



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:44 PM UTC

PDB ID : 1JYN / pdb_00001jyn
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH LACTOSE
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

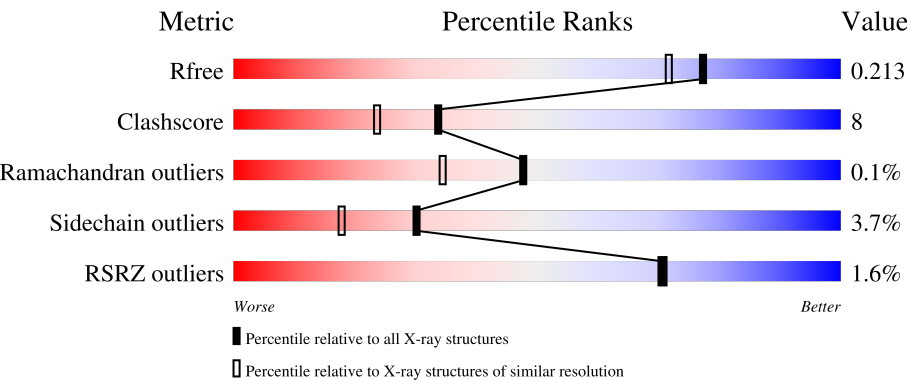
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.80 Å.

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



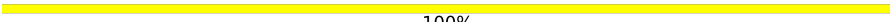
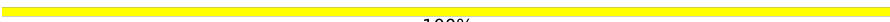
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	1023	% 78%17%..
1	B	1023	2% 77%19%..
1	C	1023	% 78%16%..
1	D	1023	2% 78%17%..
2	E	2	100%

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

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
5	DMS	A	8412	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37546 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-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? P00722
A	8	PRO	ALA	cloning artifact	? P00722
A	537	GLN	GLU	engineered mutation	? P00722
B	1	GLY	THR	cloning artifact	? P00722
B	2	SER	MET	cloning artifact	? P00722
B	3	HIS	ILE	cloning artifact	? P00722
B	4	MET	THR	cloning artifact	? P00722
B	5	LEU	ASP	cloning artifact	? P00722
B	6	GLU	SER	cloning artifact	? P00722
B	7	ASP	LEU	cloning artifact	? P00722
B	8	PRO	ALA	cloning artifact	? P00722
B	537	GLN	GLU	engineered mutation	? P00722
C	1	GLY	THR	cloning artifact	? P00722
C	2	SER	MET	cloning artifact	? P00722
C	3	HIS	ILE	cloning artifact	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
C	537	GLN	GLU	engineered mutation	? P00722
D	1	GLY	THR	cloning artifact	? P00722
D	2	SER	MET	cloning artifact	? P00722
D	3	HIS	ILE	cloning artifact	? P00722
D	4	MET	THR	cloning artifact	? P00722
D	5	LEU	ASP	cloning artifact	? P00722
D	6	GLU	SER	cloning artifact	? P00722
D	7	ASP	LEU	cloning artifact	? P00722
D	8	PRO	ALA	cloning artifact	? P00722
D	537	GLN	GLU	engineered mutation	? P00722

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	2	Total	Mg	0	0
			2	2		
3	C	4	Total	Mg	0	0
			4	4		

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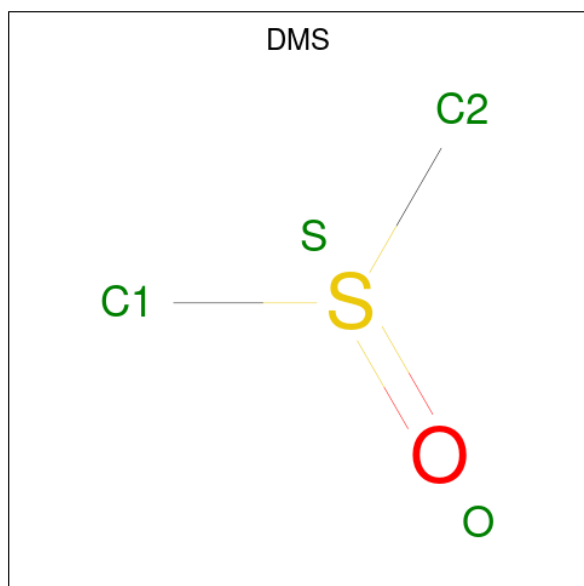
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	4	Total	Mg	0	0
			4	4		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Na	0	0
			4	4		
4	B	4	Total	Na	0	0
			4	4		
4	C	4	Total	Na	0	0
			4	4		
4	D	3	Total	Na	0	0
			3	3		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0

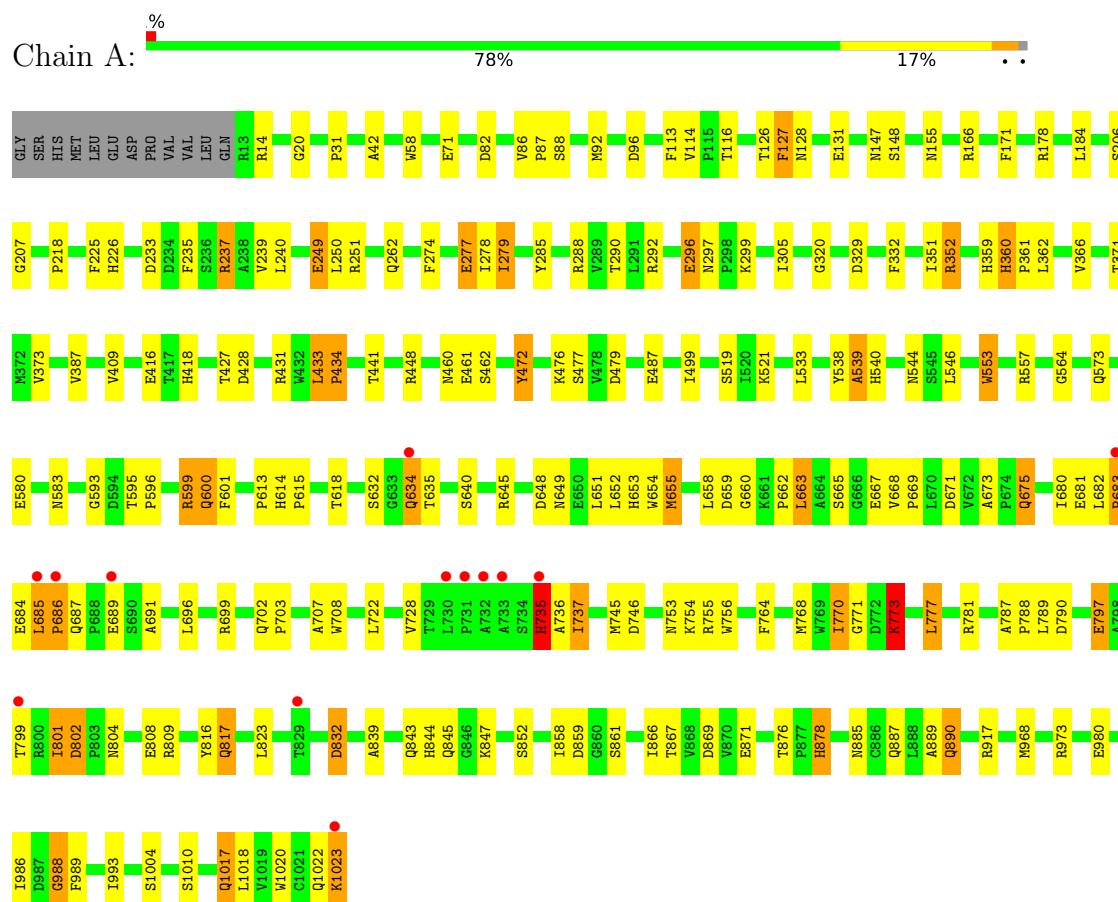
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1136	Total O 1136 1136	0	0
6	B	1151	Total O 1151 1151	0	0
6	C	1133	Total O 1133 1133	0	0
6	D	1109	Total O 1109 1109	0	0

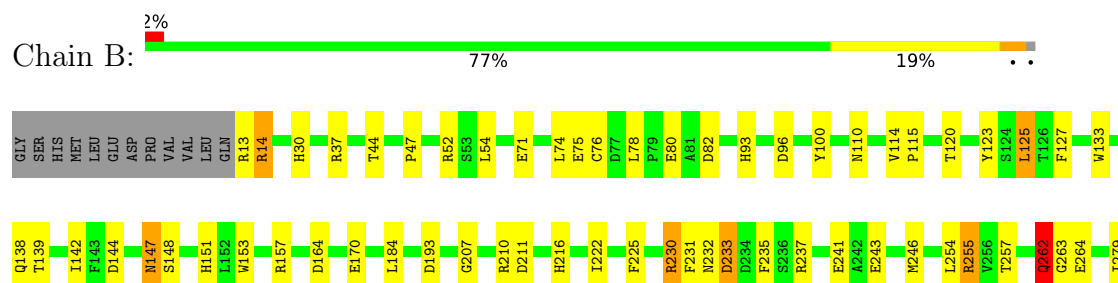
3 Residue-property plots

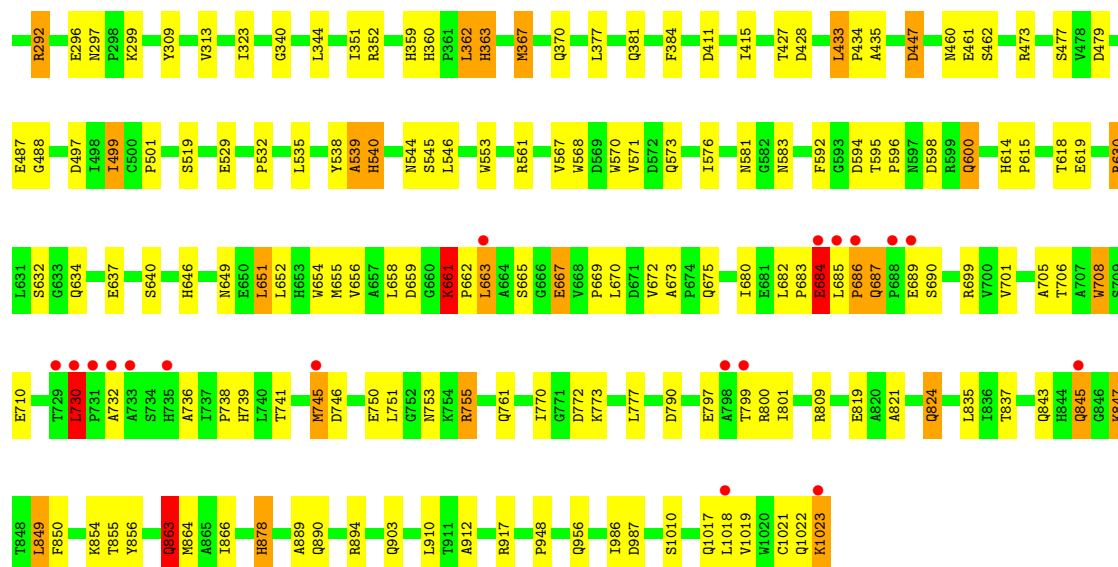
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-Galactosidase

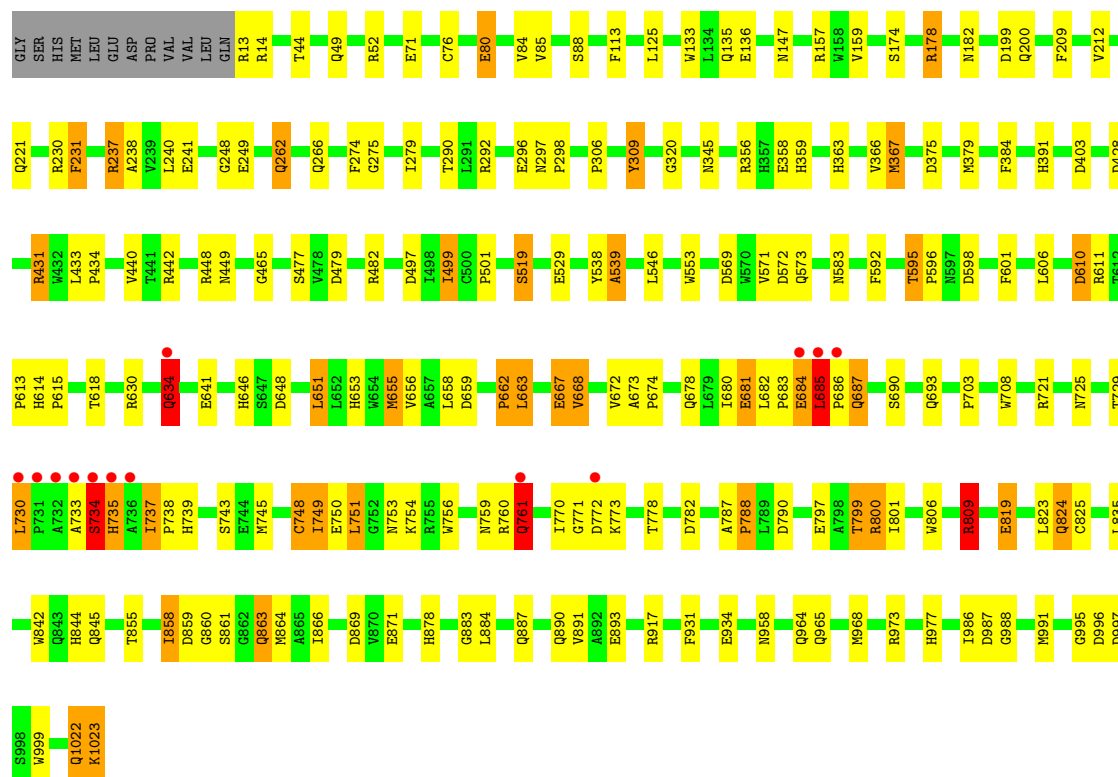
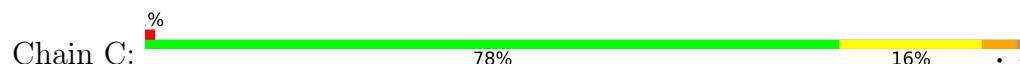


• Molecule 1: Beta-Galactosidase

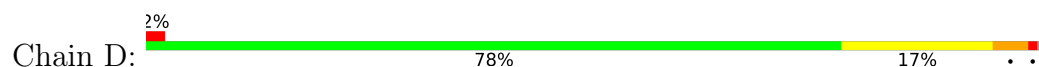


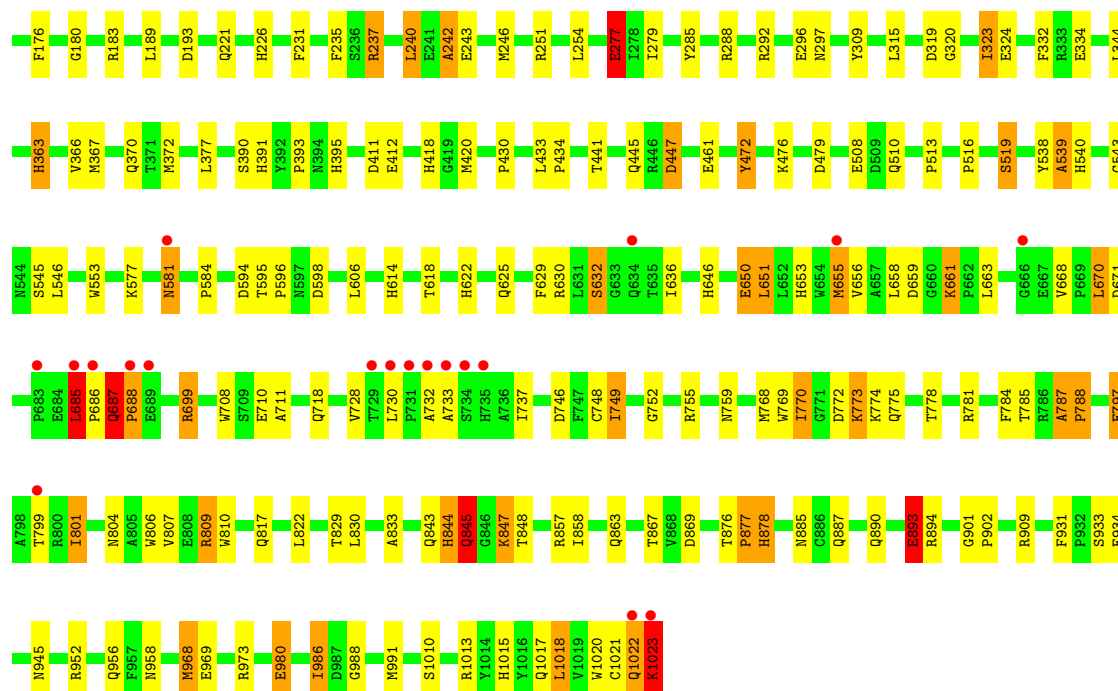


• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase





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

Chain E: 100%

BGC1
GAL2

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

Chain F: 100%

BGC1
GAL2

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

Chain G: 100%

BGC1
GAL2

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

Chain H: 100%

BGC1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.55Å 168.63Å 200.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.80 17.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (17.00-1.80) 93.3 (17.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.80Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.155 , 0.219 0.153 , 0.213	Depositor DCC
R_{free} test set	6261 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 91.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37546	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0529e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BGC, DMS, GAL, MG, NA

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	1.35	10/8383 (0.1%)	1.84	118/11437 (1.0%)
1	B	1.37	11/8383 (0.1%)	1.80	127/11437 (1.1%)
1	C	1.34	14/8383 (0.2%)	1.83	123/11437 (1.1%)
1	D	1.35	10/8383 (0.1%)	1.80	121/11437 (1.1%)
All	All	1.35	45/33532 (0.1%)	1.82	489/45748 (1.1%)

