



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:39 AM UTC

PDB ID : 2GAM / pdb_00002gam
Title : X-ray crystal structure of murine leukocyte-type Core 2 b1,6-N-acetylglucosaminyltransferase (C2GnT-L) in complex with Galb1,3GalNAc
Authors : Pak, J.E.; Rini, J.M.
Deposited on : 2006-03-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

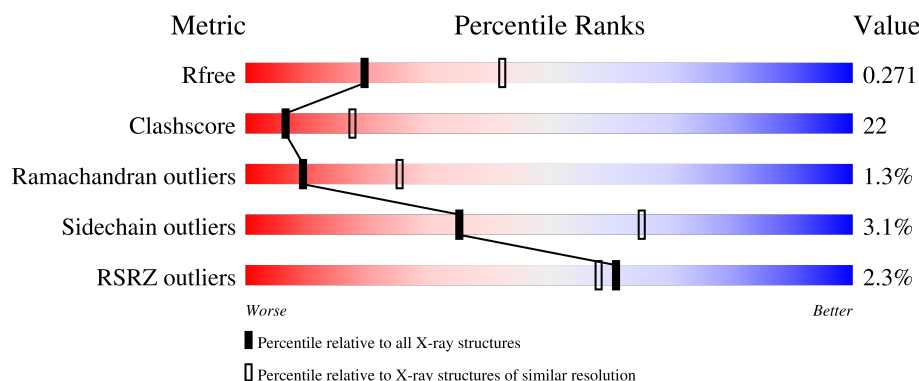
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	391	53% 37% 7%
1	B	391	53% 35% 8%
1	C	391	3% 53% 41% 2%
1	D	391	4% 57% 34% 6%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 50%50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12285 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 beta-1,6-N-acetylglucosaminyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2966	1903	505	537	21			
1	B	359	Total	C	N	O	S	0	0	0
			2919	1871	499	528	21			
1	C	374	Total	C	N	O	S	0	0	0
			3050	1958	522	549	21			
1	D	368	Total	C	N	O	S	0	0	0
			2994	1921	510	542	21			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	F	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	G	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	H	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		

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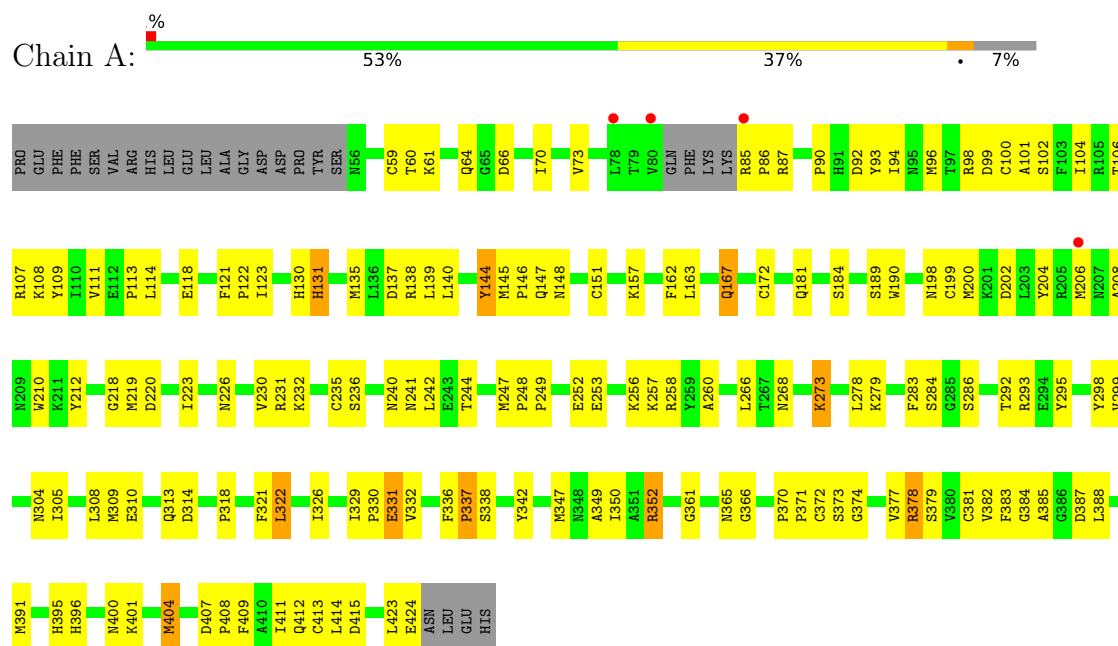
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	85	Total 85	O 85	0	0
3	C	58	Total 58	O 58	0	0
3	D	44	Total 44	O 44	0	0

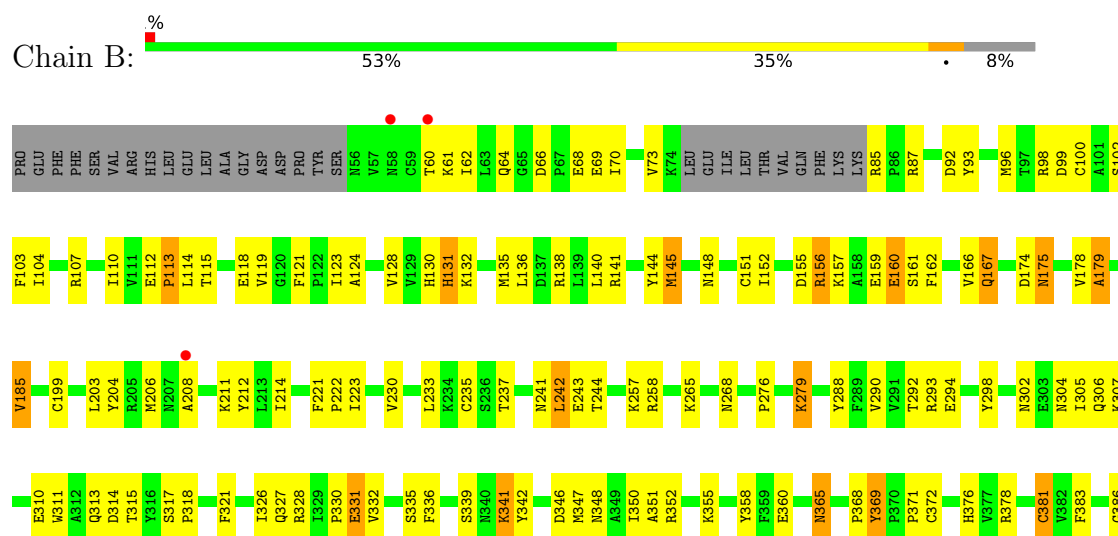
3 Residue-property plots

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: beta-1,6-N-acetylglucosaminyltransferase

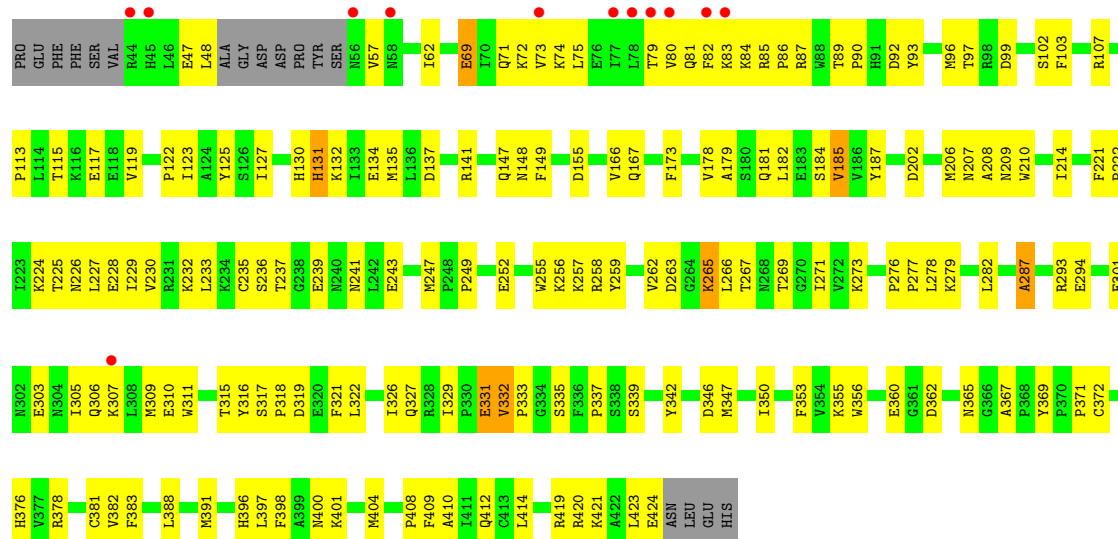


- Molecule 1: beta-1,6-N-acetylglucosaminyltransferase

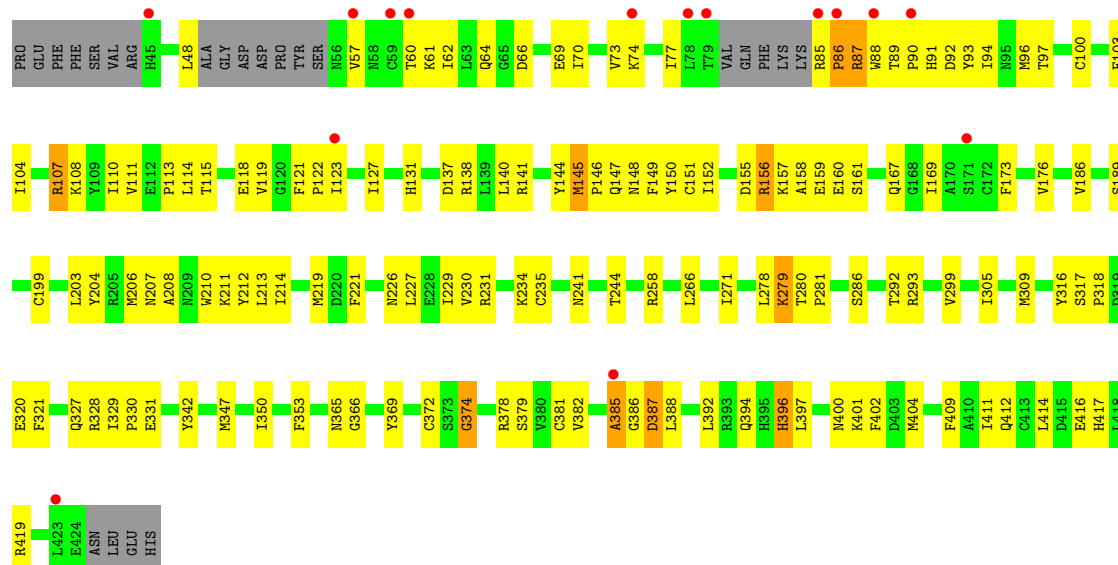




• Molecule 1: beta-1,6-N-acetylglucosaminyltransferase



• Molecule 1: beta-1,6-N-acetylglucosaminyltransferase



• Molecule 2: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

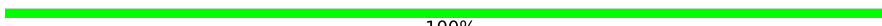


- Molecule 2: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain F:  50% 50%



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

Chain G:  100%



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

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.50Å 80.58Å 102.33Å 73.61° 76.26° 64.56°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.70) 99.3 (20.00-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.274 0.218 , 0.271	Depositor DCC
R_{free} test set	6847 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12285	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: GAL, NGA

