



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:29 PM EDT

PDB ID : 4AYJ / pdb_00004ayj
Title : Molecular structure of a metal-independent bacterial glycosyltransferase that catalyzes the synthesis of histo-blood group A antigen
Authors : Thiyagarajan, N.; Pham, T.T.K.; Stinson, B.; Sundriyal, A.; Tumbale, P.; Lizotte-Waniewskib, M.; Brewb, K.; Acharya, K.R.
Deposited on : 2012-06-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

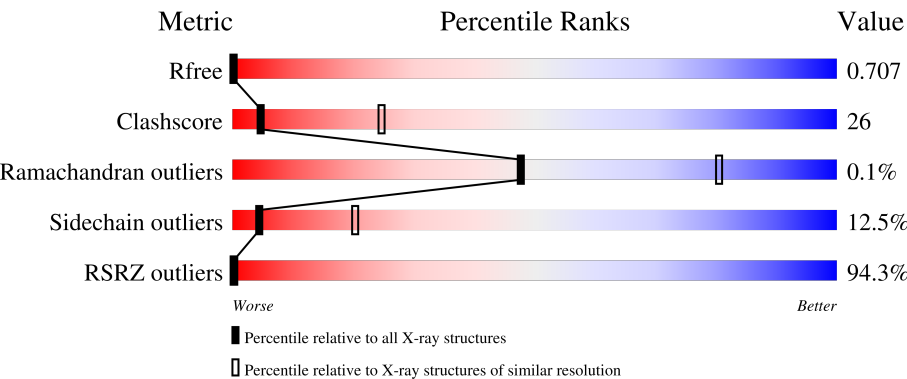
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	246	88% 48% 39% 7% 6%
1	B	246	90% 44% 46% 5% .
1	C	246	91% 44% 42% 9% 5%
1	D	246	89% 43% 43% 9% ..
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	F	3	
2	G	3	
2	H	3	

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	FUC	H	3	-	-	-	X

2 Entry composition [i](#)

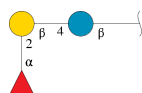
There are 2 unique types of molecules in this entry. The entry contains 7939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	4	0	0
			1928	1262	311	348	7			
1	B	235	Total	C	N	O	S	0	0	0
			1961	1282	318	354	7			
1	C	233	Total	C	N	O	S	4	0	0
			1945	1272	315	351	7			
1	D	236	Total	C	N	O	S	0	0	0
			1973	1291	319	356	7			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

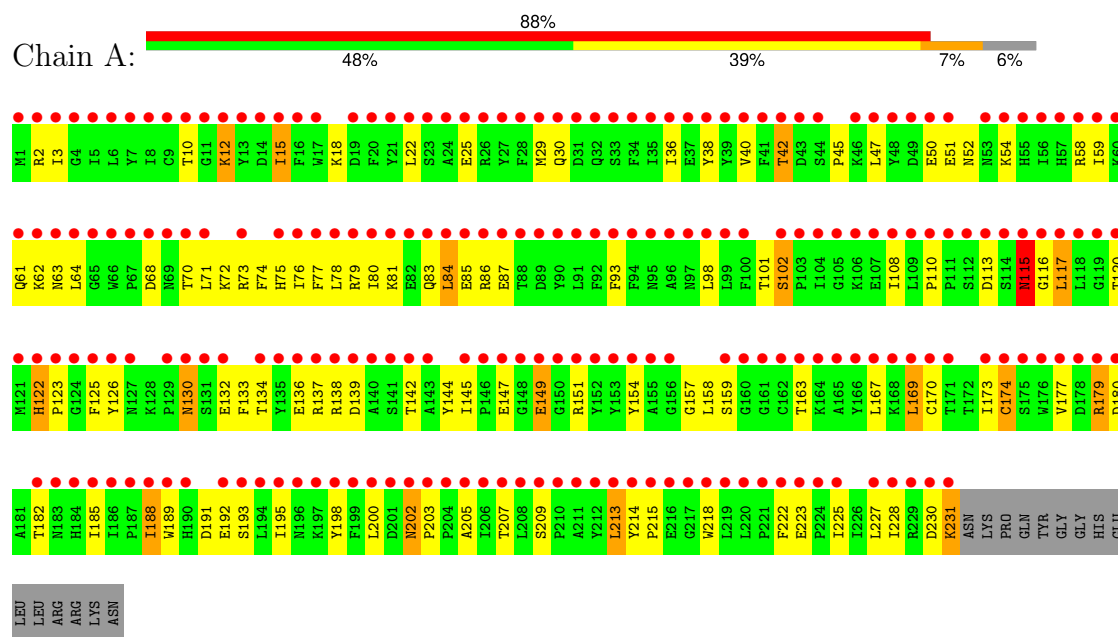


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			33	18	15			
2	F	3	Total	C	O	0	0	0
			33	18	15			
2	G	3	Total	C	O	0	0	0
			33	18	15			
2	H	3	Total	C	O	0	0	0
			33	18	15			

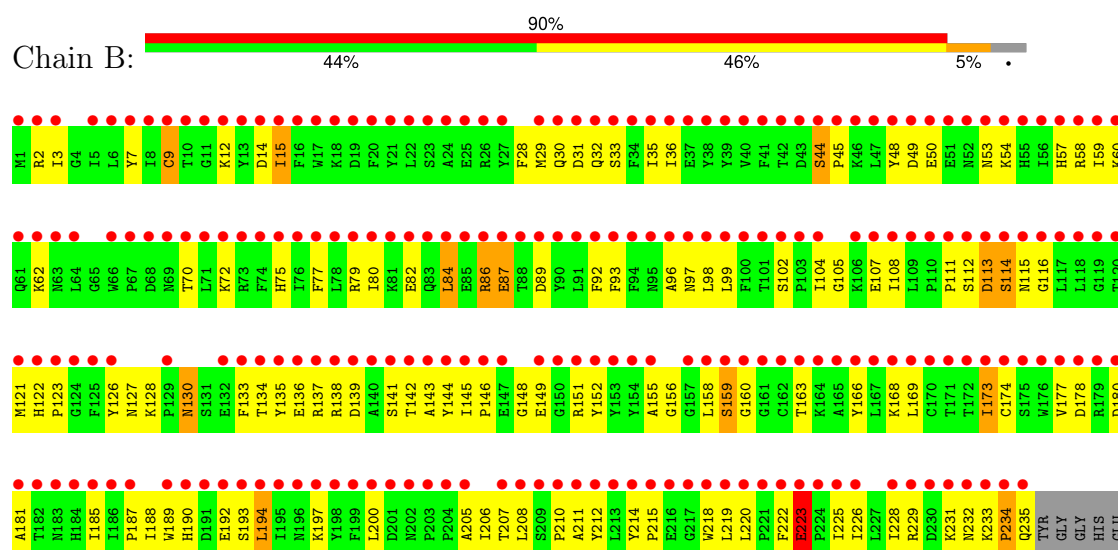
3 Residue-property plots

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

• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE



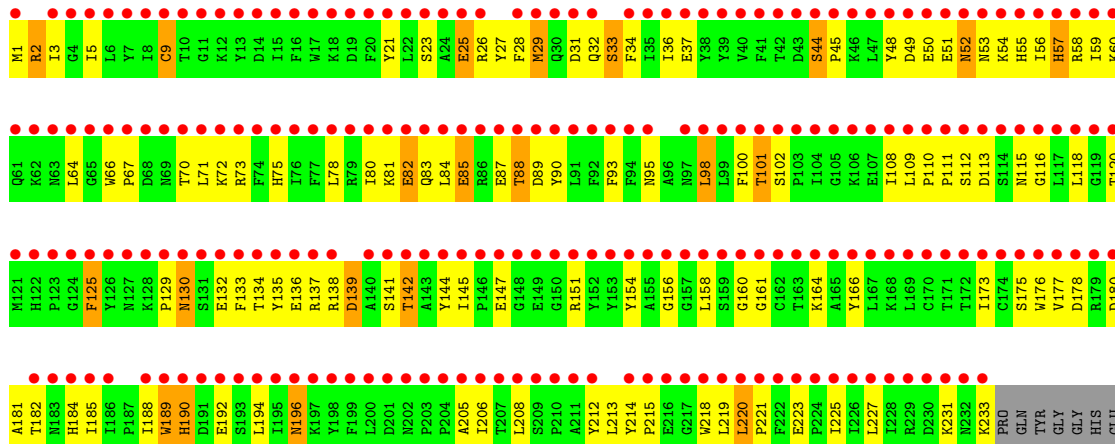
• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE



LEU
LEU
ARG
ARG
LYS
ASN

• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE

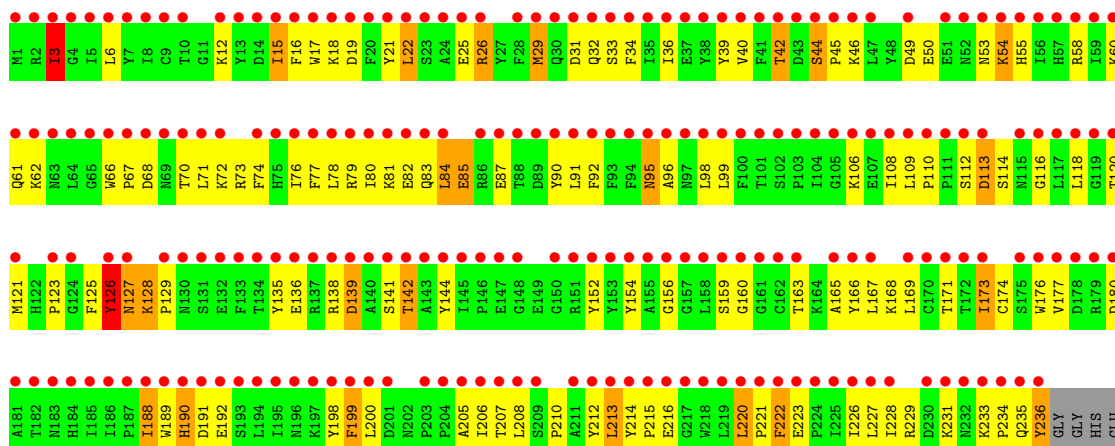
Chain C: 



LEU
LEU
ARG
ARG
LYS
ASN

• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE

Chain D: 



LEU
LEU
ARG
ARG
LYS
ASN

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranoside

Chain E: 

BGC1
GAL2
FUC3

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:  67% 33%

BGC1
GAL2
FUC3

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G:  33% 67%

BGC1
GAL2
FUC3

- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

BGC1
GAL2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.85Å 93.87Å 75.51Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	70.69 – 3.00 70.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (70.69-3.00) 91.5 (70.69-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.25 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.262 0.709 , 0.707	Depositor DCC
R_{free} test set	951 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: FUC, GAL, BGC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/1991	1.09	16/2704 (0.6%)
1	B	0.59	0/2025	1.03	9/2750 (0.3%)
1	C	0.56	0/2008	1.01	13/2726 (0.5%)
1	D	0.58	0/2038	1.03	12/2768 (0.4%)
All	All	0.59	0/8062	1.04	50/10948 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	SER	CA-C-N	8.55	129.07	119.32
1	D	44	SER	C-N-CA	8.55	129.07	119.32
1	A	202	ASN	CA-C-N	-7.61	112.54	120.38
1	A	202	ASN	C-N-CA	-7.61	112.54	120.38
1	A	102	SER	CA-C-N	6.92	127.33	119.93
1	A	102	SER	C-N-CA	6.92	127.33	119.93
1	A	115	ASN	N-CA-C	-6.90	105.20	112.93
1	C	190	HIS	CB-CA-C	-6.77	106.86	116.34
1	C	125	PHE	N-CA-C	6.69	121.61	113.38
1	C	9	CYS	N-CA-C	6.51	121.28	112.88
1	B	190	HIS	CB-CA-C	-6.39	107.39	116.34
1	D	190	HIS	CB-CA-C	-6.36	109.25	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	SER	CA-C-N	6.20	125.61	118.85
1	B	44	SER	C-N-CA	6.20	125.61	118.85
1	C	88	THR	N-CA-C	6.18	118.98	108.90
1	A	223	GLU	CA-C-N	-6.09	113.50	119.90
1	A	223	GLU	C-N-CA	-6.09	113.50	119.90
1	A	157	GLY	N-CA-C	6.05	123.25	115.32
1	D	3	ILE	CB-CA-C	-5.95	103.70	111.25
1	B	223	GLU	CA-C-N	-5.89	112.98	120.23
1	B	223	GLU	C-N-CA	-5.89	112.98	120.23
1	C	44	SER	CA-C-N	5.78	125.40	119.56
1	C	44	SER	C-N-CA	5.78	125.40	119.56
1	D	128	LYS	CA-C-N	5.71	127.09	120.98
1	D	128	LYS	C-N-CA	5.71	127.09	120.98
1	A	117	LEU	N-CA-C	-5.67	100.08	108.99
1	A	209	SER	CA-C-N	5.63	125.33	119.82
1	A	209	SER	C-N-CA	5.63	125.33	119.82
1	A	213	LEU	N-CA-C	5.62	119.44	112.59
1	B	102	SER	CA-C-N	5.49	125.80	119.93
1	B	102	SER	C-N-CA	5.49	125.80	119.93
1	A	214	TYR	CA-C-N	5.44	125.38	119.78
1	A	214	TYR	C-N-CA	5.44	125.38	119.78
1	A	122	HIS	CA-C-N	5.43	125.07	119.05
1	A	122	HIS	C-N-CA	5.43	125.07	119.05
1	C	3	ILE	N-CA-C	5.42	115.90	107.28
1	B	3	ILE	N-CA-C	5.36	115.30	107.37
1	C	29	MET	CA-C-N	-5.34	114.84	123.23
1	C	29	MET	C-N-CA	-5.34	114.84	123.23
1	C	33	SER	N-CA-C	-5.31	106.39	112.92
1	C	189	TRP	N-CA-C	5.25	119.38	112.92
1	D	68	ASP	N-CA-C	5.21	118.74	112.38
1	D	213	LEU	N-CA-C	5.16	119.26	112.92
1	D	223	GLU	CA-C-N	-5.15	114.48	119.78
1	D	223	GLU	C-N-CA	-5.15	114.48	119.78
1	B	87	GLU	N-CA-C	5.14	120.40	113.72
1	D	126	TYR	N-CA-C	5.08	117.56	111.71
1	C	102	SER	CA-C-N	5.08	124.99	119.76
1	C	102	SER	C-N-CA	5.08	124.99	119.76
1	D	33	SER	N-CA-C	-5.03	106.92	113.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Peptide

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	A	1928	0	1869	91	0
1	B	1961	0	1903	95	1
1	C	1945	0	1888	103	0
1	D	1973	0	1911	116	1
2	E	33	0	30	8	0
2	F	33	0	30	2	0
2	G	33	0	30	6	0
2	H	33	0	30	3	0
All	All	7939	0	7691	404	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 26.

