



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:14 PM BST

PDB ID : 1R46
Title : Structure of human alpha-galactosidase
Authors : Garman, S.C.; Garboczi, D.N.
Deposited on : 2003-10-03
Resolution : 3.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

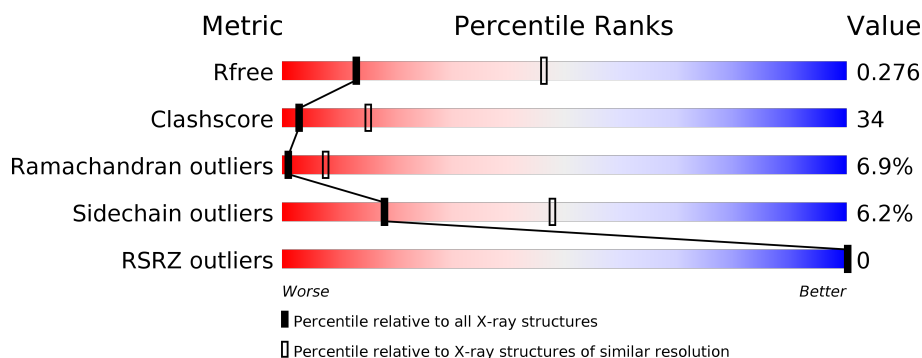
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	398	
1	B	398	
2	C	5	
3	D	2	
3	G	2	
4	E	6	

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Mol	Chain	Length	Quality of chain
5	F	4	

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
2	MAN	C	3	X	-	-	-
2	MAN	C	5	-	-	-	X
4	NAG	E	1	-	-	X	-
4	MAN	E	3	X	-	-	-
4	MAN	E	4	-	-	-	X
4	MAN	E	5	-	-	-	X
4	FUC	E	6	-	-	-	X
5	MAN	F	3	X	-	-	-

2 Entry composition [i](#)

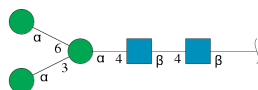
There are 8 unique types of molecules in this entry. The entry contains 6539 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-galactosidase A.

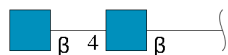
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			
1	B	391	Total	C	N	O	S	0	0	0
			3131	1993	536	576	26			

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

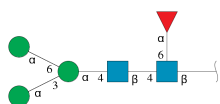
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

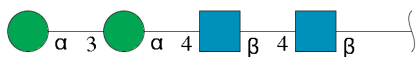
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al

pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



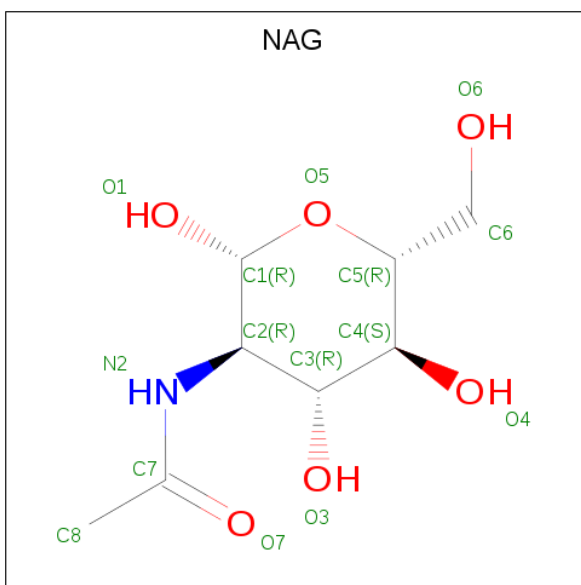
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



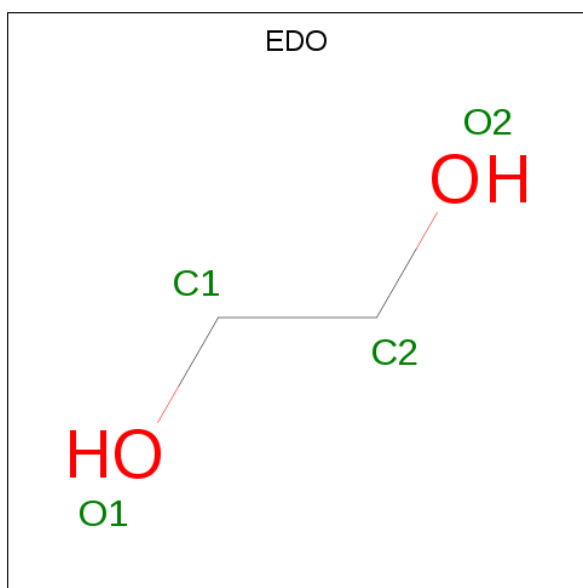
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total	O	0	0
			9	9		
8	B	9	Total	O	0	0
			9	9		

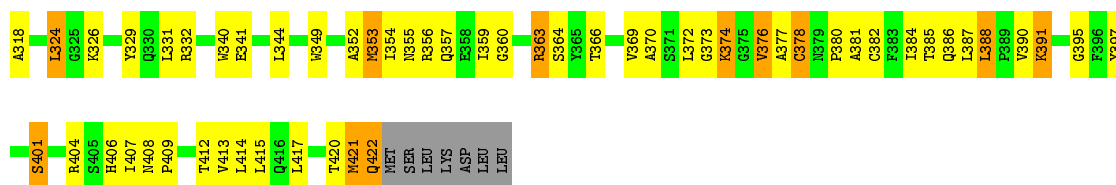
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ($\text{RSRZ} > 2$). 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.

Chain A: 43% 47% 8%

	P943	P944	L344	W849	A352	M953	R355	R356	Q357	E358	L359	ASP	L420	M421	GLN	MET	SER	LEU	LYS	ASP	LEU	L415	L416	L417	E418	W419	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L85
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Chain B:

Category	Percentage
I242	40%
G171	40%
Q99	40%
L32	40%
I245	40%
G172	40%
Q100	40%
L33	40%
I246	40%
G173	40%
Q101	40%
L34	40%
I247	40%
G174	40%
Q102	40%
L35	40%
I248	40%
G175	40%
Q103	40%
L36	40%
I249	40%
G176	40%
Q104	40%
L37	40%
I250	40%
G177	40%
Q105	40%
L38	40%
I251	40%
G178	40%
Q106	40%
L39	40%
I252	40%
G179	40%
Q107	40%
L40	40%
I253	40%
G180	40%
Q108	40%
L41	40%
I254	40%
G181	40%
Q109	40%
L42	40%
I255	40%
G182	40%
Q110	40%
L43	40%
I256	40%
G183	40%
Q111	40%
L44	40%
I257	40%
G184	40%
Q112	40%
L45	40%
G360	40%
G185	40%
Q113	40%
L46	40%
G361	40%
G186	40%
Q114	40%
L47	40%
P265	40%
G187	40%
Q115	40%
L48	40%
D266	40%
G188	40%
Q116	40%
L49	40%
M267	40%
G189	40%
Q117	40%
L50	40%
I270	40%
G190	40%
G271	40%
Q118	40%
G272	40%
Q119	40%
G273	40%
G274	40%
G275	40%
G276	40%
G277	40%
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G281	40%
G282	40%
G283	40%
G284	40%
G285	40%
G286	40%
G287	40%
M290	40%
A291	40%
D299	40%
L300	40%
R301	40%
S304	40%
Q306	40%
L310	40%
D313	40%
K314	40%
D315	40%
V316	40%
I317	40%
R180	40%
R181	40%
R182	40%
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R261	40%
R262	40%
R263	40%
R264	40%
R265	40%
R266	40%



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

Chain C: 80% 20%



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

Chain D: 100%



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

Chain G: 50% 50%



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

Chain E: 50% 50%



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

Chain F: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.46 Å 88.46 Å 215.48 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.92 – 3.25 44.23 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.92-3.25) 99.6 (44.23-2.86)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.86 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.301 0.237 , 0.276	Depositor DCC
R_{free} test set	820 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, EDO, 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	0.45	0/3209	0.69	0/4358
1	B	0.45	0/3218	0.70	1/4370 (0.0%)
All	All	0.45	0/6427	0.69	1/8728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	TRP	N-CA-C	-6.42	93.66	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3122	0	2981	195	0
1	B	3131	0	2989	230	1
2	C	61	0	52	0	0
3	D	28	0	25	0	0
3	G	28	0	25	3	0
4	E	71	0	61	14	0
5	F	50	0	43	5	0
6	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	8	0	12	1	0
7	B	8	0	12	1	0
8	A	9	0	0	1	0
8	B	9	0	0	2	0
All	All	6539	0	6213	437	1

