.06	0.54
2:L:148:GLY:HA3	2:L:154:PHE:CE2	2.42	0.54
2:L:420:ILE:HG21	2:L:423:MET:HE2	1.88	0.54
2:L:198:ILE:HG23	2:L:370:LYS:HG2	1.88	0.54
1:I:17:MET:HG2	1:I:117:ASP:HB3	1.88	0.54
1:I:76:ILE:O	1:I:77:PHE:HB2	2.08	0.54
1:I:412:ILE:O	1:I:421:ILE:HB	2.08	0.54
1:I:221:PHE:CE1	1:I:279:ILE:HG21	2.43	0.54
1:I:262:ARG:HG3	1:I:262:ARG:NH1	2.23	0.54
2:L:234:THR:HG23	2:L:251:MET:O	2.07	0.54
2:L:21:CYS:C	2:L:22:ILE:HD12	2.33	0.54
2:L:115:THR:HG23	2:L:118:GLN:CB	2.38	0.54
2:L:284:ILE:C	2:L:285:LEU:HD23	2.33	0.53
2:L:328:GLY:O	2:L:329:PHE:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:372:PHE:O	2:L:382:ALA:HA	2.08	0.53
1:I:389:VAL:HA	5:I:655:HOH:O	2.07	0.53
2:L:405:ASN:ND2	2:L:406:ARG:N	2.55	0.53
2:L:199:THR:O	2:L:200:ASP:HB3	2.08	0.53
1:I:238:LEU:HA	1:I:247:CYS:O	2.08	0.53
1:I:19:PRO:C	1:I:21:CYS:N	2.64	0.53
1:I:331:LEU:HB3	1:I:335:LEU:CD1	2.39	0.53
2:L:18:ASN:O	2:L:19:PRO:O	2.26	0.53
2:L:403:LYS:HD3	2:L:404:ALA:N	2.24	0.53
1:I:183:ARG:HB2	1:I:207:ILE:CD1	2.37	0.53
1:I:183:ARG:CA	1:I:207:ILE:HD12	2.39	0.53
2:L:221:PHE:CG	2:L:222:LYS:N	2.77	0.53
1:I:345:SER:HB3	1:I:348:LYS:HB2	1.91	0.52
2:L:105:VAL:HG21	2:L:340:LEU:HB2	1.91	0.52
1:I:182:SER:C	1:I:184:ALA:N	2.66	0.52
2:L:71:ASN:HD21	2:L:73:ASN:HB2	1.74	0.52
2:L:22:ILE:HD12	2:L:22:ILE:N	2.24	0.52
2:L:283:LEU:HD11	2:L:320:MET:CE	2.39	0.52
1:I:260:TYR:CG	1:I:261:ARG:N	2.78	0.52
2:L:130:LEU:HD23	2:L:417:LEU:HD13	1.92	0.52
2:L:283:LEU:O	2:L:284:ILE:HG13	2.08	0.52
1:I:213:LEU:HB3	1:I:364:VAL:HA	1.92	0.52
2:L:259:ARG:HD3	2:L:271:GLU:OE1	2.09	0.52
1:I:261:ARG:HD3	1:I:262:ARG:N	2.25	0.51
2:L:404:ALA:HB2	2:L:428:ASN:CG	2.33	0.51
1:I:89:MET:HA	1:I:166:TYR:CD2	2.45	0.51
1:I:170:LEU:H	1:I:170:LEU:HD23	1.76	0.51
2:L:67:ALA:O	2:L:69:SER:N	2.40	0.51
2:L:91:LYS:HE2	2:L:120:HIS:CE1	2.45	0.51
1:I:155:ASN:HB3	1:I:353:GLY:O	2.11	0.51
2:L:59:ALA:HB1	2:L:423:MET:HE1	1.93	0.51
2:L:179:ALA:HB1	2:L:207:ILE:O	2.11	0.51
2:L:404:ALA:CB	2:L:428:ASN:HB2	2.41	0.51
2:L:74:ASP:O	2:L:425:ARG:HD2	2.10	0.51
2:L:398:ASN:CG	2:L:399:ARG:H	2.19	0.51
2:L:405:ASN:O	2:L:406:ARG:C	2.54	0.51
1:I:15:ILE:N	1:I:16:PRO:HD3	2.26	0.50
1:I:154:PHE:HA	1:I:354:ILE:CG2	2.40	0.50
1:I:351:LEU:C	1:I:353:GLY:H	2.18	0.50
4:I:862:NAG:O7	4:I:862:NAG:H3	2.09	0.50
2:L:213:LEU:HG	2:L:214:VAL:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:349:SER:OG	2:L:363:TYR:HA	2.11	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.11	0.50
2:L:60:THR:O	2:L:64:GLN:HG3	2.12	0.50
1:I:71:ASN:ND2	1:I:72:ASP:N	2.58	0.50
2:L:78:LEU:N	2:L:78:LEU:HD23	2.27	0.50
2:L:304:LEU:O	2:L:308:LEU:HG	2.12	0.50
1:I:241:LYS:HD3	1:I:428:ASN:HD22	1.77	0.50
1:I:84:SER:O	1:I:88:ALA:HB2	2.12	0.49
2:L:16:PRO:O	2:L:17:MET:C	2.55	0.49
2:L:405:ASN:ND2	2:L:406:ARG:H	2.10	0.49
1:I:313:GLU:O	1:I:314:MET:HG3	2.12	0.49
2:L:292:LEU:O	2:L:295:VAL:N	2.41	0.49
1:I:331:LEU:C	1:I:335:LEU:HD12	2.38	0.49