All (404) 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:D:128:LYS:NZ	2:G:1:BGC:O5	1.79	1.15
1:C:2:ARG:NH1	1:C:89:ASP:H	1.50	1.08
1:C:2:ARG:NH1	1:C:2:ARG:O	1.93	1.02
1:A:134:THR:HG21	1:A:189:TRP:HE1	1.28	0.98
1:B:229:ARG:HD3	1:C:223:GLU:OE2	1.64	0.97
1:B:128:LYS:NZ	2:E:1:BGC:O5	2.00	0.93
1:D:80:ILE:HG13	1:D:84:LEU:HD22	1.51	0.91
1:D:128:LYS:HZ1	2:G:1:BGC:C1	1.84	0.89
1:A:136:GLU:HA	1:A:188:ILE:HD11	1.56	0.88
1:B:232:ASN:OD1	1:B:233:LYS:N	2.07	0.87
1:B:208:LEU:HB3	1:B:212:TYR:HD2	1.40	0.86
1:C:2:ARG:NH2	1:C:87:GLU:O	2.09	0.85
1:B:208:LEU:HB3	1:B:212:TYR:CD2	2.12	0.85
1:C:2:ARG:CZ	1:C:88:THR:HA	2.07	0.84
1:D:50:GLU:OE2	1:D:58:ARG:NH1	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLU:HG2	1:C:52:ASN:OD1	1.79	0.81
1:D:165:ALA:HA	1:D:168:LYS:HE2	1.65	0.79
1:A:25:GLU:O	1:A:30:GLN:NE2	2.16	0.79
1:C:134:THR:HG21	1:C:189:TRP:CD1	2.19	0.77
1:D:66:TRP:CG	1:D:67:PRO:HA	2.20	0.77
1:D:83:GLN:O	1:D:87:GLU:HG3	1.83	0.77
1:B:158:LEU:HD23	1:B:159:SER:N	2.00	0.76
1:A:80:ILE:HG13	1:A:84:LEU:HD22	1.66	0.76
1:A:134:THR:CG2	1:A:189:TRP:HE1	1.98	0.76
1:C:134:THR:O	1:C:134:THR:HG22	1.85	0.75
1:C:2:ARG:HH11	1:C:89:ASP:H	1.33	0.75
1:D:138:ARG:O	1:D:144:TYR:HB2	1.86	0.74
1:D:188:ILE:HD13	1:D:189:TRP:H	1.51	0.74
1:A:72:LYS:HD2	1:A:75:HIS:ND1	2.03	0.74
1:C:82:GLU:HA	1:C:85:GLU:HG3	1.70	0.73
1:D:74:PHE:HA	1:D:77:PHE:HD2	1.52	0.73
1:D:92:PHE:CD1	1:D:160:GLY:HA3	2.23	0.73
1:C:1:MET:O	1:C:34:PHE:HA	1.90	0.72
1:A:81:LYS:O	1:A:85:GLU:HG3	1.90	0.71
1:B:86:ARG:HG2	1:B:87:GLU:HG3	1.72	0.71
1:C:84:LEU:O	1:C:88:THR:OG1	2.06	0.71
1:A:198:TYR:O	1:A:202:ASN:HB2	1.89	0.71
1:B:75:HIS:CD2	1:B:174:CYS:SG	2.84	0.71
1:C:80:ILE:HG13	1:C:84:LEU:HD11	1.72	0.70
1:D:12:LYS:O	1:D:15:ILE:HG12	1.91	0.70
1:C:134:THR:CG2	1:C:189:TRP:CD1	2.75	0.70
1:D:26:ARG:CB	1:D:26:ARG:HH11	2.05	0.70
1:A:231:LYS:H	1:A:231:LYS:HD3	1.58	0.69
1:C:2:ARG:NH1	1:C:89:ASP:N	2.34	0.69
1:D:50:GLU:CD	1:D:58:ARG:HH11	2.01	0.69
1:C:48:TYR:CD1	1:C:49:ASP:HB2	2.29	0.68
1:A:125:PHE:HE2	2:E:2:GAL:H61	1.59	0.68
1:D:31:ASP:O	1:D:32:GLN:HG2	1.94	0.68
1:D:118:LEU:HD11	1:D:208:LEU:HD11	1.75	0.68
1:D:169:LEU:O	1:D:173:ILE:HG13	1.94	0.68
1:B:134:THR:HG21	1:B:189:TRP:HE1	1.59	0.68
1:A:62:LYS:HG2	1:A:63:ASN:N	2.09	0.67
1:A:70:THR:O	1:A:73:ARG:HG3	1.93	0.67
1:D:73:ARG:NH1	1:D:191:ASP:CG	2.52	0.67
1:C:180:ASP:HB3	1:C:185:ILE:O	1.95	0.67
1:D:128:LYS:NZ	2:G:1:BGC:C1	2.49	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:BGC:O3	2:G:2:GAL:O5	2.04	0.66
1:B:130:ASN:HD21	1:B:148:GLY:HA2	1.61	0.66
1:D:215:PRO:HA	1:D:228:ILE:HB	1.77	0.66
1:B:29:MET:HB2	1:B:36:ILE:HD11	1.76	0.66
1:A:136:GLU:O	1:A:144:TYR:HA	1.97	0.65
1:C:48:TYR:CE1	1:C:49:ASP:HB2	2.32	0.65
1:A:122:HIS:HE2	2:E:2:GAL:HO4	1.42	0.65
1:C:50:GLU:OE2	1:C:58:ARG:NH1	2.29	0.65
1:D:6:LEU:HB3	1:D:77:PHE:HE1	1.62	0.65
1:D:233:LYS:O	1:D:236:TYR:HB2	1.97	0.64
1:A:179:ARG:O	1:A:182:THR:OG1	2.13	0.64
1:D:26:ARG:HH11	1:D:26:ARG:HB2	1.62	0.64
1:D:90:TYR:O	1:D:91:LEU:HD23	1.98	0.64
1:D:126:TYR:OH	1:D:221:PRO:HG3	1.97	0.64
1:D:114:SER:HB2	1:D:205:ALA:HB2	1.80	0.64
1:D:6:LEU:HB3	1:D:77:PHE:CE1	2.33	0.64
1:D:73:ARG:HH11	1:D:191:ASP:CG	2.06	0.64
1:D:82:GLU:HA	1:D:85:GLU:HG3	1.81	0.63
1:D:53:ASN:OD1	1:D:55:HIS:N	2.20	0.62
1:D:3:ILE:HD11	1:D:34:PHE:CE1	2.34	0.62
1:C:136:GLU:HG2	1:C:141:SER:OG	2.00	0.62
1:C:139:ASP:OD1	1:C:139:ASP:N	2.28	0.62
1:A:120:THR:HG21	1:A:213:LEU:HD12	1.81	0.62
1:A:29:MET:HE2	1:A:108:ILE:HD11	1.82	0.61
1:D:73:ARG:NH1	1:D:191:ASP:OD2	2.33	0.61
1:B:121:MET:HB2	1:B:210:PRO:HD3	1.81	0.61
1:D:126:TYR:OH	1:D:221:PRO:CG	2.49	0.61
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.66	0.61
1:A:120:THR:CG2	1:A:213:LEU:HD12	2.31	0.61
1:C:2:ARG:NH2	1:C:88:THR:HA	2.15	0.61
1:C:2:ARG:CZ	1:C:2:ARG:HB2	2.27	0.61
1:A:101:THR:OG1	1:A:225:ILE:O	2.17	0.60
1:C:2:ARG:CZ	1:C:87:GLU:O	2.49	0.60
1:B:143:ALA:HB2	1:B:194:LEU:HG	1.82	0.60
1:A:134:THR:HG21	1:A:189:TRP:NE1	2.09	0.60
1:B:121:MET:HE3	1:B:152:TYR:CD1	2.36	0.60
1:D:73:ARG:HB3	1:D:77:PHE:HE2	1.66	0.60
1:A:145:ILE:HD13	1:A:200:LEU:HD22	1.83	0.60
1:B:92:PHE:CD1	1:B:160:GLY:HA3	2.37	0.60
1:A:180:ASP:HB3	1:A:185:ILE:O	2.02	0.60
1:C:181:ALA:O	1:C:184:HIS:N	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:TYR:CZ	1:C:109:LEU:HD22	2.36	0.59
1:C:134:THR:HG21	1:C:189:TRP:NE1	2.17	0.59
1:B:60:LYS:O	1:B:79:ARG:NH1	2.31	0.59
1:C:173:ILE:O	1:C:177:VAL:HG23	2.02	0.59
1:D:80:ILE:CG1	1:D:84:LEU:HD22	2.27	0.59
1:D:121:MET:HE2	1:D:126:TYR:HB2	1.83	0.59
1:D:188:ILE:HD13	1:D:189:TRP:N	2.18	0.59
1:B:208:LEU:HD22	1:B:212:TYR:CE2	2.38	0.59
1:B:128:LYS:HE2	2:E:1:BGC:O1	2.02	0.59
1:D:26:ARG:HH11	1:D:26:ARG:CG	2.15	0.59
1:B:15:ILE:CD1	1:B:235:GLN:H	2.16	0.58
1:B:28:PHE:O	1:B:30:GLN:NE2	2.34	0.58
1:C:134:THR:HG22	1:C:189:TRP:HD1	1.68	0.58
1:C:115:ASN:OD1	1:C:205:ALA:HB2	2.03	0.58
1:C:142:THR:OG1	1:C:180:ASP:OD1	2.14	0.58
1:C:90:TYR:CE2	1:C:109:LEU:HD22	2.38	0.58
1:D:73:ARG:NH1	1:D:191:ASP:OD1	2.37	0.58
1:D:212:TYR:O	1:D:226:ILE:HB	2.04	0.58
1:C:214:TYR:CE2	1:C:220:LEU:HB2	2.38	0.57
1:A:215:PRO:HA	1:A:228:ILE:HB	1.87	0.57
1:B:215:PRO:HB2	1:B:218:TRP:CG	2.39	0.57
1:D:135:TYR:OH	1:D:152:TYR:O	2.21	0.57
1:B:53:ASN:C	1:B:54:LYS:HE2	2.29	0.56
1:A:68:ASP:HA	1:A:71:LEU:HB3	1.87	0.56
1:A:123:PRO:O	1:A:126:TYR:HD1	1.87	0.56
1:B:122:HIS:NE2	2:F:2:GAL:O4	2.31	0.56
1:D:66:TRP:CD1	1:D:67:PRO:N	2.73	0.56
1:A:138:ARG:O	1:A:144:TYR:HB2	2.05	0.56
1:C:160:GLY:HA2	1:C:166:TYR:CD2	2.41	0.56
1:D:66:TRP:CD1	1:D:67:PRO:HA	2.40	0.56
1:A:154:TYR:HE1	1:A:207:THR:HG23	1.70	0.56
1:B:233:LYS:HB2	1:B:234:PRO:HD2	1.87	0.56
1:C:134:THR:CG2	1:C:189:TRP:HD1	2.19	0.56
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.21	0.55
1:A:74:PHE:O	1:A:78:LEU:HG	2.07	0.55
1:D:67:PRO:O	1:D:70:THR:HG22	2.05	0.55
1:B:138:ARG:O	1:B:144:TYR:HB2	2.07	0.55
1:D:83:GLN:HG3	1:D:87:GLU:OE2	2.07	0.55
1:B:15:ILE:HD13	1:B:235:GLN:H	1.72	0.55
1:D:66:TRP:CD1	1:D:66:TRP:C	2.85	0.55
1:D:73:ARG:O	1:D:76:ILE:HB	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:PRO:HB2	1:B:218:TRP:CD2	2.41	0.55
1:C:101:THR:HG23	1:C:225:ILE:O	2.07	0.55
1:A:134:THR:CG2	1:A:189:TRP:NE1	2.69	0.55
1:B:48:TYR:CD1	1:B:49:ASP:HB2	2.42	0.55
1:A:83:GLN:O	1:A:87:GLU:HG3	2.06	0.54
1:B:114:SER:HB2	1:B:116:GLY:H	1.72	0.54
1:A:213:LEU:O	1:A:215:PRO:HD3	2.07	0.54
1:B:126:TYR:CE1	1:B:127:ASN:HB3	2.41	0.54
1:D:6:LEU:HD13	1:D:77:PHE:CD1	2.42	0.54
1:D:139:ASP:OD1	1:D:139:ASP:N	2.36	0.54
1:A:222:PHE:HA	1:D:216:GLU:HG3	1.89	0.54
1:B:59:ILE:HG21	1:B:80:ILE:HG21	1.90	0.54
1:A:122:HIS:NE2	2:E:2:GAL:O4	2.33	0.54
1:C:25:GLU:OE1	1:C:25:GLU:HA	2.06	0.54
1:C:51:GLU:OE1	1:C:51:GLU:N	2.34	0.54
1:A:231:LYS:HD3	1:A:231:LYS:N	2.21	0.54
1:C:233:LYS:HE3	1:C:233:LYS:HA	1.90	0.54
1:C:129:PRO:HG2	1:C:132:GLU:HG2	1.88	0.54
1:C:2:ARG:NH1	1:C:88:THR:HA	2.23	0.54
1:C:134:THR:O	1:C:134:THR:CG2	2.55	0.54
1:B:197:LYS:O	1:B:200:LEU:HB3	2.07	0.53
1:B:212:TYR:O	1:B:226:ILE:HB	2.08	0.53
1:C:2:ARG:NH1	1:C:2:ARG:C	2.66	0.53
1:B:135:TYR:CD1	1:B:145:ILE:HD12	2.44	0.53
1:C:142:THR:HG21	1:C:176:TRP:CD1	2.43	0.53
1:D:15:ILE:HD12	1:D:236:TYR:HA	1.91	0.53
1:C:67:PRO:HB2	1:C:190:HIS:CD2	2.44	0.53
1:D:169:LEU:HD23	1:D:173:ILE:HG13	1.90	0.52
1:A:130:ASN:HB2	1:A:133:PHE:CD2	2.44	0.52
1:A:145:ILE:HG22	1:A:149:GLU:HB3	1.91	0.52
1:B:135:TYR:CG	1:B:145:ILE:HD12	2.44	0.52
1:D:70:THR:HG23	1:D:71:LEU:N	2.24	0.52
1:C:136:GLU:OE1	1:C:137:ARG:N	2.42	0.52
1:A:80:ILE:CG1	1:A:84:LEU:HD22	2.37	0.51
1:A:139:ASP:HA	1:A:144:TYR:CG	2.45	0.51
1:B:156:GLY:N	1:B:192:GLU:HG3	2.25	0.51
1:C:26:ARG:HG2	1:C:27:TYR:CE2	2.45	0.51
1:C:80:ILE:HG13	1:C:84:LEU:CD1	2.40	0.51
1:B:173:ILE:O	1:B:177:VAL:HG23	2.11	0.51
1:D:61:GLN:HG3	1:D:62:LYS:O	2.11	0.51
1:C:78:LEU:HD22	1:C:81:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:GLU:HG2	1:D:141:SER:OG	2.11	0.51
1:B:206:ILE:CG2	1:B:207:THR:N	2.74	0.51
1:C:156:GLY:N	1:C:192:GLU:HG3	2.26	0.51
1:D:66:TRP:CD1	1:D:67:PRO:CA	2.94	0.51
1:D:166:TYR:O	1:D:169:LEU:HB3	2.11	0.51
1:A:115:ASN:OD1	1:A:205:ALA:HB2	2.11	0.50
1:C:130:ASN:HB2	1:C:133:PHE:CE2	2.46	0.50
1:D:113:ASP:OD1	1:D:113:ASP:N	2.42	0.50
1:D:163:THR:HG22	1:D:167:LEU:HD12	1.92	0.50
1:B:211:ALA:HB2	1:B:222:PHE:HB3	1.94	0.50
1:C:75:HIS:HE1	1:C:177:VAL:HG11	1.77	0.50
1:B:104:ILE:HG21	1:B:108:ILE:HD13	1.92	0.50
1:C:51:GLU:H	1:C:51:GLU:CD	2.19	0.50
1:D:106:LYS:O	1:D:109:LEU:HD12	2.12	0.50
1:A:202:ASN:O	1:A:203:PRO:C	2.53	0.50
1:B:158:LEU:HD23	1:B:158:LEU:C	2.35	0.50
1:C:83:GLN:O	1:C:87:GLU:HG3	2.12	0.50
1:A:61:GLN:OE1	1:A:64:LEU:HD11	2.10	0.50
1:D:213:LEU:O	1:D:215:PRO:HD3	2.12	0.50
1:D:95:ASN:CB	1:D:98:LEU:HD13	2.41	0.50
1:B:134:THR:HG21	1:B:189:TRP:NE1	2.23	0.50
1:A:145:ILE:CG2	1:A:149:GLU:HB3	2.42	0.49