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	D	1	0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	ASN	C-O	-9.90	1.19	1.23
1	D	479	ASP	C-N	-8.72	1.25	1.34
1	A	479	ASP	C-N	-6.70	1.27	1.34
1	C	479	ASP	C-N	-6.54	1.27	1.34
1	D	71	GLU	CD-OE2	6.33	1.37	1.25
1	A	31	PRO	CA-C	6.24	1.57	1.52
1	B	850	PHE	N-CA	5.95	1.53	1.45
1	B	71	GLU	CD-OE2	5.88	1.36	1.25
1	C	297	ASN	CA-C	-5.88	1.49	1.53
1	A	126	THR	CA-C	-5.72	1.45	1.52
1	D	479	ASP	C-O	-5.70	1.18	1.24
1	A	114	VAL	CA-C	5.68	1.58	1.52
1	B	487	GLU	CD-OE2	5.64	1.36	1.25
1	C	465	GLY	CA-C	5.62	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	243	GLU	CD-OE2	5.57	1.35	1.25
1	C	842	TRP	CA-C	-5.56	1.46	1.52
1	B	30	HIS	ND1-CE1	5.55	1.38	1.32
1	A	296	GLU	CD-OE2	5.51	1.35	1.25
1	A	206	SER	N-CA	5.49	1.53	1.46
1	C	212	VAL	C-O	5.48	1.29	1.24
1	B	708	TRP	CA-CB	5.47	1.62	1.54
1	D	650	GLU	CD-OE2	5.46	1.35	1.25
1	C	403	ASP	CG-OD2	5.44	1.35	1.25
1	A	249	GLU	CD-OE2	5.38	1.35	1.25
1	D	1015	HIS	CE1-NE2	5.38	1.38	1.32
1	D	810	TRP	N-CA	5.35	1.52	1.46
1	C	84	VAL	N-CA	5.33	1.52	1.46
1	A	487	GLU	CD-OE2	5.29	1.35	1.25
1	C	751	LEU	CA-C	-5.28	1.46	1.52
1	C	529	GLU	CD-OE2	5.25	1.35	1.25
1	D	277	GLU	CD-OE2	5.23	1.35	1.25
1	D	334	GLU	CD-OE2	5.22	1.35	1.25
1	A	418	HIS	CE1-NE2	5.17	1.37	1.32
1	A	479	ASP	CA-CB	5.16	1.59	1.53
1	C	80	GLU	CD-OE2	5.16	1.35	1.25
1	D	154	CYS	C-O	5.14	1.29	1.23
1	C	693	GLN	CA-CB	5.12	1.60	1.53
1	C	297	ASN	CA-CB	5.12	1.57	1.52
1	B	497	ASP	C-O	5.10	1.30	1.24
1	B	540[A]	HIS	ND1-CE1	5.10	1.37	1.32
1	B	540[B]	HIS	ND1-CE1	5.10	1.37	1.32
1	B	210	ARG	NE-CZ	5.09	1.38	1.33
1	B	488	GLY	CA-C	-5.09	1.47	1.52
1	C	965	GLN	C-O	-5.06	1.18	1.24
1	B	222	ILE	C-O	5.02	1.29	1.24

