



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 AM UTC

PDB ID : 5TJ4 / pdb_00005tj4
Title : Gasdermin-B C-terminal domain containing the polymorphism residues
Gly299:Pro306 fused to maltose binding protein
Authors : Chao, L.K.; Herzberg, O.
Deposited on : 2016-10-03
Resolution : 3.50 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:

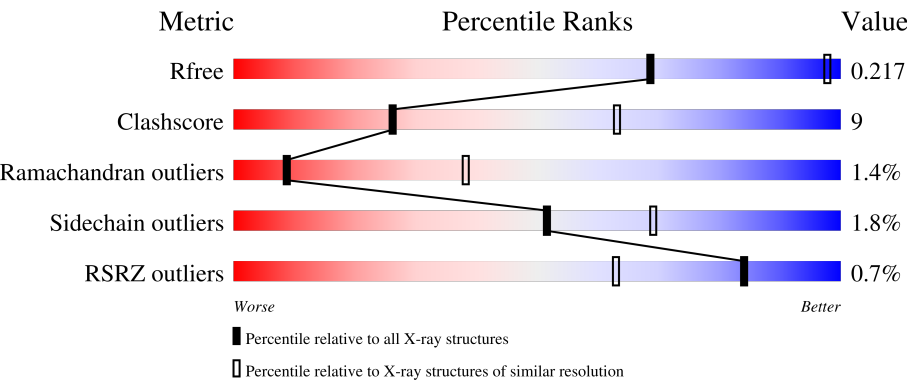
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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.



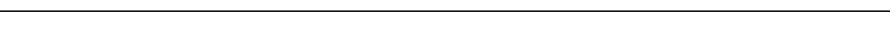
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	561	% 81%14% . .
1	B	561	83%13% ..
1	C	561	% 79%16% . .
1	D	561	% 81%14% ..
1	E	561	% 84%13% ..

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Mol	Chain	Length	Quality of chain
1	F	561	 82% 13% . .
1	G	561	 82% 12% . . .
1	H	561	 % 80% 14% . .
1	I	561	 % 80% 13% . 5%
1	J	561	 2% 85% 11% . .
2	K	2	 50% 50%
2	L	2	 100%
2	M	2	 50% 50%
2	N	2	 100%
2	O	2	 100%
2	P	2	 50% 50%
2	Q	2	 100%
2	R	2	 100%
2	S	2	 50% 50%
2	T	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39838 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 Sugar ABC transporter substrate-binding protein, Gasdermin-B fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4066	2613	658	781	14			
1	B	554	Total	C	N	O	S	0	0	0
			4064	2603	664	784	13			
1	C	554	Total	C	N	O	S	0	0	0
			4070	2608	664	785	13			
1	D	541	Total	C	N	O	S	0	0	0
			3959	2542	643	762	12			
1	E	556	Total	C	N	O	S	0	0	0
			4077	2618	669	777	13			
1	F	541	Total	C	N	O	S	0	0	0
			3956	2546	633	765	12			
1	G	543	Total	C	N	O	S	0	0	0
			3885	2504	629	740	12			
1	H	537	Total	C	N	O	S	0	0	0
			3832	2459	623	739	11			
1	I	535	Total	C	N	O	S	0	0	0
			3795	2437	619	727	12			
1	J	548	Total	C	N	O	S	0	0	0
			3902	2500	638	754	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	see remark 999	UNP A0A178SBV6
A	83	ALA	LYS	see remark 999	UNP A0A178SBV6
A	172	ALA	GLU	see remark 999	UNP A0A178SBV6
A	173	ALA	ASN	see remark 999	UNP A0A178SBV6
A	239	ALA	LYS	see remark 999	UNP A0A178SBV6
A	362	ALA	LYS	see remark 999	UNP A0A178SBV6
A	363	ALA	ASP	see remark 999	UNP A0A178SBV6
A	367	ASN	-	linker	UNP A0A178SBV6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	-	linker	UNP A0A178SBV6
A	369	ALA	-	linker	UNP A0A178SBV6
A	370	ALA	-	linker	UNP A0A178SBV6
A	1220	MET	MET	linker	UNP Q8TAX9
B	82	ALA	ASP	see remark 999	UNP A0A178SBV6
B	83	ALA	LYS	see remark 999	UNP A0A178SBV6
B	172	ALA	GLU	see remark 999	UNP A0A178SBV6
B	173	ALA	ASN	see remark 999	UNP A0A178SBV6
B	239	ALA	LYS	see remark 999	UNP A0A178SBV6
B	362	ALA	LYS	see remark 999	UNP A0A178SBV6
B	363	ALA	ASP	see remark 999	UNP A0A178SBV6
B	367	ASN	-	linker	UNP A0A178SBV6
B	368	ALA	-	linker	UNP A0A178SBV6
B	369	ALA	-	linker	UNP A0A178SBV6
B	370	ALA	-	linker	UNP A0A178SBV6
B	1220	MET	MET	linker	UNP Q8TAX9
C	82	ALA	ASP	see remark 999	UNP A0A178SBV6
C	83	ALA	LYS	see remark 999	UNP A0A178SBV6
C	172	ALA	GLU	see remark 999	UNP A0A178SBV6
C	173	ALA	ASN	see remark 999	UNP A0A178SBV6
C	239	ALA	LYS	see remark 999	UNP A0A178SBV6
C	362	ALA	LYS	see remark 999	UNP A0A178SBV6
C	363	ALA	ASP	see remark 999	UNP A0A178SBV6
C	367	ASN	-	linker	UNP A0A178SBV6
C	368	ALA	-	linker	UNP A0A178SBV6
C	369	ALA	-	linker	UNP A0A178SBV6
C	370	ALA	-	linker	UNP A0A178SBV6
C	1220	MET	MET	linker	UNP Q8TAX9
D	82	ALA	ASP	see remark 999	UNP A0A178SBV6
D	83	ALA	LYS	see remark 999	UNP A0A178SBV6
D	172	ALA	GLU	see remark 999	UNP A0A178SBV6
D	173	ALA	ASN	see remark 999	UNP A0A178SBV6
D	239	ALA	LYS	see remark 999	UNP A0A178SBV6
D	362	ALA	LYS	see remark 999	UNP A0A178SBV6
D	363	ALA	ASP	see remark 999	UNP A0A178SBV6
D	367	ASN	-	linker	UNP A0A178SBV6
D	368	ALA	-	linker	UNP A0A178SBV6
D	369	ALA	-	linker	UNP A0A178SBV6
D	370	ALA	-	linker	UNP A0A178SBV6
D	1220	MET	MET	linker	UNP Q8TAX9
E	82	ALA	ASP	see remark 999	UNP A0A178SBV6
E	83	ALA	LYS	see remark 999	UNP A0A178SBV6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	172	ALA	GLU	see remark 999	UNP A0A178SBV6
E	173	ALA	ASN	see remark 999	UNP A0A178SBV6
E	239	ALA	LYS	see remark 999	UNP A0A178SBV6
E	362	ALA	LYS	see remark 999	UNP A0A178SBV6
E	363	ALA	ASP	see remark 999	UNP A0A178SBV6
E	367	ASN	-	linker	UNP A0A178SBV6
E	368	ALA	-	linker	UNP A0A178SBV6
E	369	ALA	-	linker	UNP A0A178SBV6
E	370	ALA	-	linker	UNP A0A178SBV6
E	1220	MET	MET	linker	UNP Q8TAX9
F	82	ALA	ASP	see remark 999	UNP A0A178SBV6
F	83	ALA	LYS	see remark 999	UNP A0A178SBV6
F	172	ALA	GLU	see remark 999	UNP A0A178SBV6
F	173	ALA	ASN	see remark 999	UNP A0A178SBV6
F	239	ALA	LYS	see remark 999	UNP A0A178SBV6
F	362	ALA	LYS	see remark 999	UNP A0A178SBV6
F	363	ALA	ASP	see remark 999	UNP A0A178SBV6
F	367	ASN	-	linker	UNP A0A178SBV6
F	368	ALA	-	linker	UNP A0A178SBV6
F	369	ALA	-	linker	UNP A0A178SBV6
F	370	ALA	-	linker	UNP A0A178SBV6
F	1220	MET	MET	linker	UNP Q8TAX9
G	82	ALA	ASP	see remark 999	UNP A0A178SBV6
G	83	ALA	LYS	see remark 999	UNP A0A178SBV6
G	172	ALA	GLU	see remark 999	UNP A0A178SBV6
G	173	ALA	ASN	see remark 999	UNP A0A178SBV6
G	239	ALA	LYS	see remark 999	UNP A0A178SBV6
G	362	ALA	LYS	see remark 999	UNP A0A178SBV6
G	363	ALA	ASP	see remark 999	UNP A0A178SBV6
G	367	ASN	-	linker	UNP A0A178SBV6
G	368	ALA	-	linker	UNP A0A178SBV6
G	369	ALA	-	linker	UNP A0A178SBV6
G	370	ALA	-	linker	UNP A0A178SBV6
G	1220	MET	MET	linker	UNP Q8TAX9
H	82	ALA	ASP	see remark 999	UNP A0A178SBV6
H	83	ALA	LYS	see remark 999	UNP A0A178SBV6
H	172	ALA	GLU	see remark 999	UNP A0A178SBV6
H	173	ALA	ASN	see remark 999	UNP A0A178SBV6
H	239	ALA	LYS	see remark 999	UNP A0A178SBV6
H	362	ALA	LYS	see remark 999	UNP A0A178SBV6
H	363	ALA	ASP	see remark 999	UNP A0A178SBV6
H	367	ASN	-	linker	UNP A0A178SBV6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	368	ALA	-	linker	UNP A0A178SBV6
H	369	ALA	-	linker	UNP A0A178SBV6
H	370	ALA	-	linker	UNP A0A178SBV6
H	1220	MET	MET	linker	UNP Q8TAX9
I	82	ALA	ASP	see remark 999	UNP A0A178SBV6
I	83	ALA	LYS	see remark 999	UNP A0A178SBV6
I	172	ALA	GLU	see remark 999	UNP A0A178SBV6
I	173	ALA	ASN	see remark 999	UNP A0A178SBV6
I	239	ALA	LYS	see remark 999	UNP A0A178SBV6
I	362	ALA	LYS	see remark 999	UNP A0A178SBV6
I	363	ALA	ASP	see remark 999	UNP A0A178SBV6
I	367	ASN	-	linker	UNP A0A178SBV6
I	368	ALA	-	linker	UNP A0A178SBV6
I	369	ALA	-	linker	UNP A0A178SBV6
I	370	ALA	-	linker	UNP A0A178SBV6
I	1220	MET	MET	linker	UNP Q8TAX9
J	82	ALA	ASP	see remark 999	UNP A0A178SBV6
J	83	ALA	LYS	see remark 999	UNP A0A178SBV6
J	172	ALA	GLU	see remark 999	UNP A0A178SBV6
J	173	ALA	ASN	see remark 999	UNP A0A178SBV6
J	239	ALA	LYS	see remark 999	UNP A0A178SBV6
J	362	ALA	LYS	see remark 999	UNP A0A178SBV6
J	363	ALA	ASP	see remark 999	UNP A0A178SBV6
J	367	ASN	-	linker	UNP A0A178SBV6
J	368	ALA	-	linker	UNP A0A178SBV6
J	369	ALA	-	linker	UNP A0A178SBV6
J	370	ALA	-	linker	UNP A0A178SBV6
J	1220	MET	MET	linker	UNP Q8TAX9

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C	O	0	0	0
			23	12	11			
2	T	2	Total	C	O	0	0	0
			23	12	11			

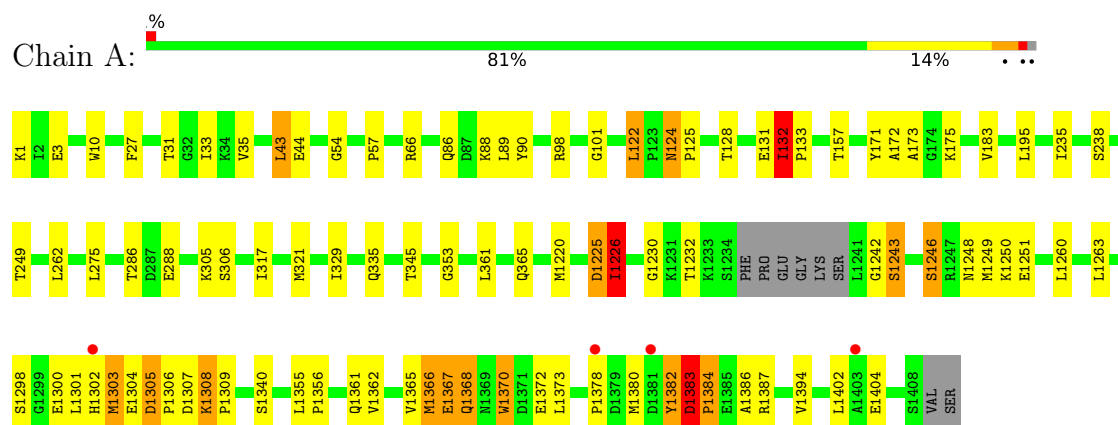
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

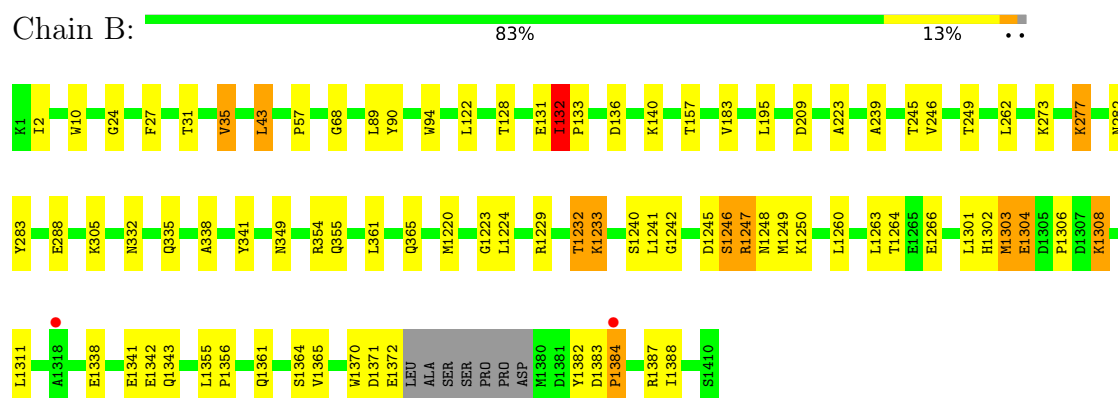
3 Residue-property plots

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.