1:B:105:GLY:H	1:B:107:GLU:CD	2.20	0.49
1:C:57:HIS:N	1:C:57:HIS:CD2	2.80	0.49
2:G:1:BGC:O3	2:G:2:GAL:O6	2.27	0.49
1:B:104:ILE:CG2	1:B:108:ILE:HD13	2.42	0.49
1:D:72:LYS:O	1:D:73:ARG:C	2.55	0.49
1:C:70:THR:O	1:C:73:ARG:HG3	2.12	0.49
1:D:91:LEU:O	1:D:160:GLY:HA2	2.13	0.49
1:A:80:ILE:HG13	1:A:84:LEU:CD2	2.40	0.49
1:B:128:LYS:NZ	2:E:1:BGC:C1	2.75	0.49
1:C:158:LEU:HB2	1:C:213:LEU:HD21	1.95	0.49
1:A:136:GLU:OE1	1:A:137:ARG:N	2.45	0.49
1:C:59:ILE:O	1:C:60:LYS:C	2.55	0.49
1:D:142:THR:HG21	1:D:176:TRP:CG	2.48	0.49
1:D:110:PRO:HB2	1:D:116:GLY:HA2	1.95	0.48
1:C:135:TYR:CG	1:C:145:ILE:HD12	2.49	0.48
1:D:66:TRP:HA	1:D:67:PRO:C	2.38	0.48
1:B:115:ASN:OD1	1:B:205:ALA:HB2	2.13	0.48
1:D:40:VAL:HG12	1:D:42:THR:HG22	1.95	0.48
1:A:163:THR:O	1:A:167:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LYS:HD2	1:C:75:HIS:ND1	2.29	0.48
1:C:178:ASP:O	1:C:182:THR:HG23	2.13	0.48
1:A:50:GLU:O	1:A:50:GLU:HG2	2.12	0.48
1:B:97:ASN:ND2	1:B:228:ILE:CG2	2.77	0.48
1:A:40:VAL:O	1:A:42:THR:HG22	2.14	0.48
1:B:29:MET:HE2	1:B:108:ILE:HD11	1.95	0.48
1:C:26:ARG:HG2	1:C:27:TYR:CD2	2.49	0.48
1:D:81:LYS:O	1:D:84:LEU:HB2	2.13	0.48
1:A:70:THR:OG1	1:A:191:ASP:OD2	2.31	0.48
1:C:164:LYS:HB3	1:C:164:LYS:HE2	1.68	0.48
1:A:169:LEU:C	1:A:169:LEU:HD23	2.39	0.48
1:C:215:PRO:HB2	1:C:218:TRP:CG	2.49	0.48
1:D:95:ASN:HB3	1:D:98:LEU:HD13	1.95	0.47
1:B:187:PRO:HG2	1:B:194:LEU:HD11	1.96	0.47
1:C:208:LEU:HB3	1:C:212:TYR:CD2	2.49	0.47
1:B:225:ILE:HG22	1:B:226:ILE:HG13	1.95	0.47
1:A:192:GLU:HA	1:A:195:ILE:HG22	1.97	0.47
1:D:12:LYS:O	1:D:15:ILE:CG1	2.62	0.47
1:A:173:ILE:O	1:A:177:VAL:HG23	2.15	0.47
1:D:156:GLY:N	1:D:192:GLU:HG3	2.30	0.47
1:B:72:LYS:HD3	1:B:75:HIS:ND1	2.30	0.47
1:B:159:SER:HB2	1:B:166:TYR:HE1	1.79	0.47
1:C:36:ILE:N	1:C:36:ILE:HD12	2.30	0.47
1:D:99:LEU:HD22	1:D:229:ARG:HD3	1.97	0.47
1:A:125:PHE:CE2	2:E:2:GAL:H61	2.46	0.47
1:B:141:SER:HB2	1:B:185:ILE:HG21	1.97	0.47
1:C:138:ARG:O	1:C:144:TYR:HB2	2.14	0.47
1:C:120:THR:HG23	1:C:208:LEU:HB2	1.97	0.46
1:D:173:ILE:O	1:D:177:VAL:HG23	2.15	0.46
1:C:52:ASN:OD1	1:C:52:ASN:N	2.47	0.46
1:D:114:SER:HB2	1:D:205:ALA:CB	2.46	0.46
1:D:234:PRO:HA	1:D:235:GLN:HA	1.42	0.46
1:B:7:TYR:CE1	1:B:96:ALA:HA	2.51	0.46
1:A:189:TRP:HB2	1:A:193:SER:OG	2.15	0.46
1:B:36:ILE:HD12	1:B:36:ILE:N	2.30	0.46
1:D:26:ARG:HB2	1:D:26:ARG:NH1	2.30	0.46
1:A:36:ILE:HG22	1:A:38:TYR:CE1	2.51	0.46
1:B:89:ASP:C	1:B:163:THR:OG1	2.59	0.46
1:D:17:TRP:O	1:D:18:LYS:C	2.58	0.46
1:D:39:TYR:N	1:D:39:TYR:CD1	2.83	0.46
1:C:31:ASP:OD2	1:C:33:SER:OG	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LYS:O	1:A:22:LEU:HG	2.16	0.45
1:B:72:LYS:CD	1:B:75:HIS:ND1	2.79	0.45
1:C:215:PRO:HB2	1:C:218:TRP:CD2	2.51	0.45
1:D:173:ILE:O	1:D:174:CYS:C	2.59	0.45
1:C:44:SER:HA	1:C:45:PRO:HD3	1.70	0.45
1:A:98:LEU:N	1:A:98:LEU:CD1	2.79	0.45
1:C:54:LYS:O	1:C:54:LYS:HG2	2.16	0.45
1:D:198:TYR:O	1:D:198:TYR:CD1	2.70	0.45
1:A:123:PRO:O	1:A:126:TYR:CD1	2.69	0.45
1:B:134:THR:HG22	1:B:134:THR:O	2.17	0.45
1:A:77:PHE:HZ	1:A:93:PHE:CD1	2.35	0.45
1:C:21:TYR:CE1	1:C:56:ILE:HD11	2.51	0.45
1:C:71:LEU:HD13	1:C:190:HIS:HB3	1.98	0.45
1:D:80:ILE:O	1:D:81:LYS:C	2.60	0.45
1:B:92:PHE:HD1	1:B:160:GLY:HA3	1.80	0.45
1:D:29:MET:HE2	1:D:108:ILE:HD11	1.99	0.45
1:D:36:ILE:N	1:D:36:ILE:HD12	2.32	0.45
1:D:66:TRP:CZ2	1:D:190:HIS:CE1	3.05	0.45
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.16	0.45
1:A:47:LEU:HB2	1:A:50:GLU:HB2	2.00	0.44
1:C:5:ILE:HD11	1:C:28:PHE:CE2	2.52	0.44
1:C:23:SER:HB2	1:C:100:PHE:HB2	1.99	0.44
1:C:176:TRP:HE3	1:C:194:LEU:HD22	1.82	0.44
1:D:74:PHE:HA	1:D:77:PHE:CD2	2.42	0.44
1:B:178:ASP:O	1:B:181:ALA:HB3	2.16	0.44
2:H:1:BGC:O6	2:H:3:FUC:H3	2.17	0.44
1:B:50:GLU:OE2	1:B:58:ARG:NH1	2.50	0.44
1:A:12:LYS:O	1:A:15:ILE:HG12	2.18	0.44
1:C:136:GLU:O	1:C:144:TYR:HA	2.18	0.44
1:D:154:TYR:OH	1:D:207:THR:OG1	2.21	0.44
1:B:32:GLN:H	1:B:32:GLN:HG2	1.66	0.44
1:B:75:HIS:HD2	1:B:174:CYS:SG	2.38	0.44
1:B:130:ASN:HA	1:B:133:PHE:CE2	2.52	0.44
1:B:189:TRP:HB2	1:B:193:SER:OG	2.17	0.44
1:C:2:ARG:HH22	1:C:88:THR:HG22	1.82	0.44
1:B:122:HIS:HA	1:B:155:ALA:HB2	1.99	0.44
1:B:128:LYS:CE	2:E:1:BGC:O1	2.64	0.44
1:B:113:ASP:OD1	1:B:113:ASP:N	2.50	0.44
1:D:189:TRP:NE1	2:H:2:GAL:H62	2.33	0.44
1:D:214:TYR:HE2	1:D:222:PHE:O	2.00	0.44
1:A:72:LYS:O	1:A:75:HIS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ARG:HG2	1:B:35:ILE:HD12	2.00	0.43
1:B:122:HIS:ND1	1:B:123:PRO:HD2	2.33	0.43
1:C:93:PHE:CD1	1:C:93:PHE:C	2.95	0.43
1:C:116:GLY:O	1:C:161:GLY:HA3	2.18	0.43
1:C:28:PHE:CE1	1:C:29:MET:HG2	2.54	0.43
1:A:45:PRO:O	1:A:58:ARG:CZ	2.67	0.43
1:B:77:PHE:HZ	1:B:93:PHE:CD2	2.36	0.43
1:B:206:ILE:HG22	1:B:207:THR:N	2.32	0.43
1:A:75:HIS:CD2	1:A:174:CYS:SG	3.11	0.43
1:C:139:ASP:HA	1:C:144:TYR:CG	2.53	0.43
1:D:73:ARG:HB3	1:D:77:PHE:CE2	2.47	0.43
1:A:72:LYS:HD2	1:A:75:HIS:CE1	2.54	0.43
1:A:98:LEU:N	1:A:98:LEU:HD12	2.32	0.43
1:D:17:TRP:CZ2	1:D:21:TYR:HB2	2.53	0.43
1:D:53:ASN:OD1	1:D:54:LYS:N	2.52	0.43
1:C:219:LEU:HA	1:C:219:LEU:HD23	1.81	0.43
1:D:125:PHE:HZ	2:H:2:GAL:HO6	1.63	0.43
1:A:189:TRP:HA	1:A:189:TRP:CE3	2.54	0.43
1:B:80:ILE:HG13	1:B:84:LEU:HD22	1.99	0.43
1:B:84:LEU:HD12	1:B:84:LEU:HA	1.89	0.43
1:B:229:ARG:CD	1:C:223:GLU:OE2	2.52	0.43
1:B:168:LYS:HD2	1:B:168:LYS:O	2.19	0.43
1:B:231:LYS:H	1:B:231:LYS:HG3	1.58	0.43
1:D:189:TRP:HA	1:D:189:TRP:CE3	2.53	0.43
1:A:167:LEU:O	1:A:170:CYS:N	2.51	0.43
1:A:188:ILE:H	1:A:188:ILE:HG12	1.54	0.43
1:A:10:THR:HG22	1:A:42:THR:HA	2.01	0.42
1:C:189:TRP:CD1	2:G:2:GAL:H62	2.54	0.42
1:D:128:LYS:HB3	1:D:129:PRO:CD	2.49	0.42
1:B:111:PRO:HB2	1:B:114:SER:OG	2.19	0.42
1:B:189:TRP:CZ2	2:F:2:GAL:H5	2.54	0.42
1:A:29:MET:HE2	1:A:108:ILE:CD1	2.47	0.42
1:A:230:ASP:C	1:A:230:ASP:OD1	2.63	0.42
1:C:82:GLU:H	1:C:82:GLU:HG2	1.63	0.42
1:D:44:SER:HA	1:D:45:PRO:HD3	1.74	0.42
1:C:130:ASN:HB2	1:C:133:PHE:CD2	2.54	0.42
1:A:61:GLN:NE2	1:A:76:ILE:HG23	2.35	0.42
1:B:214:TYR:CE1	1:C:221:PRO:HB3	2.54	0.42
1:A:225:ILE:N	1:A:225:ILE:HD13	2.33	0.42
1:B:93:PHE:CD1	1:B:93:PHE:C	2.97	0.42
1:A:110:PRO:HB3	1:A:116:GLY:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:NH1	1:A:147:GLU:HA	2.34	0.42
1:C:125:PHE:CD1	1:C:125:PHE:N	2.87	0.42
1:D:26:ARG:CG	1:D:26:ARG:NH1	2.80	0.42
1:D:128:LYS:CB	1:D:129:PRO:CD	2.98	0.42
1:A:110:PRO:HB3	1:A:116:GLY:HA3	2.02	0.42
1:A:158:LEU:C	1:A:158:LEU:HD23	2.44	0.42
1:D:127:ASN:OD1	1:D:127:ASN:N	2.51	0.42
1:A:174:CYS:O	1:A:177:VAL:HB	2.20	0.42
1:B:9:CYS:HB2	1:B:14:ASP:HB3	2.01	0.42
1:B:12:LYS:O	1:B:15:ILE:HG13	2.19	0.42
1:B:139:ASP:OD1	1:B:139:ASP:N	2.52	0.42
1:A:130:ASN:HB2	1:A:133:PHE:CE2	2.55	0.41
1:C:110:PRO:HA	1:C:111:PRO:HD3	1.97	0.41
1:D:60:LYS:O	1:D:79:ARG:NH2	2.54	0.41
1:B:166:TYR:O	1:B:169:LEU:HB3	2.20	0.41
1:A:231:LYS:H	1:A:231:LYS:CD	2.26	0.41
1:B:29:MET:CB	1:B:36:ILE:HD11	2.45	0.41
1:C:5:ILE:HD11	1:C:28:PHE:CD2	2.55	0.41
1:C:26:ARG:HG2	1:C:27:TYR:CZ	2.56	0.41
1:C:118:LEU:HD23	1:C:118:LEU:C	2.46	0.41
1:D:110:PRO:CB	1:D:116:GLY:HA2	2.50	0.41
1:C:95:ASN:N	1:C:98:LEU:HD22	2.36	0.41
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.85	0.41
1:A:75:HIS:HD2	1:A:174:CYS:SG	2.43	0.41
1:C:233:LYS:HA	1:C:233:LYS:CE	2.46	0.41
1:A:2:ARG:NH1	1:A:86:ARG:O	2.53	0.41
1:B:233:LYS:HB2	1:B:234:PRO:CD	2.50	0.41
1:C:72:LYS:HD2	1:C:75:HIS:CE1	2.56	0.41
1:D:46:LYS:HE2	1:D:46:LYS:HB3	1.82	0.41
1:A:3:ILE:HB	1:A:36:ILE:HG13	2.02	0.41
1:B:144:TYR:CE2	1:B:146:PRO:HG3	2.56	0.41
1:C:66:TRP:CG	1:C:67:PRO:HA	2.56	0.41
1:D:76:ILE:C	1:D:78:LEU:N	2.75	0.41
1:A:215:PRO:HB2	1:A:218:TRP:CG	2.56	0.41
1:B:44:SER:OG	1:B:45:PRO:HD2	2.21	0.41
1:B:105:GLY:C	1:B:107:GLU:H	2.28	0.41
1:B:210:PRO:C	1:B:212:TYR:N	2.77	0.41
1:B:223:GLU:HB2	1:B:225:ILE:CD1	2.51	0.41
1:C:37:GLU:OE1	1:C:57:HIS:NE2	2.50	0.41
1:D:16:PHE:HB3	1:D:96:ALA:O	2.21	0.41
1:D:220:LEU:HD23	1:D:222:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:O	1:A:228:ILE:CD1	2.69	0.41
1:C:53:ASN:OD1	1:C:55:HIS:HB2	2.21	0.41
1:C:154:TYR:O	1:C:196:ASN:ND2	2.54	0.41
1:D:120:THR:HG23	1:D:208:LEU:HB2	2.03	0.41
1:A:74:PHE:CE1	1:A:173:ILE:HG21	2.56	0.40
1:A:192:GLU:O	1:A:195:ILE:HG22	2.21	0.40
1:B:135:TYR:O	1:B:137:ARG:HG2	2.21	0.40
1:C:156:GLY:H	1:C:192:GLU:HG3	1.87	0.40
1:D:66:TRP:CG	1:D:67:PRO:CA	3.00	0.40
1:A:110:PRO:CB	1:A:116:GLY:HA3	2.51	0.40
1:D:22:LEU:HD12	1:D:22:LEU:HA	1.92	0.40
1:D:31:ASP:HB2	1:D:34:PHE:HD2	1.85	0.40
1:D:84:LEU:HG	1:D:91:LEU:HD11	2.03	0.40
1:D:91:LEU:O	1:D:160:GLY:CA	2.69	0.40
1:D:199:PHE:HD1	1:D:199:PHE:HA	1.75	0.40
1:B:57:HIS:CD2	1:B:57:HIS:N	2.89	0.40
1:B:136:GLU:HG2	1:B:141:SER:HB3	2.04	0.40
1:D:70:THR:CG2	1:D:71:LEU:N	2.84	0.40
1:D:123:PRO:CA	1:D:210:PRO:HB3	2.51	0.40
1:A:74:PHE:HD2	1:A:170:CYS:SG	2.45	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:12:LYS:NZ	1:D:200:LEU:O[2_645]	2.18	0.02