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	0/3042	0.96	11/4125 (0.3%)
1	B	0.48	0/2995	0.99	12/4060 (0.3%)
1	C	0.46	0/3128	0.95	6/4238 (0.1%)
1	D	0.43	0/3070	0.91	8/4161 (0.2%)
All	All	0.46	0/12235	0.95	37/16584 (0.2%)

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 (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	TYR	CA-C-N	9.71	126.65	119.66
1	D	369	TYR	C-N-CA	9.71	126.65	119.66
1	B	332	VAL	N-CA-C	8.33	117.11	108.95
1	B	145	MET	CA-C-N	7.75	127.66	119.05
1	B	145	MET	C-N-CA	7.75	127.66	119.05
1	A	167	GLN	N-CA-C	-7.71	102.88	111.28
1	B	185	VAL	N-CA-C	7.57	119.74	108.54
1	A	383	PHE	N-CA-C	7.46	121.05	110.23
1	C	287	ALA	N-CA-C	-7.37	104.31	113.38
1	A	279	LYS	N-CA-C	-7.14	102.91	111.69
1	D	369	TYR	N-CA-C	6.81	114.35	108.22
1	C	332	VAL	N-CA-C	6.77	116.34	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	410	ALA	N-CA-C	-6.56	104.05	111.07
1	D	160	GLU	N-CA-C	-6.38	104.37	111.71
1	D	279	LYS	N-CA-C	-6.33	103.90	111.69
1	C	388	LEU	N-CA-C	5.93	117.43	110.97
1	B	279	LYS	N-CA-C	-5.76	105.35	112.90
1	A	295	TYR	N-CA-C	-5.57	105.11	111.07
1	C	185	VAL	N-CA-C	5.55	116.17	108.84
1	B	410	ALA	N-CA-C	-5.54	105.32	111.36
1	B	144	TYR	N-CA-C	5.45	118.43	109.76
1	A	218	GLY	N-CA-C	5.40	119.42	112.83
1	A	370	PRO	CA-C-N	5.39	125.40	119.90
1	A	370	PRO	C-N-CA	5.39	125.40	119.90
1	B	243	GLU	N-CA-C	-5.37	102.33	110.28
1	B	331	GLU	N-CA-C	5.34	119.42	113.01
1	A	236	SER	N-CA-C	-5.29	106.53	112.87
1	A	349	ALA	N-CA-C	-5.25	103.76	110.53
1	A	240	ASN	N-CA-C	-5.24	102.76	110.52
1	B	369	TYR	CA-C-N	5.22	125.76	120.38
1	B	369	TYR	C-N-CA	5.22	125.76	120.38
1	D	396	HIS	N-CA-C	5.22	117.86	110.50
1	B	358	TYR	N-CA-C	5.17	120.50	113.37
1	D	145	MET	CA-C-N	5.16	126.28	119.84
1	D	145	MET	C-N-CA	5.16	126.28	119.84
1	C	301	GLU	N-CA-C	5.14	120.55	113.97
1	A	396	HIS	N-CA-C	5.02	117.15	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain

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	2966	0	2937	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2919	0	2882	120	0
1	C	3050	0	3028	157	0
1	D	2994	0	2962	126	0
2	E	26	0	24	0	0
2	F	26	0	24	1	0
2	G	26	0	24	0	0
2	H	26	0	24	1	0
3	A	65	0	0	4	0
3	B	85	0	0	3	0
3	C	58	0	0	2	0
3	D	44	0	0	3	0
All	All	12285	0	11905	507	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (507) 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:151:CYS:HG	1:D:199:CYS:HG	1.10	0.96
1:D:372:CYS:HG	1:D:381:CYS:HG	0.98	0.95
1:C:79:THR:HG22	1:C:81:GLN:H	1.33	0.93
1:A:372:CYS:HG	1:A:381:CYS:HG	1.17	0.93
1:B:132:LYS:HD2	1:B:135:MET:HE2	1.48	0.92
1:D:123:ILE:HD11	1:D:230:VAL:HG22	1.51	0.92
1:C:89:THR:HG22	1:C:92:ASP:OD2	1.70	0.92
1:C:372:CYS:HG	1:C:381:CYS:HG	1.08	0.91
1:B:114:LEU:HD13	1:B:145:MET:HE1	1.50	0.90
1:C:342:TYR:OH	1:D:347:MET:HE2	1.74	0.88
1:A:347:MET:HE2	1:B:342:TYR:OH	1.74	0.87
1:C:276:PRO:HG2	1:C:282:LEU:HD11	1.57	0.86
1:D:122:PRO:HB2	1:D:210:TRP:HA	1.60	0.83
1:A:151:CYS:HG	1:A:199:CYS:HG	0.87	0.82
1:A:330:PRO:O	1:A:331:GLU:HB2	1.79	0.81
1:C:235:CYS:HG	1:D:235:CYS:HG	0.90	0.81
1:C:122:PRO:HB2	1:C:210:TRP:HA	1.62	0.81
1:A:138:ARG:NH2	1:A:412:GLN:HE22	1.79	0.80
1:C:404:MET:O	1:C:408:PRO:HG3	1.83	0.79
1:A:99:ASP:OD2	1:A:102:SER:HB2	1.83	0.78
1:C:258:ARG:HG2	1:C:273:LYS:HG2	1.65	0.77
1:A:342:TYR:OH	1:B:347:MET:HE2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:HA	1:A:293:ARG:NE	2.01	0.75
1:A:66:ASP:O	1:A:70:ILE:HG12	1.88	0.74
1:D:61:LYS:HB2	1:D:69:GLU:HG3	1.68	0.74
1:B:305:ILE:HD12	1:B:326:ILE:HD12	1.70	0.74
1:B:408:PRO:O	1:B:412:GLN:HG3	1.87	0.74
1:C:305:ILE:HD12	1:C:326:ILE:HD12	1.70	0.74
1:B:175:ASN:H	1:B:175:ASN:HD22	1.35	0.74
1:C:269:THR:OG1	1:C:271:ILE:HG12	1.89	0.73
1:C:83:LYS:HG3	1:C:84:LYS:HD3	1.72	0.72
1:B:123:ILE:H	1:B:148:ASN:ND2	1.89	0.71
1:C:135:MET:HE2	1:C:404:MET:HG3	1.71	0.71
1:A:163:LEU:O	1:A:167:GLN:HG3	1.91	0.70
1:A:70:ILE:O	1:A:73:VAL:HG22	1.91	0.69
1:C:276:PRO:HG3	1:C:311:TRP:CZ2	2.27	0.69
1:B:92:ASP:O	1:B:96:MET:HG3	1.92	0.69
1:C:149:PHE:CD1	1:C:206:MET:HE3	2.28	0.69
1:B:66:ASP:O	1:B:70:ILE:HG12	1.93	0.69
1:C:347:MET:HE2	1:D:342:TYR:OH	1.93	0.68
1:C:85:ARG:HH11	1:C:85:ARG:HG2	1.57	0.68
1:C:276:PRO:HG3	1:C:311:TRP:CH2	2.29	0.68
1:D:388:LEU:HD11	1:D:414:LEU:HD13	1.77	0.67
1:B:302:ASN:O	1:B:306:GLN:HG2	1.95	0.67
1:D:113:PRO:HB3	1:D:119:VAL:HG22	1.76	0.67
1:C:87:ARG:HH21	1:C:404:MET:HE3	1.60	0.67
1:A:122:PRO:HB2	1:A:210:TRP:HA	1.77	0.66
1:A:378:ARG:HB2	1:A:378:ARG:HH11	1.58	0.66
1:B:151:CYS:HG	1:B:199:CYS:HG	0.68	0.66
1:C:259:TYR:HB3	1:C:266:LEU:HD11	1.78	0.65
1:B:276:PRO:HG3	1:B:311:TRP:CH2	2.32	0.65
1:C:47:GLU:OE2	1:C:420:ARG:HG3	1.97	0.65
1:C:87:ARG:NH2	1:C:404:MET:HE3	2.13	0.64
1:A:92:ASP:HB3	1:A:96:MET:HE2	1.79	0.64
1:B:70:ILE:HD12	1:B:386:GLY:HA2	1.78	0.64
1:D:73:VAL:O	1:D:77:ILE:HG13	1.97	0.64
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.64	0.63
1:D:88:TRP:HZ3	1:D:96:MET:SD	2.22	0.63
1:A:100:CYS:HG	1:A:172:CYS:HG	1.46	0.63
1:A:138:ARG:NH2	1:A:412:GLN:NE2	2.45	0.63
1:C:103:PHE:CE1	1:C:107:ARG:HG3	2.33	0.63
1:C:322:LEU:O	1:C:326:ILE:HG12	1.99	0.63
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:O	1:A:235:CYS:SG	2.57	0.63
1:D:204:TYR:HA	1:D:210:TRP:HZ2	1.64	0.63
1:C:107:ARG:HD3	1:C:137:ASP:OD1	1.99	0.63
1:A:59:CYS:HG	1:A:413:CYS:HG	1.44	0.62
1:D:121:PHE:CD2	1:D:230:VAL:HG13	2.34	0.62
1:C:57:VAL:HA	1:C:72:LYS:NZ	2.14	0.62
1:D:123:ILE:CG2	1:D:214:ILE:HD13	2.30	0.61
1:B:175:ASN:H	1:B:175:ASN:ND2	1.98	0.61
1:C:134:GLU:HB3	1:C:404:MET:HE1	1.82	0.61
1:C:294:GLU:N	1:C:294:GLU:OE1	2.33	0.61
1:D:48:LEU:HD23	1:D:108:LYS:HE2	1.82	0.61
1:C:331:GLU:CD	1:C:331:GLU:H	2.07	0.61
1:C:131:HIS:CE1	1:C:132:LYS:HG3	2.36	0.61
1:A:372:CYS:CB	1:A:381:CYS:HG	2.12	0.60
1:A:92:ASP:O	1:A:96:MET:HG3	2.00	0.60
1:A:121:PHE:CD2	1:A:230:VAL:HG13	2.36	0.60
1:D:122:PRO:HD2	1:D:211:LYS:HE2	1.83	0.60
1:C:360:GLU:OE1	1:C:376:HIS:HE1	1.85	0.60
1:C:408:PRO:O	1:C:412:GLN:HB2	2.01	0.60
1:B:241:ASN:CG	1:B:350:ILE:HG12	2.27	0.60
1:D:91:HIS:HA	1:D:94:ILE:CD1	2.32	0.60
1:A:123:ILE:H	1:A:148:ASN:ND2	1.99	0.60
1:C:225:THR:OG1	1:C:228:GLU:HG3	2.02	0.60
1:A:366:GLY:O	1:B:339:SER:HB2	2.01	0.60
1:C:372:CYS:CB	1:C:381:CYS:HG	2.15	0.59
1:D:61:LYS:CB	1:D:69:GLU:HG3	2.32	0.59
1:B:131:HIS:CE1	1:B:132:LYS:HG3	2.36	0.59
1:B:214:ILE:HD12	1:B:290:VAL:HG22	1.83	0.59
1:D:70:ILE:HG23	1:D:385:ALA:HB1	1.85	0.59
1:A:365:ASN:OD1	1:B:279:LYS:HE2	2.03	0.59
1:B:61:LYS:HB2	1:B:69:GLU:HG3	1.84	0.59
1:C:247:MET:HE3	1:C:255:TRP:HE1	1.68	0.59
1:B:123:ILE:H	1:B:148:ASN:HD22	1.49	0.59
1:C:69:GLU:O	1:C:72:LYS:HB3	2.02	0.59
1:A:139:LEU:HD13	1:A:220:ASP:O	2.03	0.59
1:A:404:MET:O	1:A:408:PRO:HG3	2.03	0.59
1:D:213:LEU:C	1:D:214:ILE:HD12	2.28	0.59
1:D:404:MET:CG	1:D:411:ILE:HD12	2.33	0.59
1:C:113:PRO:HB3	1:C:119:VAL:HG22	1.85	0.58
1:C:229:ILE:O	1:C:233:LEU:HG	2.01	0.58
1:D:226:ASN:O	1:D:230:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:MET:SD	1:A:411:ILE:HD12	2.43	0.58
1:D:48:LEU:HD11	1:D:419:ARG:HE	1.68	0.58
1:C:255:TRP:CZ3	1:C:256:LYS:HE3	2.38	0.58
1:D:85:ARG:HG3	1:D:85:ARG:HH11	1.68	0.57
1:A:107:ARG:HD3	1:A:137:ASP:OD1	2.05	0.57
1:B:293:ARG:HH11	1:B:293:ARG:HG2	1.69	0.57
1:C:135:MET:CE	1:C:404:MET:H	2.18	0.57
1:A:220:ASP:OD1	1:A:400:ASN:HB2	2.05	0.57
1:B:175:ASN:HD22	1:B:175:ASN:N	1.94	0.57
1:D:374:GLY:HA3	1:D:382:VAL:O	2.05	0.57
1:C:99:ASP:OD2	1:C:102:SER:HB2	2.05	0.57
1:B:293:ARG:HG2	1:B:293:ARG:NH1	2.20	0.56
1:A:202:ASP:O	1:A:206:MET:HB2	2.05	0.56
1:C:400:ASN:OD1	1:C:401:LYS:HB3	2.05	0.56
1:B:132:LYS:HD2	1:B:135:MET:CE	2.31	0.56
1:B:152:ILE:N	1:B:152:ILE:HD12	2.21	0.56
1:C:265:LYS:NZ	1:C:265:LYS:HB3	2.20	0.56
1:D:86:PRO:O	1:D:87:ARG:HB2	2.06	0.56
1:A:181:GLN:HB3	1:A:198:ASN:ND2	2.21	0.56
1:D:286:SER:HA	1:D:320:GLU:HG2	1.87	0.56
1:B:310:GLU:HA	1:B:313:GLN:HG3	1.88	0.56
1:C:107:ARG:HE	1:C:107:ARG:HA	1.70	0.56
1:A:241:ASN:CG	1:A:350:ILE:HG12	2.31	0.56
1:C:79:THR:CG2	1:C:81:GLN:HB3	2.36	0.56
1:A:190:TRP:HA	1:A:318:PRO:HG3	1.87	0.56
1:D:123:ILE:HG23	1:D:214:ILE:HD13	1.88	0.56
1:C:276:PRO:CG	1:C:282:LEU:HD11	2.32	0.56
1:D:48:LEU:HD23	1:D:108:LYS:CE	2.35	0.56
1:A:232:LYS:HE2	1:A:395:HIS:O	2.07	0.55
1:B:372:CYS:HB3	1:B:376:HIS:HE1	1.71	0.55
1:B:87:ARG:NH2	1:B:404:MET:HB3	2.21	0.55
1:B:327:GLN:O	1:B:335:SER:HB2	2.07	0.55
1:C:262:VAL:O	1:C:263:ASP:HB2	2.06	0.55
1:B:378:ARG:HB2	1:B:378:ARG:NH1	2.21	0.55
1:C:356:TRP:O	1:C:360:GLU:HG3	2.06	0.55
1:D:151:CYS:HG	1:D:199:CYS:CB	2.20	0.55
1:D:203:LEU:HA	1:D:206:MET:HG2	1.89	0.55
1:A:388:LEU:HD22	1:A:414:LEU:HD13	1.89	0.55
1:D:115:THR:OG1	1:D:118:GLU:HG3	2.06	0.55
1:D:214:ILE:HD12	1:D:214:ILE:N	2.22	0.55
1:A:235:CYS:CB	1:B:235:CYS:HG	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PRO:HB2	1:B:331:GLU:OE2	2.07	0.55
1:B:360:GLU:OE2	1:B:372:CYS:N	2.39	0.54
1:A:310:GLU:HA	1:A:313:GLN:HG3	1.88	0.54
1:B:214:ILE:HD11	1:B:290:VAL:HG13	1.90	0.54
1:D:404:MET:HG2	1:D:411:ILE:HD12	1.88	0.54
1:A:373:SER:HB2	1:A:387:ASP:OD1	2.07	0.54
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.22	0.54
1:C:83:LYS:HG3	1:C:84:LYS:CD	2.37	0.54
1:C:92:ASP:O	1:C:96:MET:HG3	2.08	0.54
1:C:48:LEU:HD13	1:C:141:ARG:NH2	2.22	0.54
1:C:327:GLN:NE2	1:C:335:SER:HA	2.23	0.54
1:C:339:SER:HB2	1:D:366:GLY:O	2.07	0.54
1:A:318:PRO:O	1:A:322:LEU:HB2	2.06	0.54
1:B:214:ILE:CD1	1:B:290:VAL:HG13	2.37	0.54
1:C:131:HIS:ND1	1:C:132:LYS:HG3	2.23	0.54
1:C:62:ILE:HD13	1:C:69:GLU:HB3	1.88	0.54
1:A:411:ILE:O	1:A:415:ASP:HB2	2.08	0.53
1:C:135:MET:HE2	1:C:404:MET:CG	2.38	0.53
1:A:138:ARG:HH22	1:A:412:GLN:NE2	2.04	0.53
1:A:352:ARG:NH1	1:A:352:ARG:HB2	2.23	0.53
1:A:145:MET:HE3	1:A:147:GLN:HE22	1.73	0.53
1:C:265:LYS:O	1:C:267:THR:HG23	2.08	0.53
1:D:123:ILE:H	1:D:148:ASN:ND2	2.06	0.53