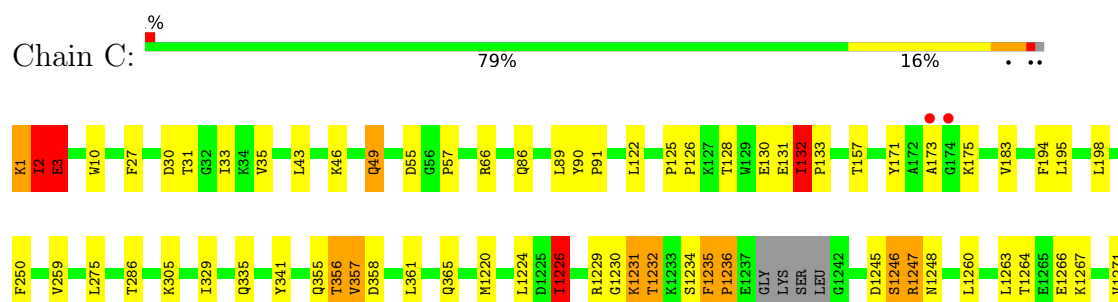
- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein



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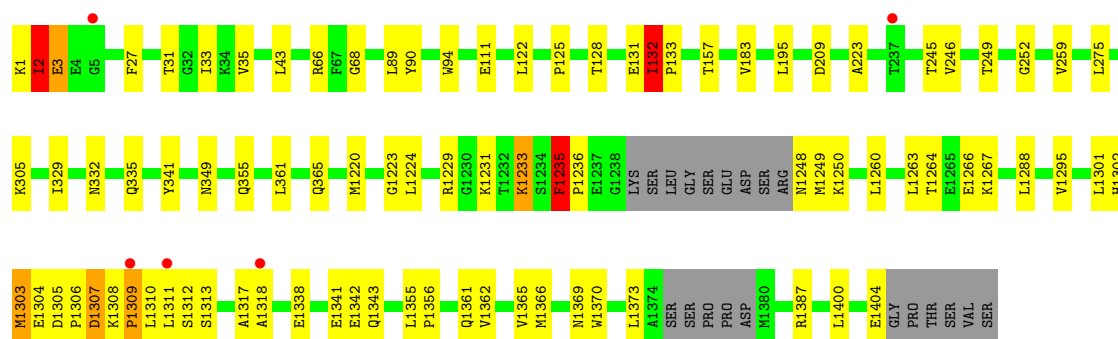
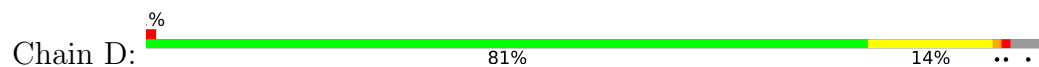


- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

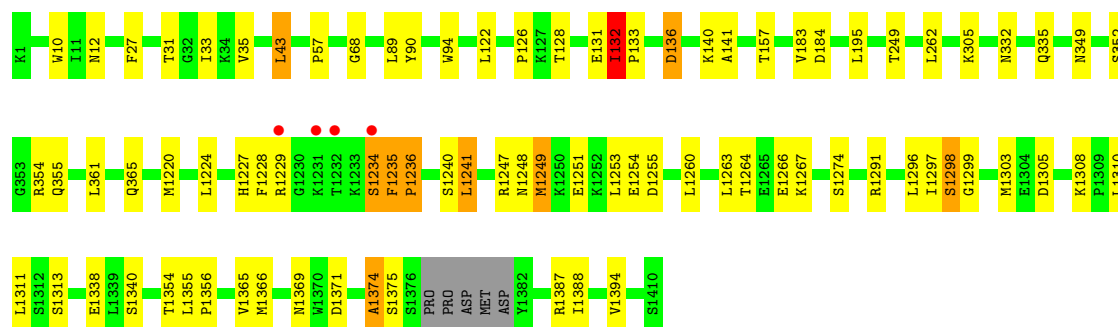
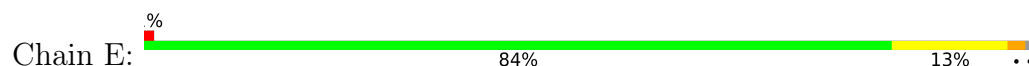




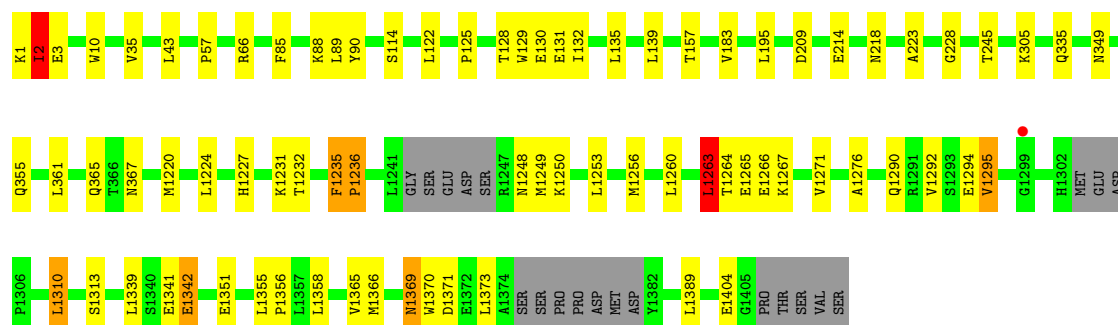
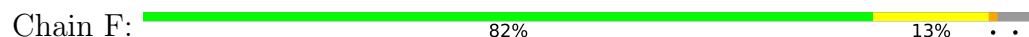
- Molecule 1: Sugar ABC transporter substrate-binding protein, Gasdermin-B fusion protein



- Molecule 1: Sugar ABC transporter substrate-binding protein, Gasdermin-B fusion protein

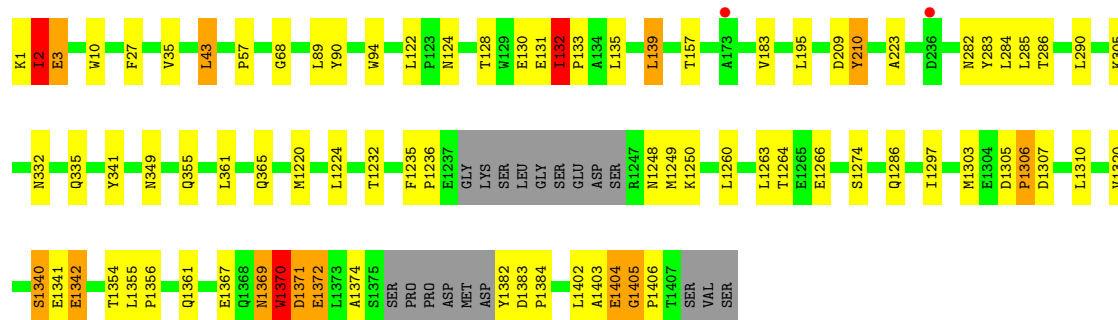


- Molecule 1: Sugar ABC transporter substrate-binding protein, Gasdermin-B fusion protein



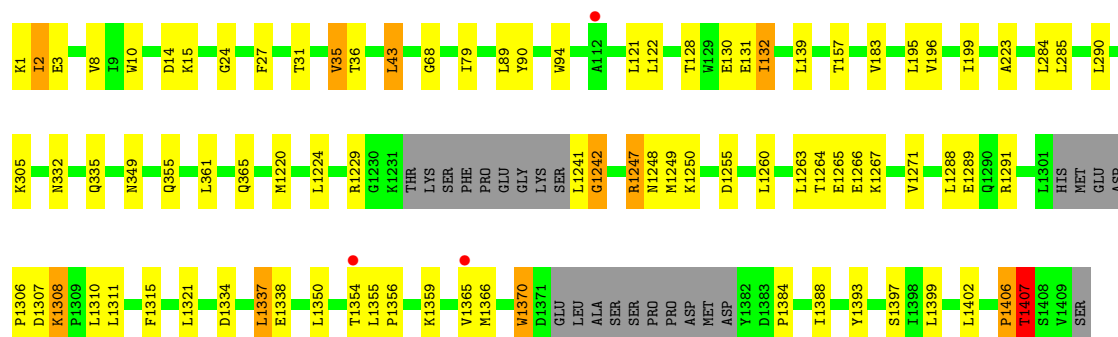
- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain G:  82% 12% ...



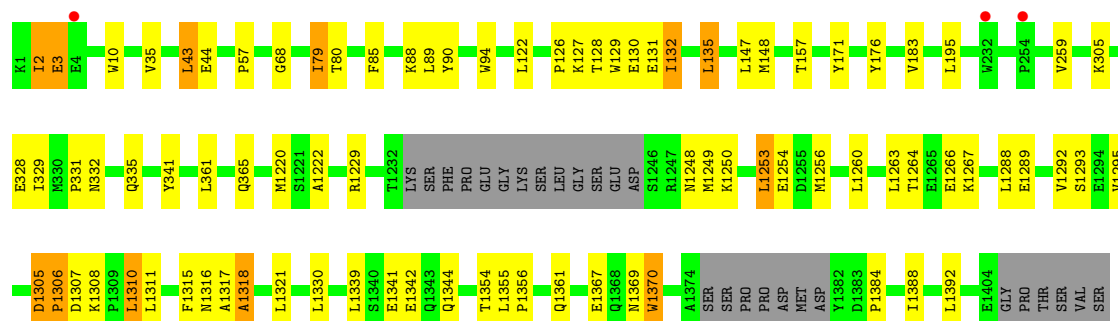
- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain H:  80% 14% ...



- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

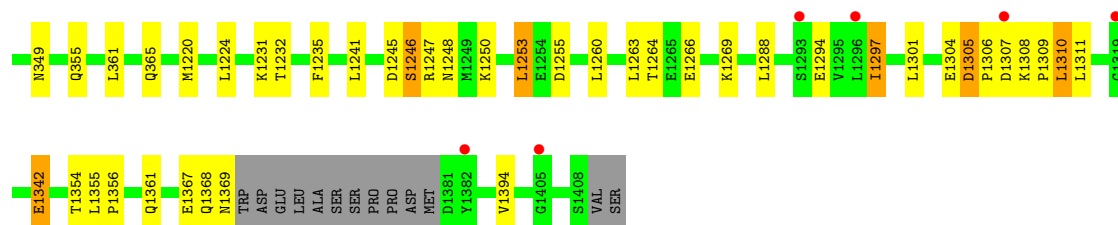
Chain I:  80% 13% 5%



- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

Chain J:  85% 11% ..



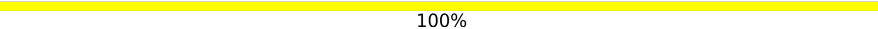


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  50%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  50%

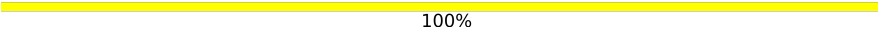


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:  50%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Q:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain R:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain S:  50%  50%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain T:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.60Å 274.57Å 174.02Å 90.00° 96.09° 90.00°	Depositor
Resolution (Å)	173.04 – 3.50 173.04 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (173.04-3.50) 99.7 (173.04-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.248 0.214 , 0.217	Depositor DCC
R_{free} test set	5232 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	39838	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: NA, GLC

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	0.77	3/4149 (0.1%)	1.09	12/5661 (0.2%)
1	B	0.76	1/4147 (0.0%)	1.08	13/5659 (0.2%)
1	C	0.75	2/4157 (0.0%)	1.15	25/5681 (0.4%)
1	D	0.72	0/4040	1.04	6/5519 (0.1%)
1	E	0.77	2/4161 (0.0%)	1.11	13/5680 (0.2%)
1	F	0.75	0/4037	1.07	10/5518 (0.2%)
1	G	0.74	3/3968 (0.1%)	1.07	11/5441 (0.2%)
1	H	0.76	4/3910 (0.1%)	1.12	15/5356 (0.3%)
1	I	0.72	0/3874	1.06	6/5318 (0.1%)
1	J	0.76	0/3984	1.09	7/5461 (0.1%)
All	All	0.75	15/40427 (0.0%)	1.09	118/55294 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1382	TYR	CA-C	9.11	1.58	1.53
1	E	1236	PRO	CA-C	8.47	1.60	1.52
1	G	1340	SER	CA-C	6.95	1.55	1.52
1	A	1305	ASP	CA-C	6.53	1.61	1.52
1	B	277	LYS	CA-C	6.38	1.61	1.52
1	H	1370	TRP	CA-C	6.01	1.60	1.52
1	H	1247	ARG	CA-C	5.84	1.60	1.52
1	A	345	THR	CA-CB	5.59	1.62	1.53
1	E	1235	PHE	C-N	5.44	1.37	1.33
1	H	1308	LYS	CA-C	5.42	1.59	1.52
1	G	124	ASN	CA-C	5.38	1.59	1.52
1	C	1246	SER	N-CA	5.22	1.52	1.46
1	G	1320	VAL	CA-CB	5.12	1.60	1.54
1	C	49	GLN	CA-CB	5.11	1.61	1.53
1	H	1407	THR	N-CA	5.06	1.52	1.46