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	229/246 (93%)	225 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/246 (95%)	221 (95%)	11 (5%)	1 (0%)	30	65
1	C	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
1	D	234/246 (95%)	223 (95%)	11 (5%)	0	100	100
All	All	927/984 (94%)	888 (96%)	38 (4%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	PRO

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	208/221 (94%)	185 (89%)	23 (11%)	6	25
1	B	212/221 (96%)	186 (88%)	26 (12%)	4	21
1	C	210/221 (95%)	184 (88%)	26 (12%)	4	20
1	D	213/221 (96%)	183 (86%)	30 (14%)	3	16
All	All	843/884 (95%)	738 (88%)	105 (12%)	4	20

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	15	ILE
1	A	42	THR
1	A	51	GLU
1	A	52	ASN
1	A	54	LYS
1	A	59	ILE
1	A	84	LEU
1	A	102	SER
1	A	113	ASP

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	130	ASN
1	A	132	GLU
1	A	142	THR
1	A	149	GLU
1	A	151	ARG
1	A	159	SER
1	A	169	LEU
1	A	174	CYS
1	A	179	ARG
1	A	188	ILE
1	A	227	LEU
1	A	231	LYS
1	B	9	CYS
1	B	15	ILE
1	B	31	ASP
1	B	33	SER
1	B	62	LYS
1	B	70	THR
1	B	82	GLU
1	B	84	LEU
1	B	86	ARG
1	B	98	LEU
1	B	99	LEU
1	B	112	SER
1	B	113	ASP
1	B	114	SER
1	B	130	ASN
1	B	142	THR
1	B	149	GLU
1	B	151	ARG
1	B	159	SER
1	B	173	ILE
1	B	180	ASP
1	B	188	ILE
1	B	194	LEU
1	B	219	LEU
1	B	220	LEU
1	B	223	GLU
1	C	2	ARG
1	C	9	CYS
1	C	25	GLU

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Mol	Chain	Res	Type
1	C	32	GLN
1	C	52	ASN
1	C	57	HIS
1	C	64	LEU
1	C	82	GLU
1	C	85	GLU
1	C	98	LEU
1	C	101	THR
1	C	108	ILE
1	C	112	SER
1	C	113	ASP
1	C	130	ASN
1	C	139	ASP
1	C	142	THR
1	C	147	GLU
1	C	151	ARG
1	C	175	SER
1	C	188	ILE
1	C	196	ASN
1	C	206	ILE
1	C	220	LEU
1	C	227	LEU
1	C	231	LYS
1	D	3	ILE
1	D	15	ILE
1	D	19	ASP
1	D	22	LEU
1	D	26	ARG
1	D	29	MET
1	D	42	THR
1	D	49	ASP
1	D	54	LYS
1	D	84	LEU
1	D	85	GLU
1	D	95	ASN
1	D	112	SER
1	D	113	ASP
1	D	126	TYR
1	D	127	ASN
1	D	139	ASP
1	D	142	THR
1	D	159	SER

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Mol	Chain	Res	Type
1	D	171	THR
1	D	173	ILE
1	D	180	ASP
1	D	188	ILE
1	D	199	PHE
1	D	206	ILE
1	D	220	LEU
1	D	222	PHE
1	D	227	LEU
1	D	231	LYS
1	D	236	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	63	ASN
1	A	75	HIS
1	B	75	HIS
1	B	130	ASN
1	B	184	HIS
1	C	75	HIS
1	C	196	ASN
1	D	61	GLN
1	D	75	HIS
1	D	95	ASN
1	D	130	ASN
1	D	190	HIS
1	D	202	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 ⓘ

12 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	BGC	E	1	2	12,12,12	1.29	2 (16%)	17,17,17	1.39	3 (17%)
2	GAL	E	2	2	11,11,12	1.82	1 (9%)	15,15,17	1.46	4 (26%)
2	FUC	E	3	2	10,10,11	2.39	4 (40%)	14,14,16	2.01	3 (21%)
2	BGC	F	1	2	12,12,12	1.22	2 (16%)	17,17,17	1.49	3 (17%)
2	GAL	F	2	2	11,11,12	1.78	1 (9%)	15,15,17	1.62	2 (13%)
2	FUC	F	3	2	10,10,11	2.57	5 (50%)	14,14,16	2.10	2 (14%)
2	BGC	G	1	2	12,12,12	1.04	2 (16%)	17,17,17	1.91	5 (29%)
2	GAL	G	2	2	11,11,12	1.75	1 (9%)	15,15,17	1.68	5 (33%)
2	FUC	G	3	2	10,10,11	2.40	5 (50%)	14,14,16	2.26	3 (21%)
2	BGC	H	1	2	12,12,12	1.43	2 (16%)	17,17,17	0.92	0
2	GAL	H	2	2	11,11,12	2.15	1 (9%)	15,15,17	1.81	3 (20%)
2	FUC	H	3	2	10,10,11	2.72	5 (50%)	14,14,16	2.08	2 (14%)

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	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	2/2/19/22	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	H	1	2	-	2/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	FUC	H	3	2	-	-	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GAL	C2-C3	6.47	1.62	1.52
2	E	2	GAL	C2-C3	5.53	1.61	1.52
2	H	3	FUC	O5-C5	5.28	1.54	1.43
2	G	2	GAL	C2-C3	5.18	1.60	1.52
2	E	3	FUC	O5-C5	5.13	1.53	1.43
2	F	2	GAL	C2-C3	5.02	1.60	1.52
2	F	3	FUC	O5-C5	4.98	1.53	1.43
2	G	3	FUC	O5-C5	4.93	1.53	1.43
2	H	3	FUC	C2-C3	3.91	1.58	1.52
2	F	3	FUC	C2-C3	3.59	1.58	1.52
2	E	1	BGC	O4-C4	3.23	1.51	1.43
2	H	1	BGC	O4-C4	3.14	1.50	1.43
2	F	3	FUC	O5-C1	3.09	1.48	1.43
2	H	3	FUC	C6-C5	3.01	1.58	1.51
2	H	3	FUC	O5-C1	2.99	1.48	1.43
2	G	3	FUC	O5-C1	2.87	1.48	1.43
2	G	3	FUC	C6-C5	2.83	1.58	1.51
2	G	3	FUC	C2-C3	2.79	1.56	1.52
2	E	3	FUC	O5-C1	2.77	1.48	1.43
2	F	3	FUC	C6-C5	2.74	1.58	1.51
2	E	3	FUC	C2-C3	2.71	1.56	1.52
2	H	1	BGC	O5-C1	2.70	1.49	1.42
2	E	3	FUC	C6-C5	2.64	1.57	1.51
2	F	3	FUC	C4-C3	2.62	1.59	1.52
2	H	3	FUC	C4-C3	2.52	1.58	1.52
2	F	1	BGC	O4-C4	2.41	1.48	1.43
2	F	1	BGC	O5-C1	2.39	1.48	1.42
2	G	3	FUC	C4-C3	2.32	1.58	1.52
2	G	1	BGC	O5-C1	2.23	1.48	1.42
2	G	1	BGC	O4-C4	2.11	1.48	1.43
2	E	1	BGC	O5-C1	2.06	1.47	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	FUC	C1-C2-C3	6.45	119.03	109.64
2	H	3	FUC	C1-C2-C3	6.17	118.62	109.64
2	F	3	FUC	C1-C2-C3	5.78	118.07	109.64
2	H	2	GAL	C1-C2-C3	-5.64	101.43	109.64
2	E	3	FUC	C1-C2-C3	5.42	117.53	109.64
2	G	1	BGC	C1-C2-C3	-4.84	100.49	110.36
2	F	2	GAL	C1-C2-C3	-4.01	103.80	109.64
2	F	1	BGC	C3-C4-C5	3.92	117.35	110.23
2	F	3	FUC	O2-C2-C3	3.88	118.19	110.15
2	H	3	FUC	O2-C2-C3	3.61	117.62	110.15
2	G	1	BGC	O5-C1-C2	-3.49	104.16	110.30
2	E	2	GAL	C1-C2-C3	-3.42	104.67	109.64
2	E	1	BGC	C1-C2-C3	-3.38	103.46	110.36
2	E	3	FUC	O2-C2-C3	3.35	117.08	110.15
2	G	3	FUC	O2-C2-C3	3.30	116.99	110.15
2	G	1	BGC	O2-C2-C1	3.05	116.28	109.25
2	E	1	BGC	O5-C1-C2	-2.81	105.36	110.30
2	G	2	GAL	C2-C3-C4	-2.65	106.20	110.86
2	G	2	GAL	C1-C2-C3	-2.63	105.82	109.64
2	G	2	GAL	C3-C4-C5	-2.55	105.60	110.23
2	E	2	GAL	C3-C4-C5	-2.39	105.90	110.23
2	G	1	BGC	C4-C3-C2	-2.36	106.69	110.83
2	G	2	GAL	O2-C2-C1	-2.34	103.87	109.22
2	H	2	GAL	O2-C2-C1	-2.33	103.88	109.22
2	F	1	BGC	O2-C2-C1	2.27	114.50	109.25
2	G	1	BGC	O4-C4-C5	-2.23	103.83	109.32
2	E	3	FUC	O2-C2-C1	2.19	114.24	109.22
2	E	2	GAL	O6-C6-C5	-2.19	103.88	111.33
2	G	3	FUC	O3-C3-C2	-2.18	105.60	110.05
2	G	2	GAL	O5-C5-C4	-2.05	105.85	110.83
2	F	2	GAL	O3-C3-C2	-2.04	105.89	110.05
2	F	1	BGC	O4-C4-C5	-2.01	104.36	109.32
2	E	2	GAL	C1-O5-C5	2.01	114.88	112.19
2	E	1	BGC	C3-C4-C5	2.01	113.88	110.23
2	H	2	GAL	O2-C2-C3	2.00	114.30	110.15