1:D:96:MET:HE2	1:D:103:PHE:CD1	2.43	0.53
1:B:258:ARG:HG3	1:B:314:ASP:OD2	2.09	0.53
1:C:85:ARG:HG2	1:C:85:ARG:NH1	2.22	0.53
1:C:226:ASN:O	1:C:230:VAL:HG23	2.09	0.53
1:C:247:MET:HE3	1:C:255:TRP:NE1	2.23	0.53
1:A:60:THR:O	1:A:64:GLN:HG3	2.08	0.53
1:B:159:GLU:O	1:B:162:PHE:N	2.42	0.53
1:D:88:TRP:CZ3	1:D:96:MET:SD	3.01	0.53
1:D:140:LEU:O	1:D:144:TYR:HB2	2.09	0.53
1:B:321:PHE:CD1	1:B:321:PHE:C	2.86	0.53
1:D:62:ILE:HD12	1:D:70:ILE:HD13	1.90	0.53
1:A:90:PRO:O	1:A:94:ILE:HG13	2.09	0.52
1:B:87:ARG:HH22	1:B:404:MET:HB3	1.73	0.52
1:D:400:ASN:CG	1:D:401:LYS:HB3	2.34	0.52
1:C:187:TYR:HE1	1:C:378:ARG:NH1	2.07	0.52
1:C:318:PRO:HA	1:C:321:PHE:CE2	2.44	0.52
1:A:219:MET:HE2	1:A:401:LYS:HD3	1.91	0.52
1:A:208:ALA:HA	1:A:293:ARG:CZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:CD1	1:B:69:GLU:HB3	2.39	0.52
1:A:86:PRO:O	1:A:87:ARG:HD2	2.10	0.52
1:A:352:ARG:HB2	1:A:352:ARG:HH11	1.75	0.52
1:B:93:TYR:HA	1:B:96:MET:HE3	1.92	0.52
1:D:69:GLU:O	1:D:73:VAL:HG23	2.10	0.52
1:A:278:LEU:HD21	1:A:308:LEU:HD22	1.92	0.52
1:D:212:TYR:CZ	1:D:292:THR:HG22	2.45	0.52
1:C:147:GLN:OE1	1:C:147:GLN:N	2.32	0.52
1:C:273:LYS:NZ	1:C:273:LYS:HB3	2.25	0.52
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.74	0.51
1:C:187:TYR:CE1	1:C:378:ARG:NH1	2.78	0.51
1:C:262:VAL:O	1:C:265:LYS:HD2	2.11	0.51
1:A:138:ARG:HH22	1:A:412:GLN:CD	2.17	0.51
1:A:299:VAL:HG12	1:A:305:ILE:HD13	1.91	0.51
1:A:374:GLY:HA3	1:A:382:VAL:O	2.11	0.51
1:A:273:LYS:HB2	3:A:503:HOH:O	2.10	0.51
1:B:411:ILE:O	1:B:415:ASP:HB2	2.11	0.51
1:C:57:VAL:HA	1:C:72:LYS:HZ3	1.75	0.51
1:C:79:THR:HG22	1:C:81:GLN:N	2.13	0.51
1:C:225:THR:O	1:C:229:ILE:HG12	2.09	0.51
1:D:186:VAL:O	1:D:189:SER:HB3	2.10	0.51
1:A:208:ALA:HA	1:A:293:ARG:HE	1.74	0.51
1:D:48:LEU:CD2	1:D:108:LYS:HE2	2.41	0.51
1:A:104:ILE:HG21	1:A:111:VAL:HG11	1.92	0.51
1:C:135:MET:HE2	1:C:404:MET:CB	2.41	0.51
1:C:202:ASP:O	1:C:206:MET:HB2	2.11	0.51
1:D:280:THR:HG23	1:D:281:PRO:HD2	1.93	0.51
1:A:260:ALA:HA	3:A:564:HOH:O	2.10	0.50
1:B:62:ILE:HD11	1:B:69:GLU:HB3	1.93	0.50
1:B:85:ARG:HH12	1:B:87:ARG:HH21	1.60	0.50
1:C:259:TYR:HB3	1:C:266:LEU:CD1	2.40	0.50
1:C:409:PHE:HA	1:C:412:GLN:HB3	1.94	0.50
1:A:85:ARG:HH11	1:A:85:ARG:HB3	1.76	0.50
1:A:93:TYR:HA	1:A:96:MET:HE3	1.93	0.50
1:C:79:THR:HG21	1:C:81:GLN:HB3	1.92	0.50
1:C:278:LEU:HD21	1:C:329:ILE:HD11	1.93	0.50
1:B:99:ASP:OD2	1:B:102:SER:HB3	2.11	0.50
1:B:372:CYS:HB3	1:B:376:HIS:CE1	2.47	0.50
1:C:222:PRO:HB3	1:C:398:PHE:CE2	2.46	0.50
1:C:123:ILE:H	1:C:148:ASN:ND2	2.10	0.50
1:D:121:PHE:CD1	1:D:211:LYS:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:PRO:HB3	1:B:398:PHE:CE2	2.47	0.49
1:C:423:LEU:O	1:C:424:GLU:HG3	2.12	0.49
1:C:115:THR:O	1:C:119:VAL:HG23	2.12	0.49
1:A:304:ASN:HD22	1:A:304:ASN:H	1.60	0.49
1:B:346:ASP:OD2	2:F:2:GAL:H4	2.12	0.49
1:D:48:LEU:CD1	1:D:419:ARG:HE	2.25	0.49
1:D:107:ARG:HD3	1:D:137:ASP:OD2	2.13	0.49
1:D:229:ILE:HG23	1:D:397:LEU:HD13	1.94	0.49
1:D:286:SER:HB2	3:D:523:HOH:O	2.12	0.49
1:D:221:PHE:HB2	1:D:402:PHE:CD2	2.48	0.49
1:A:331:GLU:HA	1:A:331:GLU:OE1	2.12	0.49
1:B:155:ASP:OD1	1:B:185:VAL:HB	2.13	0.49
1:B:223:ILE:CG2	1:B:391:MET:HE3	2.42	0.49
1:B:378:ARG:HH11	1:B:378:ARG:CB	2.25	0.49
1:C:362:ASP:C	1:C:367:ALA:HB3	2.38	0.49
1:B:208:ALA:HA	1:B:293:ARG:NE	2.28	0.49
1:C:355:LYS:HB2	1:C:381:CYS:HB3	1.94	0.49
1:A:321:PHE:C	1:A:321:PHE:CD1	2.91	0.49
1:B:103:PHE:HD2	1:B:104:ILE:HD12	1.78	0.48
1:B:112:GLU:O	1:B:113:PRO:C	2.56	0.48
1:B:257:LYS:HG3	1:B:268:ASN:HD21	1.78	0.48
1:C:80:VAL:HA	1:C:83:LYS:CD	2.42	0.48
1:D:73:VAL:HG13	1:D:409:PHE:CD1	2.48	0.48
1:A:244:THR:HG23	1:A:244:THR:O	2.12	0.48
1:A:378:ARG:O	1:A:379:SER:HB2	2.13	0.48
1:B:113:PRO:HB3	1:B:119:VAL:CG2	2.44	0.48
1:B:315:THR:O	1:B:318:PRO:HD3	2.14	0.48
1:C:360:GLU:HB3	1:C:371:PRO:HA	1.95	0.48
1:C:382:VAL:HG22	1:C:401:LYS:CG	2.43	0.48
1:D:91:HIS:HA	1:D:94:ILE:HD12	1.95	0.48
1:A:423:LEU:O	1:A:424:GLU:HB3	2.14	0.48
1:C:173:PHE:HA	3:C:538:HOH:O	2.13	0.48
1:D:70:ILE:HG23	1:D:385:ALA:CB	2.43	0.48
1:D:121:PHE:CE1	1:D:211:LYS:HG3	2.48	0.48
1:B:167:GLN:CA	1:B:167:GLN:HE21	2.26	0.48
1:D:320:GLU:OE2	2:H:1:NGA:H62	2.14	0.48
1:A:305:ILE:HG22	1:A:309:MET:HE2	1.96	0.48
1:C:307:LYS:HA	1:C:310:GLU:CD	2.39	0.48
1:C:321:PHE:CD1	1:C:321:PHE:C	2.92	0.48
1:D:400:ASN:HA	1:D:401:LYS:HA	1.53	0.48
1:B:66:ASP:OD2	1:B:68:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LYS:HA	1:C:235:CYS:SG	2.53	0.48
1:D:318:PRO:HA	1:D:321:PHE:CE2	2.49	0.48
1:B:360:GLU:HB3	1:B:371:PRO:HA	1.96	0.48
1:B:368:PRO:HB2	1:B:369:TYR:CD2	2.49	0.48
1:C:135:MET:HE2	1:C:404:MET:H	1.77	0.48
1:C:243:GLU:HG3	1:C:346:ASP:N	2.29	0.48
1:C:315:THR:OG1	1:C:318:PRO:HB3	2.14	0.48
1:A:283:PHE:O	1:A:321:PHE:HA	2.14	0.47
1:C:93:TYR:O	1:C:97:THR:HG23	2.13	0.47
1:B:178:VAL:O	1:B:179:ALA:C	2.57	0.47
1:D:62:ILE:CD1	1:D:70:ILE:HD13	2.44	0.47
1:A:61:LYS:HD3	1:A:66:ASP:OD1	2.14	0.47
1:D:97:THR:HG21	1:D:169:ILE:N	2.29	0.47
1:B:114:LEU:CD1	1:B:145:MET:HE1	2.35	0.47
1:B:265:LYS:HD3	3:B:537:HOH:O	2.14	0.47
1:C:181:GLN:O	1:C:182:LEU:HD23	2.14	0.47
1:D:91:HIS:HA	1:D:94:ILE:HG13	1.96	0.47
1:D:173:PHE:HB2	1:D:176:VAL:HB	1.96	0.47
1:D:219:MET:HB3	1:D:401:LYS:HB2	1.97	0.47
1:D:404:MET:HG3	1:D:411:ILE:HD12	1.96	0.47
1:C:178:VAL:O	1:C:179:ALA:C	2.58	0.47
1:C:278:LEU:HD11	1:C:329:ILE:CD1	2.45	0.47
1:D:66:ASP:O	1:D:70:ILE:HG12	2.15	0.47
1:D:93:TYR:CD2	1:D:169:ILE:HD11	2.50	0.46
1:A:109:TYR:O	1:A:111:VAL:HG13	2.15	0.46
1:C:130:HIS:CD2	1:C:131:HIS:ND1	2.83	0.46
1:C:135:MET:HE2	1:C:404:MET:HB2	1.97	0.46
1:D:227:LEU:O	1:D:231:ARG:HG3	2.15	0.46
1:D:327:GLN:O	1:D:328:ARG:HD2	2.15	0.46
1:B:221:PHE:CD2	1:B:414:LEU:HD23	2.51	0.46
1:C:155:ASP:OD2	1:C:185:VAL:HB	2.15	0.46
1:A:59:CYS:SG	1:A:413:CYS:SG	3.03	0.46
1:B:298:TYR:CZ	1:B:302:ASN:ND2	2.83	0.46
1:C:329:ILE:HB	1:C:332:VAL:HG23	1.98	0.46
1:A:114:LEU:HG	1:A:145:MET:HE1	1.96	0.46
1:C:303:GLU:CD	1:C:303:GLU:H	2.23	0.46
1:C:353:PHE:CD2	1:C:391:MET:HG3	2.51	0.46
1:D:57:VAL:HG11	1:D:73:VAL:CG2	2.46	0.46
1:D:113:PRO:CB	1:D:119:VAL:HG22	2.44	0.46
1:A:361:GLY:O	1:A:371:PRO:HD3	2.15	0.46
1:D:147:GLN:OE1	1:D:147:GLN:N	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HD2	1:A:184:SER:OG	2.15	0.46
1:A:407:ASP:OD1	1:A:409:PHE:HB2	2.15	0.46
1:B:107:ARG:NH2	1:B:141:ARG:HH12	2.13	0.46
1:B:128:VAL:HG13	3:B:515:HOH:O	2.15	0.46
1:C:329:ILE:HB	1:C:332:VAL:CG2	2.46	0.46
1:D:89:THR:N	1:D:92:ASP:OD2	2.45	0.46
1:D:107:ARG:HE	1:D:107:ARG:HA	1.80	0.46
1:A:85:ARG:HB3	1:A:85:ARG:NH1	2.30	0.46
1:A:140:LEU:O	1:A:144:TYR:HB2	2.16	0.46
1:C:73:VAL:HG23	1:C:74:LYS:N	2.30	0.46
1:C:257:LYS:O	1:C:273:LYS:HD2	2.16	0.46
1:C:360:GLU:OE2	1:C:372:CYS:N	2.48	0.46
1:D:321:PHE:CD1	1:D:321:PHE:C	2.93	0.46
1:B:138:ARG:HH22	1:B:412:GLN:HG2	1.81	0.46
1:C:259:TYR:CE2	1:C:316:TYR:HB2	2.51	0.46
1:B:131:HIS:ND1	1:B:132:LYS:CG	2.79	0.45
1:B:174:ASP:OD1	1:B:174:ASP:N	2.49	0.45
1:B:212:TYR:CE2	1:B:292:THR:HG22	2.51	0.45
1:B:348:ASN:O	1:B:395:HIS:HE1	1.99	0.45
1:C:221:PHE:HD2	1:C:414:LEU:HD23	1.81	0.45
1:C:241:ASN:CG	1:C:350:ILE:HG13	2.41	0.45
1:B:123:ILE:HG22	1:B:124:ALA:N	2.31	0.45
1:B:237:THR:O	1:B:237:THR:HG22	2.16	0.45
1:C:258:ARG:CG	1:C:273:LYS:HG2	2.40	0.45
1:C:382:VAL:HG22	1:C:401:LYS:HG3	1.97	0.45
1:D:208:ALA:HA	1:D:293:ARG:CZ	2.46	0.45
1:B:115:THR:OG1	1:B:118:GLU:HG3	2.16	0.45
1:B:378:ARG:HB2	1:B:378:ARG:HH11	1.82	0.45
1:A:326:ILE:HA	1:A:329:ILE:HD12	1.97	0.45
1:D:57:VAL:HG13	1:D:69:GLU:OE1	2.16	0.45
1:C:71:GLN:O	1:C:75:LEU:HG	2.17	0.45
1:C:228:GLU:OE2	1:C:421:LYS:HE2	2.16	0.45
1:A:388:LEU:CD2	1:A:414:LEU:HD13	2.46	0.45
1:C:207:ASN:OD1	1:C:209:ASN:N	2.38	0.45
1:C:273:LYS:HB3	1:C:273:LYS:HZ3	1.81	0.45
1:D:293:ARG:HH11	1:D:293:ARG:HG2	1.82	0.45
1:B:60:THR:O	1:B:64:GLN:HG3	2.16	0.45
1:C:221:PHE:CG	1:C:222:PRO:HD2	2.52	0.45