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 (437) 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:386:GLN:HE21	1:A:390:VAL:HG22	1.22	1.05
1:B:386:GLN:HE21	1:B:390:VAL:HG22	1.22	1.04
1:A:213:LYS:H	1:A:213:LYS:HD2	1.20	1.03
1:A:286:LEU:HD11	1:A:354:ILE:HD11	1.51	0.91
1:B:286:LEU:HD11	1:B:354:ILE:HD11	1.54	0.87
1:A:366:THR:HG22	1:A:404:ARG:HB2	1.58	0.84
1:B:119:GLN:HA	1:B:122:ASN:HD22	1.40	0.84
1:A:240:LYS:CE	1:A:356:ARG:HH21	1.91	0.83
1:A:386:GLN:NE2	1:A:390:VAL:HG22	1.94	0.83
1:B:386:GLN:NE2	1:B:390:VAL:HG22	1.92	0.83
3:G:1:NAG:H62	3:G:2:NAG:H82	1.59	0.81
1:A:333:GLN:HG3	1:A:334:GLY:H	1.44	0.81
1:A:359:ILE:HG12	1:A:360:GLY:H	1.46	0.81
1:B:353:MET:HG2	1:B:407:ILE:HD11	1.63	0.81
1:A:213:LYS:CD	1:A:213:LYS:H	1.94	0.80
1:A:138:GLY:HA3	1:A:173:TYR:O	1.81	0.80
1:B:359:ILE:HG12	1:B:360:GLY:H	1.47	0.79
1:B:224:ASN:HA	1:B:260:GLY:O	1.81	0.79
1:B:177:LEU:H	1:B:177:LEU:HD12	1.46	0.79
1:A:359:ILE:HG12	1:A:360:GLY:N	1.98	0.79
1:B:120:LEU:O	1:B:124:VAL:HG23	1.83	0.79
1:B:359:ILE:HG12	1:B:360:GLY:N	1.98	0.78
4:E:1:NAG:H62	4:E:6:FUC:H3	1.63	0.78
1:B:366:THR:HG22	1:B:404:ARG:HB2	1.65	0.77
1:A:177:LEU:H	1:A:177:LEU:HD12	1.48	0.77
1:A:366:THR:HG22	1:A:404:ARG:CB	2.15	0.77
1:A:240:LYS:HE3	1:A:356:ARG:HH21	1.50	0.76
1:B:174:CYS:CB	4:E:1:NAG:H81	2.14	0.76
1:B:174:CYS:HA	4:E:1:NAG:H81	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:O	1:B:274:GLY:HA3	1.84	0.76
1:A:224:ASN:HA	1:A:260:GLY:O	1.86	0.75
1:A:100:ARG:HD2	1:A:104:GLY:O	1.87	0.75
1:A:286:LEU:HD11	1:A:354:ILE:CD1	2.16	0.75
1:B:265:PRO:O	1:B:266:ASP:HB2	1.86	0.74
1:B:46:HIS:CD2	1:B:92:ASP:H	2.05	0.74
1:B:135:ALA:HB2	1:B:167:LEU:HD11	1.70	0.74
1:A:377:ALA:O	1:A:378:CYS:HB2	1.86	0.74
1:B:138:GLY:HA3	1:B:173:TYR:O	1.88	0.74
1:A:353:MET:HG2	1:A:407:ILE:HD11	1.68	0.73
1:B:366:THR:HG22	1:B:404:ARG:CB	2.19	0.72
1:B:273:PHE:CD2	1:B:273:PHE:N	2.58	0.71
1:B:315:ASP:OD2	1:B:391:LYS:HE2	1.89	0.71
1:A:135:ALA:HB2	1:A:167:LEU:HD11	1.72	0.71
1:B:203:GLU:HG3	1:B:227:ARG:HG3	1.73	0.70
1:B:324:LEU:HD22	1:B:326:LYS:HG2	1.73	0.70
1:A:140:LYS:HB2	1:A:173:TYR:CD2	2.27	0.70
1:B:240:LYS:HE3	1:B:356:ARG:HH21	1.56	0.70
1:B:422:GLN:HE21	1:B:422:GLN:N	1.89	0.69
1:B:286:LEU:HD11	1:B:354:ILE:CD1	2.20	0.69
4:E:3:MAN:O4	4:E:4:MAN:H3	1.92	0.69
1:B:240:LYS:CE	1:B:356:ARG:HH21	2.06	0.69
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.55	0.69
1:A:45:LEU:HD21	1:A:92:ASP:HB2	1.75	0.69
1:B:276:SER:O	1:B:280:GLN:HG3	1.92	0.69
1:A:381:ALA:HB3	1:A:420:THR:HB	1.75	0.69
1:A:203:GLU:HG3	1:A:227:ARG:HG3	1.75	0.68
1:B:119:GLN:HA	1:B:122:ASN:ND2	2.08	0.68
1:A:234:ASP:O	1:A:274:GLY:HA3	1.94	0.68
1:B:224:ASN:O	1:B:261:GLY:HA2	1.94	0.68
1:A:265:PRO:O	1:A:266:ASP:HB2	1.93	0.68
1:A:369:VAL:HG12	1:A:378:CYS:SG	2.33	0.68
1:A:273:PHE:CD2	1:A:273:PHE:N	2.61	0.67
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.58	0.67
1:A:324:LEU:HD22	1:A:326:LYS:HG2	1.76	0.67
1:B:110:PRO:HB2	1:B:111:GLN:NE2	2.10	0.67
4:E:1:NAG:C6	4:E:6:FUC:H3	2.25	0.67
1:A:240:LYS:HE2	1:A:356:ARG:HH21	1.60	0.66
1:B:66:GLU:O	1:B:70:MET:HG3	1.95	0.66
1:B:101:ASP:HB3	1:B:107:GLN:OE1	1.95	0.66
1:A:110:PRO:HB2	1:A:111:GLN:NE2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:O	1:A:261:GLY:HA2	1.96	0.65
1:B:127:LYS:HA	1:B:127:LYS:HE2	1.78	0.65
1:B:177:LEU:HD12	1:B:177:LEU:N	2.11	0.65
1:B:386:GLN:O	1:B:391:LYS:HA	1.96	0.65
1:B:69:PHE:CZ	1:B:91:ILE:HG23	2.32	0.65
1:B:140:LYS:HB2	1:B:173:TYR:CD2	2.29	0.65
1:A:177:LEU:N	1:A:177:LEU:HD12	2.11	0.65
1:A:369:VAL:CG1	1:A:378:CYS:SG	2.84	0.65
1:A:97:ALA:HB2	1:A:109:ASP:HA	1.78	0.64
1:A:46:HIS:CD2	1:A:92:ASP:H	2.14	0.64
1:B:300:LEU:HD12	1:B:300:LEU:H	1.62	0.64
1:B:369:VAL:HG12	1:B:378:CYS:SG	2.37	0.64
1:B:204:TRP:HB3	1:B:205:PRO:HD3	1.79	0.64
1:A:300:LEU:H	1:A:300:LEU:HD12	1.62	0.64
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.79	0.63
1:B:45:LEU:HD21	1:B:92:ASP:HB2	1.79	0.63
1:A:177:LEU:CD1	1:A:177:LEU:H	2.12	0.63
1:B:135:ALA:CB	1:B:167:LEU:HD11	2.27	0.63
1:B:177:LEU:H	1:B:177:LEU:CD1	2.11	0.63
1:B:174:CYS:CA	4:E:1:NAG:H81	2.27	0.63
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.81	0.63
1:A:386:GLN:O	1:A:391:LYS:HA	1.98	0.63
1:A:417:LEU:HD12	1:A:417:LEU:N	2.13	0.63
1:B:75:LEU:HD21	1:B:301:ARG:HG2	1.81	0.63
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.80	0.63
1:B:72:MET:O	1:B:76:MET:HG3	2.00	0.62
1:A:387:LEU:HD12	1:A:391:LYS:HG3	1.80	0.62
5:F:3:MAN:H3	5:F:4:MAN:C5	2.29	0.62
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.34	0.61
1:A:370:ALA:HB2	1:A:399:TRP:O	1.99	0.61
1:B:422:GLN:HE21	1:B:422:GLN:H	1.48	0.61
1:A:202:CYS:O	1:A:226:TRP:HA	2.00	0.61
1:B:208:MET:SD	1:B:214:PRO:HB3	2.40	0.61
1:B:377:ALA:O	1:B:378:CYS:HB2	2.01	0.61
1:A:93:ASP:O	1:A:94:CYS:HB2	1.98	0.61
1:B:359:ILE:CG1	1:B:360:GLY:H	2.12	0.61
1:A:381:ALA:HB1	1:A:420:THR:OG1	2.01	0.60
1:B:331:LEU:HD22	1:B:341:GLU:OE2	2.01	0.60
1:B:174:CYS:HA	4:E:1:NAG:O7	2.01	0.60
1:B:290:MET:O	1:B:291:ALA:C	2.40	0.60
1:A:359:ILE:CG1	1:A:360:GLY:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:HD12	1:A:404:ARG:N	2.17	0.60
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.36	0.60
1:A:34:ASN:OD1	1:A:36:LEU:HB2	2.02	0.60
1:A:330:GLN:NE2	1:A:333:GLN:HE22	1.99	0.59
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.83	0.59
1:B:213:LYS:H	1:B:213:LYS:HD2	1.65	0.59
1:B:299:ASP:OD1	1:B:301:ARG:HB2	2.02	0.59
1:B:93:ASP:O	1:B:94:CYS:HB2	2.02	0.59
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.84	0.59
1:B:100:ARG:NH1	1:B:106:LEU:HG	2.18	0.59
1:A:135:ALA:HB3	1:A:169:PHE:HD1	1.68	0.59
1:A:254:VAL:HG21	1:A:329:TYR:HB3	1.84	0.59
1:B:417:LEU:N	1:B:417:LEU:HD12	2.18	0.59
1:A:290:MET:O	1:A:291:ALA:C	2.41	0.59
1:A:51:MET:O	1:A:64:ILE:HD11	2.04	0.58
1:A:44:TRP:CD1	1:A:300:LEU:HD11	2.38	0.58
1:B:205:PRO:HG3	1:B:219:ILE:HD13	1.84	0.58
1:B:387:LEU:HD12	1:B:391:LYS:HG3	1.85	0.58
3:G:1:NAG:H62	3:G:2:NAG:C8	2.32	0.58
1:B:118:ARG:O	1:B:121:ALA:HB3	2.03	0.58
1:A:138:GLY:CA	1:A:173:TYR:O	2.52	0.58
1:B:34:ASN:OD1	1:B:36:LEU:HB2	2.04	0.57
1:B:202:CYS:O	1:B:226:TRP:HA	2.04	0.57
1:B:359:ILE:CG1	1:B:360:GLY:N	2.66	0.57
1:B:253:ILE:HG13	1:B:254:VAL:N	2.19	0.57
1:B:384:ILE:HG12	1:B:417:LEU:HG	1.86	0.57
1:A:159:PHE:O	1:A:164:VAL:HG23	2.05	0.57
1:B:234:ASP:CG	1:B:274:GLY:H	2.07	0.57
1:A:359:ILE:CG1	1:A:360:GLY:N	2.68	0.57
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.70	0.57
4:E:1:NAG:H62	4:E:6:FUC:C3	2.26	0.57