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	BGC	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	1	BGC	O5-C5-C6-O6
2	E	2	GAL	C4-C5-C6-O6
2	H	1	BGC	C4-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6

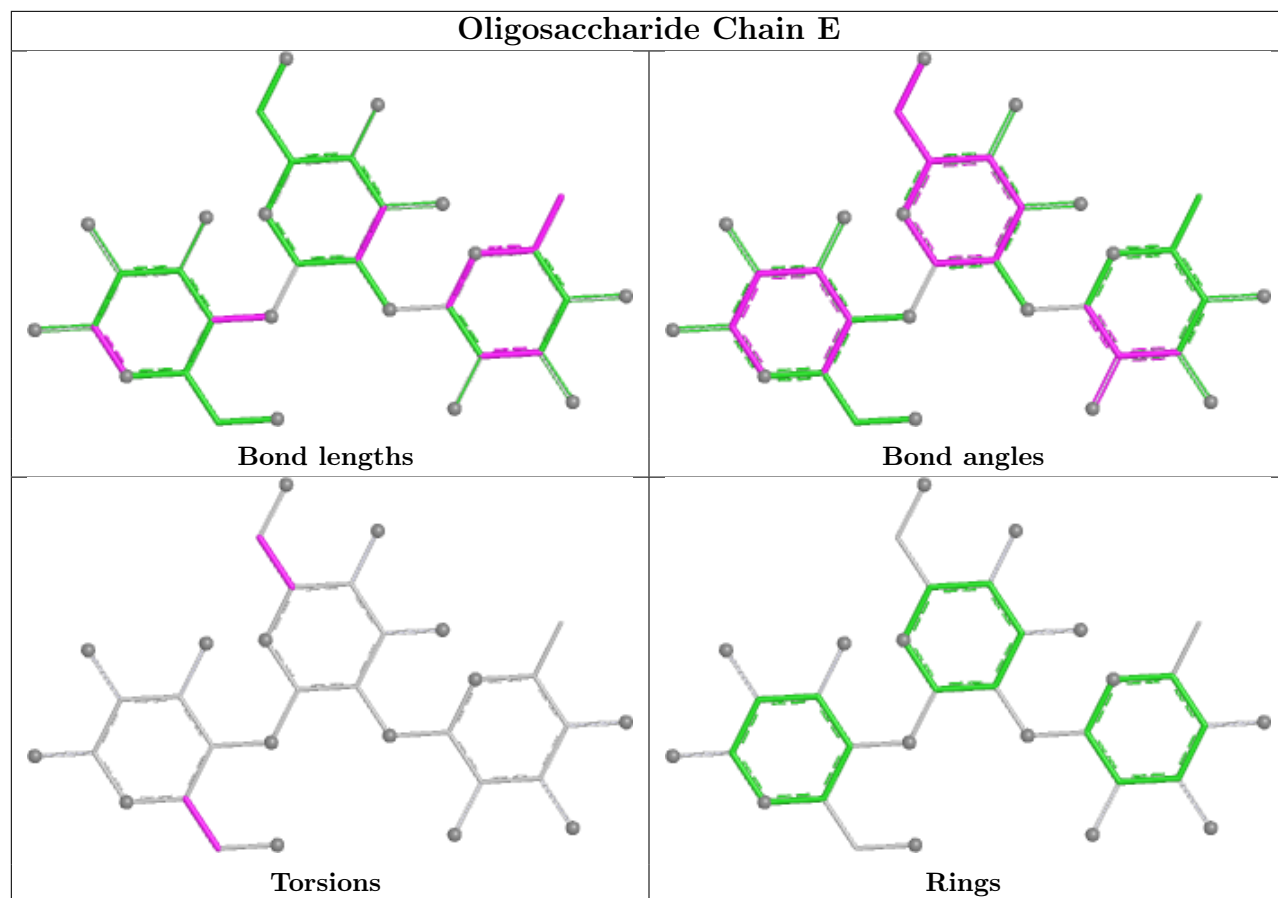
There are no ring outliers.

8 monomers are involved in 19 short contacts:

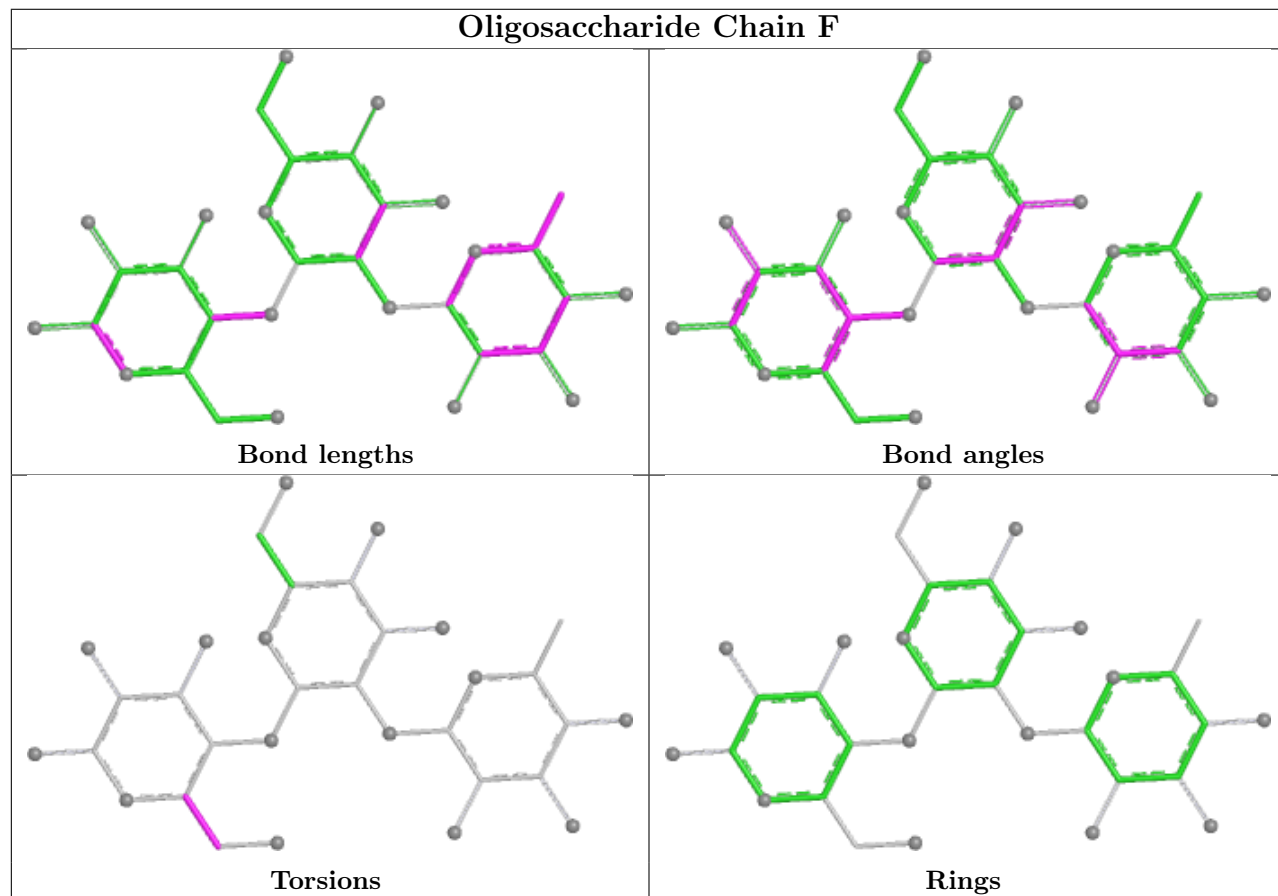
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	FUC	1	0
2	E	1	BGC	4	0
2	H	2	GAL	2	0
2	F	2	GAL	2	0
2	G	2	GAL	3	0
2	H	1	BGC	1	0
2	G	1	BGC	5	0
2	E	2	GAL	4	0

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

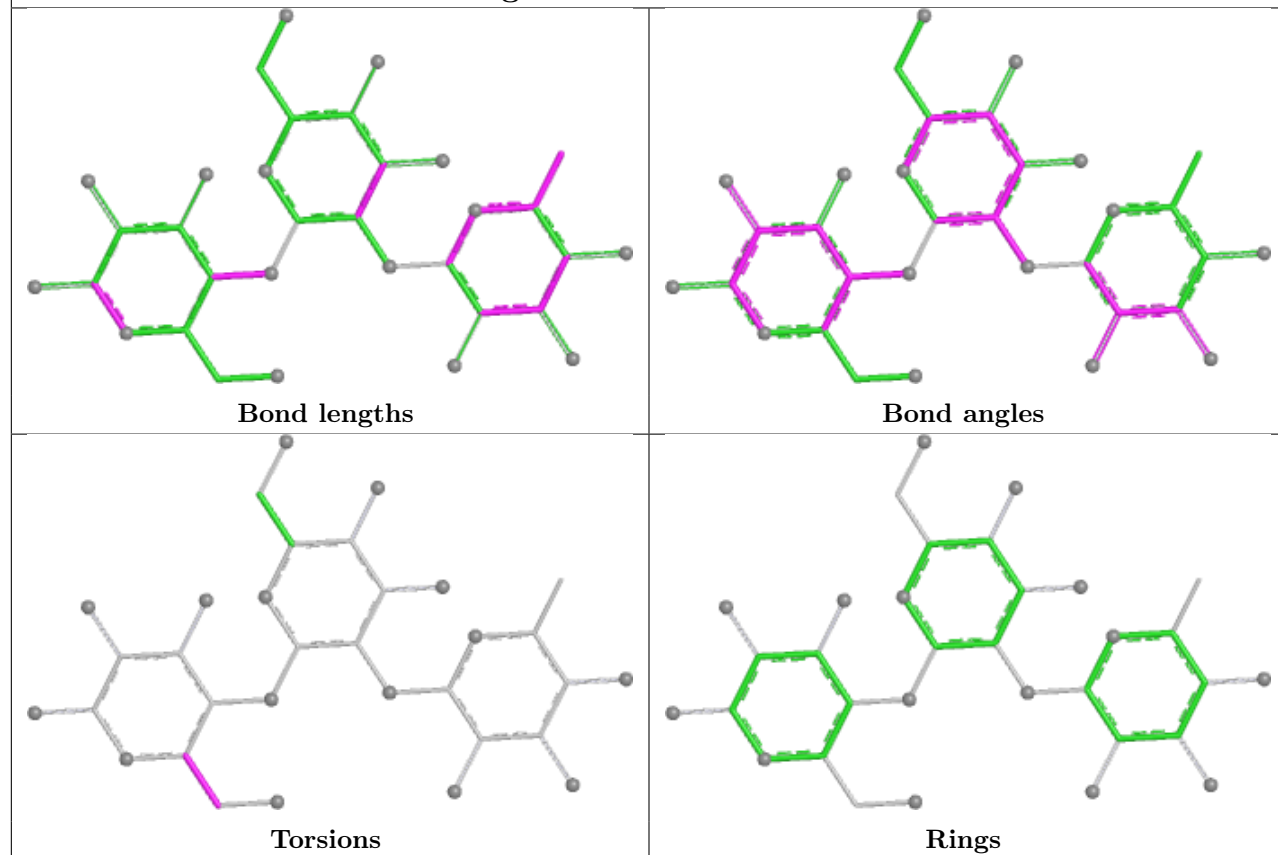
Oligosaccharide Chain E



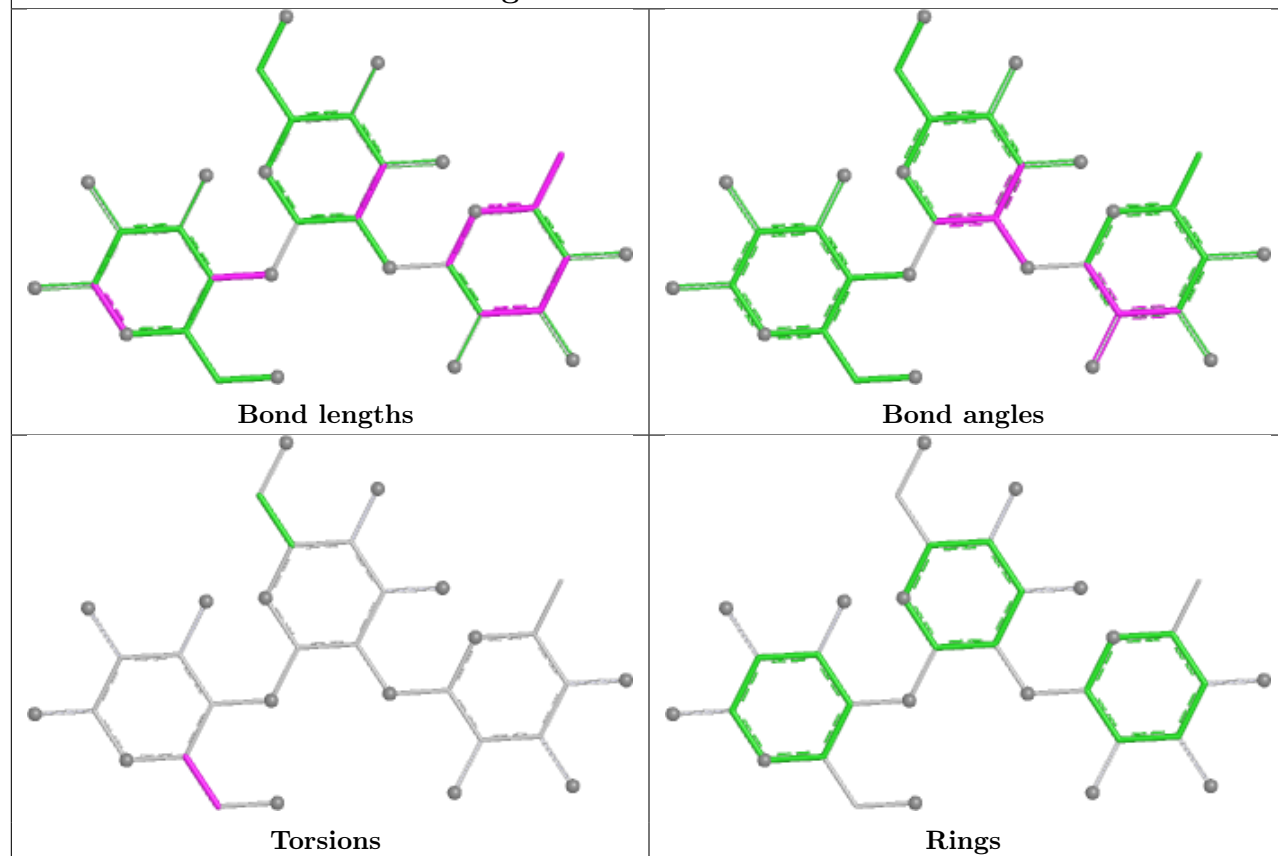
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/246 (93%)	3.78	216 (93%) 0 0	16, 28, 50, 67	1 (0%)
1	B	235/246 (95%)	4.00	222 (94%) 0 0	17, 34, 60, 74	0
1	C	233/246 (94%)	4.08	225 (96%) 0 0	18, 41, 63, 96	1 (0%)
1	D	236/246 (95%)	3.96	219 (92%) 0 0	20, 37, 60, 83	0
All	All	935/984 (95%)	3.95	882 (94%) 0 0	16, 34, 60, 96	2 (0%)