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1242	GLY	N-CA-C	-12.32	100.24	111.95
1	C	1380	MET	N-CA-C	-12.19	95.76	112.94
1	F	1227	HIS	N-CA-C	11.56	123.63	111.14
1	J	273	LYS	N-CA-C	10.59	123.81	111.11
1	H	1265	GLU	N-CA-C	-10.40	99.94	111.28
1	C	357	VAL	N-CA-C	-9.96	100.86	110.42
1	E	1298	SER	N-CA-C	9.72	121.82	111.03
1	E	1299	GLY	N-CA-C	-9.37	101.73	114.95
1	E	1227	HIS	N-CA-C	8.79	120.79	111.03
1	F	1265	GLU	N-CA-C	-8.76	101.73	111.28
1	H	35	VAL	CB-CA-C	-8.74	100.17	111.53
1	C	1307	ASP	N-CA-C	-8.21	102.14	112.90
1	C	1382	TYR	N-CA-C	8.12	119.33	108.38
1	D	1341	GLU	N-CA-C	-8.05	102.72	112.54
1	J	1310	LEU	N-CA-CB	7.83	121.72	109.82
1	H	35	VAL	N-CA-C	7.74	117.84	106.85
1	G	1307	ASP	N-CA-C	7.60	122.50	113.23
1	H	1354	THR	CB-CA-C	7.56	123.22	111.28
1	H	1263	LEU	N-CA-C	7.49	120.55	109.24
1	B	1371	ASP	N-CA-C	7.43	123.24	107.70
1	C	1374	ALA	N-CA-C	7.35	117.71	108.45
1	C	1378	PRO	N-CA-C	7.31	122.74	111.11
1	C	1377	PRO	N-CA-C	-7.29	101.80	110.70
1	B	35	VAL	CB-CA-C	-7.24	101.58	110.99
1	B	1341	GLU	N-CA-C	-7.22	103.73	112.54
1	I	44	GLU	N-CA-C	7.12	120.86	111.75
1	G	1370	TRP	N-CA-C	7.08	125.87	110.80
1	D	1343	GLN	N-CA-C	7.00	125.71	110.80
1	B	1233	LYS	N-CA-C	6.94	118.97	109.11
1	J	1367	GLU	N-CA-C	6.94	118.84	111.28
1	C	1236	PRO	N-CA-C	6.93	122.10	111.57
1	I	1318	ALA	N-CA-C	-6.90	99.73	110.42
1	C	1245	ASP	N-CA-C	6.86	122.54	114.04
1	H	1337	LEU	N-CA-CB	6.83	120.17	110.12
1	F	43	LEU	N-CA-C	6.82	118.79	111.36
1	C	43	LEU	N-CA-C	6.72	118.68	111.36
1	G	1232	THR	N-CA-C	6.69	119.41	111.71
1	F	1231	LYS	N-CA-C	-6.67	100.41	110.28
1	E	1298	SER	CB-CA-C	-6.63	100.67	110.95
1	A	1372	GLU	N-CA-C	6.62	120.95	113.01
1	A	44	GLU	N-CA-C	6.62	120.22	111.75
1	A	1366	MET	N-CA-C	-6.60	100.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLY	N-CA-C	-6.60	106.63	114.48
1	D	132	ILE	CB-CA-C	-6.58	107.38	114.35
1	H	15	LYS	N-CA-C	6.51	118.26	110.19
1	J	3	GLU	N-CA-C	6.49	119.18	110.35
1	A	1226	ILE	N-CA-C	6.49	122.84	109.34
1	D	43	LEU	N-CA-C	6.47	118.42	111.36
1	B	1343	GLN	N-CA-C	6.42	124.48	110.80
1	B	132	ILE	CB-CA-C	-6.42	107.55	114.35
1	B	43	LEU	N-CA-C	6.39	118.24	111.28
1	C	132	ILE	CB-CA-C	-6.37	107.60	114.35
1	H	132	ILE	CB-CA-C	-6.35	107.62	114.35
1	F	1263	LEU	N-CA-C	6.35	118.82	109.24
1	H	79	ILE	CB-CA-C	-6.34	102.88	111.63
1	G	132	ILE	CB-CA-C	-6.31	107.67	114.35
1	C	1226	ILE	N-CA-C	6.29	122.42	109.34
1	F	89	LEU	CB-CG-CD2	6.24	129.42	110.70
1	G	1405	GLY	CA-C-N	6.21	126.70	119.99
1	G	1405	GLY	C-N-CA	6.21	126.70	119.99
1	E	1249	MET	N-CA-C	6.18	119.29	111.69
1	E	43	LEU	N-CA-C	6.17	118.08	111.36
1	A	132	ILE	CB-CA-C	-6.17	107.81	114.35
1	I	132	ILE	CB-CA-C	-6.16	107.82	114.35
1	C	89	LEU	CB-CG-CD2	6.13	129.10	110.70
1	C	1292	VAL	N-CA-C	-6.13	104.37	110.62
1	G	43	LEU	N-CA-C	6.12	117.95	111.28
1	H	1265	GLU	N-CA-CB	6.08	119.06	110.12
1	A	89	LEU	CB-CG-CD2	6.06	128.88	110.70
1	E	132	ILE	CB-CA-C	-6.06	107.93	114.35
1	E	1253	LEU	N-CA-C	-6.05	104.60	111.14
1	B	1372	GLU	N-CA-CB	6.05	120.78	110.50
1	I	79	ILE	CB-CA-C	-6.04	103.29	111.63
1	C	1370	TRP	N-CA-C	5.99	119.05	111.69
1	H	14	ASP	CB-CA-C	-5.98	100.86	110.79
1	E	136	ASP	N-CA-C	-5.93	104.73	111.14
1	C	1231	LYS	N-CA-C	5.90	120.50	113.12
1	E	1227	HIS	CA-C-N	-5.88	114.41	123.17
1	E	1227	HIS	C-N-CA	-5.88	114.41	123.17
1	B	1308	LYS	N-CA-C	5.84	119.60	108.97
1	J	275	LEU	N-CA-C	-5.82	104.84	111.07
1	J	1309	PRO	CB-CA-C	-5.77	103.89	112.55
1	C	1341	GLU	N-CA-C	5.77	118.52	111.82
1	B	1382	TYR	N-CA-C	5.71	117.79	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	43	LEU	N-CA-C	5.71	117.51	111.28
1	B	1247	ARG	CA-C-N	5.67	129.32	120.75
1	B	1247	ARG	C-N-CA	5.67	129.32	120.75
1	H	1289	GLU	N-CA-C	-5.65	105.20	111.36
1	A	43	LEU	N-CA-C	5.61	117.07	111.07
1	C	1231	LYS	CB-CA-C	-5.59	100.34	109.56
1	J	1269	LYS	N-CA-CB	5.59	118.11	110.01
1	C	1343	GLN	N-CA-C	-5.55	105.13	111.07
1	F	228	GLY	CA-C-N	5.54	125.00	119.24
1	F	228	GLY	C-N-CA	5.54	125.00	119.24
1	I	43	LEU	N-CA-C	5.49	116.95	111.07
1	H	1289	GLU	N-CA-CB	5.49	118.28	110.16
1	G	1297	ILE	CA-CB-CG2	5.47	119.81	110.50
1	A	1298	SER	N-CA-C	5.47	122.45	110.80
1	F	1265	GLU	N-CA-CB	5.47	118.16	110.12
1	G	210	TYR	N-CA-C	-5.46	105.33	111.28
1	D	125	PRO	O-C-N	5.45	123.71	121.15
1	C	357	VAL	N-CA-CB	5.42	116.89	110.55
1	I	1317	ALA	N-CA-C	5.38	117.89	111.71
1	A	1383	ASP	N-CA-C	5.35	121.62	109.81
1	A	1232	THR	N-CA-C	5.33	116.76	107.49
1	C	1232	THR	N-CA-C	5.30	123.89	113.29
1	E	1228	PHE	N-CA-C	-5.29	103.67	111.81
1	D	1235	PHE	N-CA-C	-5.23	98.25	109.81
1	G	1297	ILE	N-CA-C	5.18	115.40	110.53
1	G	2	ILE	N-CA-C	5.15	120.05	109.34
1	E	1253	LEU	N-CA-CB	5.10	117.46	110.07
1	A	124	ASN	CB-CA-C	-5.10	102.91	110.71
1	F	125	PRO	O-C-N	5.05	123.52	121.15
1	C	1310	LEU	N-CA-C	5.04	117.43	111.33
1	C	125	PRO	O-C-N	5.04	123.52	121.15
1	C	355	GLN	N-CA-C	5.04	116.84	109.24
1	C	356	THR	N-CA-CB	5.03	117.44	110.04
1	B	239	ALA	N-CA-C	5.02	118.66	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4066	0	3871	95	0
1	B	4064	0	3833	66	0
1	C	4070	0	3841	117	0
1	D	3959	0	3729	69	0
1	E	4077	0	3874	56	0
1	F	3956	0	3714	69	0
1	G	3885	0	3583	75	0
1	H	3832	0	3525	77	0
1	I	3795	0	3444	91	1
1	J	3902	0	3567	45	1
2	K	23	0	21	1	0
2	L	23	0	21	0	0
2	M	23	0	21	1	0
2	N	23	0	21	2	0
2	O	23	0	21	0	0
2	P	23	0	21	1	0
2	Q	23	0	21	0	0
2	R	23	0	21	0	0
2	S	23	0	21	0	0
2	T	23	0	21	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
All	All	39838	0	37191	726	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 9.