All (489) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	GLY	CA-C-N	-13.83	100.25	122.79
1	A	771	GLY	C-N-CA	-13.83	100.25	122.79
1	A	685	LEU	CB-CA-C	11.02	123.99	108.68
1	C	725	ASN	CA-CB-CG	-10.91	101.69	112.60
1	B	363	HIS	CA-CB-CG	-10.43	103.37	113.80
1	C	442	ARG	NE-CZ-NH2	-9.94	110.26	119.20
1	D	183	ARG	CD-NE-CZ	-9.41	111.23	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	ASP	CA-CB-CG	-9.10	103.50	112.60
1	D	183	ARG	NE-CZ-NH1	-9.09	112.41	121.50
1	D	143	PHE	CA-CB-CG	-8.99	104.81	113.80
1	A	14	ARG	N-CA-CB	-8.97	99.59	110.53
1	A	685	LEU	CA-C-N	8.76	129.10	119.90
1	A	685	LEU	C-N-CA	8.76	129.10	119.90
1	D	878	HIS	CA-CB-CG	-8.64	105.16	113.80
1	D	845	GLN	CA-C-N	-8.60	108.53	122.20
1	D	845	GLN	C-N-CA	-8.60	108.53	122.20
1	D	614	HIS	N-CA-C	-8.39	100.49	110.13
1	B	790	ASP	CA-CB-CG	-8.21	104.39	112.60
1	C	592	PHE	CA-CB-CG	-8.09	105.71	113.80
1	B	246	MET	CG-SD-CE	-8.08	83.12	100.90
1	C	729	THR	CA-C-N	7.96	131.34	120.67
1	C	729	THR	C-N-CA	7.96	131.34	120.67
1	A	477	SER	N-CA-CB	7.96	121.61	110.07
1	B	614	HIS	N-CA-C	-7.94	101.00	110.13
1	C	614	HIS	N-CA-C	-7.92	101.03	110.13
1	A	788	PRO	N-CA-CB	7.87	110.31	103.31
1	A	832	ASP	N-CA-CB	-7.77	98.59	111.49
1	D	869	ASP	CA-CB-CG	-7.74	104.86	112.60
1	C	113	PHE	CA-CB-CG	-7.70	106.10	113.80
1	C	363	HIS	CA-CB-CG	-7.56	106.24	113.80
1	A	735	HIS	CA-CB-CG	-7.55	106.25	113.80
1	D	279	ILE	CA-CB-CG2	7.55	123.33	110.50
1	D	687	GLN	CB-CA-C	7.52	120.66	110.13
1	A	128	ASN	CA-CB-CG	-7.51	105.09	112.60
1	A	890	GLN	N-CA-CB	-7.49	98.95	109.97
1	D	164	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	689	GLU	O-C-N	7.47	129.76	122.07
1	D	890	GLN	N-CA-CB	-7.46	99.01	109.97
1	A	878	HIS	CA-CB-CG	-7.39	106.41	113.80
1	A	116	THR	CA-CB-OG1	-7.38	98.52	109.60
1	B	777	LEU	N-CA-C	-7.34	104.86	113.88
1	A	685	LEU	CA-C-O	7.32	127.00	120.19
1	D	277	GLU	N-CA-CB	-7.32	99.79	110.26
1	C	809	ARG	CG-CD-NE	7.25	127.96	112.00
1	D	319	ASP	CA-CB-CG	-7.25	105.35	112.60
1	D	867	THR	CA-C-O	-7.24	112.89	120.70
1	B	770	ILE	CA-CB-CG1	-7.20	98.15	110.40
1	B	667	GLU	CB-CG-CD	-7.18	100.39	112.60
1	C	668	VAL	N-CA-CB	-7.13	101.22	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	753	ASN	CA-C-N	-7.13	110.83	122.81
1	C	753	ASN	C-N-CA	-7.13	110.83	122.81
1	A	682	LEU	CB-CA-C	-7.12	97.82	109.27
1	C	782	ASP	CA-CB-CG	-7.10	105.50	112.60
1	A	917	ARG	NE-CZ-NH1	-7.06	114.44	121.50
1	A	771	GLY	N-CA-C	-7.06	99.33	111.47
1	D	363	HIS	CA-CB-CG	-7.05	106.75	113.80
1	B	151	HIS	CA-CB-CG	-7.05	106.75	113.80
1	C	431	ARG	CA-CB-CG	-7.03	100.03	114.10
1	C	199	ASP	CA-CB-CG	-7.02	105.58	112.60
1	B	761	GLN	CA-CB-CG	-6.99	100.12	114.10
1	C	601	PHE	CA-CB-CG	-6.97	106.83	113.80
1	D	844	HIS	CA-CB-CG	-6.95	106.85	113.80
1	D	279	ILE	CB-CG1-CD1	-6.94	99.23	113.80
1	B	986	ILE	CB-CG1-CD1	-6.93	99.24	113.80
1	C	917	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	A	816	TYR	CA-C-N	-6.91	111.51	122.29
1	A	816	TYR	C-N-CA	-6.91	111.51	122.29
1	B	235	PHE	CA-CB-CG	-6.90	106.90	113.80
1	B	878	HIS	CA-CB-CG	-6.86	106.94	113.80
1	B	843	GLN	O-C-N	6.85	132.06	123.15
1	D	877	PRO	CB-CA-C	-6.85	102.94	111.64
1	D	945	ASN	CA-CB-CG	-6.83	105.77	112.60
1	A	279	ILE	CA-CB-CG2	6.83	122.11	110.50
1	B	216	HIS	CA-CB-CG	-6.83	106.97	113.80
1	A	519	SER	N-CA-C	-6.81	100.64	110.24
1	A	601	PHE	CA-CB-CG	-6.81	106.99	113.80
1	C	685	LEU	N-CA-CB	6.80	121.61	110.05
1	B	499	ILE	CA-C-N	-6.80	114.93	123.15
1	B	499	ILE	C-N-CA	-6.80	114.93	123.15
1	C	730	LEU	CA-C-O	6.79	126.59	119.80
1	C	988	GLY	N-CA-C	-6.79	104.07	112.77
1	A	817	GLN	CB-CG-CD	-6.78	101.08	112.60
1	A	867	THR	CA-CB-OG1	-6.77	99.44	109.60
1	D	1023	LYS	N-CA-CB	6.77	122.01	110.50
1	C	598	ASP	CA-CB-CG	-6.75	105.85	112.60
1	D	770	ILE	N-CA-C	-6.75	96.55	107.28
1	A	1017	GLN	CA-CB-CG	-6.72	100.66	114.10
1	C	553	TRP	CA-CB-CG	-6.71	100.86	113.60
1	B	545	SER	N-CA-C	6.70	117.12	108.34
1	C	739	HIS	CA-CB-CG	-6.70	107.10	113.80
1	B	730	LEU	CB-CA-C	6.70	120.10	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	667	GLU	CB-CG-CD	-6.69	101.23	112.60
1	B	592	PHE	CA-CB-CG	-6.68	107.12	113.80
1	D	969	GLU	CB-CA-C	-6.68	98.88	110.17
1	D	845	GLN	CB-CA-C	-6.68	102.05	111.80
1	A	332	PHE	CA-CB-CG	-6.67	107.13	113.80
1	C	761	GLN	CB-CG-CD	6.67	123.93	112.60
1	C	274	PHE	CA-CB-CG	-6.66	107.14	113.80
1	C	306	PRO	N-CA-CB	6.64	106.90	102.25
1	B	71	GLU	CB-CG-CD	6.63	123.87	112.60
1	D	685	LEU	N-CA-C	6.62	120.20	109.15
1	A	773	LYS	N-CA-CB	6.61	121.20	110.43
1	B	384	PHE	CA-CB-CG	-6.59	107.21	113.80
1	D	980	GLU	O-C-N	-6.58	115.10	122.86
1	C	751	LEU	N-CA-CB	6.57	119.96	110.37
1	D	324	GLU	N-CA-CB	6.55	122.58	111.57
1	B	479	ASP	CA-CB-CG	-6.54	106.06	112.60
1	D	193	ASP	N-CA-C	-6.54	104.56	112.54
1	D	183	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	D	231	PHE	CA-CB-CG	-6.51	107.29	113.80
1	D	221	GLN	N-CA-CB	-6.51	101.08	111.62
1	C	76	CYS	N-CA-CB	-6.50	99.43	111.53
1	C	136	GLU	CA-C-N	-6.50	110.72	121.57
1	C	136	GLU	C-N-CA	-6.50	110.72	121.57
1	A	235	PHE	CA-CB-CG	-6.50	107.30	113.80
1	B	1018	LEU	CB-CA-C	-6.50	95.78	110.07
1	D	733	ALA	N-CA-C	6.49	119.64	110.23
1	D	606	LEU	N-CA-C	-6.48	104.64	112.54
1	C	845	GLN	CA-CB-CG	-6.47	101.15	114.10
1	A	790	ASP	CA-CB-CG	-6.44	106.16	112.60
1	A	278	ILE	CA-CB-CG1	-6.43	99.46	110.40
1	D	785	THR	CA-CB-OG1	-6.43	99.95	109.60
1	A	127	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	845	GLN	CA-CB-CG	-6.41	101.28	114.10
1	B	207	GLY	CA-C-O	-6.40	116.91	122.16
1	A	297	ASN	CA-CB-CG	-6.38	106.22	112.60
1	D	931	PHE	CA-CB-CG	-6.38	107.42	113.80
1	C	279	ILE	N-CA-C	-6.38	106.73	111.90
1	C	147	ASN	N-CA-CB	-6.38	100.54	110.55
1	A	553	TRP	CA-CB-CG	-6.36	101.52	113.60
1	D	728	VAL	CA-C-O	6.36	125.75	119.97
1	B	809	ARG	NE-CZ-NH2	-6.35	113.49	119.20
1	D	770	ILE	N-CA-CB	6.33	119.88	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	863	GLN	CB-CA-C	-6.31	98.87	109.53
1	A	746	ASP	CB-CA-C	-6.29	96.92	110.45
1	A	82	ASP	CA-CB-CG	-6.27	106.33	112.60
1	A	448	ARG	N-CA-C	6.27	120.03	112.38
1	B	233	ASP	CA-C-N	-6.27	112.64	122.49
1	B	233	ASP	C-N-CA	-6.27	112.64	122.49
1	B	144	ASP	CA-CB-CG	-6.24	106.36	112.60
1	A	614	HIS	N-CA-C	-6.22	102.03	110.36
1	C	735	HIS	N-CA-CB	6.20	119.12	110.56
1	D	277	GLU	CB-CG-CD	6.17	123.09	112.60
1	D	128	ASN	CA-CB-CG	-6.17	106.43	112.60
1	C	182	ASN	OD1-CG-ND2	6.15	128.75	122.60
1	A	691	ALA	CB-CA-C	-6.15	98.61	109.62
1	A	673	ALA	N-CA-CB	-6.15	101.56	109.55
1	A	433	LEU	CA-C-O	6.15	124.30	118.34
1	C	772	ASP	N-CA-CB	6.14	119.85	110.70
1	A	675	GLN	CB-CA-C	-6.14	101.22	111.23
1	D	309	TYR	N-CA-C	-6.12	100.44	109.81
1	C	298	PRO	CB-CA-C	-6.12	103.40	111.23
1	B	571	VAL	N-CA-C	6.11	117.56	108.46
1	B	120	THR	CA-C-N	-6.10	117.05	122.73
1	B	120	THR	C-N-CA	-6.10	117.05	122.73
1	B	661	LYS	CA-C-O	6.09	123.83	119.32
1	C	606	LEU	N-CA-C	-6.09	105.11	112.54
1	C	893	GLU	N-CA-C	6.09	118.00	111.36
1	C	136	GLU	CB-CA-C	-6.08	96.98	109.94
1	A	239	VAL	N-CA-C	-6.08	99.36	108.12
1	B	297	ASN	CA-C-O	6.07	124.66	120.47
1	C	790	ASP	CA-CB-CG	-6.07	106.53	112.60
1	B	82	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	113	PHE	CA-CB-CG	-6.04	107.76	113.80
1	C	309	TYR	N-CA-C	-6.03	101.27	110.14
1	C	788	PRO	N-CA-CB	6.03	108.70	103.27
1	B	539[A]	ALA	CB-CA-C	6.03	122.42	110.42
1	B	539[B]	ALA	CB-CA-C	6.03	122.42	110.42
1	A	770	ILE	N-CA-CB	6.02	120.00	111.82
1	D	759	ASN	CA-CB-CG	-6.02	106.58	112.60
1	B	632	SER	N-CA-CB	5.99	119.88	110.71
1	C	610	ASP	CA-C-N	-5.98	115.92	126.32
1	C	610	ASP	C-N-CA	-5.98	115.92	126.32
1	D	395	HIS	N-CA-CB	-5.98	100.96	109.75
1	D	728	VAL	N-CA-C	-5.96	106.94	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ILE	N-CA-C	-5.95	107.08	111.90
1	A	360	HIS	CA-CB-CG	-5.95	107.85	113.80
1	B	519	SER	N-CA-C	-5.95	101.85	110.24
1	D	138	GLN	N-CA-CB	-5.94	101.22	110.55
1	D	801	ILE	N-CA-CB	-5.94	100.16	110.13
1	D	598	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	686	PRO	CB-CA-C	-5.93	104.29	111.46
1	A	155	ASN	CA-CB-CG	-5.92	106.67	112.60
1	A	702	GLN	O-C-N	5.92	126.76	121.19
1	B	889	ALA	CA-C-N	-5.92	112.50	122.92
1	B	889	ALA	C-N-CA	-5.92	112.50	122.92
1	A	753	ASN	CA-C-N	-5.91	113.53	122.81
1	A	753	ASN	C-N-CA	-5.91	113.53	122.81
1	B	755	ARG	N-CA-CB	-5.91	100.53	111.52
1	C	479	ASP	CA-C-O	5.91	127.68	121.00
1	A	166	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	B	753	ASN	N-CA-CB	5.90	118.70	110.56
1	B	433	LEU	CA-C-O	5.89	124.06	118.34
1	B	649	ASN	N-CA-C	-5.89	100.70	109.83
1	D	320	GLY	CA-C-N	-5.89	113.89	122.19
1	D	320	GLY	C-N-CA	-5.89	113.89	122.19
1	D	687	GLN	N-CA-CB	5.89	121.12	110.17
1	D	1018	LEU	CB-CA-C	-5.88	97.13	110.07
1	C	869	ASP	CA-CB-CG	-5.88	106.72	112.60
1	D	447	ASP	N-CA-C	5.88	120.58	113.17
1	B	640	SER	CB-CA-C	-5.88	100.16	109.80
1	B	736	ALA	N-CA-C	5.87	117.89	109.14
1	A	777	LEU	N-CA-CB	5.87	119.04	110.47
1	C	771	GLY	CA-C-N	-5.87	113.29	122.73
1	C	771	GLY	C-N-CA	-5.87	113.29	122.73
1	D	711	ALA	CA-C-O	-5.86	114.74	121.19
1	A	889	ALA	CA-C-N	5.86	129.19	120.87
1	A	889	ALA	C-N-CA	5.86	129.19	120.87
1	B	705	ALA	CA-C-O	-5.86	115.08	121.87
1	C	680	ILE	CA-C-N	-5.86	114.98	122.77
1	C	680	ILE	C-N-CA	-5.86	114.98	122.77
1	A	329	ASP	CA-CB-CG	-5.85	106.75	112.60
1	C	159	VAL	CB-CA-C	-5.85	105.88	111.44
1	B	519	SER	N-CA-CB	-5.84	100.40	109.69
1	B	553	TRP	CA-CB-CG	-5.84	102.50	113.60
1	C	209	PHE	N-CA-C	5.81	120.49	113.17
1	C	583	ASN	CA-CB-CG	-5.81	106.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	ASP	CA-C-O	5.80	125.03	119.99
1	C	844	HIS	CA-CB-CG	-5.79	108.02	113.80
1	D	817	GLN	CB-CG-CD	-5.78	102.77	112.60
1	C	788	PRO	CB-CA-C	-5.78	104.36	111.64
1	B	351	ILE	N-CA-CB	-5.78	104.69	111.39
1	C	662	PRO	N-CA-CB	5.78	108.44	103.36
1	C	977	HIS	CA-CB-CG	-5.77	108.03	113.80
1	A	632	SER	N-CA-CB	5.77	120.27	110.87
1	A	96	ASP	N-CA-CB	5.76	120.34	111.46
1	C	964	GLN	CA-C-O	5.76	126.66	120.55
1	D	553	TRP	CA-CB-CG	-5.76	102.65	113.60
1	B	138	GLN	N-CA-CB	-5.76	101.00	110.68
1	A	274	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	207	GLY	CA-C-O	-5.74	117.45	122.16
1	B	917	ARG	CD-NE-CZ	-5.74	116.36	124.40
1	C	499	ILE	CA-C-N	-5.73	116.47	122.89
1	C	499	ILE	C-N-CA	-5.73	116.47	122.89
1	A	755	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	C	917	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	A	675	GLN	CA-C-O	-5.71	113.67	119.78
1	D	539[A]	ALA	CB-CA-C	-5.69	99.11	110.42
1	D	539[B]	ALA	CB-CA-C	-5.69	99.11	110.42
1	C	678	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	B	54	LEU	N-CA-C	-5.68	106.24	112.72
1	A	671	ASP	CA-C-N	-5.67	115.05	122.94
1	A	671	ASP	C-N-CA	-5.67	115.05	122.94
1	D	323	ILE	N-CA-C	-5.67	106.17	111.45
1	D	822	LEU	O-C-N	-5.67	116.04	123.02
1	A	593	GLY	CA-C-O	5.67	125.41	119.06
1	A	171	PHE	CA-C-N	-5.67	114.65	122.30
1	A	171	PHE	C-N-CA	-5.67	114.65	122.30
1	D	319	ASP	N-CA-C	5.67	119.82	113.02
1	D	144	ASP	CA-CB-CG	-5.66	106.94	112.60