All (882) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	PRO	12.5
1	D	97	ASN	12.2
1	A	11	GLY	11.8
1	B	210	PRO	11.0
1	C	115	ASN	10.3
1	B	120	THR	9.8
1	A	124	GLY	9.3
1	C	10	THR	9.2
1	D	206	ILE	9.2
1	C	223	GLU	9.1
1	D	78	LEU	9.0
1	D	177	VAL	9.0
1	C	193	SER	8.9
1	D	102	SER	8.8
1	D	148	GLY	8.8
1	C	8	ILE	8.6
1	B	95	ASN	8.6
1	A	75	HIS	8.3
1	C	131	SER	8.3
1	C	71	LEU	8.3
1	D	124	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	PHE	8.1
1	D	186	ILE	8.1
1	A	216	GLU	7.9
1	D	40	VAL	7.8
1	B	142	THR	7.7
1	C	157	GLY	7.5
1	D	208	LEU	7.5
1	B	166	TYR	7.5
1	D	101	THR	7.5
1	D	209	SER	7.4
1	B	3	ILE	7.4
1	D	214	TYR	7.3
1	A	125	PHE	7.3
1	D	31	ASP	7.0
1	B	195	ILE	7.0
1	C	48	TYR	7.0
1	B	60	LYS	6.9
1	C	155	ALA	6.9
1	A	185	ILE	6.9
1	D	182	THR	6.8
1	A	98	LEU	6.8
1	A	166	TYR	6.8
1	B	41	PHE	6.7
1	A	84	LEU	6.7
1	D	111	PRO	6.7
1	B	37	GLU	6.7
1	C	117	LEU	6.6
1	A	195	ILE	6.6
1	B	141	SER	6.6
1	C	146	PRO	6.6
1	A	3	ILE	6.6
1	C	138	ARG	6.6
1	B	58	ARG	6.5
1	B	172	THR	6.5
1	A	155	ALA	6.5
1	C	47	LEU	6.5
1	B	194	LEU	6.4
1	D	13	TYR	6.4
1	A	77	PHE	6.4
1	C	91	LEU	6.4
1	B	100	PHE	6.4
1	A	163	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	138	ARG	6.3
1	A	156	GLY	6.3
1	D	3	ILE	6.3
1	C	156	GLY	6.3
1	D	225	ILE	6.3
1	B	153	TYR	6.3
1	B	104	ILE	6.2
1	C	80	ILE	6.1
1	C	219	LEU	6.1
1	B	145	ILE	6.1
1	C	116	GLY	6.1
1	B	213	LEU	6.1
1	C	64	LEU	6.1
1	A	57	HIS	6.1
1	A	63	ASN	6.1
1	C	230	ASP	6.0
1	D	115	ASN	6.0
1	C	13	TYR	6.0
1	C	184	HIS	6.0
1	B	215	PRO	6.0
1	A	50	GLU	6.0
1	D	166	TYR	6.0
1	B	71	LEU	5.9
1	C	134	THR	5.9
1	A	204	PRO	5.9
1	B	77	PHE	5.9
1	A	108	ILE	5.9
1	B	59	ILE	5.9
1	D	90	TYR	5.9
1	D	117	LEU	5.9
1	A	229	ARG	5.9
1	B	155	ALA	5.9
1	C	185	ILE	5.8
1	A	134	THR	5.8
1	A	103	PRO	5.8
1	B	17	TRP	5.8
1	B	176	TRP	5.8
1	D	217	GLY	5.8
1	A	223	GLU	5.8
1	A	152	TYR	5.7
1	B	36	ILE	5.7
1	C	210	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	135	TYR	5.7
1	B	8	ILE	5.7
1	C	190	HIS	5.7
1	B	91	LEU	5.7
1	B	123	PRO	5.7
1	C	208	LEU	5.7
1	B	25	GLU	5.7
1	B	82	GLU	5.7
1	D	108	ILE	5.7
1	C	74	PHE	5.6
1	A	32	GLN	5.6
1	C	32	GLN	5.6
1	D	36	ILE	5.6
1	D	14	ASP	5.6
1	B	219	LEU	5.6
1	D	207	THR	5.6
1	C	16	PHE	5.6
1	D	123	PRO	5.6
1	A	35	ILE	5.6
1	D	235	GLN	5.5
1	C	100	PHE	5.5
1	D	136	GLU	5.5
1	B	26	ARG	5.5
1	A	123	PRO	5.5
1	B	70	THR	5.5
1	B	89	ASP	5.5
1	B	171	THR	5.5
1	D	134	THR	5.5
1	D	218	TRP	5.5
1	D	83	GLN	5.5
1	C	24	ALA	5.5
1	B	108	ILE	5.5
1	C	149	GLU	5.5
1	A	80	ILE	5.5
1	C	195	ILE	5.5
1	C	183	ASN	5.4
1	B	66	TRP	5.4
1	B	45	PRO	5.4
1	A	205	ALA	5.4
1	C	39	TYR	5.4
1	C	46	LYS	5.4
1	D	118	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	157	GLY	5.4
1	B	112	SER	5.3
1	C	120	THR	5.3
1	D	223	GLU	5.3
1	B	9	CYS	5.3
1	C	126	TYR	5.3
1	B	57	HIS	5.3
1	C	222	PHE	5.3
1	A	202	ASN	5.3
1	D	110	PRO	5.3
1	C	99	LEU	5.3
1	B	23	SER	5.3
1	D	80	ILE	5.3
1	C	63	ASN	5.3
1	D	35	ILE	5.3
1	C	6	LEU	5.3
1	C	109	LEU	5.3
1	D	147	GLU	5.3
1	A	49	ASP	5.3
1	C	122	HIS	5.3
1	D	60	LYS	5.2
1	C	35	ILE	5.2
1	A	120	THR	5.2
1	A	228	ILE	5.2
1	B	22	LEU	5.2
1	D	99	LEU	5.2
1	B	97	ASN	5.2
1	A	168	LYS	5.2
1	D	224	PRO	5.2
1	C	61	GLN	5.2
1	D	135	TYR	5.1
1	A	1	MET	5.1
1	A	230	ASP	5.1
1	D	34	PHE	5.1
1	A	19	ASP	5.1
1	B	169	LEU	5.1
1	A	16	PHE	5.1
1	C	221	PRO	5.1
1	B	233	LYS	5.1
1	D	165	ALA	5.1
1	A	136	GLU	5.1
1	B	116	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	233	LYS	5.1
1	B	226	ILE	5.1
1	C	66	TRP	5.1
1	C	82	GLU	5.1
1	C	175	SER	5.1
1	B	98	LEU	5.1
1	B	12	LYS	5.0
1	D	154	TYR	5.0
1	D	109	LEU	5.0
1	B	235	GLN	5.0
1	C	29	MET	5.0
1	A	27	TYR	5.0
1	C	224	PRO	5.0
1	D	162	CYS	5.0
1	B	178	ASP	5.0
1	B	135	TYR	5.0
1	C	104	ILE	5.0
1	D	41	PHE	5.0
1	B	32	GLN	5.0
1	D	8	ILE	4.9
1	A	200	LEU	4.9
1	B	154	TYR	4.9
1	C	12	LYS	4.9
1	C	191	ASP	4.9
1	B	173	ILE	4.9
1	C	189	TRP	4.9
1	C	79	ARG	4.9
1	B	229	ARG	4.9
1	B	48	TYR	4.9
1	B	220	LEU	4.9
1	A	171	THR	4.8
1	D	130	ASN	4.8
1	C	166	TYR	4.8
1	A	151	ARG	4.8
1	B	147	GLU	4.8
1	B	232	ASN	4.8
1	B	164	LYS	4.8
1	D	137	ARG	4.8
1	D	156	GLY	4.8
1	A	221	PRO	4.8
1	B	103	PRO	4.8
1	C	128	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	32	GLN	4.8
1	C	55	HIS	4.7
1	B	174	CYS	4.7
1	B	177	VAL	4.7
1	B	75	HIS	4.7
1	C	108	ILE	4.7
1	B	38	TYR	4.7
1	B	119	GLY	4.7
1	B	99	LEU	4.7
1	D	77	PHE	4.7
1	D	158	LEU	4.7
1	C	42	THR	4.7
1	B	68	ASP	4.7
1	B	209	SER	4.7
1	C	188	ILE	4.7
1	A	71	LEU	4.7
1	A	109	LEU	4.7
1	A	7	TYR	4.7
1	C	158	LEU	4.7
1	D	94	PHE	4.7
1	C	111	PRO	4.6
1	A	189	TRP	4.6
1	B	163	THR	4.6
1	B	78	LEU	4.6
1	D	112	SER	4.6
1	B	224	PRO	4.6
1	D	190	HIS	4.6
1	A	34	PHE	4.6
1	A	212	TYR	4.6
1	C	133	PHE	4.6
1	A	102	SER	4.6
1	C	18	LYS	4.6
1	C	186	ILE	4.6
1	A	17	TRP	4.6
1	A	126	TYR	4.6
1	B	126	TYR	4.6
1	D	236	TYR	4.6
1	C	153	TYR	4.6
1	B	72	LYS	4.6
1	D	169	LEU	4.6
1	A	162	CYS	4.5
1	C	168	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	107	GLU	4.5
1	A	47	LEU	4.5
1	D	30	GLN	4.5
1	C	161	GLY	4.5
1	C	226	ILE	4.5
1	A	37	GLU	4.5
1	D	28	PHE	4.5
1	B	88	THR	4.5
1	A	66	TRP	4.5
1	D	189	TRP	4.5
1	A	51	GLU	4.5
1	C	147	GLU	4.5
1	C	162	CYS	4.5
1	A	31	ASP	4.4
1	D	231	LYS	4.4
1	B	1	MET	4.4
1	C	218	TRP	4.4
1	D	172	THR	4.4
1	A	48	TYR	4.4
1	B	212	TYR	4.4
1	A	92	PHE	4.4
1	A	121	MET	4.4
1	D	16	PHE	4.4
1	C	124	GLY	4.4
1	C	141	SER	4.4
1	D	33	SER	4.4
1	B	140	ALA	4.4
1	D	161	GLY	4.4
1	C	57	HIS	4.4
1	C	154	TYR	4.4
1	D	39	TYR	4.4
1	D	155	ALA	4.4
1	D	181	ALA	4.4
1	D	5	ILE	4.4
1	D	71	LEU	4.4
1	D	200	LEU	4.4
1	D	219	LEU	4.4
1	B	191	ASP	4.4
1	C	9	CYS	4.4
1	C	174	CYS	4.4
1	B	234	PRO	4.4
1	C	212	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	216	GLU	4.3
1	A	208	LEU	4.3
1	C	11	GLY	4.3
1	C	15	ILE	4.3
1	A	83	GLN	4.3
1	B	79	ARG	4.3
1	B	10	THR	4.3
1	B	180	ASP	4.3
1	C	89	ASP	4.3
1	D	191	ASP	4.3
1	A	135	TYR	4.3
1	A	106	LYS	4.3
1	A	117	LEU	4.3
1	D	184	HIS	4.3
1	B	214	TYR	4.3
1	C	38	TYR	4.3
1	A	91	LEU	4.3
1	B	222	PHE	4.3
1	A	112	SER	4.3
1	C	75	HIS	4.3
1	C	123	PRO	4.3
1	D	120	THR	4.3
1	B	202	ASN	4.3
1	A	218	TRP	4.2
1	B	94	PHE	4.2
1	D	100	PHE	4.2
1	B	35	ILE	4.2
1	B	50	GLU	4.2
1	B	53	ASN	4.2
1	C	19	ASP	4.2
1	B	16	PHE	4.2
1	D	103	PRO	4.2
1	A	42	THR	4.2
1	B	27	TYR	4.2
1	A	164	LYS	4.2
1	B	92	PHE	4.2
1	B	93	PHE	4.2
1	C	62	LYS	4.2
1	B	85	GLU	4.2
1	A	68	ASP	4.2
1	B	52	ASN	4.2
1	D	54	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	51	GLU	4.2
1	D	151	ARG	4.2
1	C	98	LEU	4.2
1	A	222	PHE	4.2
1	B	115	ASN	4.1
1	D	185	ILE	4.1
1	B	29	MET	4.1
1	B	20	PHE	4.1
1	B	30	GLN	4.1
1	B	143	ALA	4.1
1	D	196	ASN	4.1
1	D	66	TRP	4.1
1	D	153	TYR	4.1
1	B	76	ILE	4.1
1	B	185	ILE	4.1
1	A	44	SER	4.1
1	B	40	VAL	4.1
1	C	169	LEU	4.1
1	D	64	LEU	4.1
1	A	15	ILE	4.1
1	A	104	ILE	4.1
1	D	127	ASN	4.1
1	B	102	SER	4.1
1	C	177	VAL	4.1
1	D	17	TRP	4.1
1	C	232	ASN	4.0
1	D	167	LEU	4.0
1	C	137	ARG	4.0
1	B	221	PRO	4.0
1	B	208	LEU	4.0
1	A	46	LYS	4.0
1	A	115	ASN	4.0
1	A	180	ASP	4.0
1	B	33	SER	4.0
1	C	20	PHE	4.0
1	A	154	TYR	4.0
1	B	118	LEU	4.0
1	D	67	PRO	4.0
1	C	225	ILE	4.0
1	C	113	ASP	4.0
1	C	73	ARG	4.0
1	D	173	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	69	ASN	4.0
1	C	192	GLU	4.0
1	D	25	GLU	4.0
1	D	105	GLY	3.9
1	A	73	ARG	3.9
1	C	58	ARG	3.9
1	D	79	ARG	3.9
1	C	95	ASN	3.9
1	D	12	LYS	3.9
1	D	212	TYR	3.9
1	A	85	GLU	3.9
1	B	146	PRO	3.9
1	A	227	LEU	3.9
1	D	194	LEU	3.9
1	C	196	ASN	3.9
1	D	192	GLU	3.9
1	A	119	GLY	3.9
1	A	217	GLY	3.9
1	C	44	SER	3.9
1	C	129	PRO	3.9
1	D	1	MET	3.9
1	A	56	ILE	3.9
1	A	194	LEU	3.9
1	B	167	LEU	3.9
1	C	194	LEU	3.9
1	C	127	ASN	3.9
1	B	62	LYS	3.9
1	D	59	ILE	3.9
1	A	86	ARG	3.8
1	C	170	CYS	3.8
1	C	1	MET	3.8
1	D	87	GLU	3.8
1	D	201	ASP	3.8
1	D	26	ARG	3.8
1	D	145	ILE	3.8
1	D	188	ILE	3.8
1	D	232	ASN	3.8
1	A	64	LEU	3.8
1	B	31	ASP	3.8
1	B	175	SER	3.8
1	C	209	SER	3.8