2:L:155:ASN:ND2	4:L:841:NAG:C7	2.76	0.49
2:L:366:ASP:OD2	2:L:368:PHE:CE1	2.66	0.49
2:L:410:VAL:O	2:L:423:MET:HA	2.13	0.49
2:L:23:TYR:HB3	2:L:116:SER:OG	2.12	0.49
2:L:200:ASP:O	2:L:201:VAL:C	2.56	0.49
1:I:284:ILE:HD13	1:I:307:TRP:CZ3	2.47	0.49
2:L:285:LEU:N	2:L:285:LEU:CD2	2.70	0.49
1:I:91:LYS:HE3	1:I:120:HIS:CE1	2.47	0.49
2:L:23:TYR:CE1	2:L:100:GLN:HG3	2.47	0.49
2:L:374:GLU:O	2:L:380:SER:HA	2.13	0.49
2:L:100:GLN:O	2:L:104:GLU:HG3	2.13	0.49
2:L:355:VAL:O	2:L:355:VAL:HG12	2.12	0.49
1:I:92:LEU:HB3	1:I:158:TYR:CE1	2.48	0.49
2:L:5:VAL:HG12	2:L:6:ASP:N	2.28	0.49
2:L:51:LEU:CD2	2:L:123:PHE:HA	2.43	0.48
2:L:62:PHE:HD1	2:L:338:MET:HE1	1.73	0.48
1:I:186:ILE:O	1:I:189:TRP:N	2.46	0.48
2:L:263:VAL:O	2:L:264:ALA:C	2.57	0.48
1:I:71:ASN:ND2	1:I:72:ASP:H	2.11	0.48
1:I:180:GLU:C	1:I:182:SER:H	2.22	0.48
1:I:170:LEU:HD23	1:I:170:LEU:N	2.28	0.48
2:L:414:GLU:OE1	2:L:416:PRO:HG2	2.14	0.48
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.79	0.48
1:I:147:PHE:CE2	1:I:186:ILE:HG12	2.49	0.48
2:L:358:GLY:O	2:L:359:ARG:C	2.57	0.48
1:I:76:ILE:HG22	1:I:77:PHE:N	2.29	0.48
1:I:89:MET:HA	1:I:166:TYR:CE2	2.49	0.48
1:I:89:MET:HE2	1:I:166:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:ASN:HB3	1:I:181:GLN:HG3	1.96	0.48
1:I:261:ARG:HD3	1:I:262:ARG:H	1.78	0.48
1:I:281:MET:HE1	1:I:320:MET:HE1	1.94	0.48
1:I:400:VAL:HG12	1:I:401:THR:N	2.28	0.48
1:I:346:PRO:HG3	1:I:363:TYR:CE2	2.49	0.47
2:L:158:TYR:HB2	2:L:353:GLY:O	2.13	0.47
2:L:326:GLU:HG2	2:L:372:PHE:HD2	1.79	0.47
1:I:396:ASN:HB2	2:L:240:TYR:CZ	2.49	0.47
1:I:260:TYR:CZ	1:I:400:VAL:HG11	2.50	0.47
2:L:96:ASN:O	2:L:97:ASP:HB2	2.14	0.47
2:L:214:VAL:HG22	2:L:389:VAL:HG22	1.97	0.47
2:L:215:LEU:H	2:L:215:LEU:CD1	2.23	0.47
1:I:14:ASP:C	1:I:16:PRO:HD3	2.40	0.47
1:I:261:ARG:NH1	5:I:658:HOH:O	2.46	0.47
1:I:87:PHE:CE1	1:I:335:LEU:HD13	2.49	0.47
1:I:154:PHE:O	1:I:155:ASN:C	2.57	0.47
2:L:308:LEU:HD13	2:L:413:ARG:NH2	2.30	0.47
2:L:355:VAL:O	2:L:357:GLU:N	2.48	0.47
2:L:355:VAL:CG2	2:L:362:LEU:HD11	2.45	0.47
1:I:261:ARG:HA	1:I:261:ARG:CZ	2.44	0.47
1:I:281:MET:HA	1:I:411:PHE:O	2.14	0.47
1:I:390:ILE:HA	2:L:319:HIS:HB2	1.96	0.47
4:I:801:NAG:O7	4:I:801:NAG:H3	2.14	0.47
2:L:119:ILE:O	2:L:122:PHE:N	2.48	0.47
2:L:208:ASN:C	2:L:208:ASN:ND2	2.73	0.47
2:L:217:ASN:ND2	2:L:218:THR:N	2.63	0.47
2:L:276:GLY:O	2:L:277:ASP:HB2	2.14	0.47
1:I:71:ASN:HB3	1:I:74:ASP:OD2	2.15	0.47
2:L:80:PRO:HG3	2:L:423:MET:HE3	1.97	0.47
2:L:146:LEU:HD11	2:L:162:SER:HB3	1.97	0.47
1:I:51:LEU:HD22	1:I:122:PHE:HB3	1.97	0.47
1:I:121:PHE:O	1:I:124:ALA:HB3	2.15	0.47
1:I:40:ILE:O	1:I:40:ILE:HG23	2.14	0.46
1:I:91:LYS:CB	1:I:102:LEU:HD13	2.42	0.46
1:I:326:GLU:CG	1:I:370:LYS:HE3	2.44	0.46
1:I:334:GLN:O	1:I:335:LEU:C	2.58	0.46
2:L:356:ALA:C	2:L:358:GLY:H	2.22	0.46
2:L:356:ALA:C	2:L:358:GLY:N	2.73	0.46
1:I:261:ARG:HA	1:I:261:ARG:HH11	1.80	0.46