1	C	221	GLN	N-CA-CB	-5.66	102.62	111.56
1	C	482	ARG	CB-CA-C	-5.66	100.71	109.20
1	C	440	VAL	CB-CA-C	-5.66	104.63	112.04
1	D	235	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	193	ASP	N-CA-C	-5.65	105.48	112.38
1	D	781	ARG	CD-NE-CZ	5.64	132.30	124.40
1	D	969	GLU	CA-C-N	-5.64	115.22	123.00
1	D	969	GLU	C-N-CA	-5.64	115.22	123.00
1	B	447	ASP	N-CA-C	5.63	120.27	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	519	SER	N-CA-C	-5.63	102.31	110.24
1	B	706	THR	CA-C-O	-5.63	115.16	121.40
1	B	987	ASP	CA-CB-CG	-5.62	106.98	112.60
1	D	176	PHE	CA-CB-CG	-5.62	108.18	113.80
1	C	772	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	893	GLU	CB-CG-CD	5.62	122.15	112.60
1	C	249	GLU	N-CA-C	5.62	117.84	109.25
1	A	42	ALA	N-CA-C	-5.61	105.24	111.36
1	A	832	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	373	VAL	CA-C-O	5.60	126.77	120.95
1	C	320	GLY	CA-C-N	-5.60	114.30	122.19
1	C	320	GLY	C-N-CA	-5.60	114.30	122.19
1	B	570	TRP	N-CA-C	5.60	117.24	111.03
1	D	632	SER	N-CA-CB	5.60	120.63	110.95
1	D	788	PRO	N-CA-C	5.59	119.87	111.14
1	C	519	SER	N-CA-CB	-5.59	100.80	109.69
1	D	147	ASN	N-CA-CB	-5.59	101.78	110.55
1	C	85	VAL	CA-CB-CG2	-5.59	100.90	110.40
1	A	1017	GLN	CB-CG-CD	5.59	122.10	112.60
1	D	430	PRO	N-CA-CB	5.58	109.06	103.48
1	A	539[A]	ALA	CB-CA-C	-5.58	99.32	110.42
1	A	539[B]	ALA	CB-CA-C	-5.58	99.32	110.42
1	C	231	PHE	N-CA-CB	-5.57	102.57	111.43
1	A	226	HIS	CA-C-N	-5.57	116.29	123.19
1	A	226	HIS	C-N-CA	-5.57	116.29	123.19
1	B	630	ARG	CA-C-N	-5.56	114.60	122.94
1	B	630	ARG	C-N-CA	-5.56	114.60	122.94
1	D	988	GLY	N-CA-C	-5.56	105.52	113.86
1	D	670	LEU	CB-CA-C	-5.54	100.17	109.48
1	B	96	ASP	CA-C-O	-5.54	115.51	121.38
1	D	710	GLU	CB-CA-C	-5.54	100.05	110.51
1	D	732	ALA	CA-C-N	5.54	128.57	120.71
1	D	732	ALA	C-N-CA	5.54	128.57	120.71
1	D	787	ALA	N-CA-C	-5.54	99.42	109.44
1	A	844	HIS	CA-C-N	-5.53	114.16	122.07
1	A	844	HIS	C-N-CA	-5.53	114.16	122.07
1	D	746	ASP	N-CA-C	5.53	117.48	109.07
1	C	178	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	D	77	ASP	N-CA-C	5.52	118.02	110.24
1	D	332	PHE	CA-CB-CG	-5.51	108.29	113.80
1	B	352	ARG	CA-C-N	-5.50	116.75	122.69
1	B	352	ARG	C-N-CA	-5.50	116.75	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	583	ASN	CA-CB-CG	-5.49	107.11	112.60
1	C	297	ASN	CB-CA-C	-5.49	105.55	110.71
1	B	323	ILE	N-CA-C	-5.49	106.34	111.45
1	C	345	ASN	CA-CB-CG	-5.49	107.11	112.60
1	C	685	LEU	CA-C-O	5.49	124.64	119.59
1	A	472	TYR	N-CA-C	-5.49	105.20	111.07
1	D	134	LEU	N-CA-C	-5.49	105.32	112.23
1	A	540[A]	HIS	N-CA-C	5.48	117.40	108.63
1	A	540[B]	HIS	N-CA-C	5.48	117.40	108.63
1	D	128	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	A	233	ASP	CA-C-N	-5.47	113.90	122.49
1	A	233	ASP	C-N-CA	-5.47	113.90	122.49
1	A	409	VAL	N-CA-C	5.47	116.36	108.48
1	A	869	ASP	CA-CB-CG	-5.46	107.14	112.60
1	D	513	PRO	CB-CA-C	-5.46	104.42	111.46
1	D	297	ASN	CA-CB-CG	-5.44	107.16	112.60
1	D	784	PHE	CA-CB-CG	-5.43	108.37	113.80
1	D	242	ALA	CB-CA-C	-5.43	101.46	110.14
1	B	100	TYR	CA-CB-CG	-5.42	104.13	113.90
1	C	685	LEU	CB-CA-C	5.42	116.18	110.17
1	B	211	ASP	N-CA-C	5.42	117.28	110.24
1	C	477	SER	N-CA-CB	-5.41	102.13	110.20
1	D	728	VAL	CB-CA-C	-5.41	105.06	111.65
1	B	352	ARG	N-CA-C	-5.40	98.46	108.24
1	C	648	ASP	CA-CB-CG	-5.40	107.20	112.60
1	A	728	VAL	CA-C-O	5.39	124.07	119.38
1	C	52	ARG	CB-CA-C	-5.39	100.43	109.48
1	B	93	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	871	GLU	CB-CG-CD	-5.38	103.45	112.60
1	D	1013	ARG	CA-CB-CG	-5.38	103.34	114.10
1	C	931	PHE	N-CA-C	-5.38	99.02	108.69
1	B	849	LEU	CB-CA-C	-5.37	100.73	110.56
1	D	752	GLY	CA-C-N	-5.37	113.74	122.65
1	D	752	GLY	C-N-CA	-5.37	113.74	122.65
1	A	1004	SER	CA-CB-OG	-5.36	100.38	111.10
1	C	871	GLU	CB-CA-C	-5.36	99.13	109.37
1	B	14	ARG	N-CA-CB	5.36	119.85	111.71
1	A	773	LYS	CB-CA-C	-5.35	100.92	109.75
1	B	801	ILE	N-CA-CB	-5.35	101.14	110.13
1	C	539[A]	ALA	CB-CA-C	-5.35	99.78	110.42
1	C	539[B]	ALA	CB-CA-C	-5.35	99.78	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	ALA	CA-C-N	-5.34	113.96	122.29
1	A	707	ALA	C-N-CA	-5.34	113.96	122.29
1	B	309	TYR	N-CA-C	-5.34	101.64	109.81
1	B	576	ILE	CB-CA-C	-5.34	104.21	111.15
1	D	100	TYR	CA-CB-CG	-5.34	104.29	113.90
1	D	668	VAL	CB-CA-C	-5.34	101.64	111.36
1	A	320	GLY	N-CA-C	5.34	122.47	114.95
1	B	684	GLU	N-CA-C	5.34	118.08	110.24
1	B	710	GLU	N-CA-CB	-5.34	101.92	110.46
1	C	721	ARG	CB-CA-C	-5.34	100.51	109.53
1	B	47	PRO	CB-CA-C	5.33	118.34	111.46
1	C	448	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	C	748	CYS	CA-CB-SG	-5.33	102.13	114.40
1	B	44	THR	OG1-CB-CG2	-5.33	98.64	109.30
1	B	71	GLU	CB-CA-C	5.32	121.43	110.31
1	B	96	ASP	CA-CB-CG	-5.32	107.28	112.60
1	A	613	PRO	CB-CA-C	-5.32	104.01	110.98
1	C	824	GLN	CA-CB-CG	-5.32	103.47	114.10
1	D	847	LYS	CA-C-N	-5.32	115.12	122.30
1	D	847	LYS	C-N-CA	-5.32	115.12	122.30
1	C	842	TRP	CA-CB-CG	-5.31	103.50	113.60
1	C	730	LEU	N-CA-CB	-5.31	99.96	109.68
1	B	856	TYR	N-CA-C	-5.31	99.75	108.41
1	B	381	GLN	CA-CB-CG	-5.31	103.48	114.10
1	B	313	VAL	N-CA-CB	-5.31	104.78	111.46
1	D	516	PRO	CB-CA-C	-5.30	104.44	111.23
1	A	416	GLU	CA-CB-CG	-5.30	103.50	114.10
1	C	248	GLY	O-C-N	-5.29	117.54	123.10
1	B	123	TYR	CB-CA-C	-5.29	99.68	109.37
1	C	681	GLU	CA-C-N	-5.29	110.68	121.48
1	C	681	GLU	C-N-CA	-5.29	110.68	121.48
1	B	544	ASN	N-CA-CB	-5.29	102.57	110.24
1	D	656	VAL	CA-CB-CG2	-5.28	101.42	110.40
1	B	499	ILE	N-CA-C	-5.28	101.87	108.84
1	B	125	LEU	CB-CA-C	-5.28	100.83	109.80
1	C	358	GLU	CA-CB-CG	-5.28	103.55	114.10
1	B	262	GLN	N-CA-CB	5.26	119.45	110.87
1	D	958	ASN	N-CA-CB	5.26	120.84	111.69
1	B	686	PRO	N-CA-CB	5.26	107.99	103.31
1	D	968	MET	N-CA-CB	-5.25	101.68	110.39
1	A	689	GLU	CA-C-N	5.25	129.74	121.56
1	A	689	GLU	C-N-CA	5.25	129.74	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	80	GLU	CG-CD-OE2	-5.24	106.34	118.40
1	C	863	GLN	CA-CB-CG	-5.24	103.62	114.10
1	C	571	VAL	N-CA-C	5.24	116.27	108.46
1	D	718	GLN	CA-C-O	-5.24	114.88	120.75
1	B	30	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	652	LEU	CD1-CG-CD2	-5.22	99.31	110.80
1	C	363	HIS	CA-C-O	5.22	125.60	119.28
1	C	174	SER	N-CA-C	5.22	117.37	111.11
1	A	499	ILE	N-CA-C	-5.22	101.95	108.84
1	D	778	THR	CA-C-N	5.21	125.50	119.92
1	D	778	THR	C-N-CA	5.21	125.50	119.92
1	B	532	PRO	CB-CA-C	-5.21	103.18	110.63
1	B	255	ARG	CA-C-N	-5.21	115.75	122.99
1	B	255	ARG	C-N-CA	-5.21	115.75	122.99
1	B	738	PRO	CB-CA-C	-5.21	104.56	111.23
1	C	613	PRO	CB-CA-C	-5.20	104.17	110.98
1	C	384	PHE	CA-CB-CG	-5.19	108.61	113.80
1	C	729	THR	N-CA-CB	5.19	118.89	110.43
1	C	772	ASP	CB-CA-C	5.19	119.51	110.94
1	B	567	VAL	CB-CA-C	-5.18	103.46	111.08
1	B	821	ALA	O-C-N	-5.18	117.18	123.29
1	B	147	ASN	N-CA-CB	-5.18	101.88	110.47
1	B	741	THR	CA-CB-OG1	-5.18	101.84	109.60
1	A	876	THR	N-CA-C	-5.17	103.62	110.40
1	B	661	LYS	N-CA-CB	-5.17	103.46	110.23
1	C	449	ASN	CA-CB-CG	-5.17	107.44	112.60
1	A	171	PHE	CA-CB-CG	-5.16	108.64	113.80
1	B	854	LYS	CB-CA-C	-5.16	98.72	110.07
1	C	479	ASP	CA-CB-CG	-5.16	107.44	112.60
1	D	510	GLN	CA-C-O	5.16	126.83	121.00
1	A	797	GLU	CB-CG-CD	-5.16	103.84	112.60
1	B	139	THR	CA-C-N	-5.15	114.15	122.81
1	B	139	THR	C-N-CA	-5.15	114.15	122.81
1	C	690	SER	N-CA-C	5.15	115.09	108.34
1	D	420	MET	CA-C-N	-5.15	118.37	122.85
1	D	420	MET	C-N-CA	-5.15	118.37	122.85
1	C	684	GLU	CB-CA-C	-5.14	101.18	109.72
1	D	659	ASP	N-CA-CB	5.14	118.97	111.62
1	C	842	TRP	CB-CA-C	-5.14	100.83	109.72
1	D	651	LEU	N-CA-CB	-5.14	101.70	111.00
1	A	434	PRO	CB-CA-C	-5.14	104.89	113.06
1	B	751	LEU	N-CA-CB	5.13	118.57	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLY	N-CA-C	-5.13	108.60	115.32
1	C	884	LEU	CA-C-N	-5.13	112.87	121.75
1	C	884	LEU	C-N-CA	-5.13	112.87	121.75
1	C	958	ASN	N-CA-CB	5.13	120.61	111.69
1	D	315	LEU	N-CA-C	-5.13	100.37	108.73
1	D	472	TYR	CA-C-O	5.12	126.20	120.82
1	D	931	PHE	CA-C-O	5.12	123.66	119.36
1	C	497	ASP	CA-CB-CG	-5.11	107.49	112.60
1	C	279	ILE	CA-CB-CG2	5.11	119.19	110.50
1	D	807	VAL	N-CA-C	5.11	115.83	110.62
1	D	89	ASN	N-CA-C	-5.11	100.91	109.24
1	D	540[A]	HIS	N-CA-C	-5.11	98.69	107.23
1	D	540[B]	HIS	N-CA-C	-5.11	98.69	107.23
1	A	218	PRO	CB-CA-C	-5.11	104.26	110.95
1	B	110	ASN	CA-CB-CG	-5.10	107.50	112.60
1	D	176	PHE	N-CA-C	-5.10	107.44	113.97
1	D	688	PRO	CB-CA-C	-5.10	105.14	111.11
1	B	257	THR	CA-C-N	-5.10	116.46	123.14
1	B	257	THR	C-N-CA	-5.10	116.46	123.14
1	A	351	ILE	N-CA-C	5.09	115.67	107.98
1	C	687	GLN	CB-CA-C	5.09	117.65	109.41
1	B	670	LEU	CA-C-N	-5.09	114.02	122.92
1	B	670	LEU	C-N-CA	-5.09	114.02	122.92
1	B	797	GLU	CA-CB-CG	-5.08	103.94	114.10
1	A	544	ASN	N-CA-CB	-5.08	102.88	110.24
1	B	52	ARG	CB-CA-C	-5.08	100.25	109.38
1	B	415	ILE	CB-CA-C	-5.07	104.70	110.73
1	B	680	ILE	CA-C-N	-5.07	116.03	122.77
1	B	680	ILE	C-N-CA	-5.07	116.03	122.77
1	C	630	ARG	N-CA-CB	5.07	120.96	111.53
1	B	279	ILE	CA-CB-CG2	5.07	119.11	110.50
1	C	733	ALA	N-CA-C	5.06	117.64	110.10
1	A	823	LEU	N-CA-CB	5.06	117.32	110.59
1	B	746	ASP	CB-CA-C	-5.06	99.58	110.45
1	B	753	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	564	GLY	CA-C-N	-5.05	112.67	120.86
1	A	564	GLY	C-N-CA	-5.05	112.67	120.86
1	A	225	PHE	N-CA-CB	5.05	119.93	110.99
1	C	770	ILE	CA-C-O	5.04	126.03	120.48
1	B	435	ALA	CA-C-N	-5.04	113.13	120.29
1	B	435	ALA	C-N-CA	-5.04	113.13	120.29
1	D	581	ASN	CA-C-O	5.04	125.56	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	540[A]	HIS	N-CA-C	5.04	116.69	108.63
1	B	540[B]	HIS	N-CA-C	5.04	116.69	108.63
1	C	787	ALA	N-CA-C	-5.04	100.33	109.44
1	B	296	GLU	CA-C-N	-5.03	118.27	123.10
1	B	296	GLU	C-N-CA	-5.03	118.27	123.10
1	C	799	THR	CA-C-O	5.03	125.36	119.28
1	D	126	THR	CA-CB-OG1	-5.03	102.06	109.60
1	A	441	THR	N-CA-C	5.02	116.76	111.28
1	C	572	ASP	CB-CA-C	-5.02	101.38	109.72
1	B	292	ARG	CA-C-O	-5.02	114.94	120.36
1	B	894	ARG	CB-CA-C	-5.01	99.93	109.66
1	D	240	LEU	CA-C-N	-5.01	115.93	123.00
1	D	240	LEU	C-N-CA	-5.01	115.93	123.00
1	A	352	ARG	CA-C-N	-5.01	117.28	122.69
1	A	352	ARG	C-N-CA	-5.01	117.28	122.69
1	C	641	GLU	N-CA-CB	5.01	117.88	110.56
1	A	988	GLY	N-CA-C	-5.01	106.36	112.77
1	C	634	GLN	N-CA-C	-5.00	106.48	112.59
1	D	797	GLU	O-C-N	-5.00	117.09	123.24
1	B	684	GLU	N-CA-CB	5.00	117.23	109.48

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	687	GLN	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8128	0	7712	121	0
1	B	8128	0	7712	119	0
1	C	8128	0	7712	112	0
1	D	8128	0	7712	123	0
2	E	23	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	23	0	20	0	0
2	G	23	0	20	0	0
2	H	23	0	20	0	0
3	A	4	0	0	1	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
5	A	92	0	138	15	0
5	B	96	0	144	16	0
5	C	100	0	150	17	0
5	D	96	0	144	9	0
6	A	1136	0	0	18	1
6	B	1151	0	0	23	0
6	C	1133	0	0	14	0
6	D	1109	0	0	10	1
All	All	37546	0	31504	496	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 8.