All (726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:259:VAL:CG2	1:I:329:ILE:HA	1.73	1.18
1:E:184:ASP:CB	1:E:365:GLN:OE1	1.96	1.14
1:H:1241:LEU:HD23	1:H:1242:GLY:H	1.07	1.12
1:D:2:ILE:HG22	1:D:3:GLU:H	1.03	1.12
1:C:1247:ARG:HH22	1:C:1327:LYS:HE3	1.01	1.11
1:F:1271:VAL:HG22	1:F:1310:LEU:CD1	1.82	1.10
1:I:1288:LEU:HD11	1:I:1310:LEU:HD21	1.13	1.10
1:A:1303:MET:HG3	1:A:1304:GLU:H	1.06	1.10
1:D:1366:MET:O	1:D:1370:TRP:N	1.84	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:ASN:HB3	1:A:1251:GLU:CG	1.82	1.09
1:A:1340:SER:HB3	1:C:173:ALA:O	1.51	1.09
1:B:1245:ASP:OD1	1:B:1247:ARG:N	1.84	1.09
1:A:1307:ASP:C	1:A:1309:PRO:HD2	1.76	1.08
1:I:1305:ASP:HB3	1:I:1306:PRO:CD	1.82	1.08
1:H:1:LYS:O	1:H:2:ILE:HG22	1.55	1.06
1:B:1245:ASP:OD1	1:B:1246:SER:N	1.88	1.05
1:I:259:VAL:HG22	1:I:329:ILE:HA	1.37	1.05
1:I:1292:VAL:HG13	1:I:1330:LEU:HD21	1.33	1.05
1:H:1220:MET:HE1	1:H:1365:VAL:HG21	1.31	1.05
1:I:1305:ASP:HB3	1:I:1306:PRO:HD2	1.13	1.05
1:C:1231:LYS:O	1:C:1232:THR:HG22	1.56	1.04
1:F:1220:MET:HE1	1:F:1365:VAL:HG21	1.32	1.04
1:D:1317:ALA:HB3	1:J:90:TYR:OH	1.57	1.04
1:J:1305:ASP:CB	1:J:1306:PRO:CD	2.36	1.04
1:E:184:ASP:HB3	1:E:365:GLN:OE1	1.57	1.03
1:I:1305:ASP:CB	1:I:1306:PRO:CD	2.36	1.03
1:E:1220:MET:HE1	1:E:1365:VAL:HG21	1.41	1.02
1:B:1223:GLY:HA2	1:B:1342:GLU:OE2	1.57	1.02
1:F:1271:VAL:HG22	1:F:1310:LEU:HD13	1.39	1.02
1:D:1288:LEU:HD11	1:D:1310:LEU:HD23	1.41	1.01
1:H:35:VAL:HG23	1:H:35:VAL:O	1.59	1.01
1:C:1401:GLU:O	1:C:1405:GLY:HA3	1.60	1.00
1:D:1223:GLY:HA2	1:D:1342:GLU:OE2	1.62	1.00
1:C:1375:SER:O	1:C:1377:PRO:HD3	1.59	1.00
1:C:1247:ARG:NH2	1:C:1327:LYS:HE3	1.75	0.99
1:I:1292:VAL:CG1	1:I:1330:LEU:HD21	1.93	0.98
1:B:35:VAL:HG23	1:B:35:VAL:O	1.63	0.97
1:I:1305:ASP:CB	1:I:1306:PRO:HD2	1.93	0.97
1:J:195:LEU:O	1:J:199:ILE:HD12	1.64	0.96
1:E:184:ASP:HB2	1:E:365:GLN:OE1	1.63	0.96
1:I:1288:LEU:HD11	1:I:1310:LEU:CD2	1.95	0.96
1:H:1229:ARG:HH22	1:H:1388:ILE:HD12	1.30	0.96
1:A:1340:SER:CB	1:C:173:ALA:O	2.14	0.95
1:I:1288:LEU:CD1	1:I:1310:LEU:HD21	1.94	0.95
1:B:1308:LYS:CB	1:B:1311:LEU:HD12	1.96	0.95
1:A:1366:MET:HE1	1:A:1370:TRP:CE3	2.02	0.95
1:H:1308:LYS:CB	1:H:1311:LEU:HD12	1.97	0.95
1:C:1301:LEU:HD22	1:C:1315:PHE:HE2	1.31	0.94
1:E:1229:ARG:HH11	1:E:1388:ILE:HD13	1.33	0.93
1:H:1229:ARG:NH2	1:H:1388:ILE:HD12	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:MET:HE1	1:J:340:TRP:HE1	1.34	0.92
1:H:1241:LEU:CD2	1:H:1242:GLY:H	1.83	0.92
1:I:2:ILE:HG22	1:I:3:GLU:N	1.83	0.92
1:A:1242:GLY:O	1:A:1243:SER:HB2	1.69	0.92
1:I:2:ILE:HG22	1:I:3:GLU:H	1.34	0.91
1:H:1241:LEU:HD23	1:H:1242:GLY:N	1.85	0.89
1:J:1305:ASP:CB	1:J:1306:PRO:HD3	1.98	0.89
1:D:2:ILE:HG22	1:D:3:GLU:N	1.84	0.89
1:I:1305:ASP:CG	1:I:1306:PRO:HD3	1.98	0.89
1:E:1248:ASN:HA	1:E:1374:ALA:HB2	1.54	0.88
1:H:10:TRP:HB3	1:H:43:LEU:HD11	1.56	0.88
1:I:128:THR:CG2	1:I:131:GLU:HG3	2.04	0.88
1:I:1305:ASP:O	1:I:1307:ASP:N	2.07	0.88
1:C:1247:ARG:HH22	1:C:1327:LYS:CE	1.86	0.87
1:A:1303:MET:HG3	1:A:1304:GLU:N	1.88	0.87
1:C:194:PHE:CE1	1:C:198:LEU:HD11	2.08	0.87
1:D:2:ILE:CG2	1:D:3:GLU:H	1.87	0.86
1:A:1308:LYS:N	1:A:1309:PRO:CD	2.39	0.86
1:G:10:TRP:HB3	1:G:43:LEU:HD11	1.57	0.85
1:A:1366:MET:HE1	1:A:1370:TRP:CZ3	2.12	0.85
1:C:1363:LYS:HA	1:C:1366:MET:HG2	1.57	0.85
1:A:1308:LYS:N	1:A:1309:PRO:HD2	1.90	0.85
1:F:1:LYS:O	1:F:2:ILE:HG22	1.76	0.85
1:E:1229:ARG:NH1	1:E:1388:ILE:HD13	1.92	0.84
1:H:2:ILE:HG13	1:H:3:GLU:H	1.42	0.84
1:D:1235:PHE:CB	1:D:1236:PRO:HD2	2.07	0.84
1:D:128:THR:OG1	1:D:131:GLU:HG3	1.78	0.84
1:E:128:THR:OG1	1:E:131:GLU:HG3	1.78	0.83
1:H:1260:LEU:HD13	1:H:1402:LEU:HD11	1.61	0.83
1:A:1220:MET:HE2	1:A:1361:GLN:HE21	1.43	0.83
1:B:10:TRP:HB3	1:B:43:LEU:HD11	1.57	0.83
1:G:1370:TRP:CD1	1:G:1371:ASP:H	1.95	0.83
1:J:1301:LEU:HD21	1:J:1308:LYS:HE3	1.61	0.83
1:G:1370:TRP:O	1:G:1372:GLU:N	2.13	0.82
1:C:1247:ARG:NH2	1:C:1327:LYS:CE	2.42	0.82
1:C:1301:LEU:CD2	1:C:1315:PHE:HE2	1.92	0.82
1:D:1305:ASP:HB3	1:D:1306:PRO:HD3	1.62	0.81
1:I:1292:VAL:CG1	1:I:1330:LEU:CD2	2.58	0.81
1:G:290:LEU:HD12	1:G:290:LEU:H	1.46	0.81
1:I:259:VAL:HG23	1:I:329:ILE:HA	1.58	0.81
1:E:1247:ARG:NH1	1:E:1255:ASP:OD2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1378:PRO:O	1:C:1379:ASP:O	1.99	0.80
1:D:1301:LEU:HD12	1:D:1303:MET:HE3	1.63	0.80
1:I:128:THR:HG22	1:I:131:GLU:HG3	1.63	0.80
1:I:128:THR:OG1	1:I:130:GLU:OE1	1.98	0.80
1:F:1370:TRP:CD1	1:F:1371:ASP:H	2.00	0.79
1:D:1400:LEU:O	1:D:1404:GLU:N	2.14	0.79
1:F:1264:THR:HB	1:F:1267:LYS:HG3	1.65	0.79
1:B:128:THR:OG1	1:B:131:GLU:HG3	1.83	0.78
1:D:1235:PHE:CB	1:D:1236:PRO:CD	2.62	0.78
1:A:86:GLN:OE1	1:C:1380:MET:HG3	1.82	0.78
1:I:259:VAL:CG2	1:I:329:ILE:CA	2.59	0.78
1:A:128:THR:OG1	1:A:131:GLU:HG3	1.83	0.78
1:F:1292:VAL:O	1:F:1295:VAL:HG23	1.84	0.77
1:I:1292:VAL:HG11	1:I:1330:LEU:CD2	2.14	0.77
1:F:1342:GLU:OE1	1:F:1342:GLU:N	2.12	0.77
1:F:85:PHE:HA	1:F:88:LYS:HD2	1.67	0.77
1:E:1264:THR:HG22	1:E:1266:GLU:H	1.49	0.76
1:I:1305:ASP:CG	1:I:1306:PRO:CD	2.58	0.76
1:H:1220:MET:HE1	1:H:1365:VAL:CG2	2.14	0.76
1:I:1264:THR:HG22	1:I:1266:GLU:H	1.49	0.76
1:J:153:GLU:OE1	1:J:344:ARG:NH1	2.20	0.75
1:C:1231:LYS:O	1:C:1232:THR:CG2	2.34	0.75
1:G:1405:GLY:N	1:G:1406:PRO:HD3	2.02	0.75
1:H:196:VAL:O	1:H:199:ILE:HG13	1.85	0.75
1:J:1288:LEU:HD11	1:J:1310:LEU:HD23	1.68	0.75
1:B:27:PHE:HD1	1:B:283:TYR:CD2	2.04	0.74
1:F:1366:MET:HG3	1:F:1389:LEU:CD2	2.17	0.74
1:G:27:PHE:HD1	1:G:283:TYR:CD2	2.05	0.74
1:C:1235:PHE:H	1:C:1236:PRO:HD3	1.51	0.74
1:F:1220:MET:HE1	1:F:1365:VAL:CG2	2.16	0.74
1:A:1303:MET:CG	1:A:1304:GLU:H	1.89	0.73
1:F:1271:VAL:HG22	1:F:1310:LEU:HD11	1.68	0.73
1:D:1307:ASP:OD1	1:D:1308:LYS:N	2.21	0.73
1:G:1:LYS:C	1:G:2:ILE:HG12	2.13	0.73
1:J:1304:GLU:HB2	1:J:1308:LYS:HD3	1.71	0.73
1:A:1220:MET:CE	1:A:1361:GLN:HE21	2.01	0.73
1:C:1301:LEU:HD22	1:C:1315:PHE:CE2	2.20	0.72
1:C:1307:ASP:OD1	1:C:1308:LYS:N	2.22	0.72
1:G:286:THR:O	1:G:290:LEU:CD1	2.37	0.72
1:D:1369:ASN:O	1:D:1370:TRP:HB2	1.90	0.72
1:G:1367:GLU:O	1:G:1370:TRP:HE3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:259:VAL:HG23	1:I:329:ILE:HG13	1.71	0.72
1:I:1292:VAL:HG11	1:I:1330:LEU:HD23	1.70	0.72
1:G:1370:TRP:C	1:G:1372:GLU:H	1.97	0.72
1:H:1:LYS:O	1:H:2:ILE:CG2	2.37	0.72
1:H:1308:LYS:CB	1:H:1311:LEU:CD1	2.68	0.71
1:E:1220:MET:HE1	1:E:1365:VAL:CG2	2.20	0.71
1:B:136:ASP:OD2	1:B:140:LYS:HE2	1.91	0.71
1:G:286:THR:O	1:G:290:LEU:HD12	1.91	0.71
1:I:128:THR:HG23	1:I:131:GLU:HG3	1.73	0.71
1:I:259:VAL:HG22	1:I:329:ILE:CA	2.18	0.70
1:I:1264:THR:HG22	1:I:1266:GLU:N	2.06	0.70
1:D:1264:THR:HG22	1:D:1266:GLU:H	1.56	0.70
1:H:1334:ASP:O	1:H:1337:LEU:HG	1.91	0.70
1:A:122:LEU:HD21	1:A:124:ASN:O	1.91	0.70
1:B:341:TYR:CD2	1:B:1361:GLN:HG2	2.26	0.70
1:C:1365:VAL:C	1:C:1367:GLU:N	2.48	0.70
1:F:1366:MET:HG3	1:F:1389:LEU:HD23	1.72	0.70
1:A:317:ILE:O	1:A:321:MET:HG3	1.91	0.70
1:I:1305:ASP:OD1	1:I:1306:PRO:HD3	1.92	0.70
1:A:1302:HIS:O	1:A:1303:MET:HB2	1.92	0.69
1:A:98:ARG:NH1	1:C:1380:MET:O	2.24	0.69
1:G:341:TYR:CD2	1:G:1361:GLN:HG2	2.28	0.69
1:G:1370:TRP:CD1	1:G:1371:ASP:N	2.61	0.69
1:B:341:TYR:HD2	1:B:1361:GLN:HG2	1.57	0.69
1:B:1264:THR:HG22	1:B:1266:GLU:H	1.57	0.69
1:I:10:TRP:HB3	1:I:43:LEU:HD11	1.75	0.69
1:B:35:VAL:O	1:B:35:VAL:CG2	2.37	0.68
1:B:1302:HIS:O	1:B:1303:MET:HB2	1.94	0.68
1:I:341:TYR:CD2	1:I:1361:GLN:HG2	2.28	0.68
1:A:10:TRP:HB3	1:A:43:LEU:HD11	1.75	0.68
1:F:129:TRP:HA	1:F:132:ILE:HD12	1.75	0.68
1:B:1308:LYS:CB	1:B:1311:LEU:CD1	2.70	0.68
1:A:1383:ASP:OD2	1:A:1387:ARG:NE	2.20	0.68
1:J:195:LEU:O	1:J:199:ILE:CD1	2.39	0.68
1:A:1365:VAL:O	1:A:1367:GLU:N	2.28	0.67
1:C:49:GLN:HA	1:C:1368:GLN:HA	1.75	0.67
1:F:1271:VAL:CG2	1:F:1310:LEU:HD13	2.20	0.67
1:J:1305:ASP:CB	1:J:1306:PRO:HD2	2.22	0.67
1:G:341:TYR:HD2	1:G:1361:GLN:HG2	1.58	0.67
1:I:341:TYR:HD2	1:I:1361:GLN:HG2	1.59	0.67
1:H:1271:VAL:HG22	1:H:1310:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:MET:CE	1:J:340:TRP:HE1	2.07	0.66
1:D:1308:LYS:O	1:D:1312:SER:OG	2.12	0.66
1:A:88:LYS:HE3	1:E:352:SER:HB2	1.76	0.66
1:G:1264:THR:HG22	1:G:1266:GLU:H	1.60	0.66
1:A:1300:GLU:O	1:F:1351:GLU:HG2	1.94	0.66
1:B:89:LEU:HD12	1:B:94:TRP:CZ2	2.30	0.66
1:D:1307:ASP:OD1	1:D:1308:LYS:HG2	1.95	0.66
1:B:1232:THR:OG1	1:B:1233:LYS:N	2.28	0.66
1:C:1271:VAL:HG22	1:C:1310:LEU:HD12	1.78	0.66
1:I:1253:LEU:HA	1:I:1256:MET:HE2	1.78	0.66
1:F:214:GLU:O	1:F:218:ASN:ND2	2.27	0.66
1:F:1370:TRP:CG	1:F:1371:ASP:H	2.14	0.66
1:C:1365:VAL:C	1:C:1367:GLU:H	2.02	0.66
1:G:290:LEU:HD12	1:G:290:LEU:N	2.11	0.65
1:G:1248:ASN:ND2	1:G:1374:ALA:HB2	2.10	0.65
1:C:1376:SER:O	1:C:1378:PRO:HD3	1.96	0.65
1:C:1229:ARG:HH12	1:C:1388:ILE:HD13	1.59	0.65
1:G:1340:SER:OG	1:G:1341:GLU:N	2.14	0.65
1:H:1229:ARG:NH2	1:H:1388:ILE:CD1	2.59	0.65
1:H:1307:ASP:OD1	1:H:1308:LYS:N	2.30	0.65
1:C:1365:VAL:O	1:C:1367:GLU:N	2.30	0.65
1:G:1:LYS:O	1:G:2:ILE:HG12	1.97	0.65
1:H:122:LEU:HD11	1:H:139:LEU:HD11	1.79	0.65
1:B:1223:GLY:CA	1:B:1342:GLU:OE2	2.40	0.65
1:H:35:VAL:O	1:H:35:VAL:CG2	2.33	0.65
1:B:24:GLY:CA	1:B:35:VAL:HG21	2.27	0.65
1:A:128:THR:HG22	1:A:249:THR:OG1	1.97	0.64
1:C:1374:ALA:C	1:C:1376:SER:H	2.05	0.64
1:A:1230:GLY:O	1:C:171:TYR:OH	2.14	0.64
1:F:1253:LEU:HA	1:F:1256:MET:HE2	1.78	0.64
1:H:1264:THR:HG22	1:H:1266:GLU:H	1.60	0.64
1:F:114:SER:OG	1:F:245:THR:O	2.14	0.64
1:H:1271:VAL:HA	1:H:1310:LEU:HD13	1.79	0.64
1:C:1271:VAL:HA	1:C:1310:LEU:HD13	1.79	0.64
1:C:1301:LEU:CD2	1:C:1315:PHE:CE2	2.79	0.64
1:I:89:LEU:HD12	1:I:94:TRP:CZ2	2.33	0.64
1:B:24:GLY:C	1:B:35:VAL:HG21	2.23	0.63
1:I:128:THR:HG22	1:I:131:GLU:CG	2.28	0.63
1:J:149:PHE:O	1:J:151:LEU:CD1	2.45	0.63
1:J:1247:ARG:NH1	1:J:1255:ASP:OD2	2.32	0.63
1:F:1373:LEU:C	1:F:1373:LEU:HD12	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:PHE:CE1	1:C:198:LEU:CD1	2.82	0.63
1:J:330:MET:HE1	1:J:340:TRP:NE1	2.09	0.63
1:A:171:TYR:HE2	1:C:1232:THR:HG21	1.63	0.63
1:C:1373:LEU:HD23	1:C:1373:LEU:O	1.99	0.63
1:E:89:LEU:HD12	1:E:94:TRP:CZ2	2.33	0.63
1:H:1264:THR:HG22	1:H:1266:GLU:N	2.14	0.63
1:G:89:LEU:HD12	1:G:94:TRP:CZ2	2.33	0.63
1:A:1248:ASN:CB	1:A:1251:GLU:CG	2.70	0.62
1:A:122:LEU:HD21	1:A:124:ASN:C	2.23	0.62
1:H:89:LEU:HD12	1:H:94:TRP:CZ2	2.34	0.62
1:B:128:THR:HG22	1:B:249:THR:OG1	1.99	0.62
1:B:273:LYS:O	1:B:277:LYS:HG3	1.99	0.62
1:A:1220:MET:HE2	1:A:1361:GLN:NE2	2.14	0.62
1:A:1382:TYR:O	1:A:1383:ASP:HB2	2.00	0.62
1:A:1373:LEU:HD23	1:A:1373:LEU:O	1.99	0.62
1:D:128:THR:OG1	1:D:131:GLU:CG	2.47	0.62
1:I:1367:GLU:O	1:I:1370:TRP:NE1	2.33	0.62
1:A:1340:SER:CA	1:C:173:ALA:O	2.48	0.61
1:F:1292:VAL:HA	1:F:1295:VAL:CG2	2.29	0.61
1:F:1310:LEU:O	1:F:1310:LEU:HD12	2.01	0.61
1:D:1304:GLU:O	1:D:1307:ASP:HB3	2.01	0.61
1:F:1341:GLU:N	1:F:1342:GLU:OE1	2.32	0.61
1:G:1340:SER:HG	1:G:1341:GLU:H	1.46	0.61
1:C:1231:LYS:C	1:C:1232:THR:HG22	2.25	0.61
1:G:128:THR:OG1	1:G:130:GLU:OE1	2.18	0.61
1:D:89:LEU:HD12	1:D:94:TRP:CZ2	2.35	0.61
1:C:2:ILE:HG23	1:C:3:GLU:N	2.16	0.61
1:H:128:THR:OG1	1:H:130:GLU:OE1	2.19	0.61
1:J:89:LEU:HD12	1:J:94:TRP:CZ2	2.35	0.61
1:A:33:ILE:HD13	1:A:275:LEU:HD22	1.83	0.61
1:A:88:LYS:CE	1:E:352:SER:HB2	2.31	0.61