1	D	19	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	164	LYS	3.8
1	C	25	GLU	3.8
1	D	152	TYR	3.8
1	A	61	GLN	3.8
1	A	143	ALA	3.8
1	B	55	HIS	3.8
1	C	49	ASP	3.8
1	B	198	TYR	3.8
1	B	84	LEU	3.8
1	C	83	GLN	3.8
1	C	114	SER	3.8
1	C	197	LYS	3.8
1	A	173	ILE	3.8
1	D	92	PHE	3.8
1	B	101	THR	3.8
1	A	33	SER	3.7
1	D	176	TRP	3.7
1	C	68	ASP	3.7
1	C	229	ARG	3.7
1	C	28	PHE	3.7
1	A	182	THR	3.7
1	B	165	ALA	3.7
1	A	118	LEU	3.7
1	A	167	LEU	3.7
1	B	150	GLY	3.7
1	B	67	PRO	3.7
1	D	234	PRO	3.7
1	C	106	LYS	3.7
1	C	143	ALA	3.7
1	B	15	ILE	3.7
1	B	225	ILE	3.7
1	C	206	ILE	3.7
1	D	65	GLY	3.7
1	D	230	ASP	3.7
1	A	129	PRO	3.7
1	A	38	TYR	3.7
1	B	87	GLU	3.7
1	C	119	GLY	3.7
1	B	7	TYR	3.7
1	B	144	TYR	3.7
1	C	216	GLU	3.7
1	A	70	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	182	THR	3.7
1	A	231	LYS	3.7
1	A	116	GLY	3.7
1	A	82	GLU	3.6
1	B	113	ASP	3.6
1	B	207	THR	3.6
1	C	182	THR	3.6
1	D	70	THR	3.6
1	D	227	LEU	3.6
1	B	69	ASN	3.6
1	B	205	ALA	3.6
1	A	198	TYR	3.6
1	D	86	ARG	3.6
1	D	187	PRO	3.6
1	C	90	TYR	3.6
1	C	59	ILE	3.6
1	D	143	ALA	3.6
1	D	81	LYS	3.6
1	D	213	LEU	3.6
1	A	79	ARG	3.6
1	C	105	GLY	3.6
1	A	215	PRO	3.6
1	A	12	LYS	3.6
1	A	113	ASP	3.6
1	A	160	GLY	3.5
1	D	96	ALA	3.5
1	D	46	LYS	3.5
1	C	125	PHE	3.5
1	A	89	ASP	3.5
1	C	67	PRO	3.5
1	C	77	PHE	3.5
1	D	23	SER	3.5
1	B	46	LYS	3.5
1	A	186	ILE	3.5
1	C	52	ASN	3.5
1	A	20	PHE	3.5
1	B	122	HIS	3.5
1	D	203	PRO	3.5
1	A	76	ILE	3.5
1	B	151	ARG	3.5
1	D	198	TYR	3.5
1	D	61	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	56	ILE	3.5
1	C	160	GLY	3.4
1	A	96	ALA	3.4
1	B	187	PRO	3.4
1	D	199	PHE	3.4
1	D	21	TYR	3.4
1	D	144	TYR	3.4
1	A	142	THR	3.4
1	D	69	ASN	3.4
1	A	138	ARG	3.4
1	B	203	PRO	3.4
1	D	45	PRO	3.4
1	B	114	SER	3.4
1	C	132	GLU	3.4
1	D	20	PHE	3.4
1	A	219	LEU	3.4
1	C	118	LEU	3.4
1	B	160	GLY	3.4
1	A	122	HIS	3.4
1	B	230	ASP	3.4
1	D	132	GLU	3.4
1	B	39	TYR	3.4
1	B	96	ALA	3.4
1	C	53	ASN	3.4
1	A	193	SER	3.4
1	B	159	SER	3.4
1	C	199	PHE	3.4
1	D	170	CYS	3.4
1	D	49	ASP	3.4
1	C	152	TYR	3.4
1	A	184	HIS	3.4
1	D	163	THR	3.4
1	C	23	SER	3.3
1	C	220	LEU	3.3
1	C	65	GLY	3.3
1	B	80	ILE	3.3
1	A	207	THR	3.3
1	A	130	ASN	3.3
1	D	133	PHE	3.3
1	B	223	GLU	3.3
1	C	85	GLU	3.3
1	A	175	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	206	ILE	3.3
1	D	7	TYR	3.3
1	C	45	PRO	3.3
1	A	53	ASN	3.3
1	B	81	LYS	3.3
1	A	165	ALA	3.3
1	C	76	ILE	3.3
1	C	150	GLY	3.3
1	D	141	SER	3.3
1	A	13	TYR	3.3
1	A	43	ASP	3.3
1	A	203	PRO	3.3
1	D	2	ARG	3.3
1	D	42	THR	3.3
1	A	6	LEU	3.3
1	B	54	LYS	3.3
1	C	17	TRP	3.3
1	D	221	PRO	3.3
1	A	147	GLU	3.3
1	C	4	GLY	3.3
1	C	7	TYR	3.2
1	C	26	ARG	3.2
1	C	92	PHE	3.2
1	A	149	GLU	3.2
1	A	2	ARG	3.2
1	A	23	SER	3.2
1	D	18	LYS	3.2
1	B	42	THR	3.2
1	A	25	GLU	3.2
1	D	150	GLY	3.2
1	D	93	PHE	3.2
1	B	49	ASP	3.2
1	C	173	ILE	3.2
1	B	217	GLY	3.2
1	B	196	ASN	3.2
1	D	63	ASN	3.2
1	A	213	LEU	3.2
1	C	110	PRO	3.2
1	C	204	PRO	3.2
1	A	137	ARG	3.2
1	B	5	ILE	3.2
1	C	36	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	104	ILE	3.2
1	D	91	LEU	3.2
1	A	21	TYR	3.2
1	B	21	TYR	3.2
1	A	146	PRO	3.2
1	D	146	PRO	3.2
1	A	178	ASP	3.1
1	C	148	GLY	3.1
1	B	189	TRP	3.1
1	C	202	ASN	3.1
1	B	129	PRO	3.1
1	C	179	ARG	3.1
1	A	209	SER	3.1
1	D	140	ALA	3.1
1	B	106	LYS	3.1
1	B	228	ILE	3.1
1	B	139	ASP	3.1
1	C	178	ASP	3.1
1	C	50	GLU	3.1
1	A	40	VAL	3.1
1	A	69	ASN	3.1
1	D	195	ILE	3.1
1	A	114	SER	3.1
1	C	43	ASP	3.1
1	D	180	ASP	3.1
1	A	62	LYS	3.1
1	A	145	ILE	3.1
1	D	22	LEU	3.1
1	A	87	GLU	3.1
1	B	168	LYS	3.1
1	B	47	LEU	3.0
1	A	30	GLN	3.0
1	D	62	LYS	3.0
1	C	145	ILE	3.0
1	A	201	ASP	3.0
1	A	95	ASN	3.0
1	A	97	ASN	3.0
1	B	190	HIS	3.0
1	D	226	ILE	3.0
1	C	84	LEU	3.0
1	C	86	ARG	3.0
1	A	127	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	231	LYS	3.0
1	C	54	LYS	3.0
1	A	132	GLU	3.0
1	D	37	GLU	3.0
1	D	58	ARG	3.0
1	D	89	ASP	3.0
1	D	72	LYS	3.0
1	D	4	GLY	3.0
1	C	101	THR	3.0
1	C	142	THR	3.0
1	B	136	GLU	3.0
1	C	37	GLU	3.0
1	C	205	ALA	3.0
1	B	152	TYR	3.0
1	C	40	VAL	3.0
1	D	55	HIS	3.0
1	A	94	PHE	3.0
1	C	41	PHE	3.0
1	A	8	ILE	3.0
1	C	172	THR	3.0
1	D	171	THR	3.0
1	B	158	LEU	2.9
1	A	67	PRO	2.9
1	D	57	HIS	2.9
1	B	74	PHE	2.9
1	A	225	ILE	2.9
1	B	2	ARG	2.9
1	C	70	THR	2.9
1	C	88	THR	2.9
1	D	82	GLU	2.9
1	A	131	SER	2.9
1	D	193	SER	2.9
1	A	174	CYS	2.9
1	D	197	LYS	2.9
1	B	132	GLU	2.9
1	D	126	TYR	2.9
1	A	65	GLY	2.9
1	B	184	HIS	2.9
1	A	59	ILE	2.9
1	D	29	MET	2.9
1	A	10	THR	2.9
1	A	196	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	24	ALA	2.9
1	A	150	GLY	2.9
1	B	6	LEU	2.9
1	B	56	ILE	2.9
1	C	180	ASP	2.9
1	C	207	THR	2.9
1	D	24	ALA	2.9
1	A	39	TYR	2.9
1	A	90	TYR	2.9
1	B	125	PHE	2.9
1	D	179	ARG	2.9
1	C	72	LYS	2.9
1	B	181	ALA	2.8
1	C	211	ALA	2.8
1	D	10	THR	2.8
1	A	148	GLY	2.8
1	B	13	TYR	2.8
1	B	117	LEU	2.8
1	C	5	ILE	2.8
1	C	144	TYR	2.8
1	A	211	ALA	2.8
1	B	107	GLU	2.8
1	A	220	LEU	2.8
1	C	217	GLY	2.8
1	B	138	ARG	2.8
1	D	68	ASP	2.8
1	D	139	ASP	2.8
1	C	97	ASN	2.8
1	A	26	ARG	2.8
1	C	159	SER	2.8
1	D	204	PRO	2.8
1	A	214	TYR	2.8
1	B	170	CYS	2.8
1	A	36	ILE	2.8
1	C	94	PHE	2.7
1	C	228	ILE	2.8
1	A	105	GLY	2.7
1	B	183	ASN	2.7
1	B	179	ARG	2.7
1	B	18	LYS	2.7
1	C	81	LYS	2.7
1	C	200	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	6	LEU	2.7
1	B	44	SER	2.7
1	D	175	SER	2.7
1	C	198	TYR	2.7
1	A	55	HIS	2.7
1	A	111	PRO	2.7
1	A	169	LEU	2.7
1	A	210	PRO	2.7
1	B	34	PHE	2.7
1	A	88	THR	2.7
1	B	193	SER	2.7
1	A	179	ARG	2.7
1	A	188	ILE	2.7
1	C	87	GLU	2.7
1	C	163	THR	2.7
1	D	205	ALA	2.7
1	D	211	ALA	2.7
1	C	56	ILE	2.7
1	A	199	PHE	2.7
1	B	137	ARG	2.7
1	A	4	GLY	2.7
1	B	211	ALA	2.7
1	B	90	TYR	2.7
1	B	14	ASP	2.7
1	D	75	HIS	2.7
1	D	95	ASN	2.7
1	C	30	GLN	2.6
1	D	129	PRO	2.6
1	A	100	PHE	2.6
1	A	192	GLU	2.6
1	C	233	LYS	2.6
1	D	74	PHE	2.6
1	D	220	LEU	2.6
1	B	111	PRO	2.6
1	C	201	ASP	2.6
1	A	9	CYS	2.6
1	C	231	LYS	2.6
1	D	131	SER	2.6
1	D	228	ILE	2.6
1	A	93	PHE	2.6
1	C	93	PHE	2.6
1	A	14	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	19	ASP	2.6
1	A	78	LEU	2.6
1	A	99	LEU	2.6
1	B	51	GLU	2.6
1	A	176	TRP	2.6
1	B	86	ARG	2.6
1	B	218	TRP	2.6
1	C	107	GLU	2.6
1	D	107	GLU	2.6
1	A	24	ALA	2.6
1	A	29	MET	2.5
1	A	153	TYR	2.5
1	B	204	PRO	2.5
1	B	61	GLN	2.5
1	B	83	GLN	2.5
1	D	119	GLY	2.5
1	B	186	ILE	2.5
1	C	176	TRP	2.5
1	B	121	MET	2.5
1	B	64	LEU	2.5
1	C	14	ASP	2.5
1	C	151	ARG	2.5
1	C	112	SER	2.5
1	D	142	THR	2.5
1	D	222	PHE	2.5
1	C	203	PRO	2.5
1	B	201	ASP	2.5
1	C	34	PHE	2.5
1	C	214	TYR	2.5
1	C	165	ALA	2.4
1	D	76	ILE	2.4
1	C	121	MET	2.4
1	D	216	GLU	2.4
1	D	106	LYS	2.4
1	B	200	LEU	2.4
1	D	160	GLY	2.4
1	C	22	LEU	2.4
1	A	139	ASP	2.4
1	B	11	GLY	2.4
1	B	124	GLY	2.4
1	C	102	SER	2.4
1	B	110	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	161	GLY	2.4
1	D	98	LEU	2.4
1	A	170	CYS	2.4
1	D	53	ASN	2.4
1	B	43	ASP	2.4
1	C	136	GLU	2.4
1	D	88	THR	2.3
1	C	167	LEU	2.3
1	D	44	SER	2.3
1	A	58	ARG	2.3
1	C	21	TYR	2.3
1	C	227	LEU	2.3
1	A	110	PRO	2.3
1	A	141	SER	2.3
1	D	159	SER	2.3
1	B	109	LEU	2.3
1	A	54	LYS	2.3
1	A	187	PRO	2.3
1	C	3	ILE	2.3
1	D	15	ILE	2.3
1	A	22	LEU	2.3
1	D	178	ASP	2.3
1	C	51	GLU	2.3
1	D	47	LEU	2.3
1	D	84	LEU	2.3
1	B	73	ARG	2.3
1	A	177	VAL	2.3
1	D	43	ASP	2.3
1	B	192	GLU	2.2
1	B	133	PHE	2.2
1	D	183	ASN	2.2
1	C	78	LEU	2.2
1	B	149	GLU	2.2
1	A	60	LYS	2.2
1	C	130	ASN	2.2
1	D	215	PRO	2.2
1	A	81	LYS	2.2
1	C	60	LYS	2.2
1	B	199	PHE	2.2
1	A	140	ALA	2.2
1	A	190	HIS	2.2
1	A	28	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	140	ALA	2.1
1	D	113	ASP	2.1
1	B	134	THR	2.1
1	C	171	THR	2.1
1	A	224	PRO	2.1
1	C	103	PRO	2.1
1	A	5	ILE	2.1
1	C	31	ASP	2.1
1	D	9	CYS	2.1
1	B	157	GLY	2.1
1	A	183	ASN	2.1
1	B	197	LYS	2.1
1	D	38	TYR	2.1
1	A	161	GLY	2.1
1	B	63	ASN	2.0
1	D	52	ASN	2.0
1	D	121	MET	2.0
1	D	116	GLY	2.0
1	A	197	LYS	2.0
1	A	159	SER	2.0
1	B	162	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