All (496) 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)
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.01	1.46
1:A:634:GLN:H	1:A:634:GLN:NE2	1.41	1.18
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.43	1.16
1:B:655:MET:HE2	1:B:665:SER:HB3	1.32	1.07
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.24	1.02
1:A:685:LEU:HD23	1:A:686:PRO:CD	1.91	1.01
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.44	1.00
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.27	0.98
1:C:761:GLN:N	1:C:761:GLN:HE21	1.65	0.95
1:A:685:LEU:CD2	1:A:686:PRO:HD2	1.96	0.94
5:A:8420:DMS:H22	6:D:9525:HOH:O	1.66	0.93
1:C:761:GLN:H	1:C:761:GLN:NE2	1.69	0.90
1:B:600:GLN:H	1:B:600:GLN:HE21	1.19	0.90
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:LYS:HD3	1:B:849:LEU:HD23	1.53	0.90
1:D:367:MET:HB3	1:D:372:MET:HE2	1.54	0.89
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.19	0.89
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.04	0.88
1:A:634:GLN:NE2	1:A:634:GLN:N	2.22	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.04	0.87
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.38	0.87
1:B:262:GLN:HE21	1:B:263:GLY:N	1.73	0.87
1:A:685:LEU:HD23	1:A:686:PRO:HD3	1.56	0.87
5:B:8410:DMS:H13	6:B:9248:HOH:O	1.75	0.85
1:A:292:ARG:HH12	5:A:8412:DMS:C2	1.91	0.84
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.55	0.84
1:A:773:LYS:H	1:A:773:LYS:HD3	1.42	0.84
5:C:8408:DMS:H22	6:C:9354:HOH:O	1.76	0.84
1:A:292:ARG:HH12	5:A:8412:DMS:H21	1.43	0.83
1:D:629:PHE:O	1:D:630:ARG:HD3	1.79	0.82
1:A:600:GLN:H	1:A:600:GLN:HE21	1.28	0.82
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.62	0.82
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.45	0.81
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.63	0.80
1:A:973:ARG:O	5:A:8423:DMS:H12	1.81	0.80
1:A:773:LYS:HD3	1:A:773:LYS:N	1.95	0.80
1:C:237:ARG:HH11	1:C:237:ARG:CB	1.94	0.80
5:A:8408:DMS:H22	6:A:9230:HOH:O	1.82	0.79
1:C:367:MET:HE3	1:C:367:MET:HA	1.63	0.79
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.64	0.79
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.13	0.79
1:C:748:CYS:C	1:C:749:ILE:HD12	2.08	0.78
1:D:658:LEU:O	1:D:661:LYS:HG3	1.83	0.78
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.10	0.77
1:B:684:GLU:O	1:B:686:PRO:HD3	1.84	0.77
1:C:44:THR:HB	6:C:9688:HOH:O	1.83	0.77
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.15	0.76
5:C:8417:DMS:H22	6:C:9247:HOH:O	1.85	0.76
1:A:1017:GLN:HG2	1:A:1018:LEU:N	1.99	0.76
1:C:761:GLN:HE21	1:C:761:GLN:H	1.23	0.75
1:D:292:ARG:HH12	5:D:8412:DMS:C2	1.98	0.75
1:D:748:CYS:C	1:D:749:ILE:HD12	2.12	0.75
1:D:130:ASP:CG	5:D:8703:DMS:H23	2.12	0.75
1:C:651:LEU:HD23	1:C:703:PRO:HG3	1.69	0.74
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.02	0.73
1:D:508:GLU:OE2	5:D:8407:DMS:H11	1.88	0.73
1:B:687:GLN:HE21	1:B:687:GLN:N	1.85	0.73
5:B:8408:DMS:H13	6:B:9340:HOH:O	1.88	0.73
1:A:797:GLU:O	1:A:801:ILE:HD13	1.89	0.73
1:C:737:ILE:HD12	1:C:738:PRO:CD	2.18	0.73
1:A:371:THR:HG22	6:A:9526:HOH:O	1.88	0.73
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.72	0.72
1:D:237:ARG:NH1	6:D:9285:HOH:O	2.23	0.72
1:B:878:HIS:HD2	6:B:8695:HOH:O	1.71	0.72
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.24	0.72
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.89	0.71
1:C:878:HIS:HD2	6:C:8704:HOH:O	1.74	0.71
1:B:262:GLN:HE21	1:B:262:GLN:C	1.98	0.71
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.22	0.70
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.73	0.69
1:D:749:ILE:HD12	1:D:749:ILE:N	2.06	0.69
1:D:857:ARG:NH1	1:D:857:ARG:HG2	2.07	0.68
1:C:634:GLN:H	1:C:634:GLN:NE2	1.92	0.68
1:A:878:HIS:HD2	6:A:8581:HOH:O	1.77	0.68
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.02	0.68
5:B:8415:DMS:H11	6:B:9646:HOH:O	1.94	0.67
1:A:277:GLU:H	1:A:277:GLU:CD	2.02	0.67
1:A:809:ARG:HG2	1:A:809:ARG:NH1	2.06	0.67
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.29	0.67
1:D:687:GLN:HB3	1:D:688:PRO:HD2	1.76	0.67
1:D:857:ARG:HG2	1:D:857:ARG:HH11	1.60	0.67
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.75	0.67
1:D:809:ARG:HH11	1:D:809:ARG:CG	2.07	0.67
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.78	0.66
1:A:654:TRP:CZ2	1:A:683:PRO:HG2	2.30	0.66
1:C:761:GLN:N	1:C:761:GLN:NE2	2.34	0.66
3:A:3105:MG:MG	6:A:9107:HOH:O	1.37	0.66
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.08	0.66
1:B:847:LYS:NZ	6:B:9679:HOH:O	2.20	0.66
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.29	0.66
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.05	0.66
1:C:651:LEU:HD11	1:C:653:HIS:HE1	1.61	0.66
1:A:634:GLN:H	1:A:634:GLN:HE21	1.38	0.65
1:A:431:ARG:HG3	6:A:9280:HOH:O	1.96	0.65
1:C:595:THR:HA	1:C:596:PRO:C	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:HIS:O	1:D:625:GLN:HG3	1.96	0.65
1:B:651:LEU:O	1:B:651:LEU:HD23	1.96	0.64
1:A:290:THR:HB	5:A:8412:DMS:H23	1.78	0.64
1:A:635:THR:OG1	1:A:681:GLU:HG3	1.97	0.64
1:B:772:ASP:OD1	1:B:773:LYS:HE3	1.97	0.64
1:C:266:GLN:HE21	5:C:8602:DMS:H23	1.62	0.64
1:C:797:GLU:O	1:C:801:ILE:HD13	1.97	0.64
1:D:829:THR:O	1:D:830:LEU:HD23	1.98	0.64
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.79	0.64
1:C:824:GLN:HG2	1:C:825:CYS:N	2.10	0.64
1:D:887:GLN:NE2	1:D:980:GLU:O	2.31	0.64
1:B:863:GLN:HG2	1:B:1019:VAL:HG13	1.80	0.63
5:B:8417:DMS:H12	6:B:9733:HOH:O	1.97	0.63
1:A:735:HIS:ND1	1:A:735:HIS:N	2.31	0.63
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.11	0.63
1:B:634:GLN:HE22	1:B:684:GLU:HA	1.64	0.62
1:D:973:ARG:O	5:D:8423:DMS:H12	1.98	0.62
1:A:680:ILE:HG12	6:A:9152:HOH:O	2.00	0.62
1:D:1022:GLN:NE2	1:D:1023:LYS:HG3	2.12	0.62
1:D:367:MET:CB	1:D:372:MET:HE2	2.30	0.61
1:A:262:GLN:NE2	1:A:299:LYS:HD3	2.16	0.61
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.30	0.61
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.81	0.61
1:A:663:LEU:CD1	1:A:686:PRO:HG2	2.31	0.61
1:B:646:HIS:HB3	6:B:9486:HOH:O	2.01	0.61
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.36	0.61
1:C:634:GLN:H	1:C:634:GLN:CD	2.08	0.61
1:B:655:MET:HE2	1:B:665:SER:CB	2.20	0.60
1:C:806:TRP:HA	1:C:809:ARG:HD3	1.82	0.60
1:A:651:LEU:C	1:A:651:LEU:HD12	2.26	0.60
1:B:658:LEU:O	1:B:661:LYS:HE2	2.00	0.60
1:C:756:TRP:CE2	1:C:858:ILE:HD12	2.36	0.60
1:D:878:HIS:HD2	6:D:8819:HOH:O	1.83	0.60
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.83	0.60
1:D:773:LYS:HG3	1:D:775:GLN:HE21	1.64	0.60
1:D:651:LEU:HG	1:D:653:HIS:CE1	2.36	0.60
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.36	0.60
1:C:667:GLU:C	1:C:668:VAL:HG23	2.27	0.60
1:D:135:GLN:O	1:D:136:GLU:HG2	2.02	0.60
1:C:615:PRO:O	1:C:618:THR:HG22	2.01	0.60
1:C:266:GLN:HB3	5:C:8602:DMS:H23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ASP:OD2	6:A:9431:HOH:O	2.17	0.59
1:B:863:GLN:HG2	1:B:1019:VAL:HG11	1.82	0.59
1:C:1023:LYS:NZ	1:C:1023:LYS:HB3	2.16	0.59
1:D:1022:GLN:HE21	1:D:1023:LYS:HG3	1.67	0.59
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.09	0.58
1:D:847:LYS:HG3	1:D:848:THR:N	2.10	0.58
1:A:685:LEU:CD2	1:A:686:PRO:CD	2.64	0.58
1:B:367:MET:HA	1:B:367:MET:HE3	1.85	0.58
1:D:651:LEU:CD2	1:D:653:HIS:HE1	2.17	0.58
1:C:749:ILE:HD12	1:C:749:ILE:N	2.18	0.58
1:A:770:ILE:O	1:A:773:LYS:HD3	2.04	0.57
1:B:699:ARG:HD2	6:B:9661:HOH:O	2.05	0.57
1:B:1017:GLN:HB2	6:B:9588:HOH:O	2.03	0.57
1:A:595:THR:HA	1:A:596:PRO:C	2.29	0.57
1:A:832:ASP:OD1	1:A:832:ASP:N	2.32	0.57
1:A:685:LEU:HD22	1:A:686:PRO:HD2	1.86	0.57
1:B:730:LEU:H	1:B:730:LEU:CD1	2.11	0.57
1:D:363:HIS:HD2	6:D:9332:HOH:O	1.87	0.57
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.57
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.04	0.57
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.87	0.56
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.35	0.56
1:B:745:MET:SD	1:B:745:MET:N	2.78	0.56
1:A:387:VAL:HG22	6:A:9584:HOH:O	2.06	0.56
1:A:737:ILE:C	1:A:737:ILE:HD13	2.30	0.56
1:B:730:LEU:H	1:B:730:LEU:HD12	1.71	0.56
1:D:797:GLU:O	1:D:801:ILE:HD13	2.07	0.56
1:B:687:GLN:HE21	1:B:687:GLN:CA	2.19	0.55
1:B:37:ARG:NH1	5:B:8504:DMS:H21	2.21	0.55
1:C:237:ARG:NH1	1:C:296:GLU:OE2	2.38	0.55
1:D:618:THR:HG23	6:D:9075:HOH:O	2.05	0.55
1:A:654:TRP:HZ2	1:A:683:PRO:HG2	1.71	0.55
1:A:735:HIS:O	1:A:736:ALA:HB2	2.06	0.55
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.26	0.55
1:B:634:GLN:NE2	1:B:684:GLU:HA	2.21	0.55
1:A:787:ALA:HA	1:A:968:MET:HG3	1.89	0.55
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.42	0.55
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.70	0.55
1:C:125:LEU:HD21	5:C:8408:DMS:H23	1.87	0.55
1:A:887:GLN:NE2	1:A:980:GLU:O	2.38	0.54
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:GLN:N	1:D:687:GLN:OE1	2.40	0.54
1:A:521:LYS:HE2	6:A:8938:HOH:O	2.07	0.54
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.43	0.54
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.71	0.54
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.42	0.54
1:B:630:ARG:HD3	1:B:637:GLU:OE1	2.07	0.54
1:C:708:TRP:CZ2	5:C:8403:DMS:H13	2.43	0.54
1:B:615:PRO:O	1:B:618:THR:HG22	2.07	0.54
1:A:699:ARG:NH2	6:A:9373:HOH:O	2.41	0.54
1:B:662:PRO:C	1:B:663:LEU:HD23	2.33	0.54
1:A:708:TRP:CZ2	5:A:8403:DMS:H13	2.43	0.53
1:D:577:LYS:O	1:D:584:PRO:HA	2.08	0.53
1:D:770:ILE:HD13	1:D:775:GLN:CG	2.38	0.53
1:B:157:ARG:HD3	6:B:9479:HOH:O	2.09	0.53
1:D:292:ARG:NH1	5:D:8412:DMS:H23	2.20	0.53
1:B:863:GLN:CG	1:B:1019:VAL:CG1	2.87	0.53
1:B:262:GLN:NE2	6:B:9167:HOH:O	2.40	0.53
1:C:788:PRO:HD3	1:C:968:MET:HE3	1.91	0.53
5:C:8415:DMS:H11	6:C:9626:HOH:O	2.09	0.53
1:C:756:TRP:CD2	1:C:858:ILE:HD12	2.43	0.53
1:D:135:GLN:C	1:D:136:GLU:HG2	2.33	0.53
1:A:615:PRO:O	1:A:618:THR:HG22	2.08	0.53
1:B:634:GLN:HG2	1:B:682:LEU:O	2.09	0.53
1:A:88:SER:HA	1:A:366:VAL:HG21	1.91	0.53
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.44	0.53
1:B:655:MET:SD	1:B:656:VAL:N	2.83	0.53
1:B:363:HIS:HD2	6:B:9206:HOH:O	1.91	0.52
1:D:770:ILE:N	1:D:770:ILE:HD12	2.25	0.52
1:B:1022:GLN:HG3	1:B:1023:LYS:O	2.09	0.52
1:A:262:GLN:HE22	1:A:299:LYS:CD	2.22	0.52
1:C:356:ARG:HD2	1:C:379:MET:CE	2.40	0.52
1:C:760:ARG:N	1:C:761:GLN:NE2	2.57	0.52
1:A:764:PHE:CE2	1:A:781:ARG:NH1	2.77	0.52
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.45	0.52
1:B:595:THR:HA	1:B:596:PRO:C	2.35	0.52
1:D:367:MET:HB3	1:D:372:MET:CE	2.34	0.52
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.92	0.52
5:C:8420:DMS:O	6:C:8630:HOH:O	2.19	0.52
1:B:262:GLN:HE21	1:B:262:GLN:CA	2.21	0.52
1:B:125:LEU:HD21	5:B:8408:DMS:H11	1.92	0.52
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.92	0.51
1:C:759:ASN:OD1	1:C:761:GLN:NE2	2.43	0.51
1:C:367:MET:HE3	1:C:367:MET:CA	2.35	0.51
1:C:859:ASP:OD1	1:C:861:SER:OG	2.26	0.51
1:B:662:PRO:O	1:B:663:LEU:HD23	2.10	0.51
1:D:277:GLU:CD	1:D:277:GLU:H	2.07	0.51
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.74	0.51
1:C:569:ASP:HB2	6:C:9438:HOH:O	2.11	0.51
1:C:858:ILE:HD13	1:C:864:MET:HB2	1.90	0.51
1:A:866:ILE:O	1:A:1017:GLN:HG3	2.10	0.51
1:D:117:GLU:HG3	6:D:9155:HOH:O	2.11	0.51
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.39	0.51
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.93	0.50
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.26	0.50
1:C:743:SER:HB3	6:C:9612:HOH:O	2.11	0.50
6:B:9406:HOH:O	5:C:8420:DMS:H22	2.11	0.50
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.76	0.50
1:D:749:ILE:N	1:D:749:ILE:CD1	2.72	0.50
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.46	0.50
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.27	0.50
1:C:745:MET:O	1:C:761:GLN:NE2	2.44	0.50
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.94	0.50
1:A:634:GLN:N	1:A:634:GLN:CD	2.68	0.50
1:A:178:ARG:HD2	6:A:9388:HOH:O	2.11	0.50
1:A:663:LEU:HD12	1:A:686:PRO:HG2	1.94	0.50
1:B:600:GLN:HE21	1:B:600:GLN:N	2.00	0.49
1:B:115:PRO:HG3	5:B:8410:DMS:H12	1.94	0.49
1:C:610:ASP:O	1:C:611:ARG:HB2	2.12	0.49
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.93	0.49
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.95	0.49
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.47	0.49
1:D:804:ASN:HA	1:D:809:ARG:CZ	2.42	0.49
1:D:809:ARG:HG2	1:D:809:ARG:NH1	2.12	0.49
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.94	0.49
1:A:801:ILE:HD12	1:A:808:GLU:OE2	2.13	0.49
1:B:669:PRO:CB	6:B:9509:HOH:O	2.60	0.49
1:D:857:ARG:HH11	1:D:857:ARG:CG	2.25	0.49
1:A:472:TYR:O	1:A:476:LYS:HG2	2.12	0.49
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.47	0.49
1:C:651:LEU:CD2	1:C:703:PRO:HG3	2.41	0.49
1:C:734:SER:CB	1:C:860:GLY:HA3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:861:SER:OG	1:C:863:GLN:HG3	2.13	0.49
1:C:428:ASP:O	5:C:8420:DMS:H11	2.13	0.48
1:D:773:LYS:CG	1:D:775:GLN:NE2	2.76	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.95	0.48
1:D:80:GLU:OE1	1:D:80:GLU:N	2.39	0.48
1:C:1023:LYS:NZ	1:C:1023:LYS:CB	2.76	0.48
1:B:262:GLN:NE2	1:B:262:GLN:CA	2.76	0.48
1:C:703:PRO:HG2	5:C:8425:DMS:H22	1.95	0.48
1:D:952:ARG:NH2	1:D:1021:CYS:SG	2.86	0.48
1:C:240:LEU:C	1:C:240:LEU:HD23	2.39	0.48
1:C:835:LEU:HD11	1:C:855:THR:HB	1.95	0.48
1:D:844:HIS:O	1:D:845:GLN:HB2	2.13	0.48
1:A:687:GLN:HG3	6:A:9362:HOH:O	2.13	0.48
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.48
1:A:237:ARG:HD2	1:A:296:GLU:OE1	2.14	0.48
1:A:262:GLN:HE22	1:A:299:LYS:HD2	1.78	0.48
1:B:359:HIS:CD2	1:B:573:GLN:HA	2.49	0.48
1:A:843:GLN:HA	1:A:847:LYS:O	2.14	0.48
5:A:8425:DMS:H22	6:A:9310:HOH:O	2.14	0.48
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.44	0.48
1:D:769:TRP:C	1:D:770:ILE:HD12	2.39	0.48
5:A:8420:DMS:H23	6:D:9255:HOH:O	2.15	0.47
1:A:660:GLY:O	1:A:662:PRO:HD3	2.14	0.47
1:C:655:MET:SD	1:C:656:VAL:N	2.87	0.47
1:B:78:LEU:HD23	6:B:9109:HOH:O	2.14	0.47
1:C:890:GLN:CG	1:C:891:VAL:N	2.78	0.47
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.29	0.47
1:A:178:ARG:HG3	6:A:9388:HOH:O	2.14	0.47
1:C:806:TRP:CD2	1:C:991:MET:HE1	2.49	0.47
1:A:754:LYS:NZ	6:A:9415:HOH:O	2.47	0.47
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.14	0.47
1:C:973:ARG:O	5:C:8423:DMS:H12	2.14	0.47
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.96	0.47
1:D:770:ILE:CD1	1:D:775:GLN:HG3	2.43	0.47
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.29	0.47
1:A:737:ILE:HD13	1:A:737:ILE:O	2.13	0.47
1:C:13:ARG:O	1:C:14:ARG:C	2.57	0.47
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.96	0.47
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.96	0.47
1:B:231:PHE:O	5:B:8417:DMS:H23	2.14	0.47
1:C:133:TRP:CD1	5:C:8504:DMS:H21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.97	0.47
1:D:240:LEU:HD23	1:D:240:LEU:C	2.40	0.47
1:A:352:ARG:HG2	1:A:553:TRP:CH2	2.50	0.46
1:D:804:ASN:HD22	1:D:809:ARG:CZ	2.19	0.46
5:A:8408:DMS:H21	6:A:9217:HOH:O	2.14	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.75	0.46
1:A:1022:GLN:C	1:A:1023:LYS:HG3	2.39	0.46
1:C:262:GLN:CG	1:C:309:TYR:CE2	2.98	0.46
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.31	0.46
1:A:292:ARG:HH12	5:A:8412:DMS:H23	1.73	0.46
1:B:230:ARG:HE	1:B:230:ARG:HB2	1.48	0.46
1:B:1023:LYS:HB3	1:B:1023:LYS:HE3	1.50	0.46
5:B:8420:DMS:H23	6:C:9140:HOH:O	2.15	0.46
1:D:538:TYR:C	1:D:539[B]:ALA:O	2.56	0.46
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.74	0.46
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.81	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.16	0.46
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.97	0.46
5:B:8410:DMS:H11	6:B:8982:HOH:O	2.16	0.46
1:C:799:THR:O	1:C:800:ARG:HG2	2.16	0.46
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.16	0.46
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.81	0.45
1:D:830:LEU:N	1:D:833:ALA:O	2.40	0.45
1:B:292:ARG:HH12	5:B:8412:DMS:H23	1.80	0.45
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.51	0.45
1:D:13:ARG:HD3	6:D:9806:HOH:O	2.15	0.45
1:A:600:GLN:HE21	1:A:600:GLN:N	2.06	0.45
1:B:262:GLN:HE21	1:B:263:GLY:H	1.60	0.45
1:B:473:ARG:NH1	1:B:477:SER:CB	2.78	0.45
1:A:557:ARG:HH11	1:A:557:ARG:HD2	1.62	0.45
1:D:787:ALA:HA	1:D:968:MET:HE2	1.97	0.45
1:A:433:LEU:N	1:A:434:PRO:CD	2.79	0.45
1:D:393:PRO:HD3	1:D:412:GLU:O	2.16	0.45
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.34	0.45
1:A:279:ILE:HG21	1:A:279:ILE:HD13	1.70	0.45
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.98	0.45
1:C:800:ARG:HE	1:C:800:ARG:HB3	1.59	0.45
1:A:262:GLN:NE2	1:A:299:LYS:CD	2.79	0.45
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.15	0.45
1:C:646:HIS:CE1	1:C:673:ALA:CB	2.99	0.45
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:LEU:O	1:A:659:ASP:C	2.59	0.45
1:A:668:VAL:HG12	1:A:669:PRO:O	2.17	0.45
1:B:675:GLN:NE2	6:B:9632:HOH:O	2.49	0.45
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.52	0.45
1:C:749:ILE:N	1:C:749:ILE:CD1	2.80	0.45
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.51	0.45
1:B:910:LEU:C	1:B:910:LEU:HD12	2.42	0.44
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.80	0.44
5:B:8508:DMS:H13	6:B:8732:HOH:O	2.15	0.44
1:C:367:MET:HA	1:C:367:MET:CE	2.42	0.44
1:C:890:GLN:HG3	1:C:891:VAL:N	2.32	0.44
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.00	0.44
1:C:231:PHE:O	5:C:8417:DMS:H12	2.18	0.44
1:D:1022:GLN:NE2	1:D:1023:LYS:CG	2.79	0.44
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.99	0.44
1:A:859:ASP:OD1	1:A:861:SER:OG	2.31	0.44
1:B:863:GLN:CG	1:B:1019:VAL:HG11	2.48	0.44
1:C:237:ARG:HH11	1:C:237:ARG:CG	2.30	0.44
1:A:745:MET:CA	1:A:745:MET:HE3	2.45	0.44
1:C:751:LEU:HD21	1:C:860:GLY:O	2.18	0.44
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.53	0.44
1:D:128:ASN:HB3	1:D:180:GLY:O	2.17	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.44
1:B:835:LEU:HD11	1:B:855:THR:HB	1.99	0.44
1:C:1023:LYS:HB3	1:C:1023:LYS:HZ3	1.83	0.44
1:D:655:MET:HE1	1:D:699:ARG:CD	2.48	0.44
1:D:472:TYR:O	1:D:476:LYS:HG2	2.17	0.43
1:A:147:ASN:HA	1:A:148:SER:HA	1.54	0.43
1:D:143:PHE:HB3	1:D:146:VAL:HG23	2.00	0.43
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.32	0.43
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.99	0.43
1:C:995:GLY:O	1:C:996:ASP:C	2.61	0.43
1:A:58:TRP:CD1	1:A:86:VAL:HB	2.54	0.43
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.99	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.18	0.43
1:B:948:PRO:O	1:B:1023:LYS:N	2.40	0.43
1:B:13:ARG:O	1:B:14:ARG:C	2.57	0.43
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.19	0.43
1:D:773:LYS:HD2	1:D:774:LYS:O	2.18	0.43
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.54	0.43
1:C:275:GLY:O	5:C:8412:DMS:H12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:NH2	6:C:9629:HOH:O	2.28	0.43
1:A:240:LEU:C	1:A:240:LEU:HD23	2.43	0.43
1:B:755:ARG:HD2	6:B:9670:HOH:O	2.17	0.43
1:D:773:LYS:HG3	1:D:773:LYS:O	2.11	0.43
1:A:640:SER:O	1:A:675:GLN:HA	2.18	0.43
1:C:883:GLY:HA3	1:C:987:ASP:HA	2.00	0.43
1:D:636:ILE:HG21	1:D:636:ILE:HD13	1.82	0.43
1:B:646:HIS:ND1	6:B:9486:HOH:O	2.37	0.43
1:B:773:LYS:HA	1:B:773:LYS:HD3	1.75	0.43
1:B:890:GLN:HB2	6:B:9722:HOH:O	2.18	0.43
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.52	0.43
1:D:804:ASN:HA	1:D:809:ARG:NH1	2.34	0.43
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.87	0.43
5:A:8503:DMS:H22	6:A:8930:HOH:O	2.19	0.43
1:C:266:GLN:O	5:C:8602:DMS:H22	2.18	0.43
1:C:655:MET:SD	1:C:656:VAL:O	2.77	0.43
1:A:428:ASP:O	5:A:8420:DMS:H11	2.19	0.42
1:C:756:TRP:CE2	1:C:858:ILE:CD1	3.02	0.42
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.34	0.42
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.29	0.42
1:D:254:LEU:CD2	1:D:323:ILE:CD1	2.97	0.42
1:C:359:HIS:CD2	1:C:573:GLN:HA	2.54	0.42
1:D:226:HIS:O	1:D:242:ALA:HA	2.18	0.42
1:A:460:ASN:O	1:A:461:GLU:C	2.62	0.42
1:A:237:ARG:NH1	1:A:296:GLU:OE2	2.52	0.42
5:A:8423:DMS:H11	6:A:9058:HOH:O	2.19	0.42
1:D:545:SER:O	1:D:909:ARG:HD3	2.19	0.42
5:D:8409:DMS:H23	6:D:9082:HOH:O	2.18	0.42
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.54	0.42
1:A:359:HIS:CD2	1:A:573:GLN:HA	2.54	0.42
1:A:696:LEU:HB2	1:A:722:LEU:HD11	2.00	0.42
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.49	0.42
5:C:8419:DMS:H13	6:C:8967:HOH:O	2.20	0.42
1:B:847:LYS:HD3	1:B:849:LEU:CD2	2.37	0.42
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.01	0.42
1:C:667:GLU:C	1:C:668:VAL:CG2	2.93	0.42
1:A:427:THR:HG21	1:A:462:SER:HB3	2.01	0.42
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.38	0.42
1:C:655:MET:SD	1:C:656:VAL:C	3.03	0.42
1:C:760:ARG:H	1:C:761:GLN:NE2	2.17	0.42
1:D:806:TRP:CD2	1:D:991:MET:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.48	0.42
1:D:687:GLN:HB3	1:D:688:PRO:CD	2.47	0.41
1:D:1022:GLN:HE21	1:D:1023:LYS:CG	2.33	0.41
1:B:655:MET:SD	1:B:655:MET:C	3.03	0.41
1:D:833:ALA:HB1	1:D:858:ILE:O	2.20	0.41
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.09	0.41
1:A:988:GLY:C	1:A:989:PHE:CD1	2.98	0.41
1:C:655:MET:HE1	1:C:662:PRO:HB3	2.03	0.41
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.83	0.41
1:A:533:LEU:C	1:A:533:LEU:HD23	2.45	0.41
1:B:646:HIS:ND1	1:B:673:ALA:HA	2.35	0.41
1:B:684:GLU:HG2	1:B:685:LEU:N	2.34	0.41
1:C:538:TYR:C	1:C:539[B]:ALA:O	2.58	0.41
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.03	0.41
1:B:538:TYR:C	1:B:539[B]:ALA:O	2.60	0.41
1:B:658:LEU:O	1:B:659:ASP:C	2.62	0.41
1:C:864:MET:HE3	1:C:866:ILE:HD11	2.02	0.41
1:D:441:THR:O	1:D:445:GLN:HG3	2.20	0.41
1:D:650:GLU:HB3	1:D:670:LEU:HD12	2.02	0.41
1:A:92:MET:HA	1:A:92:MET:HE2	2.03	0.41
1:A:285:TYR:HB3	1:A:288:ARG:HG3	2.02	0.41
1:A:538:TYR:C	1:A:539[B]:ALA:O	2.60	0.41
1:B:596:PRO:HB3	6:B:9424:HOH:O	2.20	0.41
1:A:839:ALA:HA	1:A:852:SER:O	2.21	0.41
1:B:127:PHE:CD1	1:B:127:PHE:N	2.89	0.41
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.51	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.02	0.41
1:C:367:MET:HE1	6:C:9629:HOH:O	2.20	0.41
1:C:819:GLU:H	1:C:819:GLU:HG2	1.58	0.41
1:D:251:ARG:HD2	5:D:8416:DMS:H13	2.02	0.41
1:D:687:GLN:CB	1:D:688:PRO:HD2	2.47	0.41
1:A:127:PHE:CD1	1:A:127:PHE:N	2.88	0.41
1:B:254:LEU:C	1:B:255:ARG:HG2	2.45	0.41
1:B:433:LEU:HB3	1:B:434:PRO:HD3	2.03	0.41
1:D:246:MET:SD	1:D:246:MET:C	3.03	0.41
1:A:649:ASN:HA	5:A:8425:DMS:H12	2.01	0.41
1:A:770:ILE:O	1:A:773:LYS:HE2	2.21	0.41
1:B:427:THR:HG21	1:B:462:SER:HB3	2.02	0.41
1:B:581:ASN:HB2	1:B:583:ASN:ND2	2.36	0.41
1:B:646:HIS:CE1	1:B:673:ALA:CA	3.04	0.41
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:MET:HE3	1:B:866:ILE:HD11	2.03	0.41
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.95	0.41
1:C:823:LEU:O	1:D:730:LEU:HD21	2.21	0.41
1:D:418:HIS:CE1	1:D:461:GLU:CD	2.99	0.41
1:D:788:PRO:HD2	1:D:968:MET:HG3	2.03	0.41
1:B:340:GLY:O	1:B:561:ARG:HG2	2.21	0.41
1:C:375:ASP:O	1:C:379:MET:HG3	2.21	0.41
1:C:431:ARG:HB3	6:C:9587:HOH:O	2.20	0.41
1:D:16:TRP:CE3	1:D:189:LEU:HD11	2.55	0.41
1:D:92:MET:HA	1:D:92:MET:HE2	2.02	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.95	0.41
1:D:543:GLY:N	6:D:9750:HOH:O	2.43	0.41
1:A:768:MET:CE	1:A:1020:TRP:CZ2	3.02	0.40
1:B:428:ASP:OD2	5:B:8420:DMS:H11	2.21	0.40
1:B:540[A]:HIS:HA	1:B:568:TRP:O	2.21	0.40
1:C:760:ARG:C	1:C:761:GLN:HE21	2.26	0.40
1:B:903:GLN:HB2	6:B:8832:HOH:O	2.20	0.40
1:C:230:ARG:O	1:C:238:ALA:HA	2.21	0.40
1:D:88:SER:HA	1:D:366:VAL:HG21	2.03	0.40
1:D:773:LYS:HG2	1:D:775:GLN:NE2	2.37	0.40
1:B:634:GLN:HE21	1:B:683:PRO:C	2.29	0.40
1:D:933:SER:O	1:D:934:GLU:C	2.64	0.40
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.86	0.40
1:A:802:ASP:OD1	1:A:802:ASP:C	2.63	0.40
1:B:460:ASN:O	1:B:461:GLU:C	2.64	0.40
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.04	0.40
1:B:634:GLN:CG	1:B:682:LEU:O	2.69	0.40
1:C:157:ARG:HD3	6:C:9706:HOH:O	2.21	0.40
1:D:986:ILE:HG23	1:D:986:ILE:HD13	1.72	0.40
1:D:670:LEU:HD23	1:D:670:LEU:HA	1.82	0.40
1:D:956:GLN:N	1:D:956:GLN:CD	2.79	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)
6:A:9583:HOH:O	6:D:9783:HOH:O[4_545]	2.05	0.15