1:A:253:ILE:HG13	1:A:254:VAL:N	2.19	0.56
1:B:97:ALA:HB2	1:B:109:ASP:HA	1.87	0.56
1:B:136:ASP:OD2	1:B:141:THR:HA	2.05	0.56
1:B:278:ASN:OD1	1:B:408:ASN:HB2	2.05	0.56
1:A:331:LEU:HD22	1:A:341:GLU:OE2	2.06	0.56
1:B:208:MET:CE	1:B:214:PRO:HA	2.35	0.56
1:A:115:HIS:HB3	1:A:119:GLN:OE1	2.05	0.56
1:A:324:LEU:HD12	1:A:344:LEU:O	2.05	0.56
1:A:395:GLY:HA2	7:A:1102:EDO:H22	1.86	0.56
1:A:376:VAL:HG12	1:A:377:ALA:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD12	1:A:54:LEU:N	2.21	0.56
1:A:238:SER:O	1:A:242:ILE:HG13	2.06	0.56
1:B:159:PHE:O	1:B:164:VAL:HG23	2.06	0.56
4:E:1:NAG:H62	4:E:6:FUC:O2	2.06	0.56
1:B:238:SER:O	1:B:242:ILE:HG13	2.05	0.56
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.41	0.56
1:B:376:VAL:HG12	1:B:377:ALA:N	2.18	0.56
1:B:324:LEU:HD12	1:B:344:LEU:O	2.05	0.56
1:B:369:VAL:CG1	1:B:378:CYS:SG	2.94	0.56
1:A:234:ASP:CG	1:A:274:GLY:H	2.08	0.55
1:A:135:ALA:CB	1:A:167:LEU:HD11	2.35	0.55
1:A:66:GLU:O	1:A:70:MET:HB2	2.05	0.55
1:B:72:MET:SD	1:B:300:LEU:HD13	2.46	0.55
1:B:200:TYR:HD2	1:B:222:TYR:O	1.90	0.55
1:A:276:SER:O	1:A:280:GLN:HG3	2.06	0.55
1:A:372:LEU:O	1:A:374:LYS:N	2.40	0.55
1:A:71:GLU:O	1:A:75:LEU:HD13	2.06	0.55
1:B:51:MET:O	1:B:64:ILE:HD11	2.07	0.55
1:A:377:ALA:O	1:A:378:CYS:CB	2.52	0.55
1:A:417:LEU:CD1	1:A:417:LEU:N	2.69	0.55
1:A:101:ASP:HB3	1:A:107:GLN:OE1	2.07	0.55
1:B:54:LEU:HD12	1:B:54:LEU:N	2.22	0.54
1:B:366:THR:HG22	1:B:404:ARG:CG	2.38	0.54
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.23	0.54
1:B:340:TRP:HB2	1:B:352:ALA:HB3	1.89	0.54
1:B:278:ASN:O	1:B:281:VAL:HG22	2.07	0.54
1:A:359:ILE:HG13	1:B:48:GLU:OE2	2.06	0.54
1:B:77:VAL:HG21	1:B:127:LYS:HB3	1.90	0.54
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.90	0.54
1:A:170:ASP:OD1	1:A:171:GLY:N	2.42	0.53
1:A:276:SER:H	1:A:279:GLN:HB2	1.74	0.53
1:B:248:PHE:O	1:B:248:PHE:CG	2.60	0.53
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.73	0.53
1:A:388:LEU:HB2	1:A:414:LEU:HB3	1.89	0.53
1:A:366:THR:HG22	1:A:404:ARG:CG	2.38	0.53
1:B:81:TRP:CD1	1:B:300:LEU:HD23	2.44	0.53
1:B:45:LEU:CD2	1:B:92:ASP:HB2	2.38	0.53
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.91	0.53
1:B:135:ALA:HB3	1:B:169:PHE:HD1	1.73	0.53
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.91	0.52
1:B:112:ARG:NH2	8:B:18:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:HA	4:E:1:NAG:C8	2.39	0.52
1:B:229:PHE:CD2	1:B:242:ILE:HG12	2.43	0.52
1:B:44:TRP:CD1	1:B:300:LEU:HD11	2.44	0.52
1:B:377:ALA:O	1:B:378:CYS:CB	2.58	0.52
1:B:384:ILE:HD12	1:B:397:TYR:CD1	2.45	0.52
1:A:213:LYS:N	1:A:213:LYS:HD2	2.04	0.52
1:B:380:PRO:HG2	1:B:381:ALA:H	1.75	0.52
1:A:381:ALA:HB3	1:A:420:THR:CB	2.39	0.52
1:B:270:ILE:HG23	1:B:280:GLN:OE1	2.10	0.52
1:A:45:LEU:CD2	1:A:92:ASP:HB2	2.39	0.52
1:B:229:PHE:HD2	1:B:242:ILE:HG12	1.74	0.52
1:A:205:PRO:HG3	1:A:219:ILE:HD13	1.92	0.52
5:F:3:MAN:H3	5:F:4:MAN:H5	1.91	0.52
1:A:265:PRO:HB2	1:A:287:TRP:CZ2	2.45	0.51
1:B:179:ASN:HD22	1:B:179:ASN:N	2.08	0.51
1:A:340:TRP:HB2	1:A:352:ALA:HB3	1.93	0.51
1:A:100:ARG:NH1	1:A:106:LEU:HG	2.26	0.51
1:B:32:LEU:N	1:B:220:ARG:O	2.44	0.51
1:B:420:THR:OG1	1:B:421:MET:N	2.44	0.51
1:B:174:CYS:HB2	4:E:1:NAG:H81	1.88	0.51
1:A:119:GLN:O	1:A:122:ASN:HB3	2.11	0.51
1:A:270:ILE:HG23	1:A:280:GLN:OE1	2.10	0.51
1:B:387:LEU:O	1:B:388:LEU:HD13	2.11	0.51
1:A:333:GLN:HA	1:A:333:GLN:NE2	2.25	0.51
1:B:388:LEU:HB2	1:B:414:LEU:HB3	1.91	0.51
1:A:200:TYR:HD2	1:A:222:TYR:O	1.93	0.50
1:A:220:ARG:NH1	1:A:256:VAL:O	2.44	0.50
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.75	0.50
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.27	0.50
1:B:123:TYR:O	1:B:126:SER:HB3	2.12	0.50
1:B:363:ARG:NH1	1:B:363:ARG:HG2	2.25	0.50
1:B:417:LEU:CD1	1:B:417:LEU:N	2.74	0.50
1:A:42:MET:HE3	1:A:317:ILE:HG23	1.92	0.50
1:B:220:ARG:NH1	1:B:256:VAL:O	2.44	0.50
1:B:113:PHE:N	1:B:114:PRO:HD3	2.26	0.50
1:B:117:ILE:O	1:B:119:GLN:N	2.45	0.50
1:A:214:PRO:HB2	1:A:219:ILE:HD11	1.93	0.49
1:A:277:TRP:HA	1:A:277:TRP:CE3	2.47	0.49
1:B:315:ASP:CG	1:B:391:LYS:HE2	2.33	0.49
1:B:353:MET:HG2	1:B:407:ILE:CD1	2.36	0.49
1:A:284:MET:HG2	1:A:310:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:CYS:O	1:B:173:TYR:HB2	2.12	0.49
1:A:44:TRP:NE1	1:A:300:LEU:HD11	2.27	0.49
1:B:373:GLY:O	1:B:376:VAL:N	2.44	0.49
1:A:205:PRO:O	1:A:209:TRP:HD1	1.96	0.49
1:A:97:ALA:HB2	1:A:110:PRO:HD3	1.95	0.49
1:B:304:SER:HB2	1:B:306:GLN:HG2	1.94	0.49
1:A:335:ASP:O	1:A:336:ASN:C	2.50	0.49
1:B:284:MET:HG2	1:B:310:LEU:CD2	2.43	0.49
4:E:3:MAN:O4	4:E:4:MAN:H2	2.12	0.49
1:A:179:ASN:N	1:A:179:ASN:HD22	2.10	0.49
1:A:236:TRP:NE1	1:A:240:LYS:HD2	2.27	0.49
1:A:388:LEU:HD22	1:A:414:LEU:HD23	1.95	0.49
1:A:387:LEU:O	1:A:388:LEU:HD13	2.13	0.48
1:A:381:ALA:CB	1:A:420:THR:OG1	2.60	0.48
1:B:164:VAL:HG12	1:B:166:LEU:H	1.78	0.48
1:B:313:ASP:O	1:B:317:ILE:HG13	2.12	0.48
1:A:151:TYR:O	1:A:152:TYR:C	2.51	0.48
1:A:332:ARG:HB2	1:A:339:VAL:HB	1.95	0.48
1:B:127:LYS:HA	1:B:127:LYS:CE	2.42	0.48
1:A:136:ASP:OD2	1:A:141:THR:HA	2.12	0.48
1:B:164:VAL:HG12	1:B:165:ASP:N	2.28	0.48
1:B:82:LYS:HE3	1:B:128:GLY:HA3	1.94	0.48
1:B:380:PRO:HG2	1:B:381:ALA:N	2.28	0.48
1:B:170:ASP:OD1	1:B:171:GLY:N	2.46	0.48
1:A:172:CYS:O	1:A:173:TYR:HB2	2.13	0.48
1:A:145:PHE:CB	1:A:146:PRO:HD2	2.44	0.47
1:B:93:ASP:OD1	1:B:94:CYS:N	2.47	0.47
1:B:349:TRP:CD1	1:B:377:ALA:HB2	2.50	0.47
1:A:45:LEU:CD2	1:A:47:TRP:H	2.27	0.47
1:B:136:ASP:O	1:B:148:SER:HB2	2.14	0.47
1:B:281:VAL:HG23	1:B:282:THR:N	2.29	0.47
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.79	0.47
1:B:45:LEU:CD2	1:B:47:TRP:H	2.27	0.47
1:B:412:THR:HG22	1:B:413:VAL:N	2.29	0.47
1:A:304:SER:HB2	1:A:306:GLN:HG2	1.95	0.47
1:B:151:TYR:O	1:B:152:TYR:C	2.52	0.47
1:B:95:TRP:CD2	1:B:133:ILE:HD11	2.50	0.47
1:B:315:ASP:O	1:B:318:ALA:HB3	2.15	0.47
1:B:205:PRO:O	1:B:207:TYR:N	2.48	0.47
1:B:64:ILE:O	1:B:112:ARG:NH1	2.47	0.47
1:B:299:ASP:C	1:B:301:ARG:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:MET:O	1:B:412:THR:HA	2.14	0.47
1:A:366:THR:CG2	1:A:404:ARG:HB2	2.37	0.46
1:B:71:GLU:O	1:B:75:LEU:HD13	2.16	0.46
1:A:216:TYR:HB3	1:A:256:VAL:HG21	1.98	0.46
1:A:244:ASP:HA	8:A:1:HOH:O	2.15	0.46
1:B:117:ILE:O	1:B:120:LEU:N	2.44	0.46
1:B:236:TRP:NE1	1:B:240:LYS:HD2	2.30	0.46
1:B:81:TRP:NE1	1:B:300:LEU:HD23	2.31	0.46
1:A:281:VAL:HG23	1:A:282:THR:N	2.31	0.46
1:B:270:ILE:HG13	1:B:283:GLN:OE1	2.15	0.46
1:A:364:SER:HB3	1:A:406:HIS:CE1	2.50	0.46
1:B:133:ILE:HG22	1:B:164:VAL:HG11	1.98	0.46