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

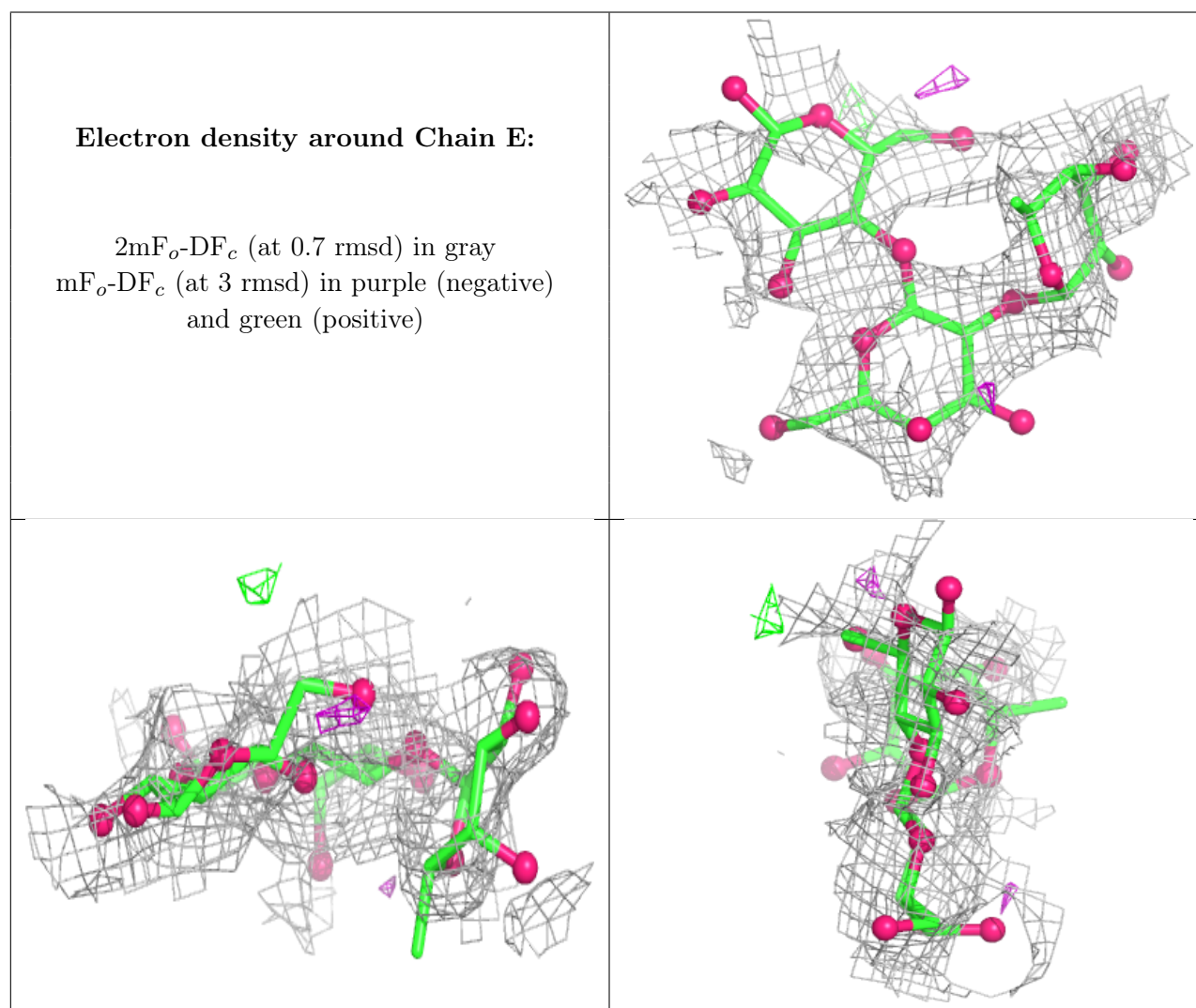
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	H	3	10/11	-0.05	0.41	48,54,62,64	0
2	GAL	H	2	11/12	0.20	0.31	44,47,58,62	0
2	BGC	H	1	12/12	0.29	0.34	42,53,59,60	0
2	BGC	E	1	12/12	0.38	0.32	25,28,32,36	0
2	FUC	E	3	10/11	0.42	0.21	13,19,30,33	0
2	GAL	E	2	11/12	0.52	0.21	21,23,26,27	0
2	GAL	F	2	11/12	0.52	0.32	27,29,30,32	0

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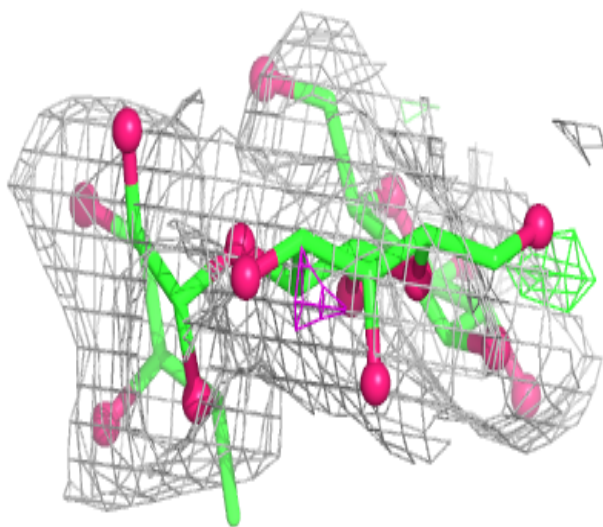
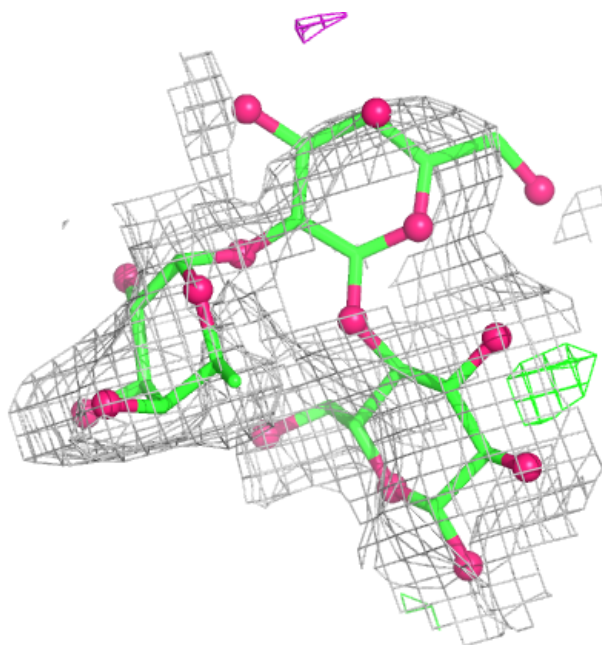
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	G	2	11/12	0.52	0.23	31,33,39,43	0
2	FUC	G	3	10/11	0.53	0.29	23,31,36,41	0
2	BGC	G	1	12/12	0.53	0.23	28,33,39,46	0
2	BGC	F	1	12/12	0.54	0.23	26,29,33,33	0
2	FUC	F	3	10/11	0.56	0.26	26,35,41,41	0

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.



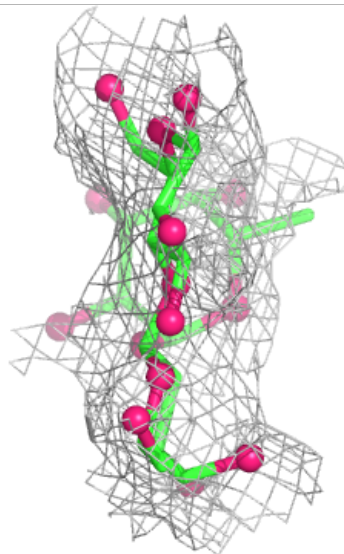
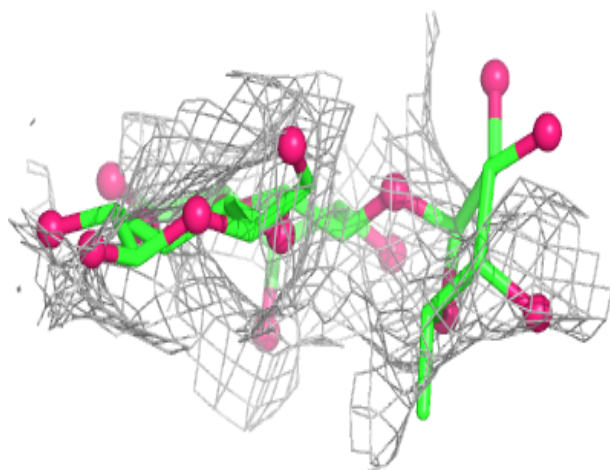
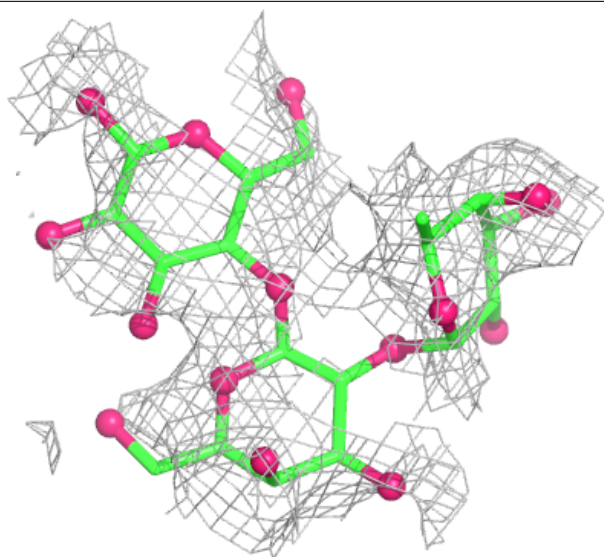
Electron density around Chain F:

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



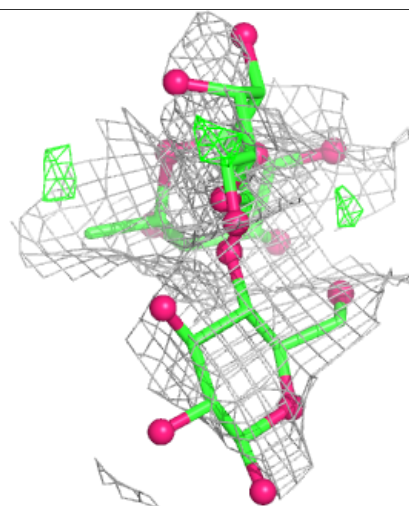
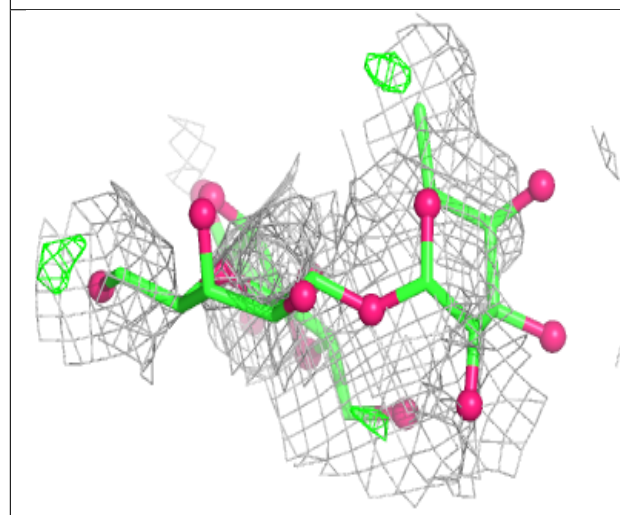
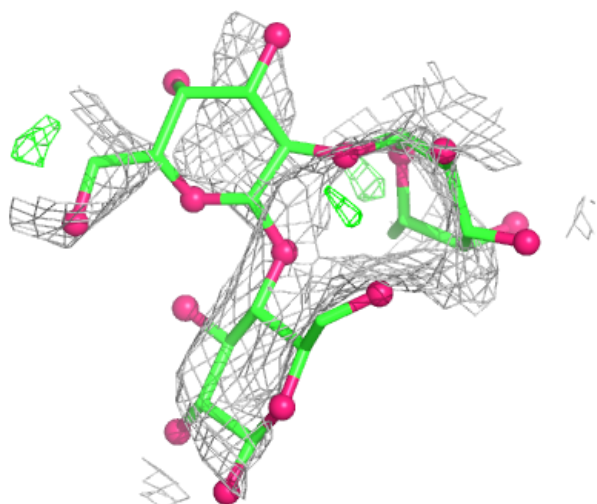
Electron density around Chain G:

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



Electron density around Chain H:

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.