1:A:1365:VAL:C	1:A:1367:GLU:N	2.57	0.61
1:H:8:VAL:HG13	1:H:36:THR:HG23	1.83	0.61
1:H:284:LEU:O	1:H:290:LEU:HD22	2.01	0.61
1:C:66:ARG:NH2	2:M:2:GLC:O4	2.34	0.60
1:J:1253:LEU:HD12	1:J:1394:VAL:HG22	1.82	0.60
1:F:1292:VAL:O	1:F:1295:VAL:CG2	2.49	0.60
1:D:1313:SER:OG	1:D:1313:SER:O	2.19	0.60
1:G:1354:THR:O	1:G:1354:THR:HG22	2.01	0.60
1:E:128:THR:OG1	1:E:131:GLU:CG	2.47	0.60
1:G:2:ILE:O	1:G:3:GLU:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:CD2	1:A:124:ASN:C	2.75	0.60
1:C:33:ILE:HD13	1:C:275:LEU:HD22	1.84	0.60
1:J:1354:THR:HG22	1:J:1354:THR:O	2.02	0.60
1:B:1338:GLU:OE1	1:B:1387:ARG:NH1	2.35	0.60
1:G:285:LEU:HA	1:G:290:LEU:HD11	1.82	0.59
1:C:1301:LEU:HB2	1:C:1315:PHE:CZ	2.37	0.59
1:I:1295:VAL:HG21	1:I:1311:LEU:HD21	1.83	0.59
1:D:1366:MET:O	1:D:1370:TRP:CA	2.51	0.59
1:H:1288:LEU:C	1:H:1288:LEU:HD12	2.27	0.59
1:D:1223:GLY:CA	1:D:1342:GLU:OE2	2.46	0.59
1:D:1306:PRO:O	1:D:1307:ASP:O	2.21	0.59
1:D:33:ILE:HD13	1:D:275:LEU:HD22	1.84	0.58
1:E:1338:GLU:OE1	1:E:1387:ARG:NH1	2.35	0.58
1:A:1362:VAL:O	1:A:1366:MET:HG3	2.02	0.58
1:F:1290:GLN:O	1:F:1294:GLU:HG2	2.03	0.58
1:A:1225:ASP:OD2	1:C:175:LYS:NZ	2.37	0.58
1:H:24:GLY:C	1:H:35:VAL:HG21	2.28	0.58
1:A:1301:LEU:HD23	1:A:1302:HIS:N	2.18	0.58
1:H:122:LEU:HD13	1:H:223:ALA:HB1	1.84	0.58
1:I:1253:LEU:C	1:I:1253:LEU:HD12	2.28	0.58
1:J:1232:THR:HG23	1:J:1232:THR:O	2.01	0.58
1:I:1310:LEU:C	1:I:1310:LEU:HD12	2.28	0.58
1:A:1307:ASP:CA	1:A:1309:PRO:HD2	2.32	0.58
1:E:1229:ARG:HH21	1:E:1340:SER:HB3	1.68	0.58
1:H:1229:ARG:NH2	1:H:1338:GLU:O	2.37	0.58
1:H:1271:VAL:HG22	1:H:1310:LEU:CD1	2.34	0.58
1:C:128:THR:OG1	1:C:130:GLU:OE1	2.20	0.58
1:F:128:THR:OG1	1:F:130:GLU:OE1	2.20	0.58
1:F:1264:THR:HG22	1:F:1266:GLU:H	1.67	0.58
1:A:86:GLN:OE1	1:C:1380:MET:CG	2.51	0.57
1:I:2:ILE:HD12	1:I:2:ILE:N	2.19	0.57
1:C:1271:VAL:HG22	1:C:1310:LEU:CD1	2.35	0.57
1:I:128:THR:HG23	1:I:131:GLU:H	1.69	0.57
1:I:1354:THR:O	1:I:1354:THR:HG22	2.04	0.57
1:E:1264:THR:HG22	1:E:1266:GLU:N	2.17	0.57
1:G:128:THR:CG2	1:G:131:GLU:HG3	2.34	0.57
1:J:10:TRP:HB3	1:J:43:LEU:HD11	1.85	0.57
1:E:1354:THR:HG22	1:E:1354:THR:O	2.05	0.57
1:I:1305:ASP:CB	1:I:1306:PRO:HD3	2.27	0.57
1:A:1380:MET:HE1	1:C:91:PRO:HB3	1.86	0.57
1:G:1370:TRP:C	1:G:1372:GLU:N	2.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:THR:HG22	1:D:249:THR:OG1	2.04	0.57
1:F:1260:LEU:HA	1:F:1263:LEU:HD12	1.86	0.57
1:G:1369:ASN:HB3	1:G:1372:GLU:HG2	1.87	0.57
1:C:194:PHE:CD2	1:C:250:PHE:CE1	2.93	0.57
1:C:1378:PRO:C	1:C:1379:ASP:O	2.48	0.57
1:G:1305:ASP:H	1:G:1306:PRO:HD2	1.69	0.57
1:A:171:TYR:HE2	1:C:1232:THR:CG2	2.17	0.57
1:B:24:GLY:HA3	1:B:35:VAL:HG21	1.85	0.57
1:D:1231:LYS:O	1:D:1233:LYS:N	2.38	0.57
1:D:1305:ASP:HB3	1:D:1306:PRO:CD	2.34	0.57
1:E:128:THR:HG1	1:E:131:GLU:HG3	1.70	0.57
1:C:1363:LYS:O	1:C:1366:MET:HB2	2.04	0.57
1:C:1375:SER:O	1:C:1377:PRO:CD	2.46	0.57
1:C:1401:GLU:O	1:C:1405:GLY:CA	2.44	0.57
1:F:1342:GLU:H	1:F:1342:GLU:CD	1.98	0.57
1:I:1253:LEU:HA	1:I:1256:MET:CE	2.35	0.57
1:F:1292:VAL:HA	1:F:1295:VAL:HG22	1.87	0.56
1:E:128:THR:HG22	1:E:249:THR:OG1	2.05	0.56
1:H:1393:TYR:HD1	1:H:1393:TYR:O	1.88	0.56
1:B:1229:ARG:NH1	1:B:1388:ILE:HD12	2.21	0.56
1:B:1246:SER:CB	1:H:1255:ASP:CG	2.78	0.56
1:I:1289:GLU:O	1:I:1292:VAL:HG12	2.05	0.56
1:I:1292:VAL:HG13	1:I:1293:SER:N	2.20	0.56
1:G:1370:TRP:CG	1:G:1371:ASP:N	2.70	0.56
1:H:128:THR:CG2	1:H:131:GLU:HG3	2.35	0.56
1:D:1304:GLU:O	1:D:1307:ASP:CB	2.54	0.56
1:F:1370:TRP:CD1	1:F:1371:ASP:N	2.73	0.56
1:F:1253:LEU:HA	1:F:1256:MET:CE	2.35	0.56
1:H:1350:LEU:CD1	1:H:1399:LEU:HD22	2.36	0.56
1:A:1301:LEU:HD23	1:A:1302:HIS:O	2.06	0.56
1:A:353:GLY:O	1:I:127:LYS:CB	2.53	0.55
1:D:1338:GLU:OE1	1:D:1387:ARG:NH1	2.38	0.55
1:C:1220:MET:SD	1:C:1361:GLN:HB3	2.46	0.55
1:C:1368:GLN:O	1:C:1369:ASN:OD1	2.24	0.55
1:E:1308:LYS:HB3	1:E:1311:LEU:HD12	1.89	0.55
1:I:259:VAL:HG22	1:I:328:GLU:O	2.07	0.55
1:J:1308:LYS:O	1:J:1308:LYS:HG3	2.07	0.55
1:H:2:ILE:HG13	1:H:3:GLU:N	2.17	0.55
1:F:1339:LEU:HB3	1:F:1342:GLU:HG2	1.89	0.55
1:G:27:PHE:HD1	1:G:283:TYR:HD2	1.55	0.54
1:H:1247:ARG:HG2	1:H:1247:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:LEU:HD13	1:I:135:LEU:HD21	1.89	0.54
1:B:27:PHE:HD1	1:B:283:TYR:HD2	1.54	0.54
1:E:1249:MET:HE2	1:E:1394:VAL:HG21	1.88	0.54
1:I:128:THR:CG2	1:I:131:GLU:CG	2.81	0.54
1:I:1229:ARG:HH12	1:I:1388:ILE:HG21	1.73	0.54
1:A:86:GLN:OE1	1:C:1380:MET:HB2	2.06	0.54
1:B:1245:ASP:OD2	1:B:1247:ARG:NH1	2.40	0.54
1:G:1260:LEU:HA	1:G:1263:LEU:HD12	1.90	0.54
1:B:1303:MET:O	1:B:1304:GLU:HB2	2.06	0.54
1:E:1235:PHE:N	1:E:1236:PRO:CD	2.71	0.54
1:E:1308:LYS:CB	1:E:1311:LEU:HD12	2.38	0.54
1:B:128:THR:OG1	1:B:131:GLU:CG	2.53	0.54
1:G:286:THR:N	1:G:290:LEU:HD11	2.21	0.54
1:I:1260:LEU:HA	1:I:1263:LEU:HD12	1.90	0.54
1:A:1383:ASP:N	1:A:1384:PRO:CD	2.70	0.54
1:G:1404:GLU:C	1:G:1406:PRO:HD3	2.33	0.54
1:A:1305:ASP:CB	1:A:1306:PRO:CD	2.86	0.54
1:C:1373:LEU:HD22	1:C:1390:CYS:SG	2.48	0.54
1:F:1264:THR:HB	1:F:1267:LYS:CG	2.37	0.54
1:I:2:ILE:CG2	1:I:3:GLU:N	2.58	0.53
1:A:128:THR:OG1	1:A:131:GLU:CG	2.53	0.53
1:C:1374:ALA:O	1:C:1375:SER:HB3	2.07	0.53
1:D:1260:LEU:HA	1:D:1263:LEU:HD12	1.91	0.53
1:I:1264:THR:HB	1:I:1267:LYS:HB2	1.90	0.53
1:J:1264:THR:HG22	1:J:1266:GLU:H	1.72	0.53
1:C:1220:MET:O	1:C:1224:LEU:HD12	2.09	0.53
1:D:66:ARG:NH2	2:N:2:GLC:O4	2.41	0.53
1:F:1370:TRP:CG	1:F:1371:ASP:N	2.75	0.53
1:G:282:ASN:O	1:G:283:TYR:HD1	1.91	0.53
1:A:1248:ASN:OD1	1:A:1250:LYS:N	2.41	0.53
1:D:1264:THR:HG22	1:D:1266:GLU:N	2.24	0.53
1:C:1234:SER:O	1:C:1235:PHE:HB2	2.08	0.53
1:A:1383:ASP:N	1:A:1384:PRO:HD3	2.24	0.53
1:D:1288:LEU:HD11	1:D:1310:LEU:CD2	2.26	0.53
1:H:285:LEU:HA	1:H:290:LEU:HD21	1.90	0.53
1:I:147:LEU:HD12	1:I:148:MET:N	2.24	0.53
1:I:1220:MET:CE	1:I:1361:GLN:HB3	2.39	0.53
1:I:1316:ASN:O	1:I:1318:ALA:O	2.27	0.53
1:J:1260:LEU:HA	1:J:1263:LEU:HD12	1.90	0.53
1:A:171:TYR:OH	1:C:1230:GLY:O	2.27	0.53
1:A:1366:MET:CE	1:A:1370:TRP:CE3	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:THR:HG22	1:C:357:VAL:N	2.23	0.53
1:B:1260:LEU:HA	1:B:1263:LEU:HD12	1.90	0.53
1:F:367:ASN:OD1	1:F:1358:LEU:HA	2.09	0.53
1:F:66:ARG:NH2	2:P:2:GLC:O4	2.41	0.52
1:J:1245:ASP:O	1:J:1246:SER:HB2	2.09	0.52
1:C:1260:LEU:HA	1:C:1263:LEU:HD12	1.91	0.52
1:A:1249:MET:HE2	1:A:1394:VAL:HG21	1.91	0.52
1:A:1366:MET:HE1	1:A:1370:TRP:HE3	1.66	0.52
1:B:282:ASN:O	1:B:283:TYR:HD1	1.93	0.52
1:F:1248:ASN:OD1	1:F:1250:LYS:N	2.43	0.52
1:G:286:THR:O	1:G:290:LEU:HD13	2.09	0.52
1:J:1307:ASP:O	1:J:1311:LEU:HD12	2.09	0.52
1:H:1393:TYR:CD1	1:H:1397:SER:OG	2.62	0.52
1:H:1393:TYR:CE1	1:H:1397:SER:OG	2.63	0.52
1:A:1260:LEU:HA	1:A:1263:LEU:HD12	1.92	0.52
1:J:1220:MET:SD	1:J:1361:GLN:NE2	2.83	0.52
1:E:1260:LEU:HA	1:E:1263:LEU:HD12	1.91	0.52
1:A:1246:SER:HB3	1:B:140:LYS:HG3	1.91	0.52
1:C:128:THR:CG2	1:C:131:GLU:HG3	2.40	0.52
1:D:1248:ASN:OD1	1:D:1250:LYS:N	2.43	0.52
1:A:86:GLN:OE1	1:C:1380:MET:CB	2.58	0.51
1:H:1359:LYS:HE3	1:H:1393:TYR:HE1	1.75	0.51
1:B:1245:ASP:OD2	1:B:1247:ARG:HB3	2.10	0.51
1:H:1366:MET:SD	1:H:1393:TYR:HD2	2.33	0.51
1:I:1248:ASN:OD1	1:I:1250:LYS:N	2.43	0.51
1:G:335:GLN:N	1:G:335:GLN:OE1	2.44	0.51
1:B:1248:ASN:OD1	1:B:1250:LYS:N	2.44	0.51
1:G:128:THR:HG23	1:G:131:GLU:HG3	1.92	0.51
1:D:90:TYR:CE1	1:D:305:LYS:HG2	2.46	0.51
1:F:2:ILE:HG23	1:F:3:GLU:N	2.25	0.51
1:F:90:TYR:CE1	1:F:305:LYS:HG2	2.46	0.51
1:C:49:GLN:HG3	1:C:1367:GLU:O	2.10	0.51
1:J:1248:ASN:OD1	1:J:1250:LYS:N	2.44	0.50
1:B:1384:PRO:O	1:B:1388:ILE:HG12	2.11	0.50
1:C:356:THR:HG22	1:C:358:ASP:H	1.75	0.50
1:G:1274:SER:HB2	1:G:1310:LEU:HD12	1.92	0.50
1:H:1248:ASN:OD1	1:H:1250:LYS:N	2.44	0.50
1:C:1:LYS:HG2	1:C:55:ASP:OD1	2.12	0.50
1:G:284:LEU:O	1:G:290:LEU:CD1	2.60	0.50
1:C:122:LEU:HD21	1:C:126:PRO:HD3	1.93	0.50
1:G:1383:ASP:OD1	1:G:1384:PRO:HD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ILE:HG23	1:C:3:GLU:H	1.77	0.50
1:F:1271:VAL:HA	1:F:1310:LEU:HD13	1.93	0.50
1:H:90:TYR:CE1	1:H:305:LYS:HG2	2.47	0.50
1:B:1220:MET:CE	1:B:1361:GLN:HB3	2.41	0.50
1:F:128:THR:CG2	1:F:131:GLU:HG3	2.41	0.50
1:G:1342:GLU:CD	1:G:1342:GLU:H	2.20	0.50
1:H:128:THR:HG23	1:H:131:GLU:HG3	1.93	0.50
1:C:1247:ARG:NH1	1:E:141:ALA:HA	2.27	0.49
1:A:1366:MET:O	1:A:1368:GLN:N	2.45	0.49
1:B:1301:LEU:C	1:B:1301:LEU:HD12	2.36	0.49
1:G:1248:ASN:OD1	1:G:1250:LYS:N	2.46	0.49
1:H:1247:ARG:NH2	1:H:1255:ASP:OD2	2.43	0.49
1:I:335:GLN:N	1:I:335:GLN:OE1	2.46	0.49
1:J:349:ASN:HB3	1:J:355:GLN:HG2	1.95	0.49
1:H:1306:PRO:O	1:H:1307:ASP:HB3	2.12	0.49
1:C:194:PHE:HD2	1:C:250:PHE:CE1	2.29	0.49
1:J:335:GLN:OE1	1:J:335:GLN:N	2.44	0.49
1:F:1264:THR:HG22	1:F:1266:GLU:N	2.27	0.49
1:G:209:ASP:OD1	1:G:210:TYR:N	2.43	0.49
1:G:1367:GLU:O	1:G:1370:TRP:CE3	2.61	0.49
1:H:2:ILE:HG23	1:H:3:GLU:O	2.12	0.49
1:A:101:GLY:HA3	1:C:1384:PRO:HG3	1.95	0.49
1:E:90:TYR:CE1	1:E:305:LYS:HG2	2.48	0.49
1:H:1247:ARG:HH22	1:H:1255:ASP:CG	2.20	0.49
1:A:1302:HIS:O	1:A:1303:MET:CB	2.61	0.49
1:C:335:GLN:OE1	1:C:335:GLN:N	2.45	0.49
1:H:349:ASN:HB3	1:H:355:GLN:HG2	1.95	0.49
1:I:1222:ALA:HB3	1:I:1342:GLU:HG3	1.95	0.49
1:E:122:LEU:HD21	1:E:126:PRO:HD3	1.94	0.49
1:E:128:THR:HG1	1:E:131:GLU:CG	2.24	0.49
1:J:1342:GLU:H	1:J:1342:GLU:CD	2.19	0.49
1:G:1264:THR:HG22	1:G:1266:GLU:N	2.25	0.49
1:H:121:LEU:O	1:H:122:LEU:HD12	2.13	0.49
1:E:335:GLN:OE1	1:E:335:GLN:N	2.46	0.48
1:F:349:ASN:HB3	1:F:355:GLN:HG2	1.95	0.48
1:F:1373:LEU:C	1:F:1373:LEU:CD1	2.86	0.48
1:B:349:ASN:HB3	1:B:355:GLN:HG2	1.95	0.48
1:G:1402:LEU:C	1:G:1404:GLU:N	2.69	0.48
1:H:1350:LEU:HD12	1:H:1399:LEU:HD22	1.94	0.48
1:I:1339:LEU:HD21	1:I:1392:LEU:HD13	1.94	0.48
1:H:335:GLN:OE1	1:H:335:GLN:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:O	1:C:49:GLN:HB2	2.13	0.48
1:C:1406:PRO:O	1:C:1407:THR:HG22	2.14	0.48
1:C:1301:LEU:HB2	1:C:1315:PHE:CE2	2.48	0.48
1:C:1373:LEU:CD2	1:C:1390:CYS:SG	3.02	0.48
1:G:286:THR:H	1:G:290:LEU:CD1	2.26	0.48
1:G:349:ASN:HB3	1:G:355:GLN:HG2	1.96	0.48
1:A:27:PHE:O	1:A:31:THR:HG22	2.14	0.48
1:I:1292:VAL:CG1	1:I:1293:SER:N	2.77	0.48
1:J:149:PHE:O	1:J:151:LEU:HD13	2.12	0.48
1:A:90:TYR:CE1	1:A:305:LYS:HG2	2.48	0.48
1:G:286:THR:N	1:G:290:LEU:CD1	2.77	0.48
1:B:1229:ARG:HH22	1:B:1342:GLU:CD	2.21	0.48
1:G:1403:ALA:O	1:G:1404:GLU:CB	2.61	0.48
1:J:90:TYR:CE1	1:J:305:LYS:HG2	2.49	0.48
1:E:1366:MET:O	1:E:1369:ASN:O	2.32	0.48
1:I:1310:LEU:HD12	1:I:1311:LEU:N	2.29	0.48
1:A:1366:MET:O	1:A:1367:GLU:HB2	2.14	0.48
1:H:1384:PRO:O	1:H:1388:ILE:HG12	2.14	0.48
1:I:122:LEU:HD21	1:I:126:PRO:HD3	1.95	0.47
1:I:1341:GLU:O	1:I:1344:GLN:HG2	2.14	0.47
1:J:1253:LEU:CD1	1:J:1394:VAL:HA	2.44	0.47
1:A:335:GLN:N	1:A:335:GLN:OE1	2.47	0.47
1:B:335:GLN:N	1:B:335:GLN:OE1	2.47	0.47
1:A:1305:ASP:CB	1:A:1306:PRO:HD2	2.44	0.47
1:D:1229:ARG:HH22	1:D:1342:GLU:CD	2.21	0.47
1:E:349:ASN:HB3	1:E:355:GLN:HG2	1.97	0.47
1:I:176:TYR:CE2	1:I:331:PRO:HG3	2.50	0.47
1:F:1366:MET:CG	1:F:1389:LEU:HD23	2.43	0.47
1:G:90:TYR:CE1	1:G:305:LYS:HG2	2.50	0.47
1:I:90:TYR:CE1	1:I:305:LYS:HG2	2.48	0.47
1:C:27:PHE:O	1:C:31:THR:HG22	2.15	0.47
1:C:1301:LEU:CB	1:C:1315:PHE:CE2	2.98	0.47
1:C:1365:VAL:O	1:C:1366:MET:C	2.55	0.47