1:C:255:TRP:CH2	1:C:256:LYS:HE3	2.51	0.45
1:C:279:LYS:HA	1:C:279:LYS:HD2	1.87	0.45
1:D:353:PHE:HB2	1:D:396:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:GLU:HA	1:D:159:GLU:OE1	2.17	0.45
1:B:276:PRO:HG3	1:B:311:TRP:CZ2	2.52	0.45
1:B:327:GLN:NE2	1:B:335:SER:HA	2.31	0.45
1:B:339:SER:C	1:B:341:LYS:H	2.25	0.45
1:C:259:TYR:CB	1:C:266:LEU:HD11	2.45	0.45
1:D:100:CYS:O	1:D:104:ILE:HD13	2.17	0.45
1:B:100:CYS:O	1:B:104:ILE:HD13	2.17	0.45
1:B:155:ASP:C	1:B:157:LYS:H	2.25	0.45
1:D:60:THR:O	1:D:64:GLN:HG3	2.17	0.44
1:D:103:PHE:CE1	1:D:107:ARG:HG3	2.52	0.44
1:D:386:GLY:O	1:D:387:ASP:C	2.60	0.44
1:A:106:THR:O	1:A:108:LYS:HG3	2.16	0.44
1:B:241:ASN:ND2	1:B:350:ILE:HG12	2.32	0.44
1:A:219:MET:HG3	3:A:562:HOH:O	2.17	0.44
1:C:214:ILE:N	1:C:214:ILE:HD12	2.33	0.44
1:C:350:ILE:C	1:C:350:ILE:HD12	2.41	0.44
1:D:417:HIS:C	1:D:417:HIS:CD2	2.93	0.44
1:B:346:ASP:O	1:B:396:HIS:HE1	2.01	0.44
1:A:252:GLU:O	1:A:256:LYS:HG2	2.18	0.44
1:B:288:TYR:CG	1:B:352:ARG:NH2	2.85	0.44
1:A:131:HIS:ND1	1:A:131:HIS:C	2.76	0.44
1:B:167:GLN:NE2	1:B:167:GLN:HA	2.33	0.44
1:C:409:PHE:HA	1:C:412:GLN:CB	2.47	0.44
1:D:241:ASN:CG	1:D:350:ILE:HG12	2.43	0.44
1:C:346:ASP:O	1:C:396:HIS:HE1	2.01	0.44
1:A:372:CYS:HB2	1:A:381:CYS:SG	2.58	0.44
1:B:131:HIS:ND1	1:B:131:HIS:C	2.75	0.44
1:C:208:ALA:HA	1:C:293:ARG:NE	2.33	0.44
1:A:219:MET:CE	1:A:401:LYS:HD3	2.48	0.44
1:B:103:PHE:CE1	1:B:107:ARG:HG3	2.53	0.44
1:D:90:PRO:HG3	3:D:532:HOH:O	2.18	0.44
1:D:155:ASP:OD2	1:D:157:LYS:HB2	2.17	0.43
1:B:420:ARG:O	1:B:424:GLU:HG3	2.18	0.43
1:D:150:TYR:N	1:D:150:TYR:CD2	2.85	0.43
1:A:131:HIS:HA	1:A:162:PHE:CE1	2.52	0.43
1:A:200:MET:O	1:A:204:TYR:HB2	2.17	0.43
1:A:258:ARG:HG2	1:A:314:ASP:OD2	2.18	0.43
1:B:98:ARG:HD3	1:B:98:ARG:HA	1.72	0.43
1:A:100:CYS:O	1:A:101:ALA:C	2.61	0.43
1:C:48:LEU:HG	1:C:419:ARG:HG2	2.00	0.43
1:D:96:MET:HE2	1:D:103:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:C	1:D:146:PRO:HG2	2.44	0.43
1:D:221:PHE:HB3	1:D:402:PHE:CE2	2.53	0.43
1:D:387:ASP:HA	3:D:531:HOH:O	2.18	0.43
1:D:388:LEU:CD1	1:D:414:LEU:HD13	2.48	0.43
1:A:377:VAL:HG12	1:A:378:ARG:NH1	2.34	0.43
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.87	0.43
1:A:256:LYS:O	1:A:273:LYS:HG2	2.19	0.43
1:B:121:PHE:CE1	1:B:211:LYS:HG3	2.54	0.43
1:D:107:ARG:O	1:D:108:LYS:HB2	2.18	0.43
1:D:258:ARG:HB3	1:D:271:ILE:HB	2.00	0.43
1:A:85:ARG:O	1:A:87:ARG:HG2	2.19	0.43
1:C:400:ASN:HA	1:C:401:LYS:HA	1.68	0.43
1:D:123:ILE:HD13	1:D:226:ASN:HD21	1.84	0.43
1:D:299:VAL:HG13	1:D:305:ILE:HG21	2.01	0.43
1:A:87:ARG:HG3	1:A:87:ARG:HH11	1.84	0.43
1:C:130:HIS:O	1:C:131:HIS:HB3	2.17	0.43
1:C:369:TYR:HE2	3:C:510:HOH:O	2.01	0.43
1:A:223:ILE:HG22	1:A:391:MET:HE3	2.01	0.43
1:B:304:ASN:ND2	3:B:588:HOH:O	2.51	0.43
1:C:82:PHE:O	1:C:83:LYS:C	2.61	0.43
1:C:305:ILE:O	1:C:309:MET:HG3	2.18	0.43
1:C:331:GLU:CD	1:C:331:GLU:N	2.75	0.43
1:D:145:MET:HG3	1:D:147:GLN:OE1	2.18	0.43
1:A:247:MET:HA	1:A:248:PRO:HD3	1.90	0.42
1:D:74:LYS:HA	1:D:77:ILE:HD12	2.01	0.42
1:A:248:PRO:HD3	1:A:284:SER:HB2	2.00	0.42
1:A:336:PHE:O	1:A:337:PRO:C	2.63	0.42
1:B:136:LEU:HD23	1:B:166:VAL:HG22	2.02	0.42
1:B:244:THR:HG23	1:B:244:THR:O	2.19	0.42
1:B:328:ARG:HD2	1:B:336:PHE:HB2	2.01	0.42
1:D:230:VAL:O	1:D:234:LYS:HG3	2.20	0.42
1:D:378:ARG:O	1:D:379:SER:HB2	2.20	0.42
1:C:241:ASN:ND2	1:C:350:ILE:HG13	2.34	0.42
1:C:276:PRO:HA	1:C:277:PRO:HD3	1.85	0.42
1:C:332:VAL:HA	1:C:333:PRO:HD3	1.86	0.42
1:D:74:LYS:O	1:D:77:ILE:HB	2.19	0.42
1:D:392:LEU:HD23	1:D:392:LEU:HA	1.93	0.42
1:B:130:HIS:O	1:B:131:HIS:HB3	2.19	0.42
1:B:355:LYS:HB2	1:B:381:CYS:HB3	2.00	0.42
1:B:400:ASN:HA	1:B:401:LYS:HA	1.64	0.42
1:C:117:GLU:OE1	1:C:227:LEU:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:CYS:SG	1:D:199:CYS:HA	2.60	0.42
1:A:298:TYR:CE1	1:A:332:VAL:HG22	2.54	0.42
1:B:203:LEU:HA	1:B:206:MET:HG2	2.02	0.42
1:B:417:HIS:CE1	1:B:421:LYS:HD2	2.55	0.42
1:C:208:ALA:HA	1:C:293:ARG:CZ	2.49	0.42
1:D:208:ALA:HA	1:D:293:ARG:NE	2.35	0.42
1:D:416:GLU:O	1:D:419:ARG:HB3	2.18	0.42
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.85	0.42
1:B:131:HIS:ND1	1:B:132:LYS:HG3	2.34	0.42
1:B:221:PHE:CD2	1:B:222:PRO:HD2	2.55	0.42
1:D:127:ILE:HD12	1:D:152:ILE:CD1	2.50	0.42
1:A:226:ASN:O	1:A:230:VAL:HG23	2.20	0.42
1:C:79:THR:HG22	1:C:81:GLN:HB3	2.02	0.42
1:C:252:GLU:O	1:C:256:LYS:HG2	2.19	0.42
1:D:85:ARG:HG3	1:D:85:ARG:NH1	2.35	0.42
1:A:118:GLU:OE1	1:A:145:MET:HE2	2.20	0.42
1:B:123:ILE:N	1:B:123:ILE:HD12	2.35	0.42
1:C:125:TYR:HB3	1:C:127:ILE:HD11	2.02	0.42
1:C:236:SER:O	1:C:239:GLU:HB2	2.20	0.42
1:A:113:PRO:HG3	1:A:146:PRO:HG2	2.02	0.41
1:A:223:ILE:CG2	1:A:391:MET:HE3	2.49	0.41
1:B:212:TYR:CD1	1:B:233:LEU:HD22	2.55	0.41
1:A:408:PRO:O	1:A:412:GLN:HB2	2.19	0.41
1:B:61:LYS:CB	1:B:69:GLU:HG3	2.49	0.41
1:B:155:ASP:C	1:B:157:LYS:N	2.77	0.41
1:B:204:TYR:CE1	1:B:293:ARG:NH1	2.88	0.41
1:C:249:PRO:HA	1:C:252:GLU:OE1	2.19	0.41
1:C:360:GLU:HG2	1:C:369:TYR:CE1	2.55	0.41
1:D:138:ARG:HH22	1:D:412:GLN:HB2	1.86	0.41
1:D:330:PRO:O	1:D:331:GLU:HB2	2.20	0.41
1:A:130:HIS:HD2	3:A:510:HOH:O	2.04	0.41
1:A:293:ARG:HG2	1:A:293:ARG:NH1	2.35	0.41
1:D:85:ARG:HG3	1:D:85:ARG:O	2.21	0.41
1:D:244:THR:HG23	1:D:244:THR:O	2.20	0.41
1:B:110:ILE:HG21	1:B:114:LEU:HD11	2.02	0.41
1:C:89:THR:OG1	1:C:90:PRO:HD2	2.20	0.41
1:C:265:LYS:HB3	1:C:265:LYS:HZ2	1.84	0.41
1:D:210:TRP:CD1	1:D:210:TRP:H	2.38	0.41
1:B:242:LEU:HD23	1:B:242:LEU:N	2.35	0.41
1:C:113:PRO:HB3	1:C:119:VAL:CG2	2.48	0.41
1:C:362:ASP:O	1:C:367:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:H	1:A:304:ASN:ND2	2.18	0.41
1:A:400:ASN:HA	1:A:401:LYS:HA	1.56	0.41
1:D:156:ARG:C	1:D:158:ALA:H	2.29	0.41
1:D:397:LEU:N	1:D:397:LEU:HD23	2.35	0.41
1:C:166:VAL:O	1:C:167:GLN:C	2.62	0.41
1:D:57:VAL:HG11	1:D:73:VAL:HG22	2.02	0.41
1:D:91:HIS:HA	1:D:94:ILE:CG1	2.50	0.41
1:C:350:ILE:HD13	1:C:397:LEU:HG	2.03	0.41
1:A:212:TYR:CZ	1:A:292:THR:HG22	2.56	0.41
1:A:257:LYS:HG3	1:A:268:ASN:HD21	1.86	0.41
1:A:384:GLY:O	1:A:385:ALA:C	2.64	0.41
1:B:160:GLU:HG3	1:B:161:SER:N	2.35	0.41
1:B:222:PRO:O	1:B:418:LEU:HD11	2.20	0.41
1:B:294:GLU:H	1:B:294:GLU:CD	2.27	0.41
1:C:278:LEU:HD11	1:C:329:ILE:HD11	2.03	0.41
1:C:337:PRO:HD2	1:C:342:TYR:CG	2.56	0.41
1:D:149:PHE:CZ	1:D:207:ASN:ND2	2.89	0.41
1:D:266:LEU:HD23	1:D:316:TYR:CD1	2.56	0.41
1:D:280:THR:HB	1:D:329:ILE:CD1	2.51	0.41
1:D:350:ILE:O	1:D:397:LEU:HG	2.21	0.41
1:C:79:THR:HG22	1:C:80:VAL:N	2.36	0.41
1:C:257:LYS:HA	1:C:271:ILE:O	2.20	0.41
1:C:57:VAL:HA	1:C:72:LYS:HZ1	1.86	0.40
1:C:224:LYS:HB2	1:C:229:ILE:CD1	2.51	0.40
1:D:107:ARG:O	1:D:141:ARG:HD2	2.21	0.40
1:C:287:ALA:HB2	1:C:319:ASP:OD2	2.20	0.40
1:C:303:GLU:CD	1:C:303:GLU:N	2.79	0.40
1:D:293:ARG:HG2	1:D:293:ARG:NH1	2.36	0.40
1:A:342:TYR:HE1	1:B:368:PRO:HA	1.86	0.40
1:B:121:PHE:CG	1:B:230:VAL:HG13	2.57	0.40
1:B:304:ASN:C	1:B:306:GLN:N	2.79	0.40
1:C:80:VAL:HG13	1:C:83:LYS:HD2	2.03	0.40
1:D:394:GLN:HB3	1:D:396:HIS:HD2	1.86	0.40
1:C:318:PRO:HA	1:C:321:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/391 (92%)	341 (94%)	20 (6%)	0	100	100
1	B	355/391 (91%)	321 (90%)	27 (8%)	7 (2%)	6	16
1	C	370/391 (95%)	339 (92%)	27 (7%)	4 (1%)	11	29
1	D	362/391 (93%)	322 (89%)	32 (9%)	8 (2%)	5	14
All	All	1448/1564 (93%)	1323 (91%)	106 (7%)	19 (1%)	9	25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	383	PHE
1	D	87	ARG
1	D	114	LEU
1	C	365	ASN
1	D	86	PRO
1	D	365	ASN
1	C	237	THR
1	D	385	ALA
1	B	383	PHE
1	D	387	ASP
1	B	156	ARG
1	B	351	ALA
1	B	113	PRO
1	B	179	ALA
1	B	365	ASN
1	C	86	PRO
1	D	110	ILE
1	D	374	GLY
1	B	73	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/351 (93%)	313 (96%)	14 (4%)	26	54
1	B	321/351 (92%)	310 (97%)	11 (3%)	32	62
1	C	336/351 (96%)	329 (98%)	7 (2%)	47	75
1	D	330/351 (94%)	321 (97%)	9 (3%)	39	69
All	All	1314/1404 (94%)	1273 (97%)	41 (3%)	35	65