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	1011/1023 (99%)	972 (96%)	38 (4%)	1 (0%)	48	34
1	B	1011/1023 (99%)	974 (96%)	35 (4%)	2 (0%)	43	31
1	C	1011/1023 (99%)	979 (97%)	31 (3%)	1 (0%)	48	34
1	D	1011/1023 (99%)	973 (96%)	37 (4%)	1 (0%)	48	34
All	All	4044/4092 (99%)	3898 (96%)	141 (4%)	5 (0%)	48	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA
1	D	164	ASP
1	B	164	ASP
1	C	734	SER
1	A	683	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	865/875 (99%)	840 (97%)	25 (3%)	37	25
1	B	865/875 (99%)	830 (96%)	35 (4%)	28	15
1	C	865/875 (99%)	829 (96%)	36 (4%)	26	14
1	D	865/875 (99%)	833 (96%)	32 (4%)	30	18
All	All	3460/3500 (99%)	3332 (96%)	128 (4%)	30	18

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	131	GLU
1	A	237	ARG
1	A	250	LEU
1	A	277	GLU
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN
1	A	634	GLN
1	A	653	HIS
1	A	655	MET
1	A	663	LEU
1	A	665	SER
1	A	667	GLU
1	A	684	GLU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	801	ILE
1	A	817	GLN
1	A	885	ASN
1	A	890	GLN
1	A	986	ILE
1	A	1023	LYS
1	B	76	CYS
1	B	80	GLU
1	B	230	ARG
1	B	262	GLN
1	B	264	GLU
1	B	299	LYS
1	B	344	LEU
1	B	362	LEU
1	B	367	MET
1	B	370	GLN
1	B	535	LEU
1	B	546	LEU
1	B	594	ASP
1	B	600	GLN
1	B	651	LEU
1	B	652	LEU
1	B	661	LYS

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Mol	Chain	Res	Type
1	B	663	LEU
1	B	667	GLU
1	B	672	VAL
1	B	684	GLU
1	B	687	GLN
1	B	689	GLU
1	B	690	SER
1	B	730	LEU
1	B	745	MET
1	B	799	THR
1	B	800	ARG
1	B	819	GLU
1	B	824	GLN
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	956	GLN
1	B	1023	LYS
1	C	49	GLN
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	237	ARG
1	C	262	GLN
1	C	367	MET
1	C	519	SER
1	C	546	LEU
1	C	595	THR
1	C	634	GLN
1	C	651	LEU
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE

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Mol	Chain	Res	Type
1	C	749	ILE
1	C	750	GLU
1	C	761	GLN
1	C	773	LYS
1	C	800	ARG
1	C	809	ARG
1	C	819	GLU
1	C	858	ILE
1	C	934	GLU
1	C	986	ILE
1	C	1022	GLN
1	C	1023	LYS
1	D	112	PRO
1	D	116	THR
1	D	237	ARG
1	D	277	GLU
1	D	344	LEU
1	D	370	GLN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	594	ASP
1	D	632	SER
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	685	LEU
1	D	687	GLN
1	D	699	ARG
1	D	737	ILE
1	D	749	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	799	THR
1	D	809	ARG
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU
1	D	986	ILE
1	D	1017	GLN
1	D	1018	LEU

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Mol	Chain	Res	Type
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	262	GLN
1	A	266	GLN
1	A	294	ASN
1	A	445	GLN
1	A	485	GLN
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	757	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	A	903	GLN
1	A	977	HIS
1	B	262	GLN
1	B	294	ASN
1	B	363	HIS
1	B	370	GLN
1	B	485	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	634	GLN
1	B	653	HIS
1	B	675	GLN
1	B	687	GLN
1	B	704	ASN
1	B	804	ASN
1	B	817	GLN
1	B	843	GLN
1	B	878	HIS
1	B	885	ASN
1	B	977	HIS
1	C	128	ASN

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	266	GLN
1	C	363	HIS
1	C	445	GLN
1	C	485	GLN
1	C	646	HIS
1	C	653	HIS
1	C	687	GLN
1	C	704	ASN
1	C	761	GLN
1	C	824	GLN
1	C	878	HIS
1	C	903	GLN
1	C	977	HIS
1	D	135	GLN
1	D	163	GLN
1	D	266	GLN
1	D	294	ASN
1	D	297	ASN
1	D	363	HIS
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	653	HIS
1	D	804	ASN
1	D	843	GLN
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS
1	D	1022	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	BGC	E	1	2	12,12,12	0.60	0	17,17,17	1.63	6 (35%)
2	GAL	E	2	4,2	11,11,12	0.81	0	15,15,17	1.24	2 (13%)
2	BGC	F	1	2	12,12,12	0.75	0	17,17,17	1.87	5 (29%)
2	GAL	F	2	4,2	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
2	BGC	G	1	2	12,12,12	0.96	0	17,17,17	1.51	3 (17%)
2	GAL	G	2	4,2	11,11,12	1.21	1 (9%)	15,15,17	0.72	0
2	BGC	H	1	2	12,12,12	0.86	0	17,17,17	1.23	1 (5%)
2	GAL	H	2	4,2	11,11,12	1.04	1 (9%)	15,15,17	1.07	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GAL	E	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GAL	G	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	4,2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	GAL	O5-C1	-3.73	1.37	1.43
2	H	2	GAL	O5-C1	-2.66	1.39	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	BGC	O5-C1-C2	-3.93	103.38	110.30
2	F	1	BGC	O1-C1-C2	-3.70	98.24	108.98
2	G	1	BGC	O1-C1-O5	-3.44	100.20	110.41
2	E	1	BGC	O3-C3-C2	-3.06	103.17	110.38
2	F	2	GAL	O5-C5-C4	-2.61	104.47	110.83
2	F	1	BGC	O4-C4-C5	-2.61	102.90	109.32
2	H	1	BGC	O4-C4-C5	-2.56	103.03	109.32
2	H	2	GAL	C1-O5-C5	-2.46	108.89	112.19
2	E	1	BGC	O5-C1-C2	-2.40	106.07	110.30
2	E	1	BGC	O2-C2-C3	-2.39	104.74	110.38
2	E	2	GAL	C1-C2-C3	2.38	113.11	109.64
2	E	1	BGC	O4-C4-C5	-2.24	103.80	109.32
2	G	1	BGC	O5-C5-C6	-2.24	100.88	106.44
2	E	1	BGC	O2-C2-C1	2.24	114.42	109.25
2	E	1	BGC	O1-C1-O5	-2.22	103.81	110.41
2	F	1	BGC	O3-C3-C2	-2.14	105.34	110.38
2	G	1	BGC	O5-C1-C2	-2.13	106.55	110.30
2	F	2	GAL	O3-C3-C2	-2.07	105.84	110.05
2	E	2	GAL	O3-C3-C2	-2.07	105.84	110.05
2	F	1	BGC	C6-C5-C4	-2.06	107.96	113.02

There are no chirality outliers.

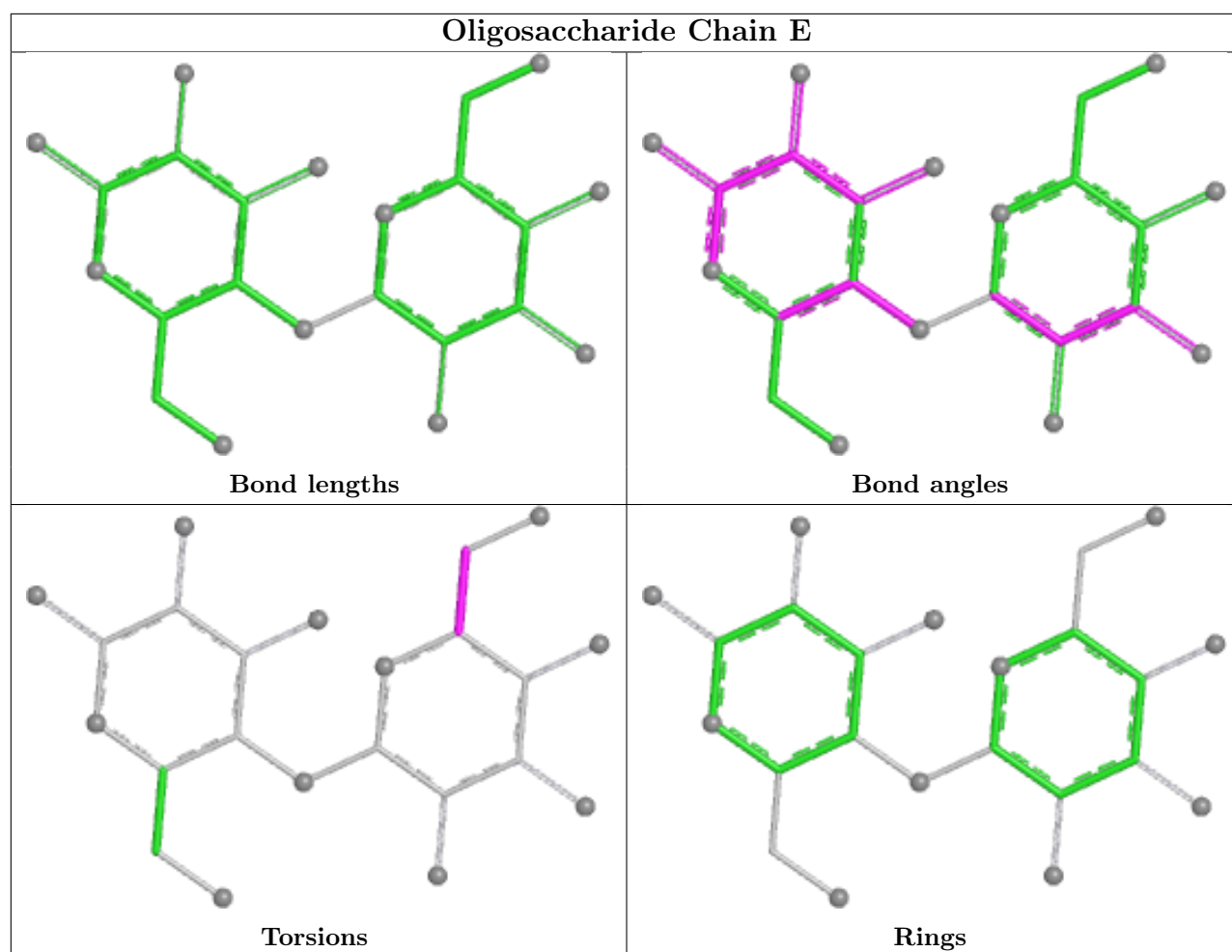
All (4) torsion outliers are listed below:

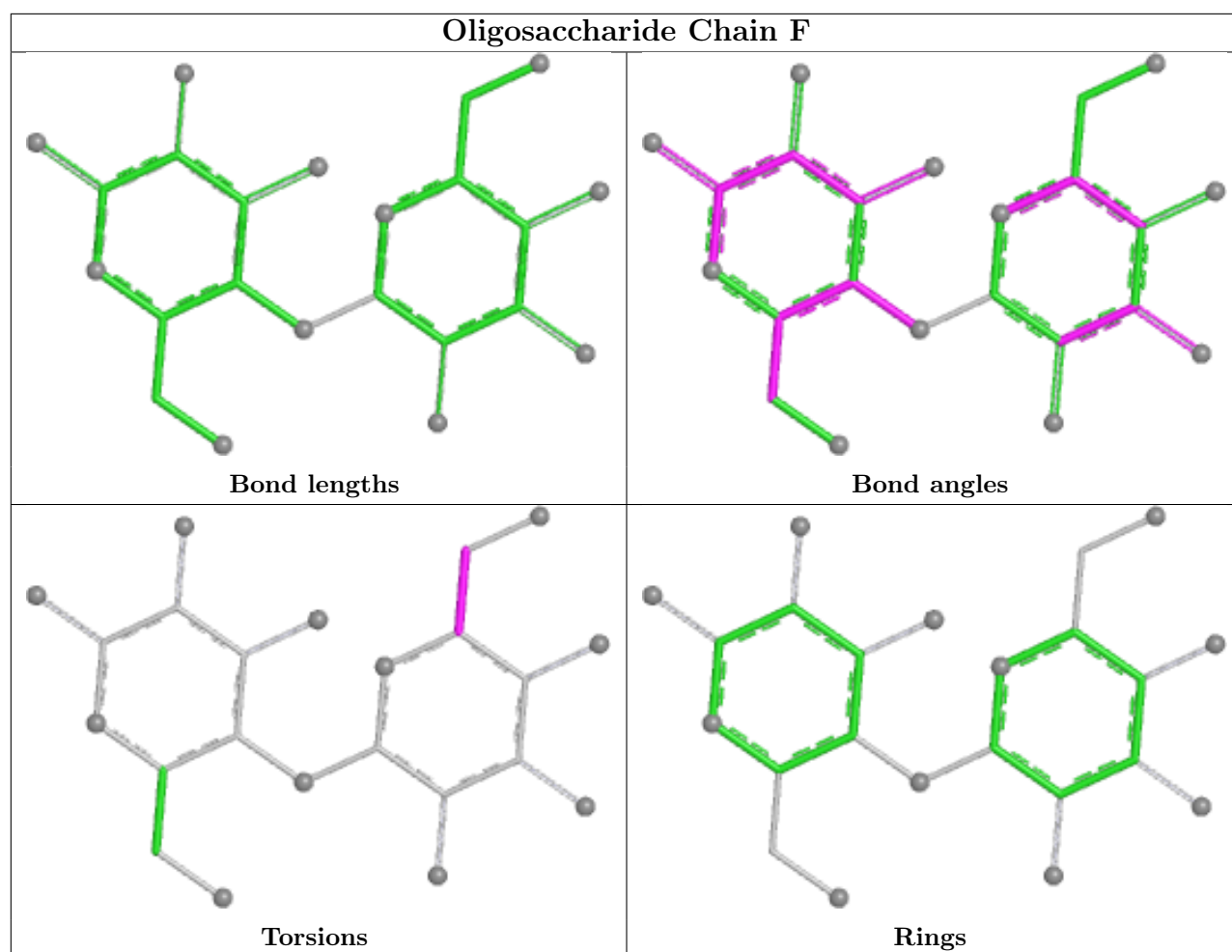
Mol	Chain	Res	Type	Atoms
2	G	2	GAL	O5-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6

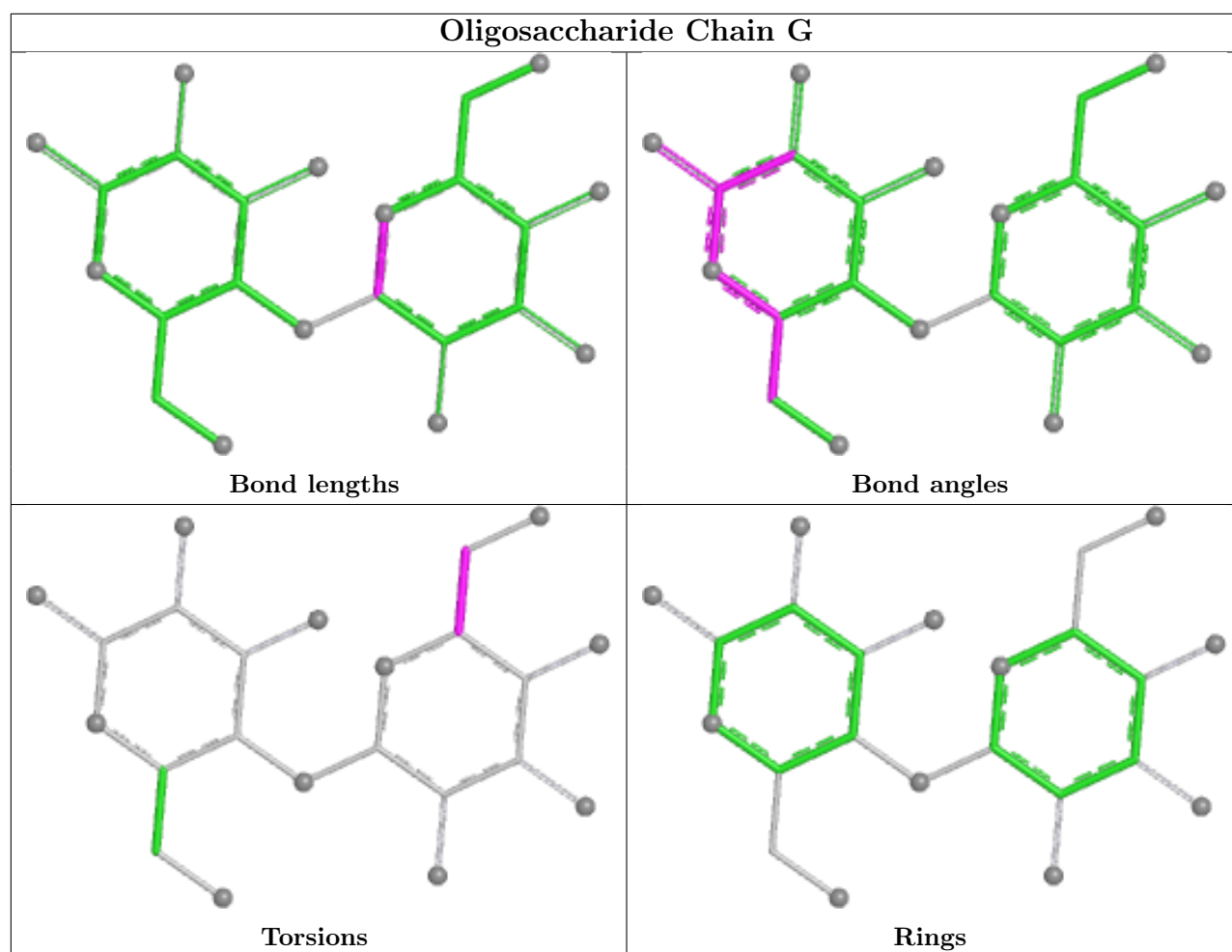
There are no ring outliers.