1:B:42:MET:HE3	1:B:317:ILE:HG23	1.98	0.46
1:B:372:LEU:O	1:B:374:LYS:N	2.42	0.46
1:B:369:VAL:HG23	1:B:401:SER:O	2.16	0.46
1:A:164:VAL:HG12	1:A:165:ASP:N	2.31	0.46
1:B:117:ILE:O	1:B:118:ARG:C	2.53	0.46
1:B:248:PHE:O	1:B:249:ASN:ND2	2.49	0.46
1:B:247:SER:O	1:B:250:GLN:HG2	2.15	0.46
1:B:60:PRO:O	1:B:63:CYS:HB3	2.15	0.46
1:B:101:ASP:OD1	1:B:103:GLU:HB3	2.16	0.45
1:A:270:ILE:HG13	1:A:283:GLN:OE1	2.16	0.45
1:A:373:GLY:O	1:A:376:VAL:N	2.49	0.45
1:A:379:ASN:HA	1:A:380:PRO:HA	1.66	0.45
1:A:166:LEU:C	1:A:166:LEU:HD23	2.37	0.45
1:A:92:ASP:HA	1:A:134:TYR:HB2	1.98	0.45
1:B:248:PHE:O	1:B:249:ASN:CG	2.54	0.45
1:B:355:ASN:ND2	1:B:409:PRO:HA	2.31	0.45
5:F:3:MAN:HO4	5:F:4:MAN:C1	2.30	0.45
1:B:133:ILE:HG13	1:B:134:TYR:N	2.32	0.45
1:B:214:PRO:HB2	1:B:219:ILE:HD11	1.99	0.45
1:A:239:ILE:HD13	1:A:283:GLN:HB2	1.99	0.45
1:A:412:THR:HG22	1:A:413:VAL:N	2.32	0.45
1:A:120:LEU:O	1:A:121:ALA:C	2.54	0.45
1:B:253:ILE:CG1	1:B:254:VAL:N	2.80	0.45
1:B:366:THR:CG2	1:B:404:ARG:HB2	2.43	0.45
1:B:76:MET:SD	1:B:89:LEU:HD13	2.56	0.45
1:A:301:ARG:O	1:A:302:HIS:HD2	1.99	0.45
1:A:357:GLN:OE1	1:A:363:ARG:HD2	2.16	0.45
1:B:200:TYR:CD2	1:B:222:TYR:O	2.69	0.45
1:B:69:PHE:CZ	1:B:91:ILE:HG12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:HIS:HE1	1:B:165:ASP:OD2	1.99	0.45
1:A:255:ASP:C	1:A:257:ALA:H	2.20	0.44
1:A:82:LYS:HA	1:A:86:TYR:O	2.18	0.44
1:B:166:LEU:C	1:B:166:LEU:HD23	2.37	0.44
1:A:299:ASP:OD1	1:A:301:ARG:HB2	2.18	0.44
1:B:240:LYS:HE2	1:B:356:ARG:HH21	1.79	0.44
1:A:95:TRP:CD2	1:A:133:ILE:HD11	2.52	0.44
1:A:228:ASN:HB3	1:A:245:TRP:CZ3	2.52	0.44
1:B:66:GLU:HB3	1:B:113:PHE:CD1	2.51	0.44
1:A:81:TRP:CD1	1:A:300:LEU:HD23	2.51	0.44
1:B:138:GLY:CA	1:B:173:TYR:O	2.63	0.44
1:B:281:VAL:CG2	1:B:282:THR:N	2.81	0.44
1:A:300:LEU:N	1:A:300:LEU:HD12	2.32	0.44
1:A:420:THR:O	1:A:421:MET:HG2	2.18	0.44
1:A:333:GLN:HG3	1:A:334:GLY:N	2.23	0.43
1:B:44:TRP:NE1	1:B:300:LEU:HD11	2.33	0.43
4:E:3:MAN:O4	4:E:4:MAN:C3	2.62	0.43
1:B:170:ASP:OD2	7:B:1103:EDO:H12	2.17	0.43
1:B:387:LEU:HA	1:B:391:LYS:HA	2.00	0.43
1:B:52:CYS:SG	1:B:54:LEU:HD11	2.58	0.43
1:A:404:ARG:NH2	1:B:58:GLU:O	2.50	0.43
1:A:164:VAL:HG12	1:A:166:LEU:H	1.83	0.43
1:A:322:ASP:OD1	1:A:323:PRO:HD2	2.18	0.43
1:A:363:ARG:NH1	1:A:363:ARG:HG2	2.27	0.43
1:B:315:ASP:HB3	1:B:387:LEU:HD11	1.99	0.43
1:B:193:ARG:O	1:B:195:GLY:N	2.51	0.43
3:G:1:NAG:H62	3:G:2:NAG:C7	2.49	0.43
1:B:134:TYR:HE2	1:B:141:THR:HB	1.82	0.43
1:A:281:VAL:HA	1:A:310:LEU:HD11	1.99	0.43
1:A:281:VAL:CG2	1:A:282:THR:N	2.81	0.43
1:B:254:VAL:HG21	1:B:329:TYR:HB3	2.01	0.43
1:B:255:ASP:C	1:B:257:ALA:H	2.22	0.43
1:A:101:ASP:OD1	1:A:103:GLU:N	2.52	0.43
1:B:179:ASN:ND2	1:B:179:ASN:N	2.67	0.43
1:B:234:ASP:OD2	1:B:273:PHE:HD2	2.00	0.43
1:A:136:ASP:O	1:A:148:SER:HB2	2.19	0.43
1:A:247:SER:O	1:A:250:GLN:HG2	2.19	0.43
1:A:123:TYR:O	1:A:124:VAL:C	2.57	0.43
1:A:213:LYS:CD	1:A:213:LYS:N	2.72	0.43
1:A:82:LYS:HE3	1:A:128:GLY:HA3	2.01	0.42
1:A:200:TYR:CD2	1:A:222:TYR:O	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:CD1	1:A:177:LEU:N	2.78	0.42
1:A:232:ILE:HG13	1:A:238:SER:OG	2.19	0.42
1:A:333:GLN:CG	1:A:334:GLY:H	2.22	0.42
1:A:381:ALA:O	1:A:419:ASN:HA	2.17	0.42
1:B:229:PHE:CG	1:B:230:ALA:N	2.87	0.42
1:B:364:SER:HA	1:B:406:HIS:HA	2.01	0.42
1:B:45:LEU:HD21	1:B:92:ASP:CB	2.49	0.42
1:A:75:LEU:O	1:A:78:SER:N	2.52	0.42
5:F:3:MAN:O4	5:F:4:MAN:C1	2.67	0.42
1:A:125:HIS:CE1	1:A:165:ASP:OD2	2.70	0.42
1:A:390:VAL:O	1:A:391:LYS:C	2.58	0.42
1:A:65:SER:O	1:A:68:LEU:N	2.52	0.42
1:B:422:GLN:HE21	1:B:422:GLN:CA	2.29	0.42
1:B:82:LYS:HA	1:B:86:TYR:O	2.18	0.42
1:A:177:LEU:HA	1:A:180:LEU:HB3	2.02	0.42
1:A:93:ASP:OD1	1:A:94:CYS:N	2.53	0.42
1:B:285:ALA:HB2	1:B:388:LEU:HD23	2.00	0.42
1:B:390:VAL:O	1:B:391:LYS:C	2.57	0.42
1:A:255:ASP:O	1:A:257:ALA:N	2.52	0.42
1:A:277:TRP:O	1:A:281:VAL:HG13	2.20	0.42
1:A:179:ASN:ND2	1:A:179:ASN:N	2.68	0.42
1:A:326:LYS:O	1:A:342:ARG:HG3	2.19	0.42
1:A:65:SER:C	1:A:67:LYS:N	2.74	0.42
1:B:101:ASP:OD2	1:B:105:ARG:HB2	2.20	0.42
1:B:180:LEU:O	1:B:183:GLY:N	2.52	0.42
1:B:208:MET:O	1:B:211:PHE:HB2	2.20	0.42
1:B:253:ILE:O	1:B:255:ASP:N	2.52	0.42
1:B:75:LEU:O	1:B:78:SER:N	2.53	0.42
1:A:239:ILE:CD1	1:A:283:GLN:HB2	2.49	0.42
1:B:388:LEU:HD22	1:B:414:LEU:HD23	2.02	0.42
1:B:97:ALA:HB2	1:B:110:PRO:HD3	2.02	0.41
1:B:137:VAL:HG12	1:B:171:GLY:HA2	2.02	0.41
1:A:99:GLN:N	1:A:99:GLN:OE1	2.53	0.41
1:B:32:LEU:HB2	1:B:223:CYS:N	2.35	0.41
1:B:93:ASP:O	1:B:94:CYS:CB	2.68	0.41
1:A:133:ILE:HG13	1:A:134:TYR:N	2.36	0.41
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.55	0.41
1:B:66:GLU:OE2	1:B:113:PHE:HA	2.20	0.41
1:A:193:ARG:O	1:A:195:GLY:N	2.53	0.41
1:A:237:LYS:HE3	1:B:237:LYS:HE3	2.01	0.41
1:A:332:ARG:HD3	1:A:365:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:HG22	1:B:247:SER:N	2.35	0.41
1:B:267:MET:H	1:B:267:MET:HG3	1.70	0.41
1:B:300:LEU:HD12	1:B:300:LEU:N	2.32	0.41
1:A:382:CYS:HA	1:A:418:GLU:O	2.21	0.41
1:A:75:LEU:C	1:A:77:VAL:N	2.73	0.41
1:A:387:LEU:HA	1:A:391:LYS:HA	2.03	0.41
1:B:265:PRO:HB2	1:B:287:TRP:CZ2	2.56	0.41
1:A:180:LEU:O	1:A:183:GLY:N	2.53	0.41
1:A:272:ASN:HB3	1:A:273:PHE:H	1.60	0.41
1:B:145:PHE:CB	1:B:146:PRO:HD2	2.44	0.41
1:B:56:CYS:HB2	8:B:11:HOH:O	2.20	0.41
1:B:115:HIS:HB3	1:B:119:GLN:OE1	2.21	0.41
1:B:216:TYR:HB3	1:B:256:VAL:HG21	2.03	0.41
1:B:199:VAL:HA	1:B:224:ASN:OD1	2.21	0.41
1:B:239:ILE:O	1:B:240:LYS:C	2.58	0.41
1:B:250:GLN:CB	1:B:254:VAL:HB	2.51	0.41
1:B:50:PHE:O	1:B:51:MET:C	2.60	0.41
1:B:53:ASN:HB3	1:B:62:SER:O	2.20	0.41
1:B:99:GLN:OE1	1:B:99:GLN:N	2.54	0.41
1:A:42:MET:HG2	1:A:294:LEU:HB2	2.03	0.41
1:A:353:MET:O	1:A:412:THR:HA	2.21	0.41
1:A:76:MET:SD	1:A:89:LEU:HD13	2.61	0.41
1:B:357:GLN:OE1	1:B:363:ARG:HD2	2.21	0.41
1:B:422:GLN:CG	1:B:422:GLN:O	2.68	0.41
5:F:1:NAG:H61	5:F:2:NAG:N2	2.36	0.41
1:A:39:THR:HB	1:A:321:GLN:OE1	2.21	0.40
1:B:205:PRO:C	1:B:207:TYR:N	2.75	0.40
1:B:364:SER:HB3	1:B:406:HIS:CE1	2.56	0.40
1:A:97:ALA:CB	1:A:110:PRO:HD3	2.51	0.40
1:A:209:TRP:HA	1:A:210:PRO:HA	1.91	0.40
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.84	0.40
1:B:174:CYS:HA	4:E:1:NAG:C7	2.50	0.40
1:B:185:LYS:HG2	1:B:222:TYR:CE2	2.57	0.40
1:B:37:ALA:C	1:B:39:THR:H	2.25	0.40
1:B:60:PRO:HA	1:B:63:CYS:HB3	2.03	0.40
1:B:376:VAL:O	1:B:377:ALA:C	2.59	0.40
1:B:53:ASN:C	1:B:54:LEU:HD12	2.42	0.40
1:A:253:ILE:CG1	1:A:254:VAL:N	2.83	0.40
1:B:47:TRP:O	1:B:51:MET:N	2.41	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLU:OE2	1:B:58:GLU:OE2[4_556]	1.96	0.24