1:D:1305:ASP:CB	1:D:1306:PRO:HD3	2.40	0.47
1:F:335:GLN:N	1:F:335:GLN:OE1	2.45	0.47
1:C:1290:GLN:O	1:C:1293:SER:HB2	2.14	0.47
1:E:1220:MET:O	1:E:1224:LEU:HD12	2.15	0.47
1:E:1235:PHE:N	1:E:1236:PRO:HD3	2.30	0.47
1:H:1315:PHE:HD1	1:H:1321:LEU:HA	1.78	0.47
1:I:128:THR:OG1	1:I:129:TRP:N	2.47	0.47
1:J:1355:LEU:N	1:J:1356:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ASP:OD2	1:E:140:LYS:NZ	2.48	0.47
1:B:27:PHE:O	1:B:31:THR:HG22	2.15	0.47
1:F:129:TRP:HA	1:F:132:ILE:CD1	2.43	0.47
1:I:79:ILE:HG22	1:I:80:THR:N	2.30	0.47
1:I:1253:LEU:HD12	1:I:1254:GLU:N	2.30	0.47
1:I:1384:PRO:O	1:I:1388:ILE:HG12	2.13	0.47
1:C:90:TYR:CE1	1:C:305:LYS:HG2	2.50	0.46
1:D:1:LYS:HB3	1:D:2:ILE:H	1.60	0.46
1:D:349:ASN:HB3	1:D:355:GLN:HG2	1.96	0.46
1:I:1295:VAL:CG2	1:I:1311:LEU:HD21	2.46	0.46
1:C:1374:ALA:C	1:C:1376:SER:N	2.72	0.46
1:D:27:PHE:O	1:D:31:THR:HG22	2.15	0.46
1:E:1355:LEU:N	1:E:1356:PRO:CD	2.78	0.46
1:D:1220:MET:CE	1:D:1365:VAL:HG21	2.45	0.46
1:A:172:ALA:O	1:A:173:ALA:HB3	2.14	0.46
1:I:341:TYR:HD2	1:I:1361:GLN:CG	2.28	0.46
1:I:1315:PHE:HD1	1:I:1321:LEU:HA	1.80	0.46
1:C:128:THR:HG23	1:C:131:GLU:HG3	1.98	0.46
1:F:1220:MET:O	1:F:1224:LEU:HD12	2.16	0.46
1:G:1248:ASN:OD1	1:G:1249:MET:N	2.49	0.46
1:H:157:THR:HG23	1:H:195:LEU:HD22	1.98	0.46
1:G:1402:LEU:C	1:G:1404:GLU:H	2.24	0.46
1:A:1380:MET:HE1	1:C:91:PRO:CB	2.46	0.46
1:D:1309:PRO:HG2	1:D:1310:LEU:H	1.81	0.46
1:F:1235:PHE:HA	1:F:1236:PRO:HA	1.66	0.46
1:G:128:THR:HG22	1:G:131:GLU:HG3	1.98	0.46
1:D:1220:MET:O	1:D:1224:LEU:HD12	2.16	0.45
1:H:27:PHE:O	1:H:31:THR:HG22	2.15	0.45
1:A:1384:PRO:C	1:A:1386:ALA:N	2.73	0.45
1:B:1232:THR:HG1	1:B:1233:LYS:H	1.60	0.45
1:G:157:THR:HG23	1:G:195:LEU:HD22	1.98	0.45
1:J:330:MET:HE3	1:J:340:TRP:CZ2	2.51	0.45
1:A:183:VAL:O	1:A:361:LEU:HD22	2.17	0.45
1:B:90:TYR:CE1	1:B:305:LYS:HG2	2.50	0.45
1:C:2:ILE:CG2	1:C:3:GLU:N	2.78	0.45
1:D:1318:ALA:HB2	1:J:90:TYR:CE2	2.51	0.45
1:F:1:LYS:O	1:F:2:ILE:CG2	2.57	0.45
1:H:1359:LYS:HE3	1:H:1393:TYR:CE1	2.51	0.45
1:H:1393:TYR:O	1:H:1393:TYR:CD1	2.69	0.45
1:J:1220:MET:O	1:J:1224:LEU:HD12	2.17	0.45
1:B:1356:PRO:HB3	1:C:30:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:THR:HG23	1:I:195:LEU:HD22	1.99	0.45
1:I:1229:ARG:NH1	1:I:1388:ILE:HG21	2.30	0.45
1:I:1295:VAL:HG21	1:I:1311:LEU:CD2	2.47	0.45
1:C:183:VAL:O	1:C:361:LEU:HD22	2.17	0.45
1:D:341:TYR:CD1	1:D:1361:GLN:HG3	2.51	0.45
1:D:1301:LEU:CD1	1:D:1303:MET:HE3	2.42	0.45
1:E:27:PHE:O	1:E:31:THR:HG22	2.15	0.45
1:E:1251:GLU:O	1:E:1254:GLU:HB2	2.16	0.45
1:G:1248:ASN:ND2	1:G:1374:ALA:CB	2.79	0.45
1:C:2:ILE:O	1:C:3:GLU:CB	2.64	0.45
1:D:1365:VAL:HG12	1:D:1365:VAL:O	2.16	0.45
1:I:341:TYR:CD2	1:I:1361:GLN:CG	2.98	0.45
1:A:1355:LEU:N	1:A:1356:PRO:CD	2.79	0.45
1:B:183:VAL:O	1:B:361:LEU:HD22	2.16	0.45
1:C:1235:PHE:H	1:C:1236:PRO:CD	2.26	0.45
1:D:157:THR:HG23	1:D:195:LEU:HD22	1.99	0.45
1:E:31:THR:HG23	1:E:33:ILE:HD12	1.99	0.45
1:E:1297:ILE:HG13	1:E:1298:SER:N	2.31	0.45
1:F:128:THR:HG23	1:F:131:GLU:HG3	1.98	0.45
1:G:1220:MET:O	1:G:1224:LEU:HD12	2.17	0.45
1:A:1365:VAL:C	1:A:1367:GLU:H	2.17	0.45
1:C:356:THR:CG2	1:C:357:VAL:N	2.80	0.45
1:E:10:TRP:CD2	1:E:57:PRO:HG3	2.52	0.45
1:G:1370:TRP:CG	1:G:1371:ASP:H	2.24	0.45
1:H:1220:MET:O	1:H:1224:LEU:HD12	2.16	0.45
1:A:1380:MET:HB2	1:C:86:GLN:NE2	2.32	0.45
1:D:122:LEU:HD23	1:D:223:ALA:HB1	1.99	0.45
1:B:341:TYR:CD2	1:B:1361:GLN:CG	2.98	0.45
1:C:49:GLN:HG2	1:C:1368:GLN:O	2.17	0.45
1:C:1355:LEU:N	1:C:1356:PRO:CD	2.80	0.45
1:D:31:THR:HG23	1:D:33:ILE:HD12	1.99	0.45
1:C:1291:ARG:HG2	1:C:1311:LEU:HD21	1.98	0.44
1:D:1355:LEU:N	1:D:1356:PRO:CD	2.79	0.44
1:F:1264:THR:HB	1:F:1267:LYS:HB2	1.99	0.44
1:H:183:VAL:O	1:H:361:LEU:HD22	2.17	0.44
1:J:330:MET:CE	1:J:340:TRP:NE1	2.76	0.44
1:J:1294:GLU:O	1:J:1297:ILE:HG13	2.17	0.44
1:D:335:GLN:N	1:D:335:GLN:OE1	2.47	0.44
1:C:1308:LYS:CB	1:C:1311:LEU:HD12	2.47	0.44
1:D:183:VAL:O	1:D:361:LEU:HD22	2.18	0.44
1:G:1355:LEU:N	1:G:1356:PRO:CD	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:THR:HG22	1:H:131:GLU:HG3	1.99	0.44
1:I:183:VAL:O	1:I:361:LEU:HD22	2.17	0.44
1:A:157:THR:HG23	1:A:195:LEU:HD22	1.99	0.44
1:F:1267:LYS:HD2	1:F:1313:SER:HA	1.99	0.44
1:C:31:THR:HG23	1:C:33:ILE:HD12	2.00	0.44
1:F:1369:ASN:O	1:F:1370:TRP:HB3	2.18	0.44
1:G:341:TYR:CD2	1:G:1361:GLN:CG	2.98	0.44
1:J:247:LEU:HD12	1:J:247:LEU:N	2.32	0.44
1:B:354:ARG:NH1	1:C:286:THR:HG22	2.32	0.44
1:C:1267:LYS:HD2	1:C:1313:SER:HA	1.99	0.44
1:E:183:VAL:O	1:E:361:LEU:HD22	2.17	0.44
1:J:183:VAL:O	1:J:361:LEU:HD22	2.17	0.44
1:A:1402:LEU:C	1:A:1404:GLU:H	2.26	0.44
1:B:27:PHE:HD1	1:B:283:TYR:CE2	2.36	0.44
1:B:1355:LEU:N	1:B:1356:PRO:CD	2.80	0.44
1:C:157:THR:HG23	1:C:195:LEU:HD22	1.99	0.44
1:F:10:TRP:CD2	1:F:57:PRO:HG3	2.53	0.44
1:F:157:THR:HG23	1:F:195:LEU:HD22	1.99	0.44
1:H:8:VAL:HA	1:H:36:THR:HG23	2.00	0.44
1:A:1366:MET:CE	1:A:1370:TRP:HE3	2.28	0.44
1:B:1361:GLN:O	1:B:1365:VAL:HG23	2.18	0.44
1:F:183:VAL:O	1:F:361:LEU:HD22	2.17	0.44
1:J:157:THR:HG23	1:J:195:LEU:HD22	1.99	0.44
1:C:1:LYS:HB2	1:C:1:LYS:HE3	1.78	0.44
1:A:286:THR:HG21	1:E:354:ARG:NH2	2.33	0.43
1:A:132:ILE:N	1:A:133:PRO:CD	2.82	0.43
1:A:1303:MET:CG	1:A:1304:GLU:N	2.60	0.43
1:C:1246:SER:HB3	1:E:140:LYS:HG3	2.00	0.43
1:G:122:LEU:HD23	1:G:223:ALA:HB1	2.00	0.43
1:C:1401:GLU:OE2	1:C:1406:PRO:HA	2.17	0.43
1:D:245:THR:OG1	1:D:246:VAL:N	2.52	0.43
1:D:1362:VAL:O	1:D:1366:MET:HG3	2.18	0.43
1:I:10:TRP:CD2	1:I:57:PRO:HG3	2.53	0.43
1:I:1339:LEU:HD21	1:I:1392:LEU:CD1	2.48	0.43
1:A:1367:GLU:HG3	1:A:1373:LEU:HD12	2.00	0.43
1:B:1220:MET:O	1:B:1224:LEU:HD12	2.18	0.43
1:D:1304:GLU:O	1:D:1307:ASP:N	2.48	0.43
1:E:1274:SER:HB2	1:E:1310:LEU:HD12	1.99	0.43
1:G:183:VAL:O	1:G:361:LEU:HD22	2.17	0.43
1:G:1382:TYR:CG	1:G:1383:ASP:N	2.87	0.43
1:B:157:THR:HG23	1:B:195:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:LEU:HD23	1:F:223:ALA:HB1	1.99	0.43
1:G:1405:GLY:N	1:G:1406:PRO:CD	2.78	0.43
1:I:259:VAL:HG22	1:I:328:GLU:C	2.44	0.43
1:D:1229:ARG:NH2	1:D:1342:GLU:OE2	2.52	0.43
1:E:1264:THR:HB	1:E:1267:LYS:HG3	2.01	0.43
1:H:1247:ARG:HG3	1:H:1248:ASN:N	2.34	0.43
1:I:1249:MET:SD	1:I:1249:MET:C	3.02	0.43
1:A:31:THR:HG23	1:A:33:ILE:HD12	2.01	0.43
1:A:125:PRO:HD2	1:D:252:GLY:O	2.18	0.43
1:G:10:TRP:CD2	1:G:57:PRO:HG3	2.54	0.43
1:G:135:LEU:O	1:G:139:LEU:HD12	2.19	0.43
1:G:284:LEU:O	1:G:290:LEU:HD12	2.19	0.43
1:H:1355:LEU:N	1:H:1356:PRO:CD	2.82	0.43
1:I:1355:LEU:N	1:I:1356:PRO:CD	2.82	0.43
1:B:1264:THR:HG22	1:B:1266:GLU:N	2.29	0.42
1:D:111:GLU:OE1	2:N:1:GLC:O2	2.28	0.42
1:E:1234:SER:C	1:E:1236:PRO:HD2	2.44	0.42
1:E:1241:LEU:HD22	1:E:1296:LEU:HD23	2.00	0.42
1:E:1267:LYS:HD2	1:E:1313:SER:HA	2.01	0.42
1:C:1366:MET:O	1:C:1368:GLN:N	2.52	0.42
1:E:157:THR:HG23	1:E:195:LEU:HD22	1.99	0.42
1:A:10:TRP:CD2	1:A:57:PRO:HG3	2.55	0.42
1:B:1303:MET:CG	1:B:1304:GLU:H	2.32	0.42
1:C:1264:THR:HG22	1:C:1266:GLU:H	1.84	0.42
1:G:286:THR:H	1:G:290:LEU:HD11	1.83	0.42
1:C:2:ILE:CG2	1:C:3:GLU:H	2.32	0.42
1:D:1248:ASN:OD1	1:D:1249:MET:N	2.52	0.42
1:H:1229:ARG:CZ	1:H:1388:ILE:HD12	2.48	0.42
1:E:132:ILE:N	1:E:133:PRO:CD	2.82	0.42
1:C:10:TRP:CD2	1:C:57:PRO:HG3	2.55	0.42
1:D:1295:VAL:HG21	1:D:1311:LEU:HD23	2.01	0.42
1:F:1264:THR:HB	1:F:1267:LYS:CB	2.49	0.42
1:A:66:ARG:NH2	2:K:2:GLC:O4	2.50	0.42
1:A:122:LEU:HD21	1:A:125:PRO:HA	2.01	0.42
1:B:341:TYR:HD2	1:B:1361:GLN:CG	2.28	0.42
1:D:132:ILE:N	1:D:133:PRO:CD	2.83	0.42
1:F:1355:LEU:N	1:F:1356:PRO:CD	2.83	0.42
1:B:122:LEU:HD23	1:B:223:ALA:HB1	2.00	0.42
1:B:338:ALA:HB1	1:B:1220:MET:HB3	2.00	0.42
1:B:1248:ASN:OD1	1:B:1249:MET:N	2.52	0.42
1:F:135:LEU:O	1:F:139:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:N	1:B:133:PRO:CD	2.83	0.42
1:J:1368:GLN:HG3	1:J:1369:ASN:N	2.34	0.42
1:F:209:ASP:C	1:F:209:ASP:OD1	2.63	0.42
1:H:1393:TYR:CD1	1:H:1393:TYR:C	2.98	0.42
1:I:85:PHE:HA	1:I:88:LYS:CD	2.50	0.42
1:A:128:THR:HG22	1:A:249:THR:HG1	1.85	0.41
1:A:1220:MET:SD	1:A:1361:GLN:HB3	2.60	0.41
1:C:341:TYR:CE2	1:C:1365:VAL:HG12	2.55	0.41
1:D:209:ASP:OD1	1:D:209:ASP:C	2.63	0.41
1:E:1305:ASP:O	1:E:1308:LYS:N	2.45	0.41
1:A:1301:LEU:HD23	1:A:1301:LEU:C	2.46	0.41
1:A:1303:MET:HE1	1:F:1276:ALA:HB1	2.01	0.41
1:B:68:GLY:HA3	1:B:332:ASN:O	2.20	0.41
1:G:1235:PHE:HA	1:G:1236:PRO:HA	1.62	0.41
1:I:1248:ASN:OD1	1:I:1249:MET:N	2.54	0.41
1:C:1271:VAL:HG13	1:C:1310:LEU:CD1	2.50	0.41
1:I:1369:ASN:O	1:I:1370:TRP:HB2	2.20	0.41
1:H:8:VAL:HG13	1:H:36:THR:CG2	2.49	0.41
1:C:132:ILE:N	1:C:133:PRO:CD	2.84	0.41
1:F:1249:MET:SD	1:F:1249:MET:C	3.04	0.41
1:G:341:TYR:HD2	1:G:1361:GLN:CG	2.28	0.41
1:J:10:TRP:CD2	1:J:57:PRO:HG3	2.56	0.41
1:B:27:PHE:CD1	1:B:283:TYR:CD2	2.96	0.41
1:E:68:GLY:HA3	1:E:332:ASN:O	2.21	0.41
1:G:68:GLY:HA3	1:G:332:ASN:O	2.21	0.41
1:C:1308:LYS:HB2	1:C:1311:LEU:HD12	2.02	0.41
1:C:1379:ASP:HB2	1:C:1381:ASP:H	1.85	0.41
1:D:259:VAL:HB	1:D:329:ILE:HA	2.02	0.41
1:D:1267:LYS:HD2	1:D:1313:SER:HA	2.02	0.41
1:G:27:PHE:HD1	1:G:283:TYR:CE2	2.38	0.41
1:J:68:GLY:HA3	1:J:332:ASN:O	2.21	0.41
1:A:1340:SER:HA	1:C:173:ALA:O	2.18	0.41
1:B:10:TRP:CD2	1:B:57:PRO:HG3	2.55	0.41
1:B:209:ASP:OD1	1:B:209:ASP:C	2.64	0.41
1:B:245:THR:OG1	1:B:246:VAL:N	2.54	0.41
1:C:194:PHE:CD2	1:C:250:PHE:HE1	2.38	0.41
1:D:68:GLY:HA3	1:D:332:ASN:O	2.21	0.41
1:E:1240:SER:C	1:E:1241:LEU:O	2.62	0.41
1:F:1220:MET:CE	1:F:1365:VAL:HG21	2.25	0.41
1:F:1248:ASN:OD1	1:F:1249:MET:N	2.54	0.41
1:H:1248:ASN:OD1	1:H:1249:MET:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:GLY:HA3	1:I:332:ASN:O	2.21	0.41
1:I:1220:MET:HE3	1:I:1361:GLN:HB3	2.02	0.41
1:C:1301:LEU:HB2	1:C:1315:PHE:HZ	1.83	0.41
1:H:68:GLY:HA3	1:H:332:ASN:O	2.21	0.41
1:I:1220:MET:HE1	1:I:1361:GLN:HB3	2.02	0.41
1:H:1264:THR:HB	1:H:1267:LYS:CB	2.50	0.40
1:H:1271:VAL:HG13	1:H:1310:LEU:CD1	2.51	0.40
1:B:128:THR:HG22	1:B:249:THR:HG1	1.86	0.40
1:C:1248:ASN:OD1	1:C:1248:ASN:N	2.53	0.40
1:H:1307:ASP:O	1:H:1308:LYS:C	2.63	0.40
1:A:235:ILE:O	1:A:238:SER:HB3	2.22	0.40
1:A:1382:TYR:O	1:A:1383:ASP:CB	2.69	0.40
1:D:1305:ASP:CB	1:D:1306:PRO:CD	2.97	0.40
1:A:329:ILE:HG22	1:C:1232:THR:HA	2.03	0.40
1:C:259:VAL:HB	1:C:329:ILE:HA	2.04	0.40
1:F:1366:MET:HG3	1:F:1389:LEU:HD21	1.96	0.40
1:G:132:ILE:N	1:G:133:PRO:CD	2.84	0.40
1:E:12:ASN:HA	1:E:43:LEU:HD21	2.04	0.40
1:G:1340:SER:HG	1:G:1341:GLU:N	2.11	0.40
1:H:1406:PRO:HB2	1:H:1407:THR:H	1.76	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:171:TYR:OH	1:J:1231:LYS:O[2_444]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	547/561 (98%)	504 (92%)	30 (6%)	13 (2%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	550/561 (98%)	510 (93%)	29 (5%)	11 (2%)	6	32
1	C	550/561 (98%)	517 (94%)	21 (4%)	12 (2%)	5	30
1	D	535/561 (95%)	505 (94%)	22 (4%)	8 (2%)	8	37
1	E	552/561 (98%)	520 (94%)	27 (5%)	5 (1%)	14	47
1	F	533/561 (95%)	511 (96%)	18 (3%)	4 (1%)	16	49
1	G	537/561 (96%)	513 (96%)	17 (3%)	7 (1%)	9	39
1	H	529/561 (94%)	504 (95%)	21 (4%)	4 (1%)	16	49
1	I	529/561 (94%)	509 (96%)	14 (3%)	6 (1%)	11	43
1	J	544/561 (97%)	521 (96%)	19 (4%)	4 (1%)	18	51
All	All	5406/5610 (96%)	5114 (95%)	218 (4%)	74 (1%)	9	38