1:I:341:VAL:C	1:I:343:LEU:H	2.24	0.46
2:L:217:ASN:ND2	2:L:217:ASN:C	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:GLU:O	1:I:114:LYS:C	2.57	0.46
1:I:346:PRO:HA	1:I:363:TYR:CD1	2.50	0.46
2:L:131:TYR:CZ	2:L:142:SER:HB2	2.50	0.46
2:L:215:LEU:N	2:L:215:LEU:CD1	2.76	0.46
1:I:155:ASN:O	1:I:158:TYR:HB3	2.16	0.46
1:I:299:LEU:C	1:I:299:LEU:HD13	2.41	0.46
1:I:87:PHE:H	1:I:87:PHE:HD2	1.63	0.46
1:I:151:SER:O	1:I:152:LEU:O	2.34	0.46
1:I:229:PHE:CE2	1:I:254:GLN:HG2	2.51	0.46
2:L:163:GLU:O	2:L:163:GLU:HG2	2.15	0.46
4:I:861:NAG:H5	4:I:862:NAG:C1	2.46	0.46
2:L:95:CYS:O	2:L:350:LYS:HB2	2.16	0.46
2:L:372:PHE:CD1	2:L:372:PHE:C	2.93	0.46
1:I:51:LEU:HD22	1:I:122:PHE:HB2	1.97	0.46
1:I:190:VAL:HB	1:I:201:VAL:CG2	2.35	0.45
1:I:351:LEU:O	1:I:353:GLY:N	2.49	0.45
2:L:71:ASN:O	2:L:73:ASN:N	2.49	0.45
2:L:101:GLN:O	2:L:105:VAL:HG23	2.15	0.45
1:I:22:ILE:HG22	1:I:23:TYR:N	2.30	0.45
2:L:221:PHE:CE1	2:L:279:ILE:HD13	2.52	0.45
2:L:333:GLU:O	2:L:337:ASP:OD1	2.34	0.45
1:I:319:HIS:CB	1:I:403:LYS:HG3	2.46	0.45
2:L:326:GLU:HG2	2:L:372:PHE:CD2	2.52	0.45
2:L:172:PRO:O	2:L:173:LEU:HG	2.16	0.45
2:L:253:TYR:CD1	2:L:253:TYR:C	2.94	0.45
1:I:56:SER:OG	1:I:420:ILE:HD12	2.17	0.45
1:I:327:ASP:O	1:I:370:LYS:HD2	2.16	0.45
2:L:43:ALA:HB3	2:L:46:ARG:CB	2.47	0.45
1:I:219:ILE:HG22	1:I:220:LEU:N	2.32	0.45
5:I:609:HOH:O	2:L:239:PHE:HB2	2.17	0.45
2:L:145:ARG:HG2	2:L:147:PHE:CZ	2.51	0.44
1:I:276:GLY:O	1:I:277:ASP:HB2	2.17	0.44
2:L:294:LYS:O	2:L:294:LYS:HG2	2.18	0.44
2:L:404:ALA:HB2	2:L:428:ASN:CB	2.47	0.44
2:L:418:ASN:OD1	2:L:418:ASN:O	2.35	0.44
1:I:78:LEU:HD23	1:I:78:LEU:H	1.80	0.44
2:L:71:ASN:N	2:L:74:ASP:OD2	2.46	0.44
2:L:199:THR:O	2:L:200:ASP:CB	2.64	0.44
2:L:258:PHE:O	2:L:314:MET:N	2.49	0.44
2:L:59:ALA:HB1	2:L:423:MET:HE3	1.98	0.44
2:L:116:SER:O	2:L:117:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:258:PHE:HB2	2:L:316:LEU:HD21	2.00	0.44
1:I:346:PRO:HG3	1:I:363:TYR:CZ	2.53	0.43
2:L:91:LYS:HZ3	2:L:120:HIS:CE1	2.34	0.43
2:L:404:ALA:HB2	2:L:428:ASN:HB2	1.99	0.43
1:I:219:ILE:HB	1:I:422:PHE:CZ	2.53	0.43
1:I:285:LEU:HD12	1:I:286:PRO:HD2	2.00	0.43
1:I:332:LYS:HG3	1:I:344:PHE:CD1	2.52	0.43
2:L:245:GLU:HG2	2:L:246:SER:N	2.34	0.43
1:I:239:PHE:CD2	1:I:429:PRO:HG3	2.53	0.43
1:I:360:ASP:OD2	1:I:361:ASP:N	2.52	0.43
2:L:115:THR:O	2:L:116:SER:C	2.61	0.43
1:I:193:LYS:C	1:I:195:GLU:H	2.27	0.43
1:I:151:SER:HB3	1:I:152:LEU:H	1.54	0.43
1:I:198:ILE:HG23	1:I:370:LYS:HG2	2.01	0.43
1:I:353:GLY:C	1:I:354:ILE:HD12	2.43	0.43
1:I:417:LEU:O	1:I:418:ASN:C	2.61	0.43
1:I:192:ASN:ND2	4:I:861:NAG:C1	2.80	0.43
1:I:253:TYR:OH	1:I:255:GLU:OE2	2.34	0.43
2:L:157:THR:OG1	4:L:841:NAG:H5	2.19	0.43
2:L:258:PHE:HB2	2:L:316:LEU:CD2	2.48	0.43
1:I:288:PRO:HB2	1:I:289:GLU:OE2	2.18	0.43
2:L:157:THR:CB	4:L:841:NAG:H5	2.49	0.43
2:L:171:GLN:HA	2:L:172:PRO:HD3	1.81	0.43
1:I:153:THR:O	1:I:354:ILE:HG22	2.18	0.43
1:I:192:ASN:ND2	4:I:861:NAG:C2	2.77	0.43