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

Mol	Chain	Res	Type
1	A	131	HIS
1	A	135	MET
1	A	189	SER
1	A	242	LEU
1	A	253	GLU
1	A	273	LYS
1	A	286	SER
1	A	322	LEU
1	A	331	GLU
1	A	337	PRO
1	A	338	SER
1	A	352	ARG
1	A	378	ARG
1	A	404	MET
1	B	131	HIS
1	B	140	LEU
1	B	160	GLU
1	B	167	GLN
1	B	175	ASN
1	B	242	LEU
1	B	307	LYS
1	B	317	SER
1	B	341	LYS
1	B	365	ASN

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Mol	Chain	Res	Type
1	B	381	CYS
1	C	69	GLU
1	C	131	HIS
1	C	184	SER
1	C	265	LYS
1	C	306	GLN
1	C	317	SER
1	C	331	GLU
1	D	107	ARG
1	D	131	HIS
1	D	156	ARG
1	D	161	SER
1	D	167	GLN
1	D	278	LEU
1	D	279	LYS
1	D	309	MET
1	D	317	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	148	ASN
1	A	181	GLN
1	A	226	ASN
1	A	304	ASN
1	A	340	ASN
1	A	376	HIS
1	A	396	HIS
1	B	64	GLN
1	B	148	ASN
1	B	167	GLN
1	B	175	ASN
1	B	209	ASN
1	B	226	ASN
1	B	250	ASN
1	B	304	ASN
1	B	306	GLN
1	B	313	GLN
1	B	394	GLN
1	B	395	HIS
1	B	396	HIS

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Mol	Chain	Res	Type
1	B	412	GLN
1	B	417	HIS
1	C	58	ASN
1	C	71	GLN
1	C	95	ASN
1	C	148	ASN
1	C	226	ASN
1	C	394	GLN
1	C	396	HIS
1	D	95	ASN
1	D	148	ASN
1	D	167	GLN
1	D	181	GLN
1	D	209	ASN
1	D	226	ASN
1	D	250	ASN
1	D	313	GLN
1	D	348	ASN
1	D	365	ASN
1	D	396	HIS
1	D	412	GLN
1	D	417	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

8 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	NGA	E	1	2	15,15,15	0.52	0	21,21,21	0.79	1 (4%)
2	GAL	E	2	2	11,11,12	0.48	0	15,15,17	0.33	0
2	NGA	F	1	2	15,15,15	0.49	0	21,21,21	0.60	0
2	GAL	F	2	2	11,11,12	0.40	0	15,15,17	0.33	0
2	NGA	G	1	2	15,15,15	0.42	0	21,21,21	0.73	0
2	GAL	G	2	2	11,11,12	0.44	0	15,15,17	0.42	0
2	NGA	H	1	2	15,15,15	0.43	0	21,21,21	0.85	0
2	GAL	H	2	2	11,11,12	0.39	0	15,15,17	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NGA	E	1	2	-	2/6/26/26	0/1/1/1
2	GAL	E	2	2	-	1/2/19/22	0/1/1/1
2	NGA	F	1	2	-	1/6/26/26	0/1/1/1
2	GAL	F	2	2	-	2/2/19/22	0/1/1/1
2	NGA	G	1	2	-	2/6/26/26	0/1/1/1
2	GAL	G	2	2	-	2/2/19/22	0/1/1/1
2	NGA	H	1	2	-	2/6/26/26	0/1/1/1
2	GAL	H	2	2	-	2/2/19/22	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(°)
2	E	1	NGA	C1-C2-C3	-2.15	107.61	110.54

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	GAL	O5-C5-C6-O6
2	G	1	NGA	O5-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6
2	H	1	NGA	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6

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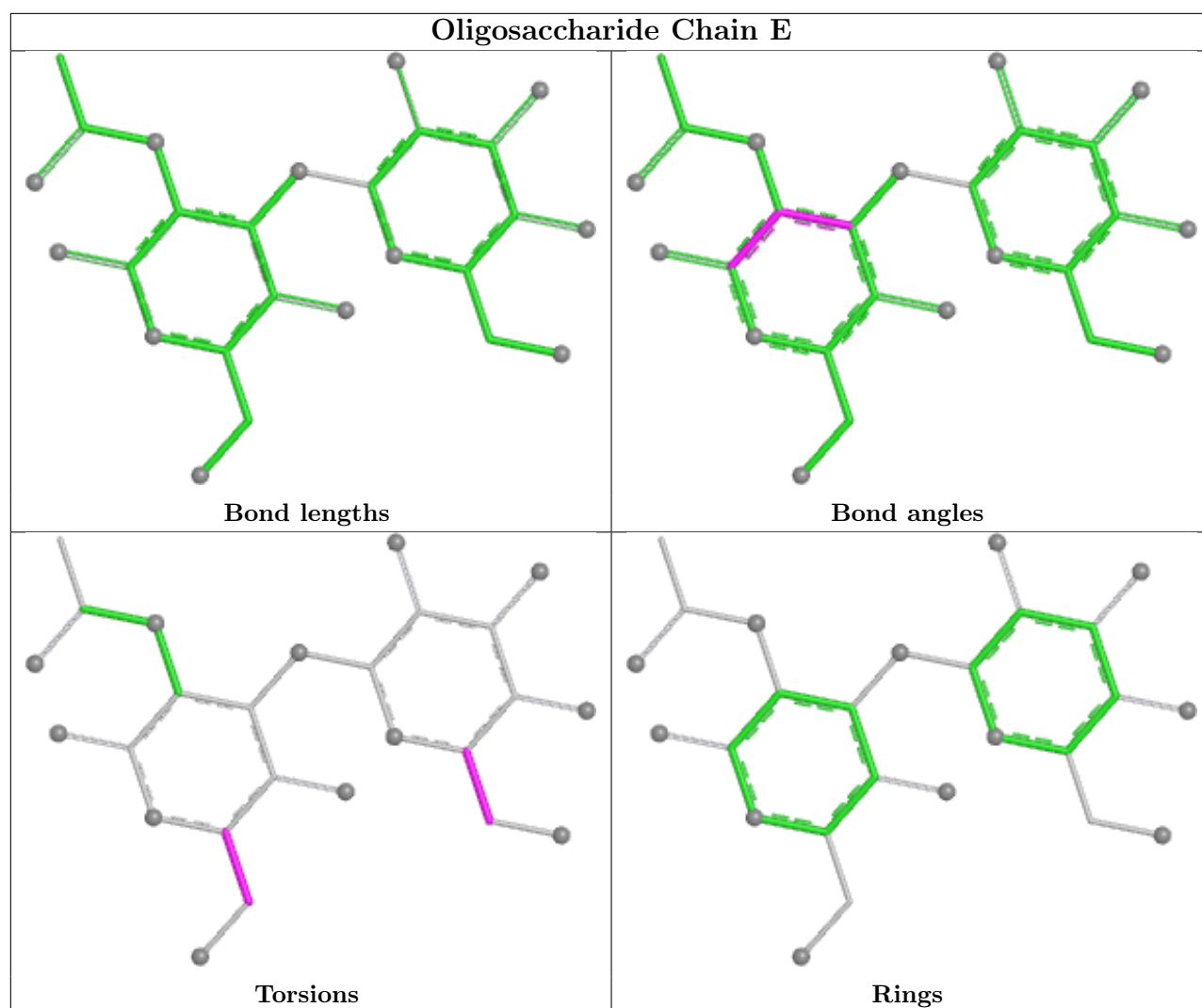
Mol	Chain	Res	Type	Atoms
2	H	1	NGA	C4-C5-C6-O6
2	G	1	NGA	C4-C5-C6-O6
2	E	1	NGA	O5-C5-C6-O6
2	G	2	GAL	C4-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	F	2	GAL	C4-C5-C6-O6
2	H	2	GAL	C4-C5-C6-O6
2	F	1	NGA	O5-C5-C6-O6
2	E	1	NGA	C4-C5-C6-O6