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1226	ILE
1	A	1303	MET
1	A	1368	GLN
1	A	1370	TRP
1	A	1383	ASP
1	B	1246	SER
1	B	1303	MET
1	B	1306	PRO
1	C	2	ILE
1	C	1226	ILE
1	C	1235	PHE
1	C	1379	ASP
1	D	2	ILE
1	D	1235	PHE
1	D	1307	ASP
1	D	1309	PRO
1	F	2	ILE
1	G	3	GLU
1	G	1404	GLU
1	H	2	ILE
1	H	1406	PRO
1	I	1305	ASP
1	J	1246	SER
1	J	1305	ASP
1	A	1243	SER

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Mol	Chain	Res	Type
1	B	2	ILE
1	B	1240	SER
1	B	1242	GLY
1	B	1370	TRP
1	B	1384	PRO
1	C	3	GLU
1	C	1366	MET
1	C	1369	ASN
1	D	1233	LYS
1	D	1302	HIS
1	D	1303	MET
1	E	1234	SER
1	F	1404	GLU
1	G	1371	ASP
1	H	1370	TRP
1	I	2	ILE
1	I	1306	PRO
1	A	3	GLU
1	A	1367	GLU
1	C	1247	ARG
1	E	1241	LEU
1	E	1303	MET
1	E	1375	SER
1	G	2	ILE
1	G	1370	TRP
1	H	1407	THR
1	A	1246	SER
1	B	1304	GLU
1	B	1383	ASP
1	D	1373	LEU
1	E	1374	ALA
1	F	1235	PHE
1	G	1303	MET
1	I	3	GLU
1	J	1235	PHE
1	A	1225	ASP
1	B	1232	THR
1	C	1302	HIS
1	C	1306	PRO
1	C	1367	GLU
1	G	1306	PRO
1	A	1384	PRO