1:I:241:LYS:CD	1:I:428:ASN:HD22	2.32	0.43
2:L:119:ILE:O	2:L:120:HIS:C	2.62	0.43
1:I:89:MET:O	1:I:92:LEU:HB2	2.19	0.42
1:I:284:ILE:HB	1:I:409:LEU:HB2	2.01	0.42
1:I:22:ILE:CG2	1:I:23:TYR:N	2.81	0.42
1:I:94:ALA:HB3	1:I:99:LEU:HD13	2.01	0.42
1:I:167:GLY:O	1:I:168:ALA:HB2	2.19	0.42
1:I:360:ASP:O	1:I:361:ASP:C	2.62	0.42
1:I:341:VAL:O	1:I:343:LEU:N	2.52	0.42
1:I:421:ILE:HG22	1:I:422:PHE:CD2	2.54	0.42
2:L:259:ARG:NH2	2:L:311:LEU:HB2	2.33	0.42
1:I:155:ASN:HA	3:A:1:NAG:C8	2.50	0.42
1:I:239:PHE:CZ	1:I:406:ARG:C	2.98	0.42
1:I:414:GLU:HB2	1:I:421:ILE:HD11	2.01	0.42
2:L:71:ASN:C	2:L:73:ASN:N	2.78	0.42
2:L:356:ALA:O	2:L:358:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:365:SER:OG	2:L:389:VAL:HG12	2.20	0.42
1:I:189:TRP:O	1:I:192:ASN:HB3	2.20	0.42
2:L:245:GLU:HG2	2:L:246:SER:H	1.85	0.42
2:L:138:SER:HB3	2:L:279:ILE:HD12	2.02	0.42
2:L:225:TRP:CD1	2:L:379:GLY:HA2	2.55	0.42
1:I:336:GLN:C	1:I:338:MET:N	2.77	0.42
1:I:81:LEU:HD21	1:I:130:LEU:CD1	2.50	0.42
1:I:337:ASP:O	1:I:337:ASP:OD2	2.37	0.42
2:L:292:LEU:O	2:L:293:ALA:C	2.63	0.42
1:I:183:ARG:NE	1:I:203:PRO:O	2.52	0.41
1:I:354:ILE:N	1:I:354:ILE:CD1	2.77	0.41
2:L:283:LEU:CD1	2:L:320:MET:HE1	2.49	0.41
2:L:136:LYS:O	2:L:137:SER:HB2	2.20	0.41
1:I:222:LYS:HB2	1:I:381:GLU:HG2	2.01	0.41
1:I:243:ASP:OD1	1:I:244:GLY:N	2.42	0.41
1:I:343:LEU:CD1	1:I:364:VAL:HG23	2.49	0.41
2:L:273:PRO:HA	2:L:280:THR:HG22	2.02	0.41
1:I:138:SER:OG	1:I:138:SER:O	2.37	0.41
1:I:305:GLN:HG2	5:I:586:HOH:O	2.21	0.41
2:L:341:VAL:CG2	2:L:342:ASP:N	2.83	0.41
1:I:48:VAL:HG13	1:I:126:LEU:HD13	2.03	0.41
1:I:86:ALA:C	1:I:88:ALA:N	2.78	0.41
1:I:131:TYR:CZ	1:I:142:SER:HB2	2.56	0.41
1:I:114:LYS:N	1:I:114:LYS:HD2	2.34	0.41
1:I:241:LYS:HD3	1:I:428:ASN:ND2	2.35	0.41
2:L:75:ASN:C	2:L:76:ILE:HG13	2.46	0.41
2:L:91:LYS:HE2	2:L:91:LYS:HB3	1.80	0.41
2:L:102:LEU:CD2	2:L:340:LEU:HD11	2.51	0.41
1:I:81:LEU:HD21	1:I:130:LEU:HD11	2.02	0.41
1:I:293:ALA:O	1:I:294:LYS:C	2.63	0.41
1:I:323:PHE:CZ	1:I:375:VAL:HG21	2.56	0.41
1:I:341:VAL:C	1:I:343:LEU:N	2.78	0.41
2:L:221:PHE:HE1	2:L:279:ILE:HD13	1.86	0.41
1:I:252:MET:HG3	1:I:322:ARG:HG2	2.01	0.41
1:I:39:LYS:O	1:I:40:ILE:C	2.64	0.40
1:I:361:ASP:OD1	1:I:361:ASP:O	2.39	0.40
1:I:75:ASN:C	1:I:76:ILE:HG13	2.46	0.40
1:I:40:ILE:HA	1:I:41:PRO:HD2	2.01	0.40
1:I:200:ASP:OD1	1:I:370:LYS:HE2	2.21	0.40
2:L:105:VAL:HG13	2:L:338:MET:HB3	2.02	0.40
2:L:136:LYS:C	2:L:138:SER:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:LYS:N	1:I:173:LEU:O	2.54	0.40
2:L:253:TYR:CE2	2:L:317:VAL:CG1	3.05	0.40
2:L:260:TYR:O	2:L:261:ARG:HB2	2.21	0.40
1:I:119:ILE:HG22	1:I:120:HIS:N	2.35	0.40
1:I:190:VAL:C	1:I:192:ASN:H	2.30	0.40
1:I:253:TYR:CD2	1:I:253:TYR:C	2.98	0.40
2:L:203:PRO:HB2	2:L:204:SER:H	1.69	0.40
2:L:251:MET:CE	2:L:319:HIS:HB3	2.52	0.40
2:L:372:PHE:N	2:L:383:ALA:O	2.54	0.40
2:L:373:LEU:HD12	2:L:374:GLU:H	1.86	0.40