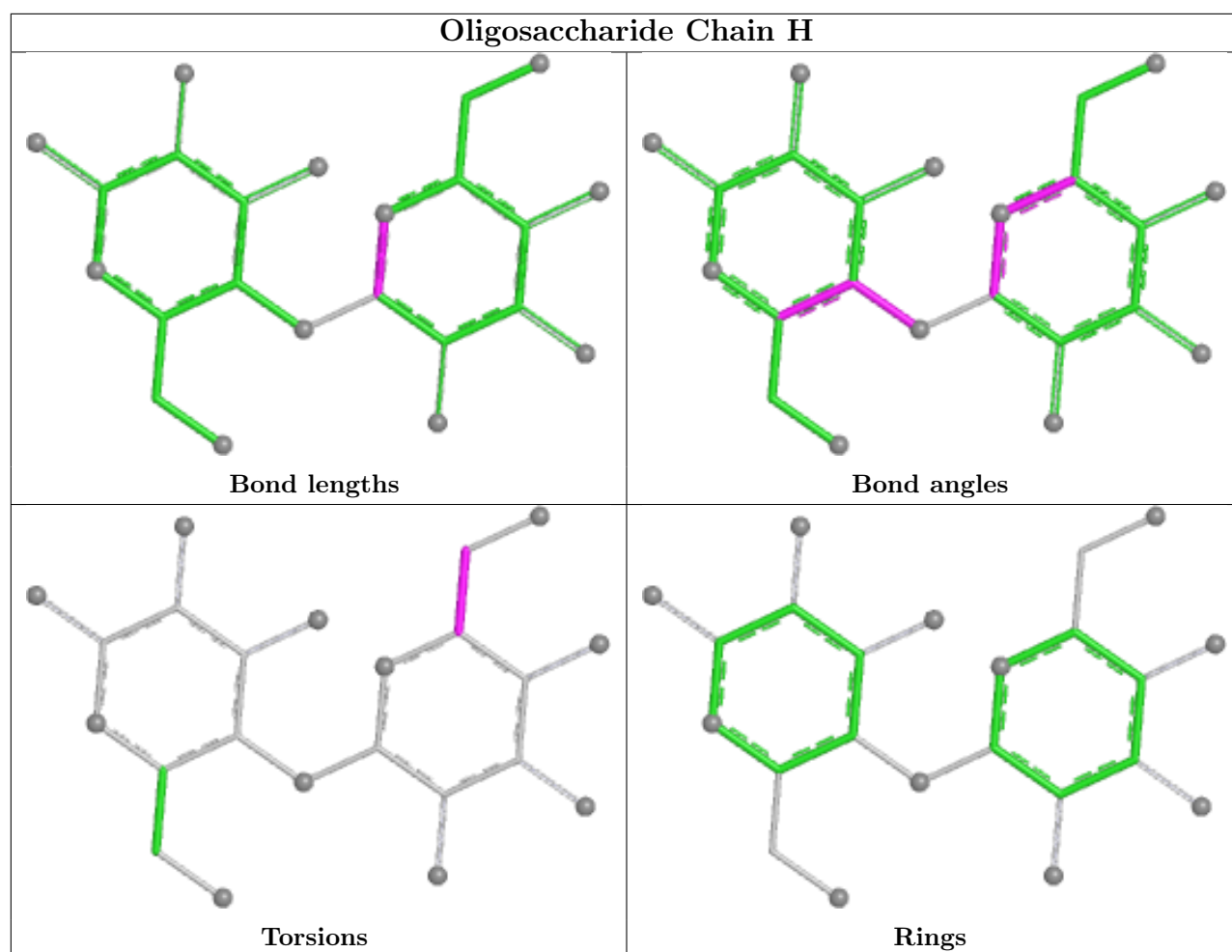
No monomer is involved in short contacts.

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](#)

Of 125 ligands modelled in this entry, 29 are monoatomic - leaving 96 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMS	A	8425	4	3,3,3	1.45	1 (33%)	3,3,3	0.29	0
5	DMS	A	8411	-	3,3,3	0.29	0	3,3,3	0.40	0
5	DMS	D	8407	-	3,3,3	1.91	2 (66%)	3,3,3	0.60	0
5	DMS	D	8414	-	3,3,3	0.15	0	3,3,3	0.26	0
5	DMS	C	8504	-	3,3,3	0.67	0	3,3,3	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8421	-	3,3,3	0.16	0	3,3,3	0.16	0
5	DMS	D	8703	-	3,3,3	0.72	0	3,3,3	0.54	0
5	DMS	B	8402	-	3,3,3	1.25	0	3,3,3	0.30	0
5	DMS	B	8504	-	3,3,3	0.12	0	3,3,3	0.26	0
5	DMS	D	8501	-	3,3,3	0.58	0	3,3,3	0.11	0
5	DMS	D	8406	-	3,3,3	0.90	0	3,3,3	0.58	0
5	DMS	A	8423	-	3,3,3	0.95	0	3,3,3	0.34	0
5	DMS	A	8410	-	3,3,3	0.25	0	3,3,3	0.29	0
5	DMS	D	8405	-	3,3,3	0.39	0	3,3,3	0.38	0
5	DMS	D	8508	-	3,3,3	0.83	0	3,3,3	0.23	0
5	DMS	B	8420	-	3,3,3	0.59	0	3,3,3	0.23	0
5	DMS	D	8411	-	3,3,3	0.48	0	3,3,3	0.53	0
5	DMS	C	8407	-	3,3,3	0.97	0	3,3,3	0.14	0
5	DMS	D	8419	-	3,3,3	0.33	0	3,3,3	0.22	0
5	DMS	A	8413	-	3,3,3	1.70	1 (33%)	3,3,3	0.44	0
5	DMS	D	8402	-	3,3,3	0.77	0	3,3,3	0.25	0
5	DMS	B	8417	-	3,3,3	0.48	0	3,3,3	0.08	0
5	DMS	C	8415	-	3,3,3	1.28	0	3,3,3	0.41	0
5	DMS	B	8409	-	3,3,3	1.19	0	3,3,3	0.31	0
5	DMS	C	8423	-	3,3,3	0.62	0	3,3,3	0.44	0
5	DMS	C	8410	-	3,3,3	0.94	0	3,3,3	0.16	0
5	DMS	D	8423	-	3,3,3	0.76	0	3,3,3	0.18	0
5	DMS	A	8501	-	3,3,3	0.92	0	3,3,3	0.13	0
5	DMS	A	8408	-	3,3,3	0.99	0	3,3,3	0.59	0
5	DMS	D	8413	-	3,3,3	1.00	0	3,3,3	0.26	0
5	DMS	B	8414	-	3,3,3	0.28	0	3,3,3	0.19	0
5	DMS	B	8411	-	3,3,3	0.85	0	3,3,3	0.23	0
5	DMS	B	8425	4	3,3,3	1.43	1 (33%)	3,3,3	0.65	0
5	DMS	C	8402	-	3,3,3	1.46	1 (33%)	3,3,3	0.32	0
5	DMS	A	8406	-	3,3,3	0.22	0	3,3,3	0.44	0
5	DMS	B	8410	-	3,3,3	1.06	0	3,3,3	0.78	0
5	DMS	A	8503	-	3,3,3	0.45	0	3,3,3	0.15	0
5	DMS	B	8502	-	3,3,3	0.93	0	3,3,3	1.16	1 (33%)
5	DMS	D	8416	-	3,3,3	0.43	0	3,3,3	0.19	0
5	DMS	C	8413	-	3,3,3	1.33	0	3,3,3	0.25	0
5	DMS	A	8412	-	3,3,3	0.19	0	3,3,3	0.19	0
5	DMS	A	8405	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	C	8420	-	3,3,3	0.53	0	3,3,3	0.25	0
5	DMS	A	8401	-	3,3,3	0.66	0	3,3,3	0.27	0
5	DMS	C	8404	-	3,3,3	0.94	0	3,3,3	0.64	0
5	DMS	B	8423	-	3,3,3	0.26	0	3,3,3	0.45	0
5	DMS	D	8704	-	3,3,3	0.35	0	3,3,3	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8408	-	3,3,3	1.07	0	3,3,3	0.37	0
5	DMS	D	8412	-	3,3,3	0.25	0	3,3,3	0.25	0
5	DMS	B	8403	-	3,3,3	1.19	0	3,3,3	0.43	0
5	DMS	B	8601	-	3,3,3	0.93	0	3,3,3	0.45	0
5	DMS	C	8417	-	3,3,3	0.65	0	3,3,3	0.36	0
5	DMS	C	8421	-	3,3,3	0.78	0	3,3,3	0.47	0
5	DMS	A	8404	-	3,3,3	0.79	0	3,3,3	0.09	0
5	DMS	C	8411	-	3,3,3	0.56	0	3,3,3	0.10	0
5	DMS	B	8416	-	3,3,3	0.78	0	3,3,3	0.17	0
5	DMS	D	8410	-	3,3,3	0.64	0	3,3,3	0.26	0
5	DMS	C	8401	-	3,3,3	0.62	0	3,3,3	0.27	0
5	DMS	A	8504	-	3,3,3	0.24	0	3,3,3	0.16	0
5	DMS	B	8415	-	3,3,3	0.87	0	3,3,3	0.54	0
5	DMS	D	8404	-	3,3,3	1.25	1 (33%)	3,3,3	0.12	0
5	DMS	C	8405	-	3,3,3	1.21	0	3,3,3	0.36	0
5	DMS	A	8414	-	3,3,3	0.86	0	3,3,3	0.16	0
5	DMS	D	8409	-	3,3,3	1.23	1 (33%)	3,3,3	0.95	0
5	DMS	C	8425	4	3,3,3	0.99	0	3,3,3	0.29	0
5	DMS	B	8401	-	3,3,3	0.83	0	3,3,3	0.40	0
5	DMS	B	8408	-	3,3,3	0.81	0	3,3,3	0.84	0
5	DMS	A	8419	-	3,3,3	0.52	0	3,3,3	0.36	0
5	DMS	C	8416	-	3,3,3	0.95	0	3,3,3	0.19	0
5	DMS	D	8408	-	3,3,3	0.95	0	3,3,3	0.06	0
5	DMS	C	8602	-	3,3,3	0.61	0	3,3,3	0.20	0
5	DMS	D	8403	-	3,3,3	0.54	0	3,3,3	0.21	0
5	DMS	B	8407	-	3,3,3	1.37	0	3,3,3	0.25	0
5	DMS	C	8403	-	3,3,3	0.53	0	3,3,3	0.39	0
5	DMS	D	8701	-	3,3,3	1.70	0	3,3,3	0.42	0
5	DMS	D	8705	-	3,3,3	1.18	0	3,3,3	0.56	0
5	DMS	A	8507	-	3,3,3	1.48	0	3,3,3	0.38	0
5	DMS	A	8421	-	3,3,3	0.51	0	3,3,3	0.56	0
5	DMS	B	8508	-	3,3,3	2.21	1 (33%)	3,3,3	0.60	0
5	DMS	B	8412	-	3,3,3	0.31	0	3,3,3	0.14	0
5	DMS	A	8409	-	3,3,3	1.07	0	3,3,3	0.17	0
5	DMS	C	8414	-	3,3,3	1.11	0	3,3,3	0.61	0
5	DMS	C	8419	-	3,3,3	0.44	0	3,3,3	0.19	0
5	DMS	A	8402	-	3,3,3	0.91	0	3,3,3	0.52	0
5	DMS	D	8401	-	3,3,3	1.13	0	3,3,3	0.36	0
5	DMS	B	8404	-	3,3,3	0.87	0	3,3,3	0.31	0
5	DMS	A	8420	-	3,3,3	0.35	0	3,3,3	0.61	0
5	DMS	B	8413	-	3,3,3	1.68	1 (33%)	3,3,3	0.39	0
5	DMS	B	8405	-	3,3,3	0.92	0	3,3,3	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8412	-	3,3,3	0.79	0	3,3,3	0.40	0
5	DMS	C	8409	-	3,3,3	0.98	0	3,3,3	0.23	0
5	DMS	A	8407	-	3,3,3	1.13	0	3,3,3	0.88	0
5	DMS	C	8501	-	3,3,3	0.58	0	3,3,3	0.60	0
5	DMS	A	8403	-	3,3,3	1.18	0	3,3,3	0.37	0
5	DMS	B	8421	-	3,3,3	0.54	0	3,3,3	0.37	0
5	DMS	C	8601	-	3,3,3	0.91	0	3,3,3	0.34	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8508	DMS	C1-S	3.61	2.01	1.76
5	D	8407	DMS	O-S	2.33	1.65	1.50
5	D	8407	DMS	C2-S	2.26	1.92	1.76
5	C	8402	DMS	C2-S	2.21	1.91	1.76
5	B	8413	DMS	O-S	2.21	1.64	1.50
5	B	8425	DMS	O-S	2.20	1.64	1.50
5	D	8409	DMS	O-S	2.05	1.63	1.50
5	A	8413	DMS	C2-S	2.05	1.90	1.76
5	D	8404	DMS	C2-S	2.04	1.90	1.76
5	A	8425	DMS	O-S	2.03	1.63	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	8502	DMS	C2-S-C1	2.02	108.75	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8425	DMS	2	0
5	D	8407	DMS	1	0
5	C	8504	DMS	1	0
5	D	8703	DMS	1	0
5	B	8504	DMS	2	0
5	A	8423	DMS	2	0
5	B	8420	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8417	DMS	3	0
5	C	8415	DMS	1	0
5	C	8423	DMS	1	0
5	D	8423	DMS	1	0
5	A	8408	DMS	2	0
5	B	8410	DMS	3	0
5	A	8503	DMS	1	0
5	D	8416	DMS	1	0
5	A	8412	DMS	4	0
5	C	8420	DMS	3	0
5	C	8408	DMS	2	0
5	D	8412	DMS	3	0
5	C	8417	DMS	2	0
5	B	8415	DMS	1	0
5	D	8409	DMS	1	0
5	C	8425	DMS	1	0
5	B	8408	DMS	2	0
5	C	8602	DMS	3	0
5	D	8403	DMS	1	0
5	C	8403	DMS	1	0
5	B	8508	DMS	2	0
5	B	8412	DMS	1	0
5	C	8419	DMS	1	0
5	A	8420	DMS	3	0
5	C	8412	DMS	1	0
5	A	8403	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.79	13 (1%) 75 75	6, 13, 41, 100	1 (0%)
1	B	1011/1023 (98%)	-0.79	18 (1%) 67 68	6, 12, 40, 94	1 (0%)
1	C	1011/1023 (98%)	-0.78	13 (1%) 75 75	6, 13, 42, 100	1 (0%)
1	D	1011/1023 (98%)	-0.75	20 (1%) 65 65	6, 13, 43, 95	1 (0%)
All	All	4044/4092 (98%)	-0.78	64 (1%) 70 71	6, 13, 42, 100	4 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	5.9
1	B	685	LEU	5.1
1	D	732	ALA	4.2
1	D	685	LEU	4.1
1	A	685	LEU	4.0
1	D	730	LEU	3.9
1	A	799	THR	3.9
1	A	1023	LYS	3.8
1	B	732	ALA	3.7
1	A	634	GLN	3.7
1	C	730	LEU	3.7
1	B	733	ALA	3.6
1	C	686	PRO	3.6
1	D	686	PRO	3.6
1	A	730	LEU	3.6
1	D	733	ALA	3.5
1	D	735	HIS	3.5
1	C	733	ALA	3.5
1	A	735	HIS	3.5
1	D	734	SER	3.5
1	B	1023	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	736	ALA	3.5
1	B	730	LEU	3.3
1	C	735	HIS	3.2
1	D	634	GLN	3.2
1	C	685	LEU	3.2
1	C	634	GLN	2.9
1	B	729	THR	2.8
1	A	731	PRO	2.8
1	B	686	PRO	2.8
1	C	732	ALA	2.8
1	A	689	GLU	2.8
1	D	688	PRO	2.7
1	B	745	MET	2.7
1	C	734	SER	2.6
1	B	845	GLN	2.5
1	D	689	GLU	2.5
1	D	1023	LYS	2.4
1	B	689	GLU	2.4
1	C	731	PRO	2.4
1	A	732	ALA	2.4
1	B	735	HIS	2.4
1	B	1018	LEU	2.3
1	A	829	THR	2.3
1	A	683	PRO	2.3
1	C	772	ASP	2.3
1	D	71	GLU	2.3
1	B	798	ALA	2.2
1	C	761	GLN	2.2
1	B	799	THR	2.2
1	A	733	ALA	2.2
1	D	666	GLY	2.2
1	B	688	PRO	2.2
1	D	731	PRO	2.2
1	D	683	PRO	2.1
1	D	655	MET	2.1
1	D	729	THR	2.1
1	B	663	LEU	2.1
1	B	731	PRO	2.1
1	C	684	GLU	2.1
1	D	1022	GLN	2.1
1	D	581	ASN	2.0
1	B	684	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	799	THR	2.0

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

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

6.3 Carbohydrates [i](#)

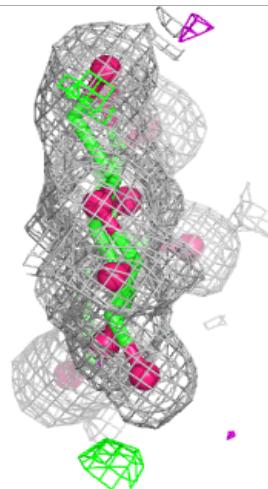
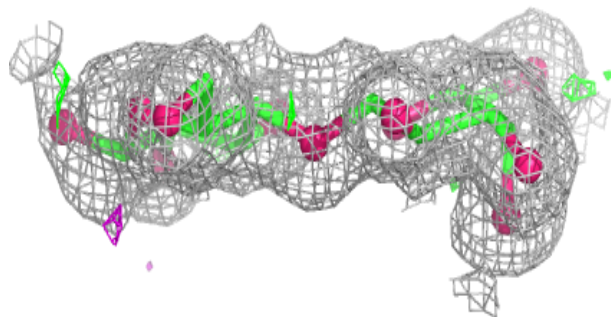
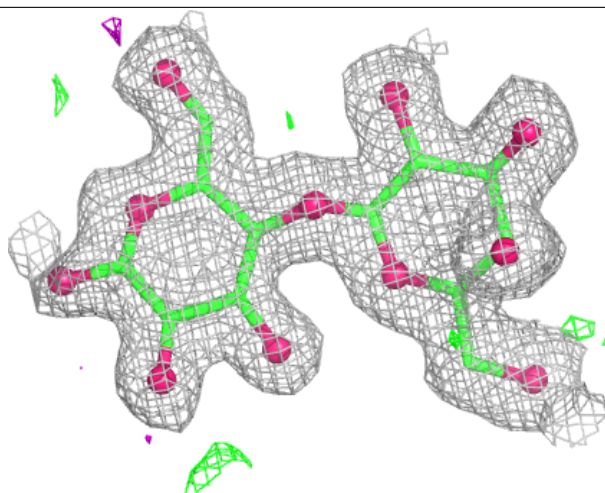
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	F	1	12/12	0.95	0.07	7,19,30,32	0
2	BGC	G	1	12/12	0.95	0.08	6,16,32,45	12
2	BGC	H	1	12/12	0.95	0.09	8,23,29,100	0
2	BGC	E	1	12/12	0.96	0.07	9,19,28,42	0
2	GAL	E	2	11/12	0.98	0.04	8,9,13,15	0
2	GAL	G	2	11/12	0.99	0.03	4,5,8,10	11
2	GAL	F	2	11/12	0.99	0.03	2,5,10,13	0
2	GAL	H	2	11/12	0.99	0.03	7,10,12,13	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.