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	388/398 (98%)	306 (79%)	56 (14%)	26 (7%)	1	8
1	B	389/398 (98%)	302 (78%)	59 (15%)	28 (7%)	1	7
All	All	777/796 (98%)	608 (78%)	115 (15%)	54 (7%)	1	8

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ALA
1	A	376	VAL
1	B	118	ARG
1	B	376	VAL
1	B	378	CYS
1	B	401	SER
1	A	47	TRP
1	A	100	ARG
1	A	175	ASP
1	A	256	VAL
1	A	266	ASP
1	A	374	LYS
1	A	395	GLY
1	A	401	SER
1	B	47	TRP
1	B	175	ASP
1	B	180	LEU
1	B	266	ASP
1	B	374	LYS
1	B	395	GLY

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Mol	Chain	Res	Type
1	A	180	LEU
1	A	313	ASP
1	B	206	LEU
1	B	249	ASN
1	B	267	MET
1	B	272	ASN
1	B	300	LEU
1	B	313	ASP
1	A	78	SER
1	A	151	TYR
1	A	210	PRO
1	A	267	MET
1	A	272	ASN
1	A	378	CYS
1	A	391	LYS
1	B	78	SER
1	B	151	TYR
1	B	256	VAL
1	A	94	CYS
1	A	146	PRO
1	A	370	ALA
1	B	146	PRO
1	B	230	ALA
1	B	391	LYS
1	A	98	PRO
1	A	206	LEU
1	B	181	ALA
1	B	194	THR
1	B	254	VAL
1	B	370	ALA
1	A	254	VAL
1	B	210	PRO
1	B	98	PRO
1	A	334	GLY

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	331/339 (98%)	310 (94%)	21 (6%)	18	47
1	B	332/339 (98%)	312 (94%)	20 (6%)	19	49
All	All	663/678 (98%)	622 (94%)	41 (6%)	18	48

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	CYS
1	A	67	LYS
1	A	70	MET
1	A	74	GLU
1	A	98	PRO
1	A	169	PHE
1	A	246	THR
1	A	250	GLN
1	A	251	GLU
1	A	254	VAL
1	A	273	PHE
1	A	287	TRP
1	A	310	LEU
1	A	324	LEU
1	A	353	MET
1	A	363	ARG
1	A	382	CYS
1	A	385	THR
1	A	388	LEU
1	A	389	PRO
1	A	421	MET
1	B	63	CYS
1	B	98	PRO
1	B	123	TYR
1	B	161	ASP
1	B	169	PHE
1	B	246	THR
1	B	250	GLN
1	B	251	GLU
1	B	254	VAL
1	B	273	PHE
1	B	287	TRP
1	B	310	LEU
1	B	324	LEU
1	B	353	MET

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Mol	Chain	Res	Type
1	B	363	ARG
1	B	382	CYS
1	B	385	THR
1	B	388	LEU
1	B	421	MET
1	B	422	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	111	GLN
1	A	125	HIS
1	A	179	ASN
1	A	212	GLN
1	A	272	ASN
1	A	302	HIS
1	A	330	GLN
1	A	333	GLN
1	A	386	GLN
1	B	46	HIS
1	B	111	GLN
1	B	122	ASN
1	B	125	HIS
1	B	179	ASN
1	B	272	ASN
1	B	386	GLN
1	B	422	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 ⓘ

19 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	C	1	1,2	14,14,15	0.64	0	17,19,21	0.68	0
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	0.68	0
2	MAN	C	3	2	11,11,12	0.57	0	15,15,17	0.84	1 (6%)
2	MAN	C	4	2	11,11,12	0.81	0	15,15,17	0.62	0
2	MAN	C	5	2	11,11,12	0.86	0	15,15,17	0.54	0
3	NAG	D	1	1,3	14,14,15	0.54	0	17,19,21	0.62	0
3	NAG	D	2	3	14,14,15	0.60	0	17,19,21	0.62	0
4	NAG	E	1	1,4	14,14,15	0.71	0	17,19,21	1.07	2 (11%)
4	NAG	E	2	4	14,14,15	0.59	0	17,19,21	0.81	1 (5%)
4	MAN	E	3	4	11,11,12	0.76	0	15,15,17	1.56	2 (13%)
4	MAN	E	4	4	11,11,12	0.98	1 (9%)	15,15,17	1.12	2 (13%)
4	MAN	E	5	4	11,11,12	0.56	0	15,15,17	0.88	2 (13%)
4	FUC	E	6	4	10,10,11	0.80	0	14,14,16	0.49	0
5	NAG	F	1	1,5	14,14,15	0.70	0	17,19,21	0.71	0
5	NAG	F	2	5	14,14,15	0.57	0	17,19,21	0.82	1 (5%)
5	MAN	F	3	5	11,11,12	0.62	0	15,15,17	1.00	1 (6%)
5	MAN	F	4	5	11,11,12	0.53	0	15,15,17	1.00	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.75	0	17,19,21	0.70	0
3	NAG	G	2	3	14,14,15	0.71	0	17,19,21	0.70	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	MAN	C	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3	4	1/1/4/5	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	FUC	E	6	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	MAN	F	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	MAN	C2-C3	2.49	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	MAN	C1-C2-C3	4.92	115.72	109.67
5	F	3	MAN	C1-C2-C3	-3.16	105.79	109.67
5	F	4	MAN	C1-C2-C3	2.65	112.93	109.67
4	E	3	MAN	O3-C3-C2	-2.55	105.11	109.99
4	E	1	NAG	C2-N2-C7	-2.52	119.31	122.90
4	E	4	MAN	C1-C2-C3	2.48	112.71	109.67
4	E	4	MAN	C6-C5-C4	2.39	118.60	113.00
4	E	5	MAN	C1-C2-C3	2.30	112.49	109.67
5	F	2	NAG	C2-N2-C7	-2.28	119.66	122.90
4	E	1	NAG	C3-C4-C5	2.21	114.19	110.24
4	E	2	NAG	C2-N2-C7	-2.17	119.81	122.90
2	C	3	MAN	O3-C3-C2	2.10	114.02	109.99
3	G	2	NAG	C2-N2-C7	-2.09	119.92	122.90
4	E	5	MAN	C1-O5-C5	2.08	115.01	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	3	MAN	C1
2	C	3	MAN	C1
5	F	3	MAN	C1

All (20) torsion outliers are listed below:

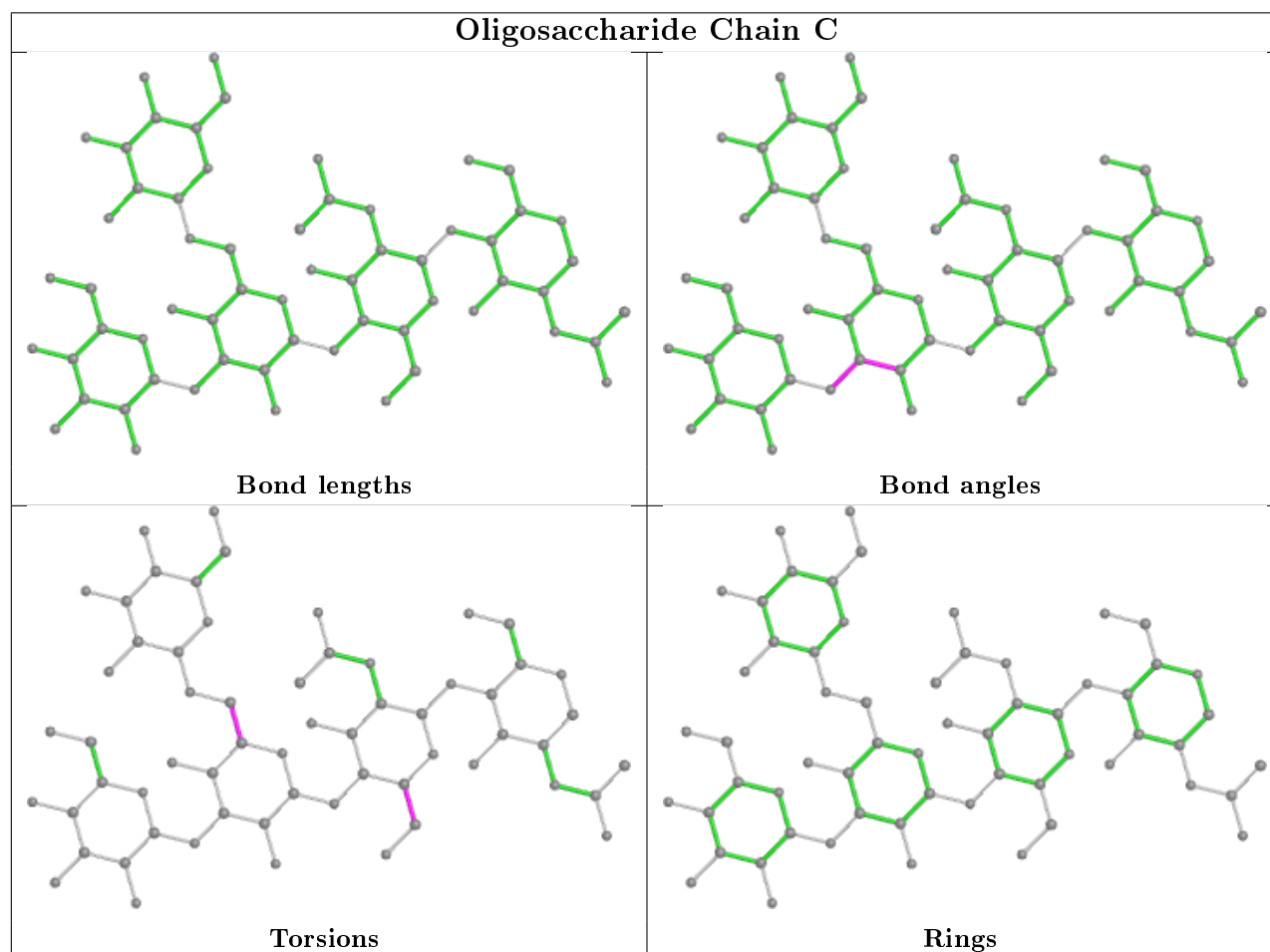
Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
5	F	3	MAN	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
5	F	3	MAN	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
5	F	4	MAN	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6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