There are no symmetry-related clashes.

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	I	405/427 (95%)	309 (76%)	65 (16%)	31 (8%)	1	2
2	L	404/427 (95%)	328 (81%)	47 (12%)	29 (7%)	1	2
All	All	809/854 (95%)	637 (79%)	112 (14%)	60 (7%)	1	2

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	42	GLU
1	I	152	LEU
1	I	170	LEU
1	I	176	LYS
1	I	430	CYS
2	L	19	PRO
2	L	96	ASN
2	L	112	SER

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Mol	Chain	Res	Type
2	L	116	SER
2	L	117	ASP
2	L	136	LYS
2	L	200	ASP
2	L	203	PRO
2	L	228	LYS
2	L	250	SER
2	L	264	ALA
2	L	356	ALA
2	L	403	LYS
1	I	184	ALA
1	I	245	GLU
1	I	350	LYS
1	I	383	ALA
1	I	384	ALA
2	L	44	THR
2	L	69	SER
2	L	72	ASP
2	L	243	ASP
1	I	77	PHE
1	I	168	ALA
1	I	183	ARG
1	I	243	ASP
1	I	244	GLY
1	I	337	ASP
1	I	342	ASP
2	L	17	MET
2	L	68	ASP
2	L	293	ALA
2	L	359	ARG
1	I	38	GLN
1	I	82	SER
1	I	158	TYR
1	I	203	PRO
1	I	352	PRO
1	I	386	THR
2	L	244	GLY
2	L	357	GLU
1	I	12	PRO
1	I	43	ALA
1	I	116	SER
1	I	130	LEU

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Mol	Chain	Res	Type
1	I	171	GLN
2	L	222	LYS
2	L	406	ARG
1	I	40	ILE
1	I	112	SER
2	L	275	LYS
2	L	333	GLU
1	I	41	PRO
2	L	263	VAL
2	L	119	ILE

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	I	341/378 (90%)	322 (94%)	19 (6%)	19	50
2	L	312/379 (82%)	298 (96%)	14 (4%)	24	58
All	All	653/757 (86%)	620 (95%)	33 (5%)	21	54

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	13	ARG
1	I	17	MET
1	I	78	LEU
1	I	92	LEU
1	I	97	ASP
1	I	105	VAL
1	I	109	ASP
1	I	119	ILE
1	I	153	THR
1	I	170	LEU
1	I	216	VAL
1	I	217	ASN
1	I	302	GLU

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Mol	Chain	Res	Type
1	I	309	ASP
1	I	310	GLU
1	I	316	LEU
1	I	322	ARG
1	I	347	GLU
1	I	354	ILE
2	L	6	ASP
2	L	7	ILE
2	L	84	SER
2	L	97	ASP
2	L	141	VAL
2	L	162	SER
2	L	201	VAL
2	L	208	ASN
2	L	217	ASN
2	L	285	LEU
2	L	316	LEU
2	L	324	ARG
2	L	397	PRO
2	L	403	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	55	ASN
1	I	71	ASN
1	I	118	GLN
1	I	178	ASN
1	I	192	ASN
1	I	217	ASN
1	I	428	ASN
2	L	55	ASN
2	L	71	ASN
2	L	96	ASN
2	L	144	ASN
2	L	208	ASN
2	L	217	ASN
2	L	254	GLN
2	L	336	GLN
2	L	405	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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1	1,3	14,14,15	0.81	0	17,19,21	1.06	1 (5%)
3	NAG	A	2	3	14,14,15	0.61	0	17,19,21	0.77	1 (5%)
3	NAG	B	1	2,3	14,14,15	0.77	0	17,19,21	0.99	1 (5%)
3	NAG	B	2	3	13,13,15	0.87	0	16,17,21	1.03	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	1,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	A	2	3	-	4/6/23/26	0/1/1/1
3	NAG	B	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/5/22/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C7-N2-C2	3.88	120.35	114.43
3	A	1	NAG	C2-N2-C7	-2.53	119.51	122.90
3	B	1	NAG	C2-N2-C7	-2.18	119.97	122.90
3	A	2	NAG	C2-N2-C7	-2.15	120.01	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	NAG	C1

All (14) torsion outliers are listed below:

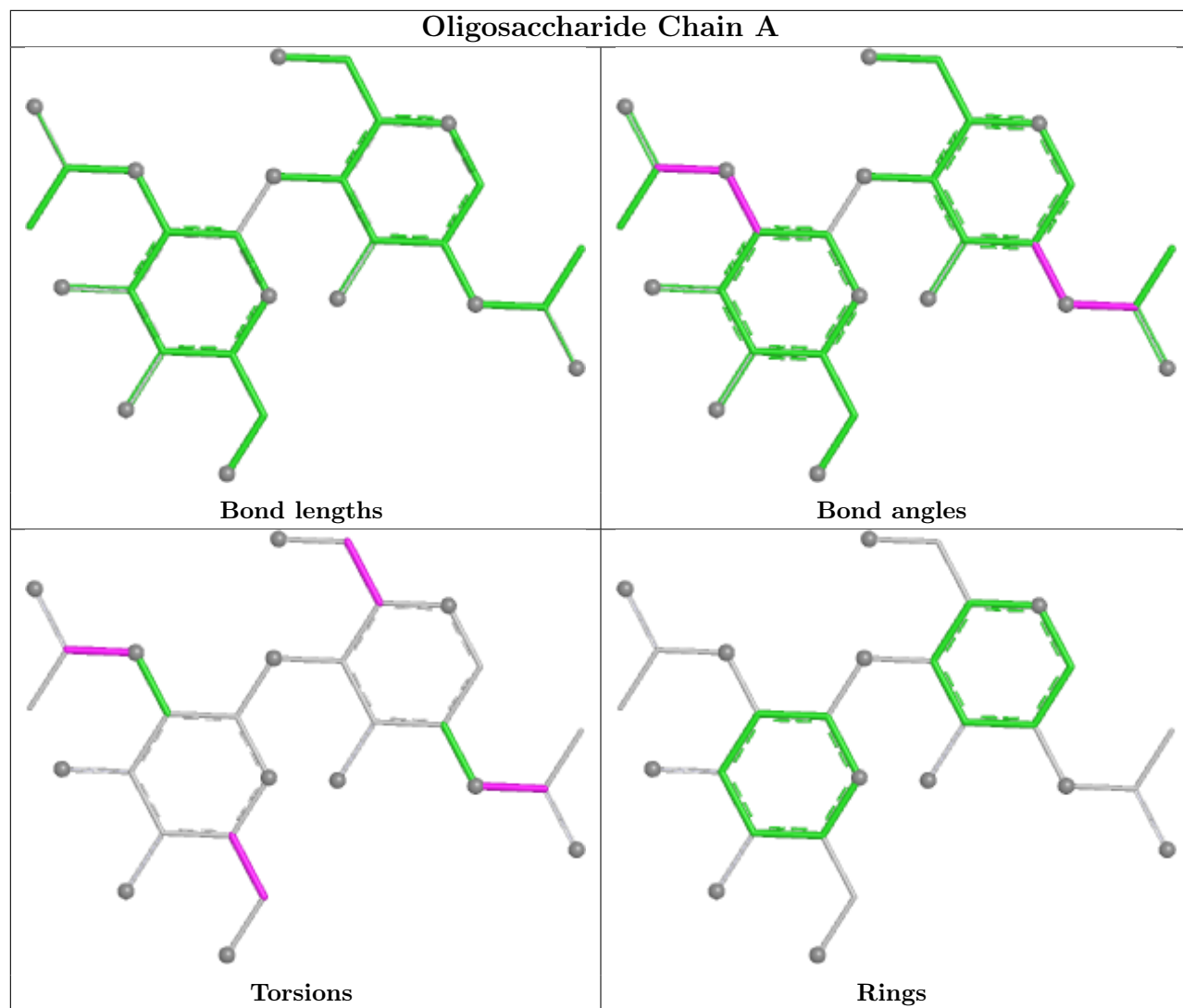
Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C8-C7-N2-C2
3	A	1	NAG	O7-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2
3	A	2	NAG	C8-C7-N2-C2
3	B	2	NAG	C1-C2-N2-C7
3	B	1	NAG	C8-C7-N2-C2
3	A	1	NAG	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	1	NAG	O7-C7-N2-C2
3	A	1	NAG	O5-C5-C6-O6
3	B	2	NAG	C8-C7-N2-C2
3	A	2	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6