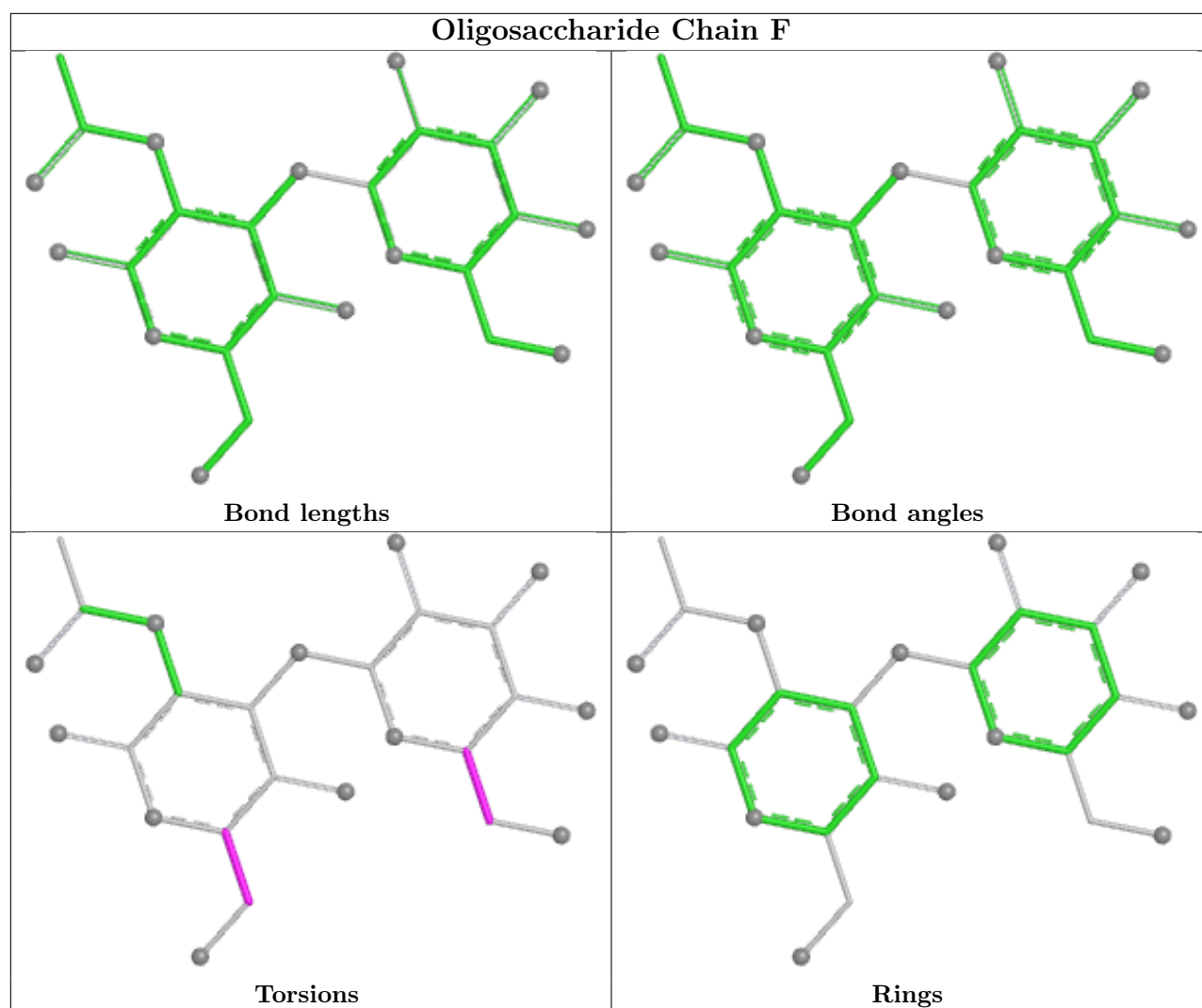
There are no ring outliers.

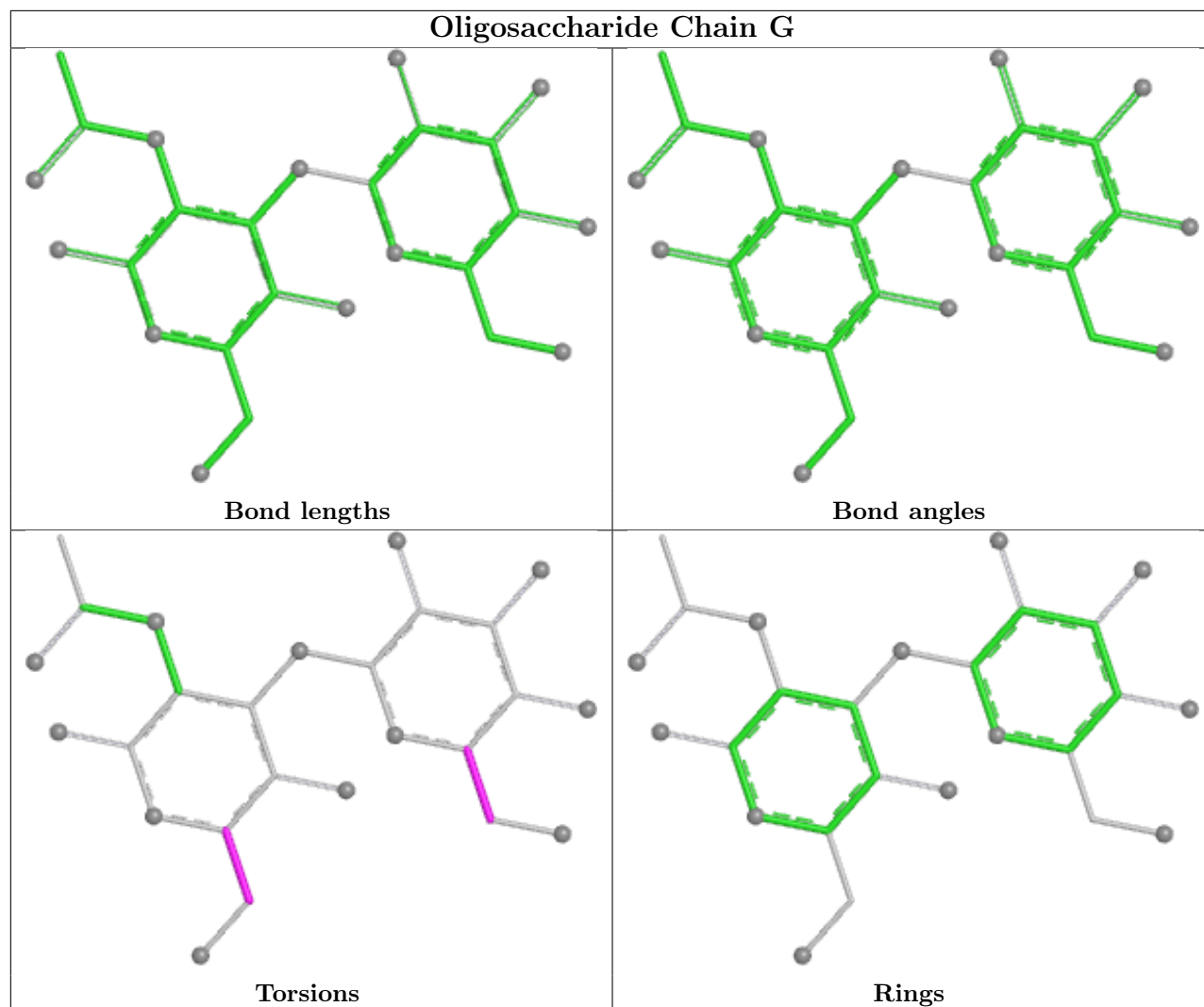
2 monomers are involved in 2 short contacts:

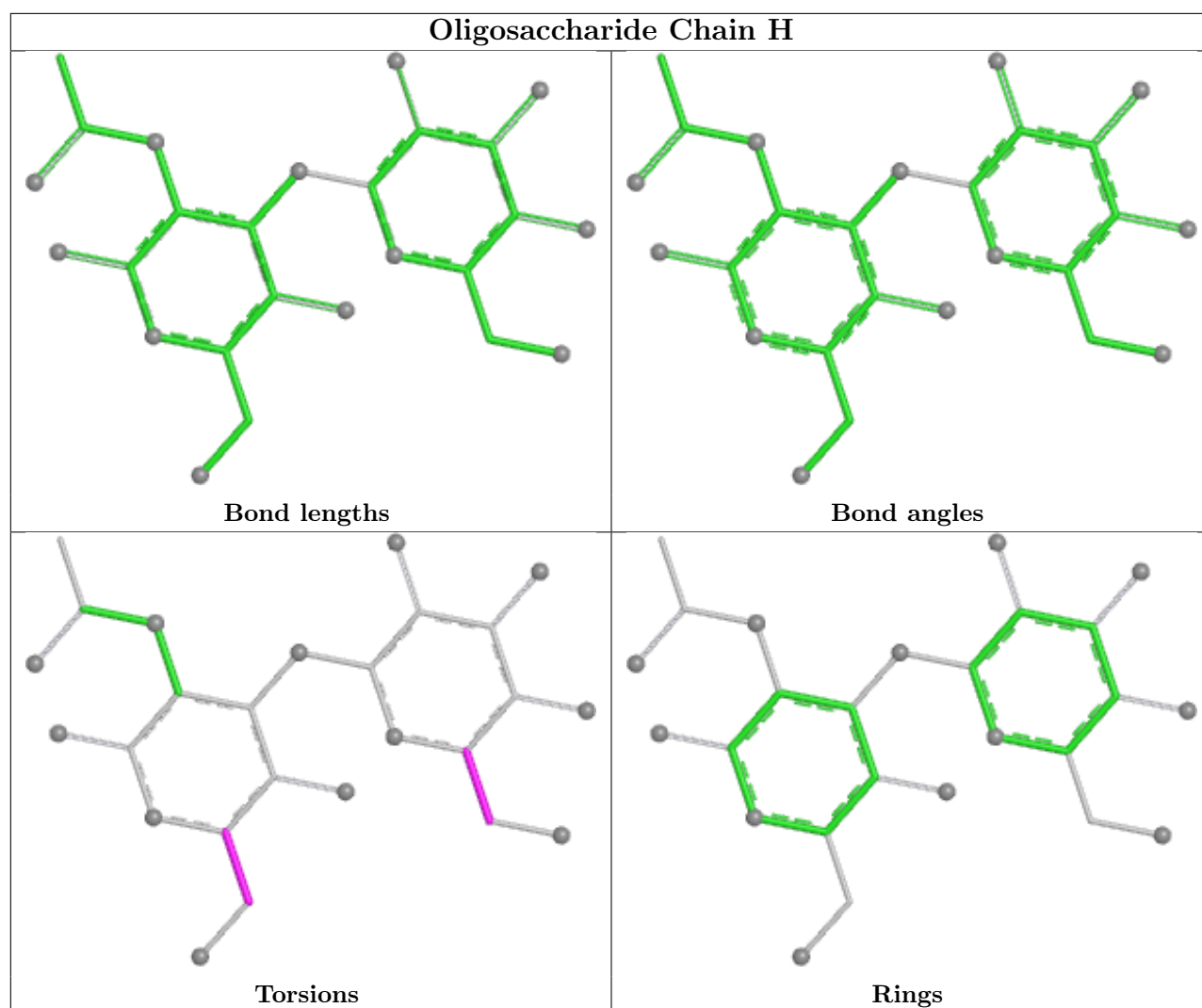
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GAL	1	0
2	H	1	NGA	1	0

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









5.6 Ligand geometry [i](#)

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	365/391 (93%)	-0.02	4 (1%) 78 76	19, 41, 72, 107	0
1	B	359/391 (91%)	-0.11	3 (0%) 82 81	18, 36, 70, 87	0
1	C	374/391 (95%)	0.10	12 (3%) 50 46	21, 41, 90, 114	0
1	D	368/391 (94%)	0.32	15 (4%) 41 37	15, 46, 93, 113	0
All	All	1466/1564 (93%)	0.08	34 (2%) 61 58	15, 40, 84, 114	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	PHE	5.0
1	A	80	VAL	4.8
1	D	59	CYS	3.9
1	D	78	LEU	3.2
1	C	80	VAL	3.2
1	D	79	THR	3.1
1	C	78	LEU	2.9
1	D	85	ARG	2.9
1	A	206	MET	2.8
1	D	385	ALA	2.7
1	C	77	ILE	2.7
1	A	78	LEU	2.7
1	D	88	TRP	2.7
1	C	79	THR	2.6
1	C	45	HIS	2.6
1	D	45	HIS	2.5
1	D	57	VAL	2.5
1	D	423	LEU	2.3
1	C	44	ARG	2.3
1	D	90	PRO	2.3
1	D	60	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	60	THR	2.2
1	C	56	ASN	2.2
1	D	74	LYS	2.2
1	B	58	ASN	2.2
1	D	86	PRO	2.2
1	B	208	ALA	2.2
1	A	85	ARG	2.2
1	C	83	LYS	2.1
1	C	307	LYS	2.1
1	D	171	SER	2.1
1	C	58	ASN	2.1
1	C	73	VAL	2.1
1	D	123	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