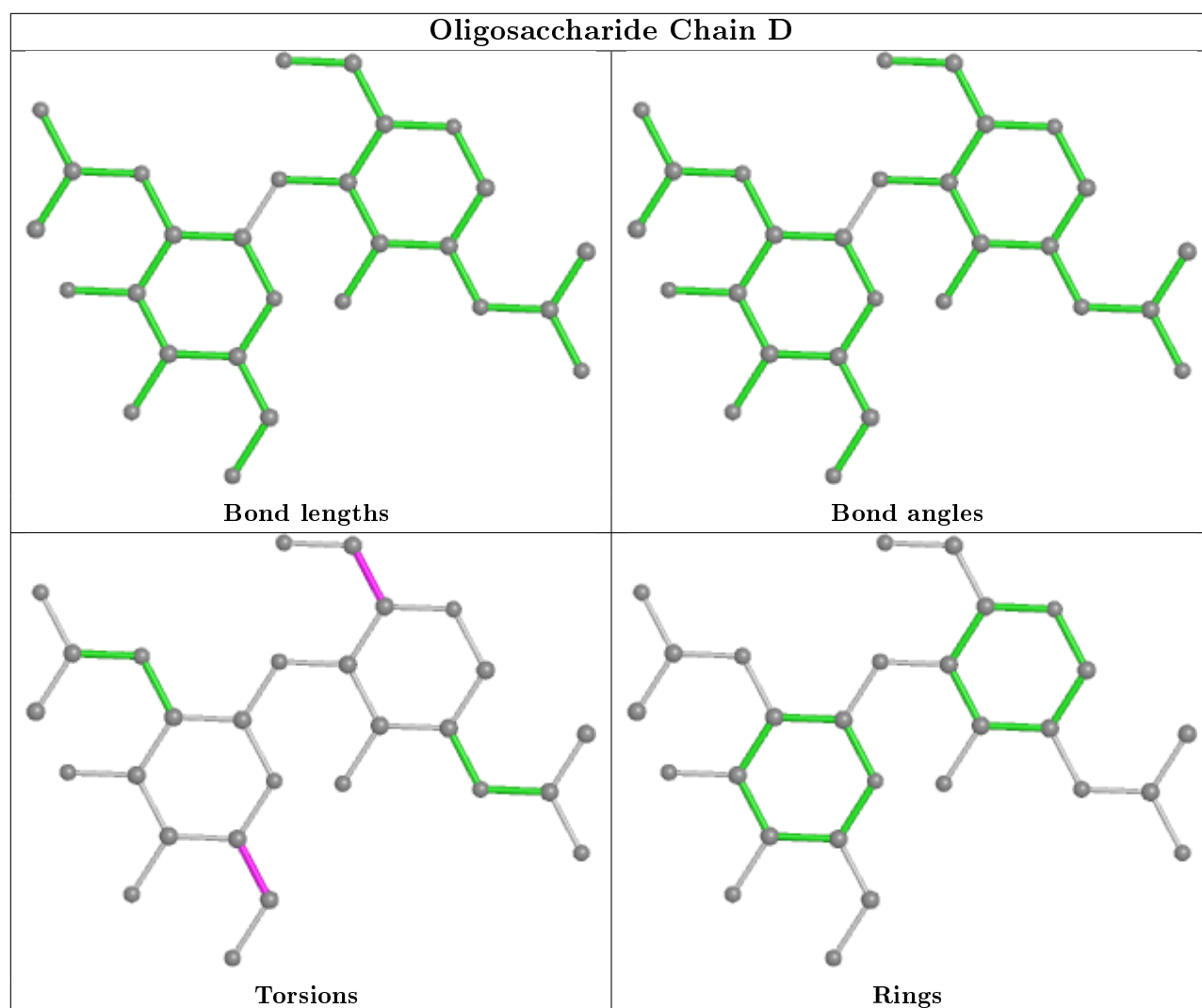
There are no ring outliers.

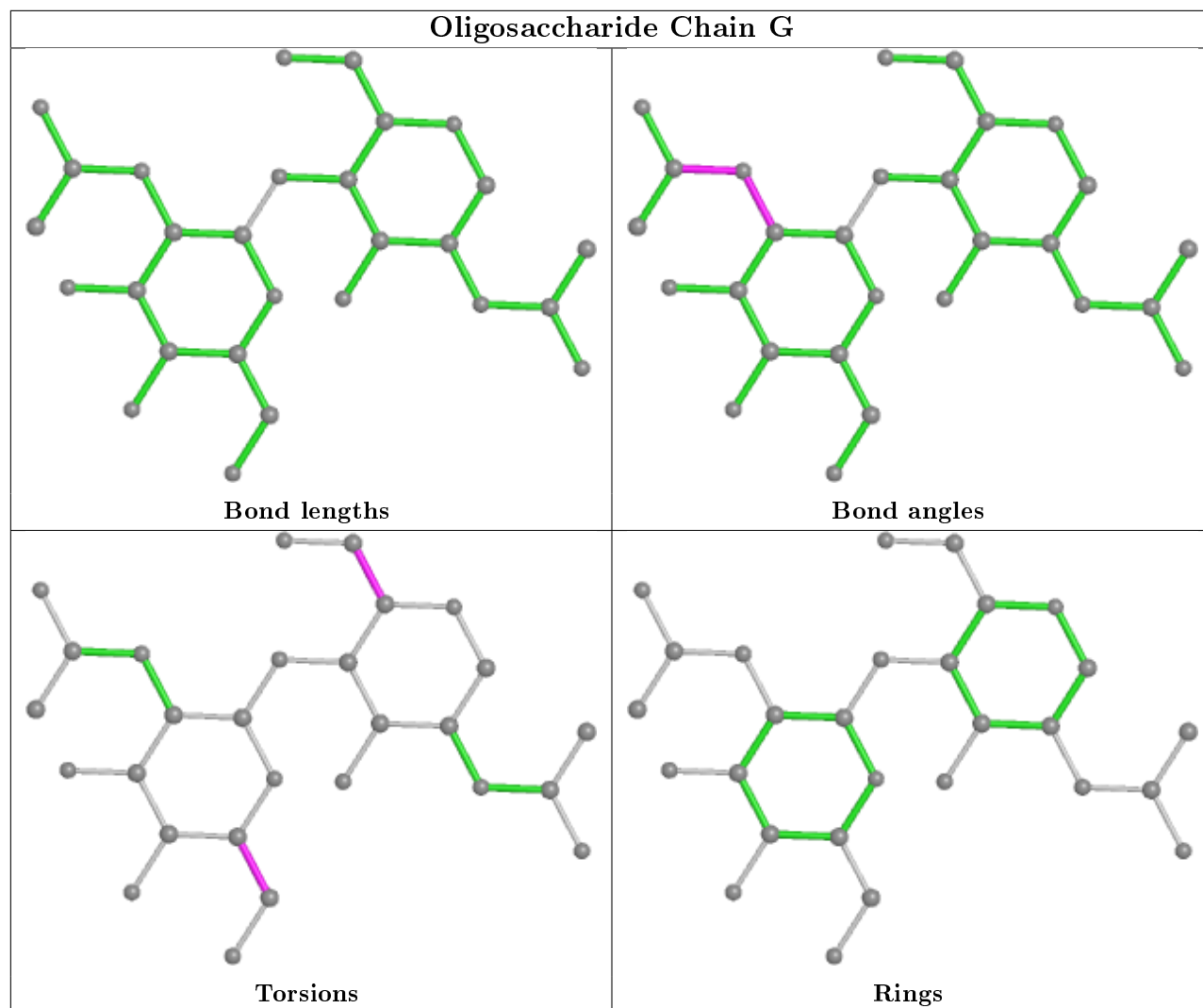
10 monomers are involved in 22 short contacts:

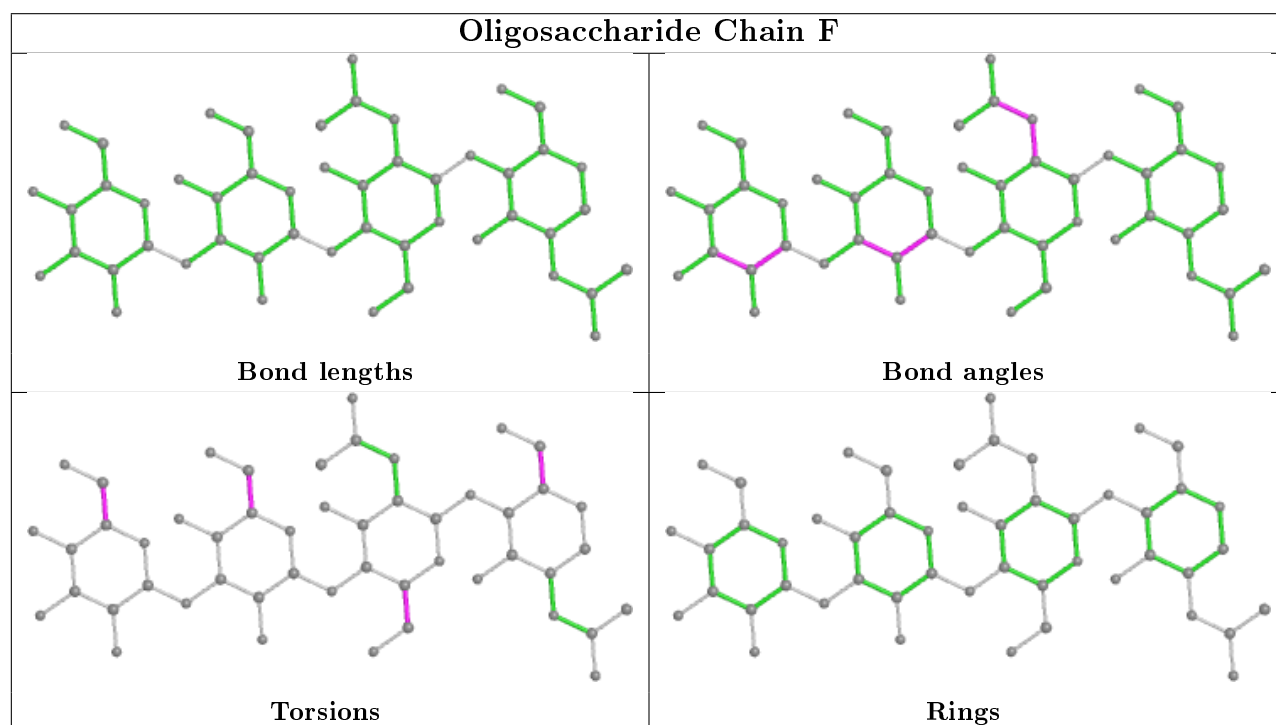
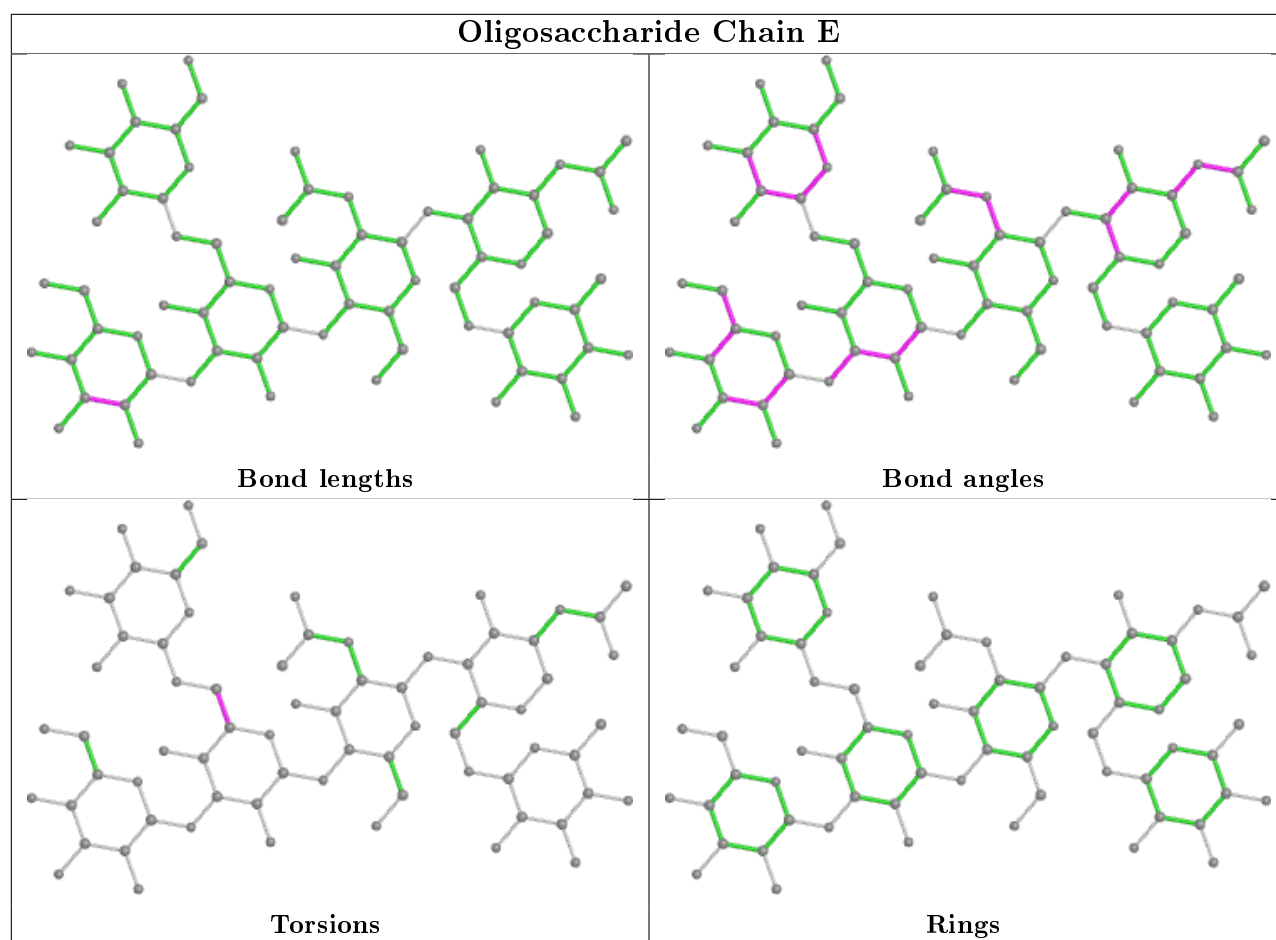
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	MAN	3	0
5	F	4	MAN	4	0
4	E	3	MAN	3	0
3	G	1	NAG	3	0
4	E	1	NAG	11	0
5	F	1	NAG	1	0
3	G	2	NAG	3	0
5	F	2	NAG	1	0
5	F	3	MAN	4	0
4	E	6	FUC	4	0

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

5 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
7	EDO	A	1102	-	3,3,3	0.86	0	2,2,2	0.04	0
7	EDO	A	1101	-	3,3,3	0.73	0	2,2,2	0.18	0
7	EDO	B	1104	-	3,3,3	0.71	0	2,2,2	0.15	0
7	EDO	B	1103	-	3,3,3	0.36	0	2,2,2	0.64	0
6	NAG	A	639	1	14,14,15	0.88	0	17,19,21	0.82	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
7	EDO	A	1102	-	-	1/1/1/1	-
7	EDO	A	1101	-	-	1/1/1/1	-
7	EDO	B	1104	-	-	1/1/1/1	-
7	EDO	B	1103	-	-	1/1/1/1	-
6	NAG	A	639	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	639	NAG	C2-N2-C7	-2.10	119.91	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1102	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	1101	EDO	O1-C1-C2-O2
7	B	1104	EDO	O1-C1-C2-O2
6	A	639	NAG	C4-C5-C6-O6
6	A	639	NAG	O5-C5-C6-O6
7	B	1103	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1102	EDO	1	0
7	B	1103	EDO	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	A	390/398 (97%)	-0.54	0 100 100	33, 58, 89, 119	0
1	B	391/398 (98%)	-0.54	0 100 100	35, 60, 94, 118	0
All	All	781/796 (98%)	-0.54	0 100 100	33, 59, 93, 119	0

There are no RSRZ outliers to report.

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.

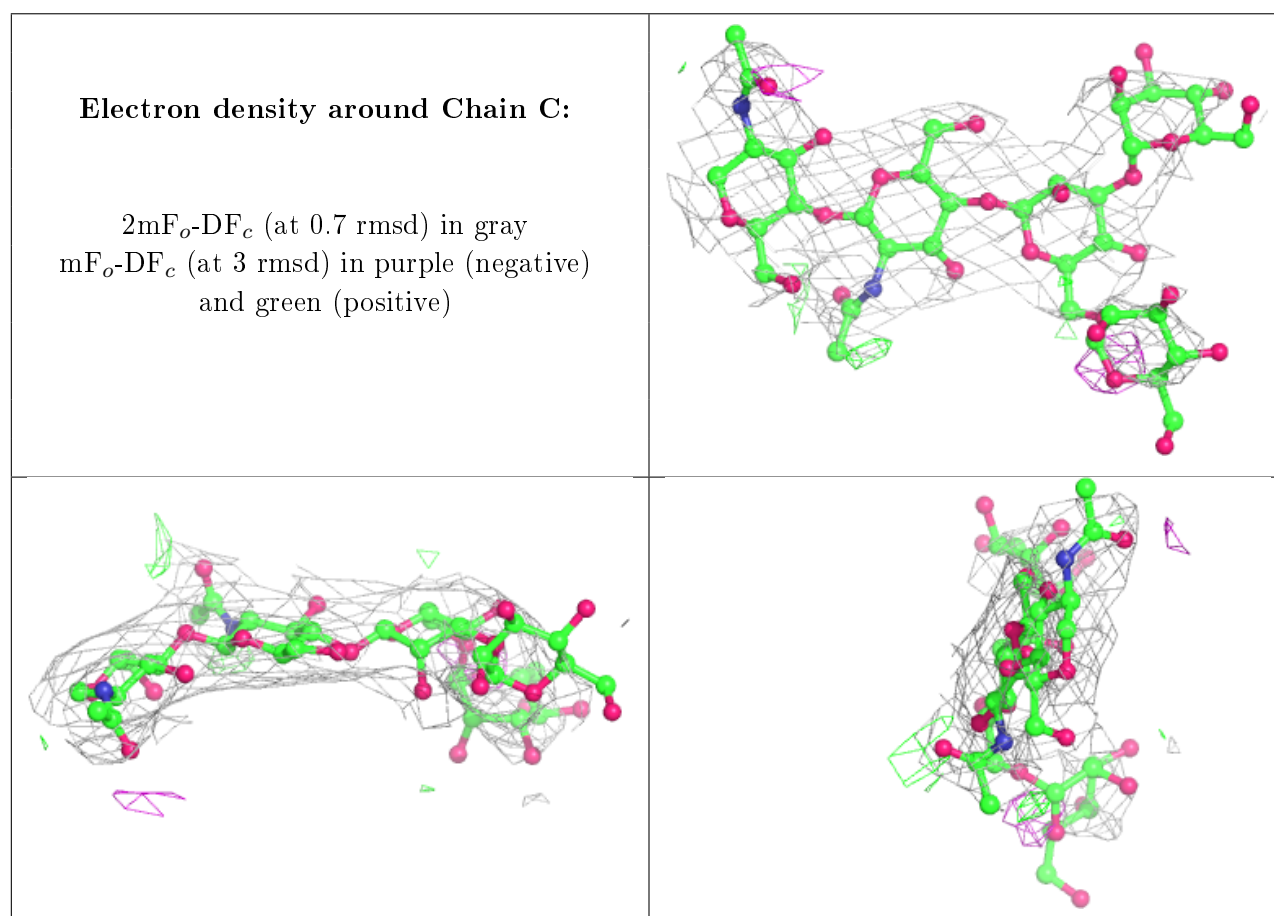
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	E	4	11/12	0.50	0.45	132,140,143,143	0
2	MAN	C	3	11/12	0.56	0.21	106,114,128,134	0
2	MAN	C	5	11/12	0.58	0.70	128,138,142,146	0
4	MAN	E	3	11/12	0.60	0.23	137,139,142,143	0
3	NAG	G	2	14/15	0.66	0.35	139,146,150,152	0
5	MAN	F	4	11/12	0.66	0.20	103,108,112,115	0
4	FUC	E	6	10/11	0.67	0.43	136,145,154,161	0
2	MAN	C	4	11/12	0.70	0.30	128,138,147,151	0
4	MAN	E	5	11/12	0.77	0.48	139,140,142,143	0
5	MAN	F	3	11/12	0.81	0.16	109,118,127,127	0
3	NAG	D	2	14/15	0.83	0.20	108,121,125,127	0