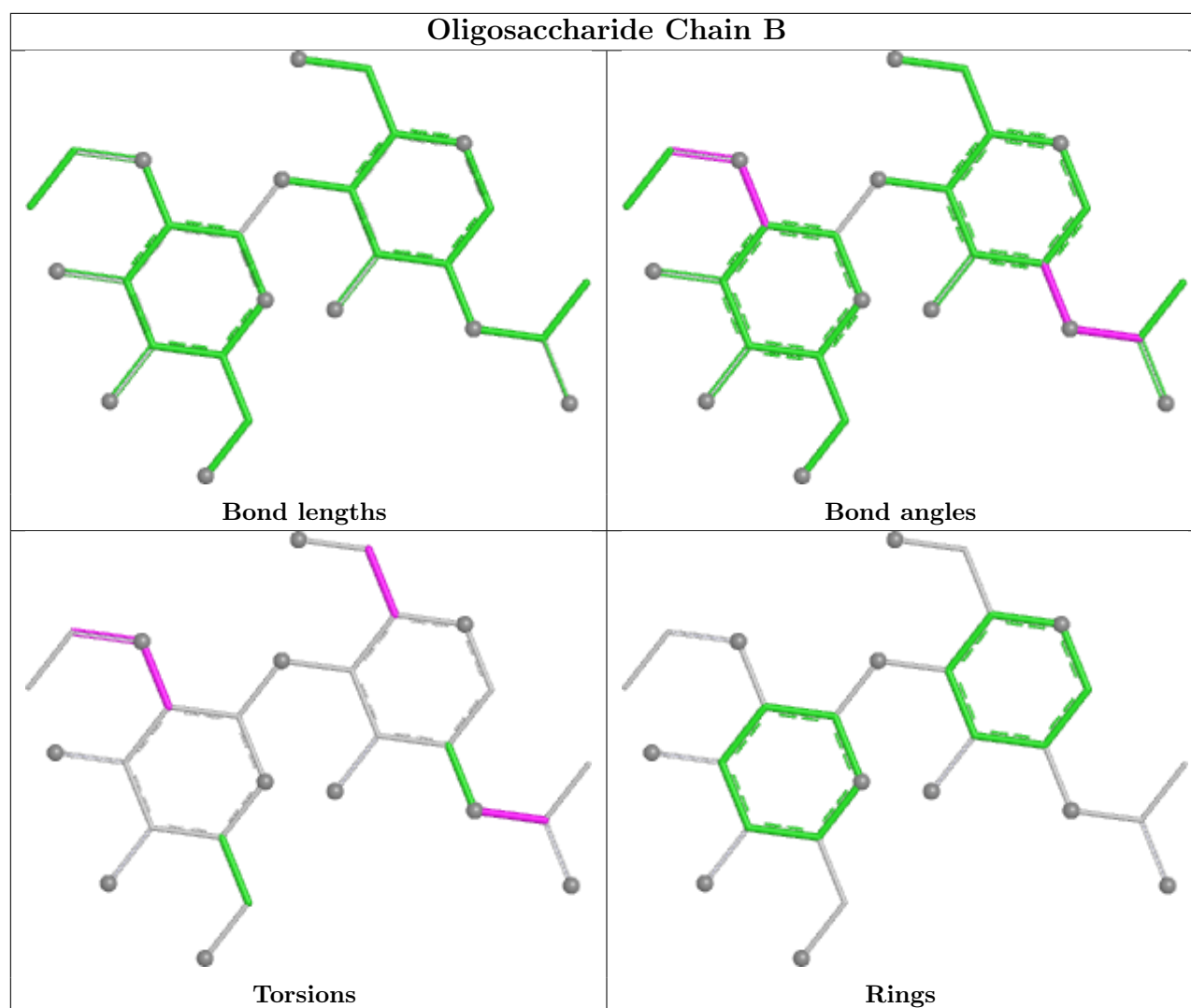
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	NAG	I	861	-	14,14,15	0.63	0	17,19,21	0.79	1 (5%)
4	NAG	L	801	-	14,14,15	0.60	0	17,19,21	0.61	0
4	NAG	I	801	1	14,14,15	0.75	1 (7%)	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	L	841	2	14,14,15	0.67	0	17,19,21	1.01	2 (11%)
4	NAG	I	862	-	14,14,15	0.57	0	17,19,21	0.59	0
4	NAG	L	842	-	14,14,15	0.47	0	17,19,21	0.59	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
4	NAG	I	861	-	-	4/6/23/26	0/1/1/1
4	NAG	L	801	-	-	5/6/23/26	0/1/1/1
4	NAG	I	801	1	-	3/6/23/26	0/1/1/1
4	NAG	L	841	2	-	6/6/23/26	0/1/1/1
4	NAG	I	862	-	-	1/6/23/26	0/1/1/1
4	NAG	L	842	-	-	6/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	801	NAG	C1-C2	2.17	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	841	NAG	C4-C3-C2	2.37	114.49	111.02
4	L	841	NAG	C3-C4-C5	2.14	114.11	110.23
4	I	861	NAG	C2-N2-C7	-2.14	120.04	122.90

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	861	NAG	O7-C7-N2-C2
4	L	801	NAG	C1-C2-N2-C7
4	L	801	NAG	C8-C7-N2-C2
4	L	801	NAG	O7-C7-N2-C2
4	L	841	NAG	C3-C2-N2-C7
4	L	841	NAG	C8-C7-N2-C2
4	L	841	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	L	842	NAG	O7-C7-N2-C2
4	I	861	NAG	C8-C7-N2-C2
4	L	842	NAG	C8-C7-N2-C2
4	L	842	NAG	O5-C5-C6-O6
4	L	842	NAG	C4-C5-C6-O6
4	L	801	NAG	O5-C5-C6-O6
4	I	861	NAG	C4-C5-C6-O6
4	L	841	NAG	O5-C5-C6-O6
4	I	861	NAG	O5-C5-C6-O6
4	L	801	NAG	C4-C5-C6-O6
4	L	841	NAG	C4-C5-C6-O6
4	I	862	NAG	C3-C2-N2-C7
4	L	841	NAG	C1-C2-N2-C7
4	L	842	NAG	C1-C2-N2-C7
4	I	801	NAG	C3-C2-N2-C7
4	I	801	NAG	O5-C5-C6-O6
4	I	801	NAG	C1-C2-N2-C7
4	L	842	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	861	NAG	7	0
4	L	801	NAG	1	0
4	I	801	NAG	1	0
4	L	841	NAG	4	0
4	I	862	NAG	2	0
4	L	842	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	I	413/427 (96%)	-0.12	2 (0%) 87 82	36, 79, 115, 151	0
2	L	410/427 (96%)	-0.21	1 (0%) 91 88	42, 77, 121, 141	0
All	All	823/854 (96%)	-0.17	3 (0%) 88 84	36, 78, 120, 151	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	207	ILE	2.7
2	L	17	MET	2.5
1	I	94	ALA	2.4

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](#)