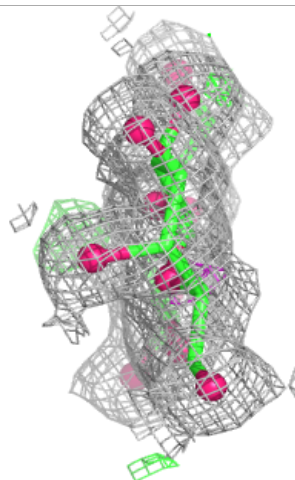
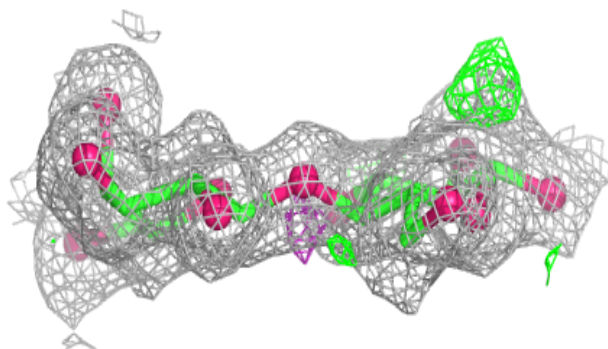
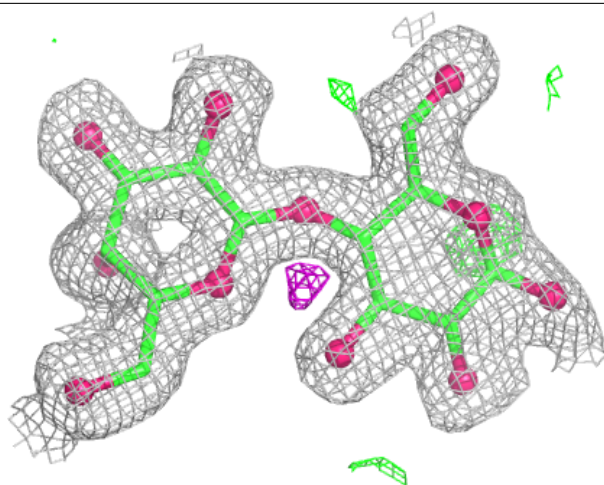
Electron density around Chain E:

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



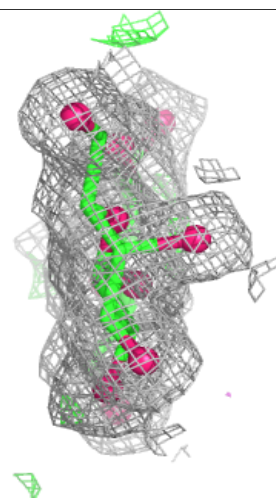
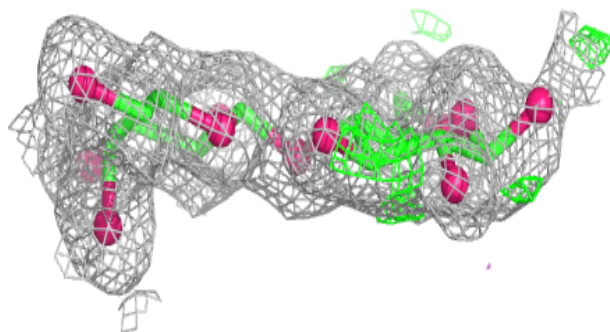
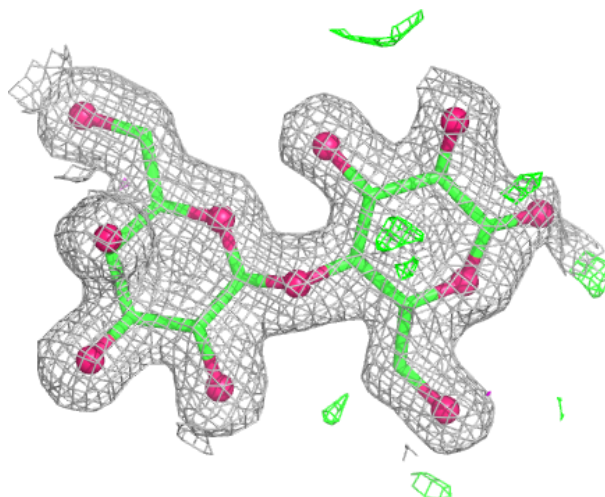
Electron density around Chain F:

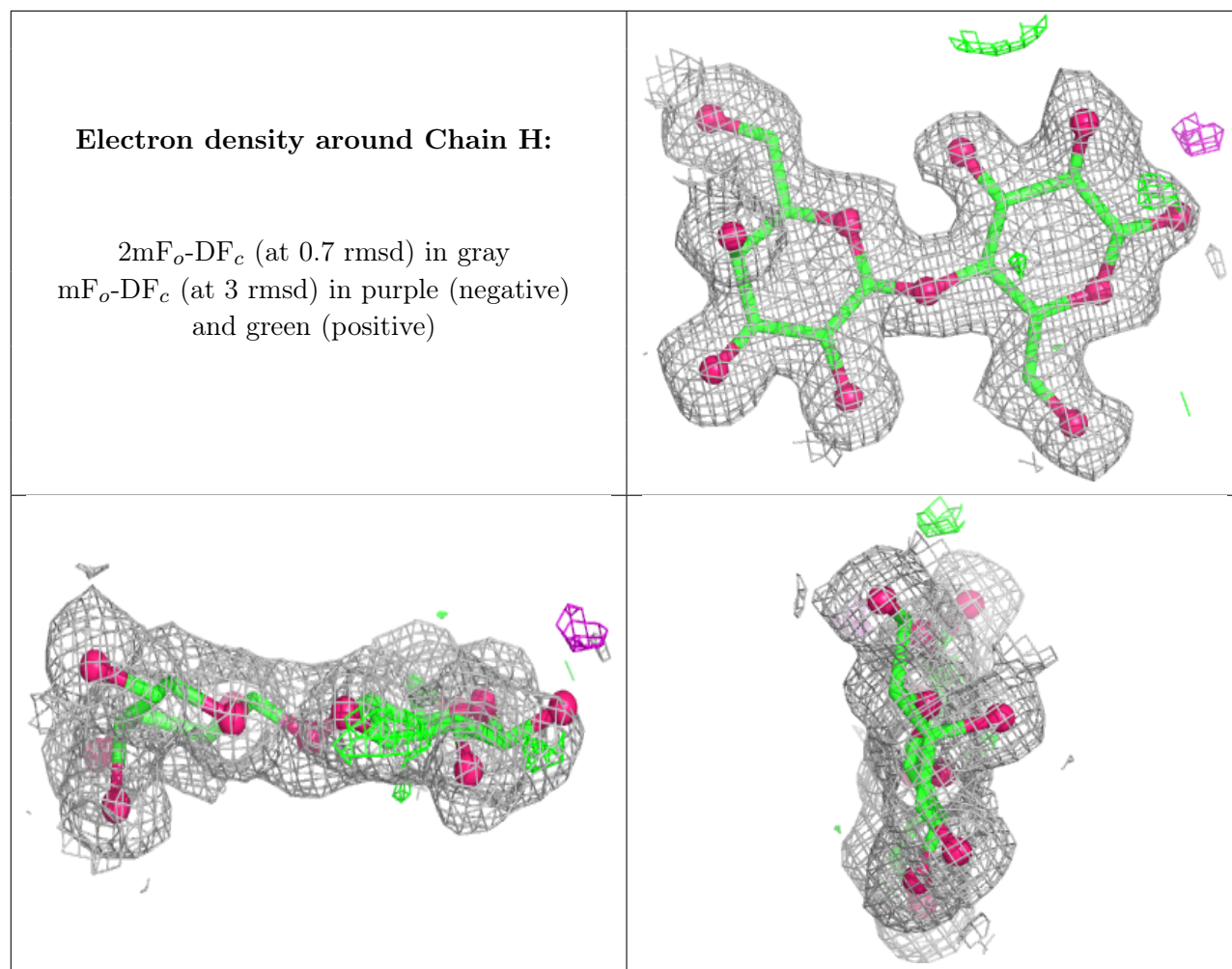
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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](#)

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
3	MG	A	3105	1/1	0.67	0.16	77,77,77,77	0
5	DMS	A	8507	4/4	0.83	0.15	23,26,35,72	0
5	DMS	D	8704	4/4	0.83	0.21	32,63,100,100	0
5	DMS	D	8423	4/4	0.85	0.17	27,46,56,65	0
5	DMS	D	8703	4/4	0.86	0.19	29,55,61,61	0
5	DMS	B	8417	4/4	0.88	0.14	22,32,68,74	0
5	DMS	D	8705	4/4	0.88	0.15	30,37,42,43	0
5	DMS	C	8417	4/4	0.89	0.15	25,27,63,74	0
5	DMS	C	8423	4/4	0.89	0.12	31,31,46,51	0
5	DMS	A	8423	4/4	0.90	0.12	27,33,43,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8406	4/4	0.90	0.16	23,42,59,61	0
5	DMS	A	8421	4/4	0.90	0.13	36,42,50,59	0
5	DMS	B	8415	4/4	0.91	0.11	21,31,32,59	0
5	DMS	B	8420	4/4	0.91	0.17	41,43,64,72	0
5	DMS	C	8415	4/4	0.91	0.13	15,33,50,60	0
5	DMS	C	8602	4/4	0.92	0.14	46,51,58,69	0
5	DMS	D	8407	4/4	0.92	0.13	27,31,37,44	0
5	DMS	D	8416	4/4	0.92	0.13	22,36,46,100	0
5	DMS	D	8421	4/4	0.92	0.15	33,46,52,100	0
5	DMS	B	8425	4/4	0.92	0.10	21,26,37,42	0
5	DMS	A	8425	4/4	0.92	0.12	26,35,37,40	0
3	MG	D	3003	1/1	0.92	0.15	55,55,55,55	0
5	DMS	B	8413	4/4	0.92	0.12	27,36,38,39	0
5	DMS	B	8423	4/4	0.93	0.14	24,28,46,100	0
5	DMS	D	8404	4/4	0.93	0.11	17,17,42,58	0
5	DMS	B	8416	4/4	0.93	0.10	28,35,43,58	0
4	NA	B	3104	1/1	0.93	0.08	27,27,27,27	0
5	DMS	B	8407	4/4	0.93	0.13	30,31,36,37	0
5	DMS	C	8420	4/4	0.93	0.11	26,32,43,64	0
5	DMS	D	8501	4/4	0.93	0.09	21,29,32,50	0
5	DMS	D	8508	4/4	0.93	0.09	29,34,36,53	0
5	DMS	C	8421	4/4	0.93	0.14	31,35,46,100	0
5	DMS	B	8421	4/4	0.93	0.11	22,46,51,73	0
5	DMS	C	8601	4/4	0.93	0.15	43,43,55,81	0
5	DMS	A	8412	4/4	0.94	0.12	34,44,51,54	0
5	DMS	A	8503	4/4	0.94	0.10	34,37,46,50	0
5	DMS	C	8419	4/4	0.94	0.10	33,39,43,54	0
5	DMS	C	8504	4/4	0.94	0.09	29,32,45,52	0
5	DMS	D	8409	4/4	0.95	0.09	25,28,30,33	0
5	DMS	D	8414	4/4	0.95	0.17	21,36,100,100	0
5	DMS	C	8413	4/4	0.95	0.11	25,31,31,32	0
5	DMS	C	8425	4/4	0.95	0.12	32,40,40,41	0
5	DMS	C	8501	4/4	0.95	0.09	18,35,37,38	0
5	DMS	A	8414	4/4	0.95	0.12	26,26,43,100	0
5	DMS	A	8420	4/4	0.95	0.12	30,33,39,44	0
4	NA	A	3104	1/1	0.95	0.06	26,26,26,26	0
5	DMS	A	8413	4/4	0.95	0.10	24,26,32,41	0
5	DMS	B	8508	4/4	0.95	0.09	15,34,46,47	0
3	MG	A	3005	1/1	0.96	0.07	31,31,31,31	0
5	DMS	A	8501	4/4	0.96	0.07	11,24,32,36	0
4	NA	C	3104	1/1	0.96	0.09	26,26,26,26	0
5	DMS	A	8504	4/4	0.96	0.14	19,33,55,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	3004	1/1	0.96	0.07	37,37,37,37	0
5	DMS	B	8502	4/4	0.96	0.09	19,24,33,33	0
5	DMS	B	8504	4/4	0.96	0.07	17,25,33,36	0
5	DMS	A	8419	4/4	0.96	0.09	34,37,38,42	0
5	DMS	D	8406	4/4	0.96	0.08	18,19,22,29	0
5	DMS	B	8601	4/4	0.96	0.10	35,35,39,48	0
5	DMS	C	8407	4/4	0.96	0.09	26,26,31,32	0
5	DMS	C	8408	4/4	0.96	0.06	15,20,28,29	0
5	DMS	C	8409	4/4	0.96	0.08	27,32,37,38	0
5	DMS	C	8412	4/4	0.96	0.09	23,29,32,56	0
5	DMS	B	8409	4/4	0.96	0.08	28,28,31,32	0
5	DMS	C	8414	4/4	0.96	0.10	16,36,37,51	0
5	DMS	A	8407	4/4	0.96	0.07	16,24,25,33	0
5	DMS	B	8414	4/4	0.96	0.14	21,42,100,100	0
5	DMS	A	8408	4/4	0.96	0.09	23,25,29,41	0
5	DMS	A	8409	4/4	0.96	0.07	26,26,26,40	0
5	DMS	D	8413	4/4	0.97	0.08	27,27,27,31	0
5	DMS	B	8410	4/4	0.97	0.08	15,37,37,38	0
5	DMS	C	8416	4/4	0.97	0.07	31,34,36,40	0
5	DMS	D	8419	4/4	0.97	0.07	22,33,39,41	0
5	DMS	B	8412	4/4	0.97	0.06	22,30,32,32	0
3	MG	C	3006	1/1	0.97	0.09	27,27,27,27	0
5	DMS	B	8404	4/4	0.97	0.06	17,25,28,31	0
4	NA	D	3103	1/1	0.97	0.05	26,26,26,26	0
5	DMS	B	8408	4/4	0.97	0.08	17,26,29,46	0
5	DMS	D	8408	4/4	0.97	0.06	16,27,27,31	0
5	DMS	A	8404	4/4	0.97	0.07	18,21,27,27	0
3	MG	D	3005	1/1	0.98	0.06	21,21,21,21	0
4	NA	A	3103	1/1	0.98	0.04	21,21,21,21	0
5	DMS	A	8402	4/4	0.98	0.07	12,19,20,21	0
4	NA	C	3103	1/1	0.98	0.04	19,19,19,19	0
5	DMS	C	8404	4/4	0.98	0.05	15,18,18,25	0
5	DMS	C	8405	4/4	0.98	0.06	16,22,25,27	0
5	DMS	A	8410	4/4	0.98	0.07	18,28,29,35	0
5	DMS	A	8405	4/4	0.98	0.08	16,22,25,57	0
5	DMS	D	8701	4/4	0.98	0.06	9,12,16,32	0
5	DMS	B	8405	4/4	0.98	0.07	22,26,31,34	0
5	DMS	C	8410	4/4	0.98	0.07	25,28,31,35	0
5	DMS	D	8410	4/4	0.98	0.05	15,25,28,34	0
5	DMS	D	8401	4/4	0.99	0.05	11,11,14,15	0
5	DMS	D	8402	4/4	0.99	0.04	13,15,18,19	0
5	DMS	D	8403	4/4	0.99	0.04	13,20,20,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8411	4/4	0.99	0.06	17,17,22,36	0
5	DMS	D	8405	4/4	0.99	0.06	21,23,31,36	0
5	DMS	A	8401	4/4	0.99	0.04	11,11,12,12	0
5	DMS	C	8411	4/4	0.99	0.04	16,21,23,28	0
5	DMS	B	8401	4/4	0.99	0.05	11,12,14,16	0
5	DMS	B	8402	4/4	0.99	0.05	9,16,17,20	0
5	DMS	B	8403	4/4	0.99	0.04	14,15,20,20	0
5	DMS	D	8411	4/4	0.99	0.07	15,17,22,48	0
5	DMS	D	8412	4/4	0.99	0.07	21,25,30,46	0
4	NA	B	3101	1/1	0.99	0.02	11,11,11,11	0
5	DMS	A	8403	4/4	0.99	0.04	15,15,16,20	0
4	NA	B	3103	1/1	0.99	0.04	19,19,19,19	0
3	MG	A	3002	1/1	0.99	0.03	12,12,12,12	0
3	MG	B	3001	1/1	0.99	0.03	8,8,8,8	0
3	MG	D	3001	1/1	0.99	0.04	9,9,9,9	0
5	DMS	C	8402	4/4	0.99	0.05	11,16,21,24	0
5	DMS	C	8403	4/4	0.99	0.04	16,17,18,18	0
5	DMS	B	8411	4/4	0.99	0.09	18,22,22,80	0
4	NA	D	3101	1/1	0.99	0.03	10,10,10,10	0
4	NA	D	3102	1/1	0.99	0.03	10,10,10,10	0
3	MG	D	3002	1/1	0.99	0.04	12,12,12,12	0
4	NA	A	3101	1/1	1.00	0.04	10,10,10,10	0
5	DMS	C	8401	4/4	1.00	0.04	8,10,16,21	0
4	NA	C	3101	1/1	1.00	0.02	9,9,9,9	0
4	NA	C	3102	1/1	1.00	0.03	11,11,11,11	0
4	NA	A	3102	1/1	1.00	0.02	12,12,12,12	0
3	MG	C	3001	1/1	1.00	0.02	10,10,10,10	0
3	MG	C	3002	1/1	1.00	0.04	9,9,9,9	0
3	MG	A	3001	1/1	1.00	0.01	10,10,10,10	0
4	NA	B	3102	1/1	1.00	0.04	10,10,10,10	0
3	MG	B	3002	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.