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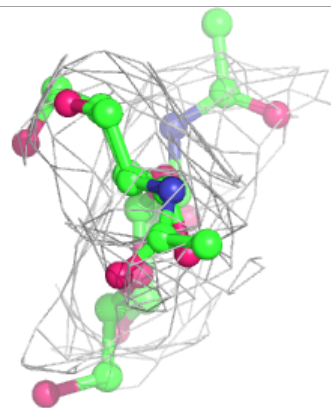
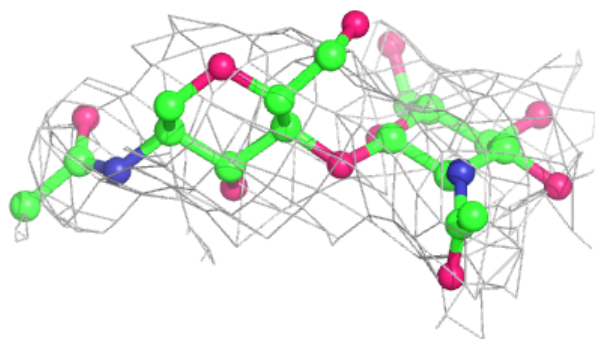
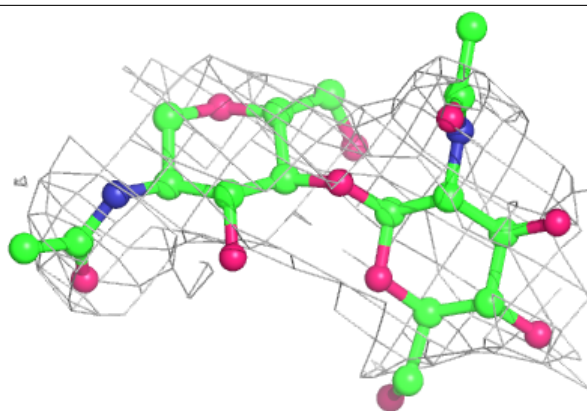
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	1	14/15	0.84	0.14	80,106,120,129	0
4	NAG	E	2	14/15	0.84	0.22	115,132,136,136	0
4	NAG	E	1	14/15	0.87	0.17	93,130,134,135	0
3	NAG	D	1	14/15	0.90	0.15	107,117,122,123	0
5	NAG	F	1	14/15	0.90	0.17	58,76,91,94	0
2	NAG	C	2	14/15	0.90	0.16	65,73,84,96	0
5	NAG	F	2	14/15	0.91	0.18	85,96,116,119	0
2	NAG	C	1	14/15	0.95	0.17	46,62,73,73	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.



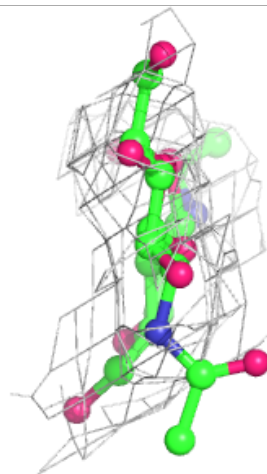
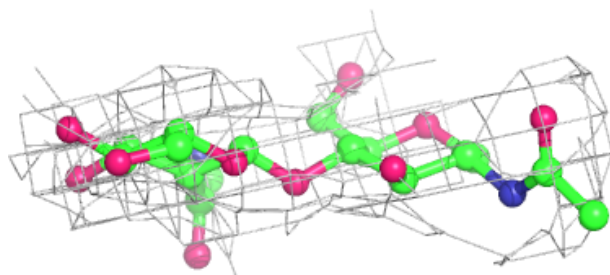
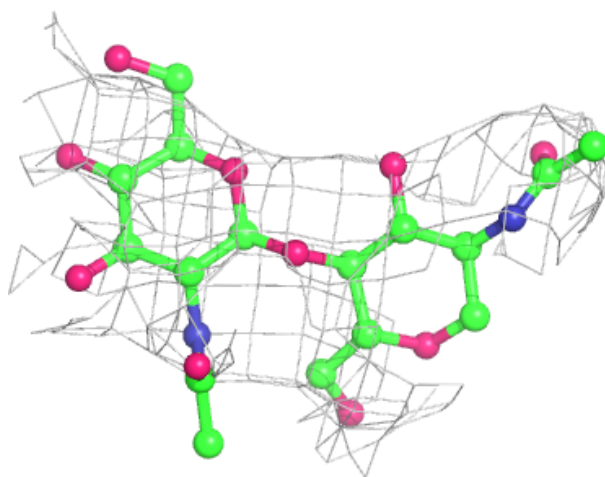
Electron density around Chain D:

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



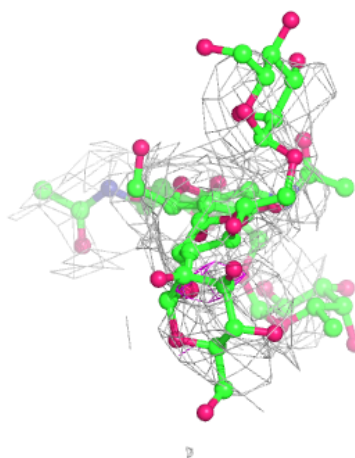
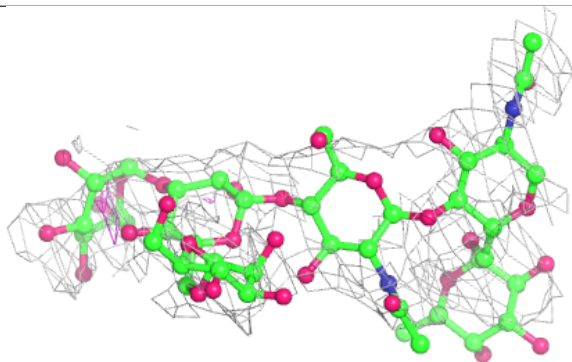
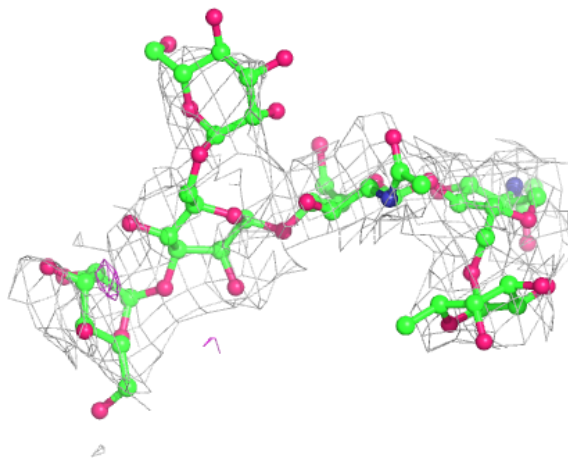
Electron density around Chain G:

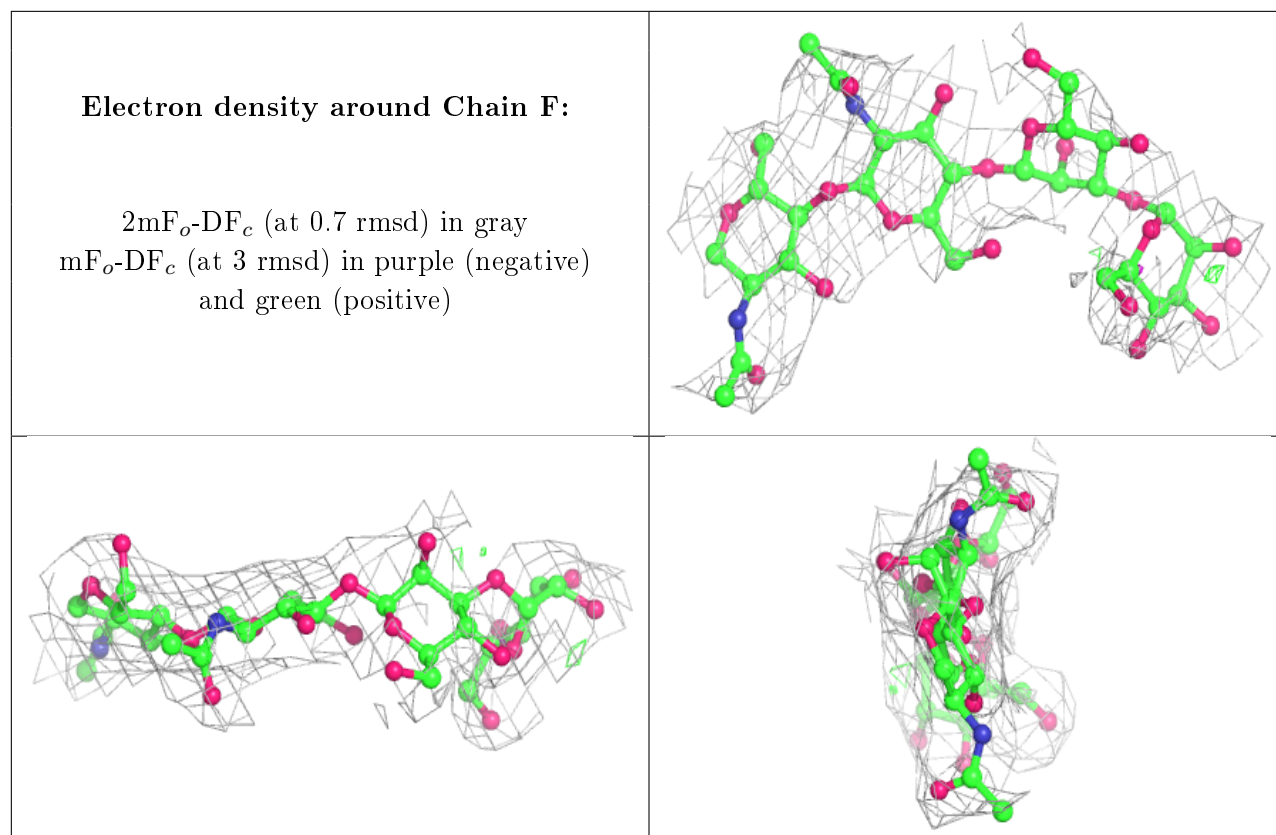
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	B	1103	4/4	0.71	0.26	24,29,39,42	0
6	NAG	A	639	14/15	0.75	0.20	67,81,95,98	0
7	EDO	A	1102	4/4	0.78	0.19	31,47,50,57	0
7	EDO	B	1104	4/4	0.92	0.12	40,41,44,46	0
7	EDO	A	1101	4/4	0.98	0.12	25,31,32,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.