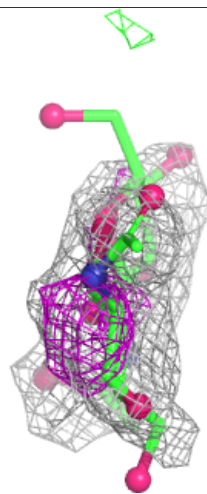
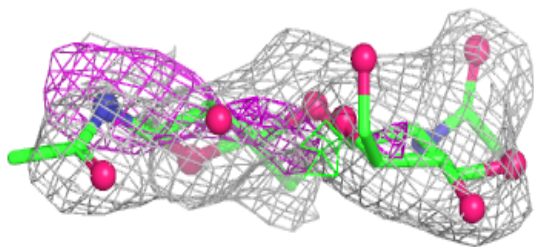
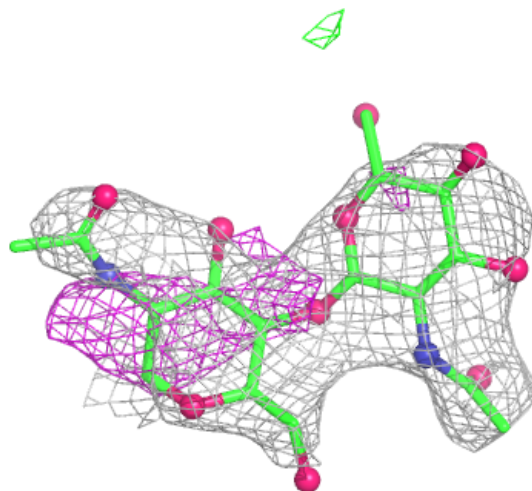
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

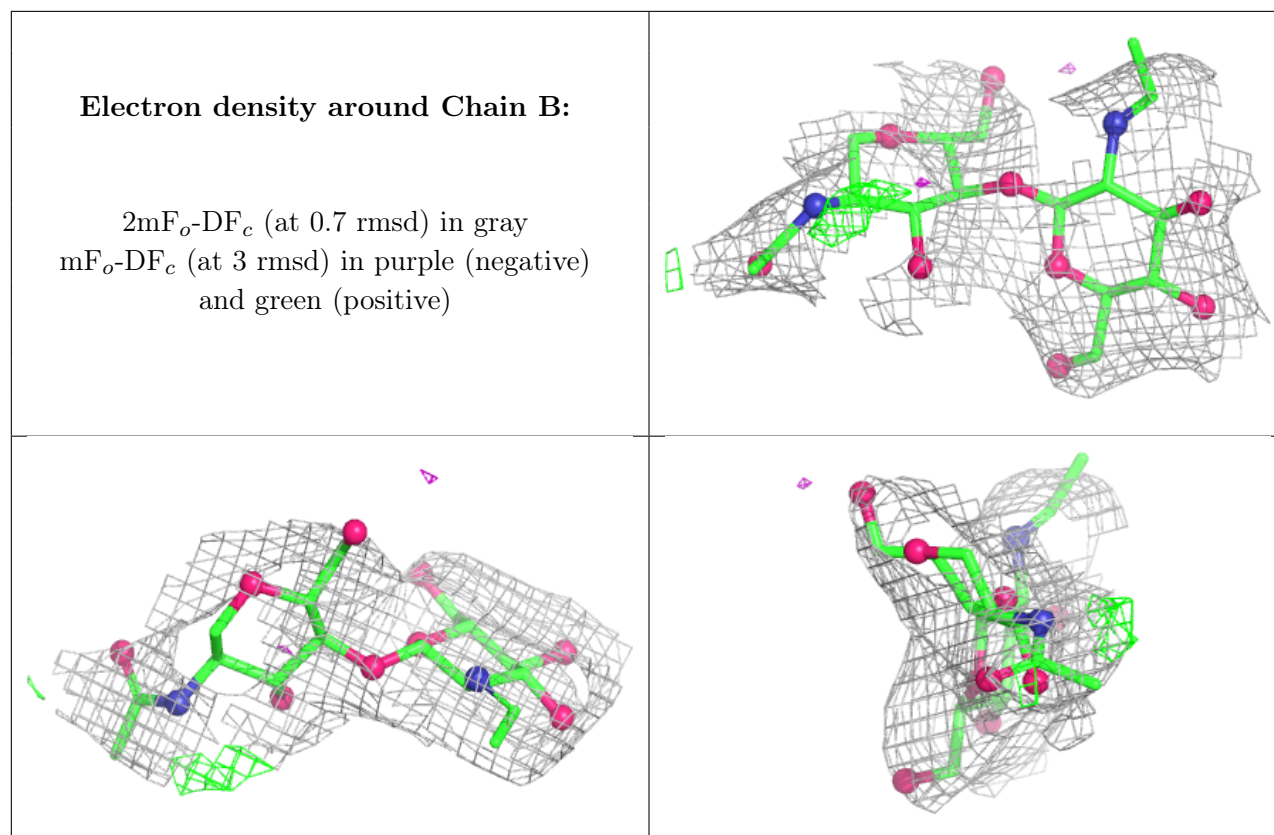
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	1	14/15	-	-	106,112,116,118	0
3	NAG	A	2	14/15	-	-	120,122,122,122	0
3	NAG	B	1	14/15	-	-	115,119,122,124	0
3	NAG	B	2	13/15	-	-	127,128,129,129	0

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 A:

$2mF_o-DF_c$ (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
4	NAG	I	801	14/15	0.31	0.12	125,128,130,130	0
4	NAG	I	862	14/15	0.31	0.12	160,162,163,163	0
4	NAG	I	861	14/15	0.48	0.14	139,143,145,147	0
4	NAG	L	801	14/15	0.59	0.13	126,128,129,129	0
4	NAG	L	842	14/15	0.70	0.11	148,150,151,152	0
4	NAG	L	841	14/15	0.84	0.08	86,93,96,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.