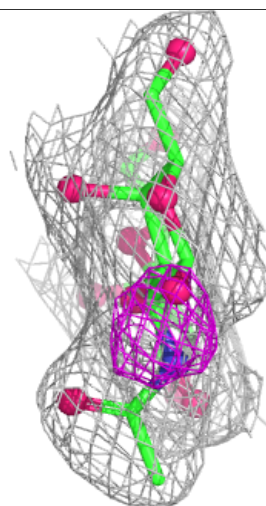
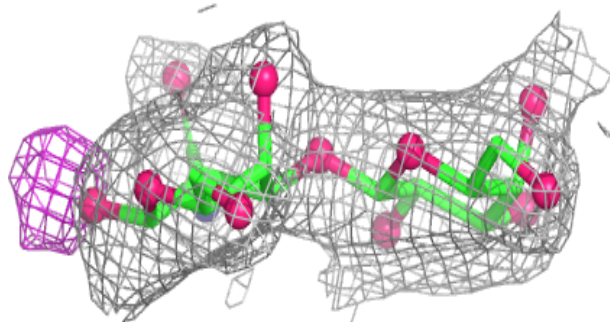
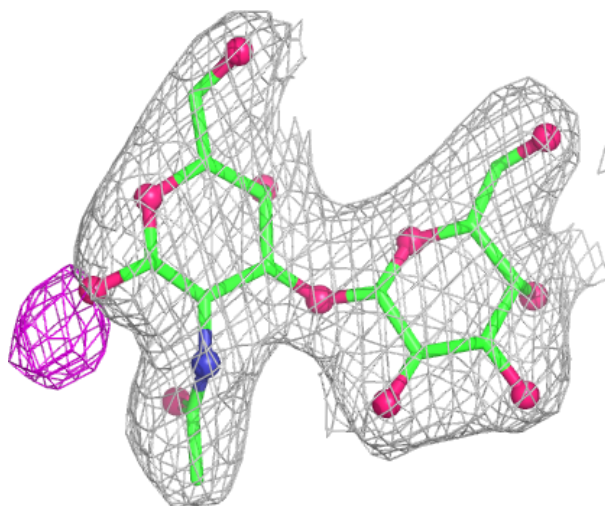
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NGA	E	1	15/15	0.90	0.08	25,31,35,38	0
2	NGA	G	1	15/15	0.92	0.09	39,41,43,44	0
2	NGA	F	1	15/15	0.94	0.07	24,29,32,33	0
2	NGA	H	1	15/15	0.94	0.08	29,32,33,37	0
2	GAL	G	2	11/12	0.95	0.08	41,43,44,45	0
2	GAL	F	2	11/12	0.95	0.07	27,30,31,32	0
2	GAL	E	2	11/12	0.96	0.06	19,23,24,24	0
2	GAL	H	2	11/12	0.96	0.07	21,25,27,28	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.

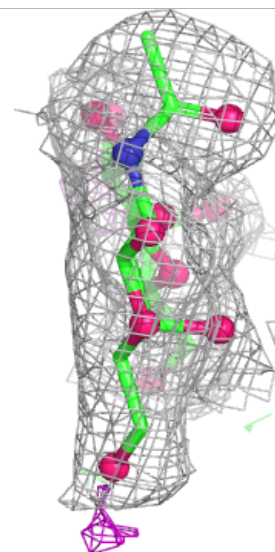
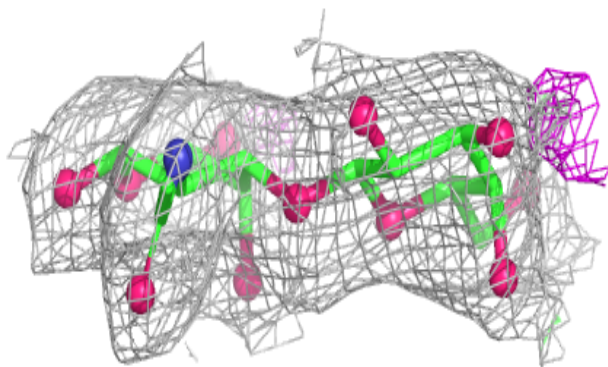
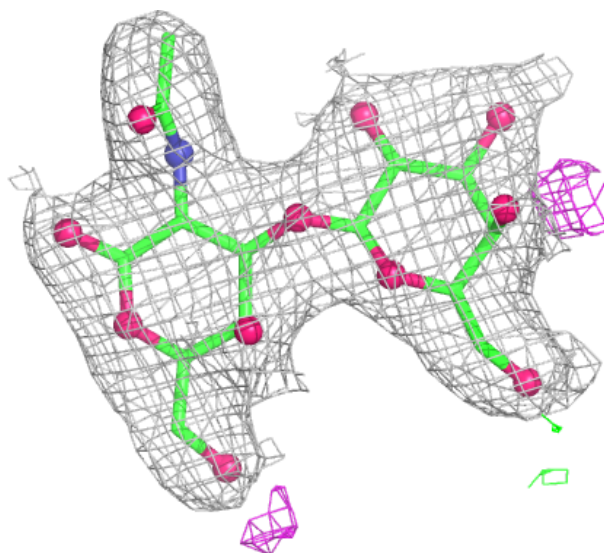
Electron density around Chain E:

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



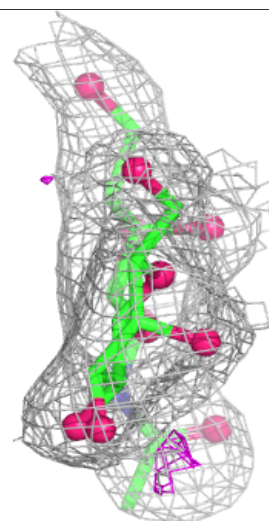
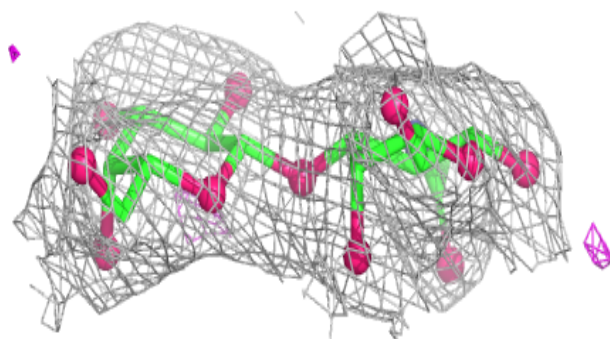
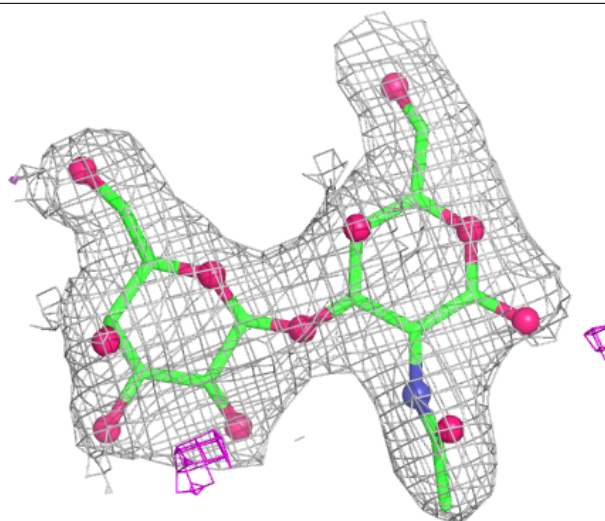
Electron density around Chain F:

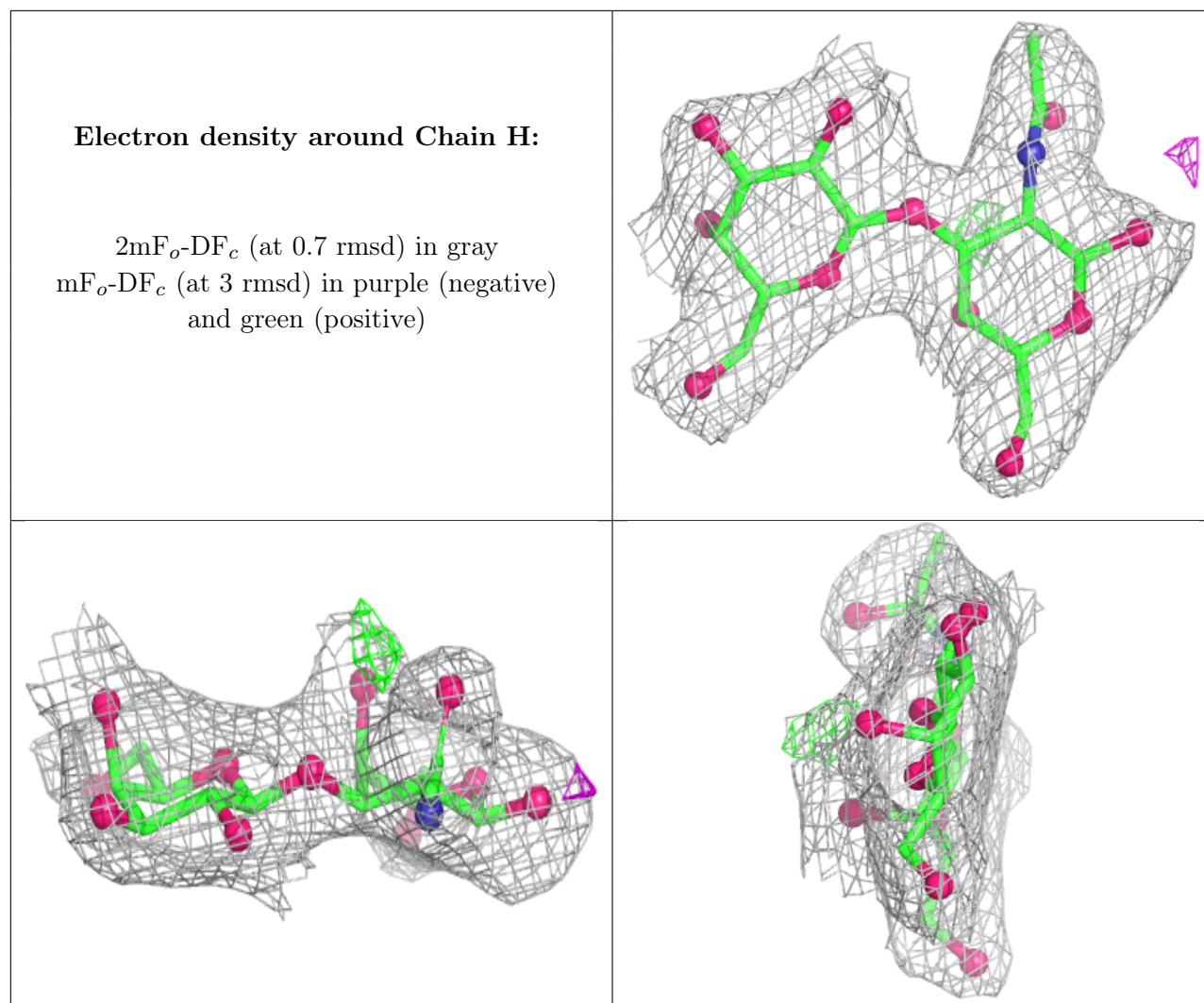
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.