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Mol	Chain	Res	Type
1	C	1376	SER
1	I	1370	TRP
1	A	1308	LYS
1	J	2	ILE
1	I	1308	LYS
1	A	1378	PRO
1	F	1236	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	388/454 (86%)	378 (97%)	10 (3%)	40	62
1	B	384/454 (85%)	378 (98%)	6 (2%)	55	70
1	C	389/454 (86%)	381 (98%)	8 (2%)	47	66
1	D	372/454 (82%)	367 (99%)	5 (1%)	61	72
1	E	385/454 (85%)	380 (99%)	5 (1%)	61	72
1	F	372/454 (82%)	363 (98%)	9 (2%)	43	64
1	G	350/454 (77%)	342 (98%)	8 (2%)	44	64
1	H	347/454 (76%)	344 (99%)	3 (1%)	70	76
1	I	335/454 (74%)	329 (98%)	6 (2%)	51	69
1	J	351/454 (77%)	345 (98%)	6 (2%)	53	70
All	All	3673/4540 (81%)	3607 (98%)	66 (2%)	51	69

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	35	VAL
1	A	122	LEU
1	A	132	ILE
1	A	175	LYS
1	A	262	LEU

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Mol	Chain	Res	Type
1	A	288	GLU
1	A	306	SER
1	A	365	GLN
1	A	1226	ILE
1	B	132	ILE
1	B	262	LEU
1	B	288	GLU
1	B	365	GLN
1	B	1241	LEU
1	B	1364	SER
1	C	1	LYS
1	C	2	ILE
1	C	3	GLU
1	C	35	VAL
1	C	132	ILE
1	C	365	GLN
1	C	1226	ILE
1	C	1344	GLN
1	D	2	ILE
1	D	3	GLU
1	D	35	VAL
1	D	132	ILE
1	D	365	GLN
1	E	35	VAL
1	E	132	ILE
1	E	262	LEU
1	E	1291	ARG
1	E	1371	ASP
1	F	2	ILE
1	F	35	VAL
1	F	365	GLN
1	F	1232	THR
1	F	1263	LEU
1	F	1295	VAL
1	F	1310	LEU
1	F	1342	GLU
1	F	1369	ASN
1	G	35	VAL
1	G	132	ILE
1	G	139	LEU
1	G	365	GLN
1	G	1286	GLN

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Mol	Chain	Res	Type
1	G	1342	GLU
1	G	1369	ASN
1	G	1372	GLU
1	H	132	ILE
1	H	365	GLN
1	H	1291	ARG
1	I	35	VAL
1	I	132	ILE
1	I	135	LEU
1	I	365	GLN
1	I	1253	LEU
1	I	1310	LEU
1	J	35	VAL
1	J	365	GLN
1	J	1241	LEU
1	J	1253	LEU
1	J	1297	ILE
1	J	1342	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	282	ASN
1	A	1361	GLN
1	B	100	ASN
1	B	272	ASN
1	B	1368	GLN
1	C	86	GLN
1	D	100	ASN
1	D	1361	GLN
1	E	1248	ASN
1	F	1273	ASN
1	H	272	ASN
1	I	124	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	GLC	K	1	2	12,12,12	1.00	0	17,17,17	1.80	3 (17%)
2	GLC	K	2	2	11,11,12	0.43	0	15,15,17	1.43	3 (20%)
2	GLC	L	1	2	12,12,12	0.67	0	17,17,17	1.22	2 (11%)
2	GLC	L	2	2	11,11,12	0.42	0	15,15,17	1.20	2 (13%)
2	GLC	M	1	2	12,12,12	0.49	0	17,17,17	1.13	1 (5%)
2	GLC	M	2	2	11,11,12	0.66	0	15,15,17	1.32	2 (13%)
2	GLC	N	1	2	12,12,12	0.67	0	17,17,17	1.14	2 (11%)
2	GLC	N	2	2	11,11,12	0.51	0	15,15,17	1.04	1 (6%)
2	GLC	O	1	2	12,12,12	0.72	0	17,17,17	1.50	4 (23%)
2	GLC	O	2	2	11,11,12	0.35	0	15,15,17	1.57	2 (13%)
2	GLC	P	1	2	12,12,12	0.66	0	17,17,17	1.17	1 (5%)
2	GLC	P	2	2	11,11,12	0.58	0	15,15,17	1.09	1 (6%)
2	GLC	Q	1	2	12,12,12	0.76	0	17,17,17	1.75	4 (23%)
2	GLC	Q	2	2	11,11,12	0.50	0	15,15,17	1.32	1 (6%)
2	GLC	R	1	2	12,12,12	0.63	0	17,17,17	1.41	3 (17%)
2	GLC	R	2	2	11,11,12	0.32	0	15,15,17	2.02	4 (26%)
2	GLC	S	1	2	12,12,12	0.60	0	17,17,17	1.00	0
2	GLC	S	2	2	11,11,12	0.82	0	15,15,17	1.44	2 (13%)
2	GLC	T	1	2	12,12,12	0.65	0	17,17,17	1.67	4 (23%)
2	GLC	T	2	2	11,11,12	0.39	0	15,15,17	0.80	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	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1
2	GLC	M	1	2	-	2/2/22/22	0/1/1/1
2	GLC	M	2	2	-	1/2/19/22	0/1/1/1
2	GLC	N	1	2	-	0/2/22/22	0/1/1/1
2	GLC	N	2	2	-	0/2/19/22	0/1/1/1
2	GLC	O	1	2	-	2/2/22/22	0/1/1/1
2	GLC	O	2	2	-	0/2/19/22	0/1/1/1
2	GLC	P	1	2	-	2/2/22/22	0/1/1/1
2	GLC	P	2	2	-	0/2/19/22	0/1/1/1
2	GLC	Q	1	2	-	2/2/22/22	0/1/1/1
2	GLC	Q	2	2	-	1/2/19/22	0/1/1/1
2	GLC	R	1	2	-	0/2/22/22	0/1/1/1
2	GLC	R	2	2	-	0/2/19/22	0/1/1/1
2	GLC	S	1	2	-	2/2/22/22	0/1/1/1
2	GLC	S	2	2	-	1/2/19/22	0/1/1/1
2	GLC	T	1	2	-	2/2/22/22	0/1/1/1
2	GLC	T	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	2	GLC	C1-O5-C5	5.83	120.00	112.19
2	Q	2	GLC	C1-O5-C5	4.07	117.64	112.19
2	O	2	GLC	C1-O5-C5	3.87	117.37	112.19
2	K	1	GLC	C1-C2-C3	3.84	118.19	110.36
2	S	2	GLC	C1-O5-C5	3.84	117.33	112.19
2	T	1	GLC	C3-C4-C5	3.67	116.89	110.23
2	T	1	GLC	C1-C2-C3	3.56	117.61	110.36
2	K	1	GLC	O3-C3-C4	3.48	118.59	110.38
2	Q	1	GLC	C4-C3-C2	3.45	116.88	110.83
2	O	1	GLC	O2-C2-C3	-3.17	102.91	110.38
2	O	1	GLC	C1-C2-C3	3.12	116.72	110.36
2	K	1	GLC	C3-C4-C5	3.05	115.76	110.23
2	Q	1	GLC	C3-C4-C5	2.87	115.44	110.23
2	M	2	GLC	C1-O5-C5	2.79	115.93	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	1	GLC	C1-C2-C3	2.75	115.95	110.36
2	K	2	GLC	C1-O5-C5	2.74	115.86	112.19
2	L	2	GLC	O3-C3-C4	-2.71	103.99	110.38
2	Q	1	GLC	C1-C2-C3	2.69	115.84	110.36
2	O	2	GLC	C6-C5-C4	-2.67	106.47	113.02
2	K	2	GLC	O3-C3-C4	-2.64	104.15	110.38
2	Q	1	GLC	O3-C3-C2	-2.59	104.26	110.38
2	S	2	GLC	O2-C2-C3	2.55	115.44	110.15
2	N	1	GLC	C1-C2-C3	2.54	115.53	110.36
2	L	1	GLC	C1-C2-C3	2.50	115.45	110.36
2	L	1	GLC	O5-C1-C2	2.50	114.69	110.30
2	R	2	GLC	C2-C3-C4	-2.48	106.50	110.86
2	P	1	GLC	C1-C2-C3	2.40	115.25	110.36
2	N	2	GLC	C1-O5-C5	2.31	115.28	112.19
2	P	2	GLC	C2-C3-C4	2.30	114.90	110.86
2	T	1	GLC	O4-C4-C3	-2.29	104.98	110.38
2	T	2	GLC	C1-O5-C5	2.28	115.24	112.19
2	K	2	GLC	O2-C2-C1	-2.25	104.06	109.22
2	T	1	GLC	C4-C3-C2	2.25	114.78	110.83
2	R	2	GLC	C1-C2-C3	-2.24	106.39	109.64
2	O	1	GLC	O3-C3-C2	-2.22	105.15	110.38
2	R	1	GLC	C3-C4-C5	2.19	114.21	110.23
2	O	1	GLC	O3-C3-C4	2.17	115.50	110.38
2	R	2	GLC	C3-C4-C5	-2.14	106.35	110.23
2	N	1	GLC	C3-C4-C5	2.13	114.10	110.23
2	R	1	GLC	C4-C3-C2	2.10	114.52	110.83
2	M	2	GLC	O5-C1-C2	-2.05	105.89	110.79
2	M	1	GLC	C3-C4-C5	2.05	113.94	110.23
2	L	2	GLC	C2-C3-C4	2.04	114.45	110.86

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	GLC	O5-C5-C6-O6
2	O	1	GLC	C4-C5-C6-O6
2	S	1	GLC	C4-C5-C6-O6
2	S	1	GLC	O5-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6
2	Q	1	GLC	O5-C5-C6-O6
2	L	2	GLC	C4-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6

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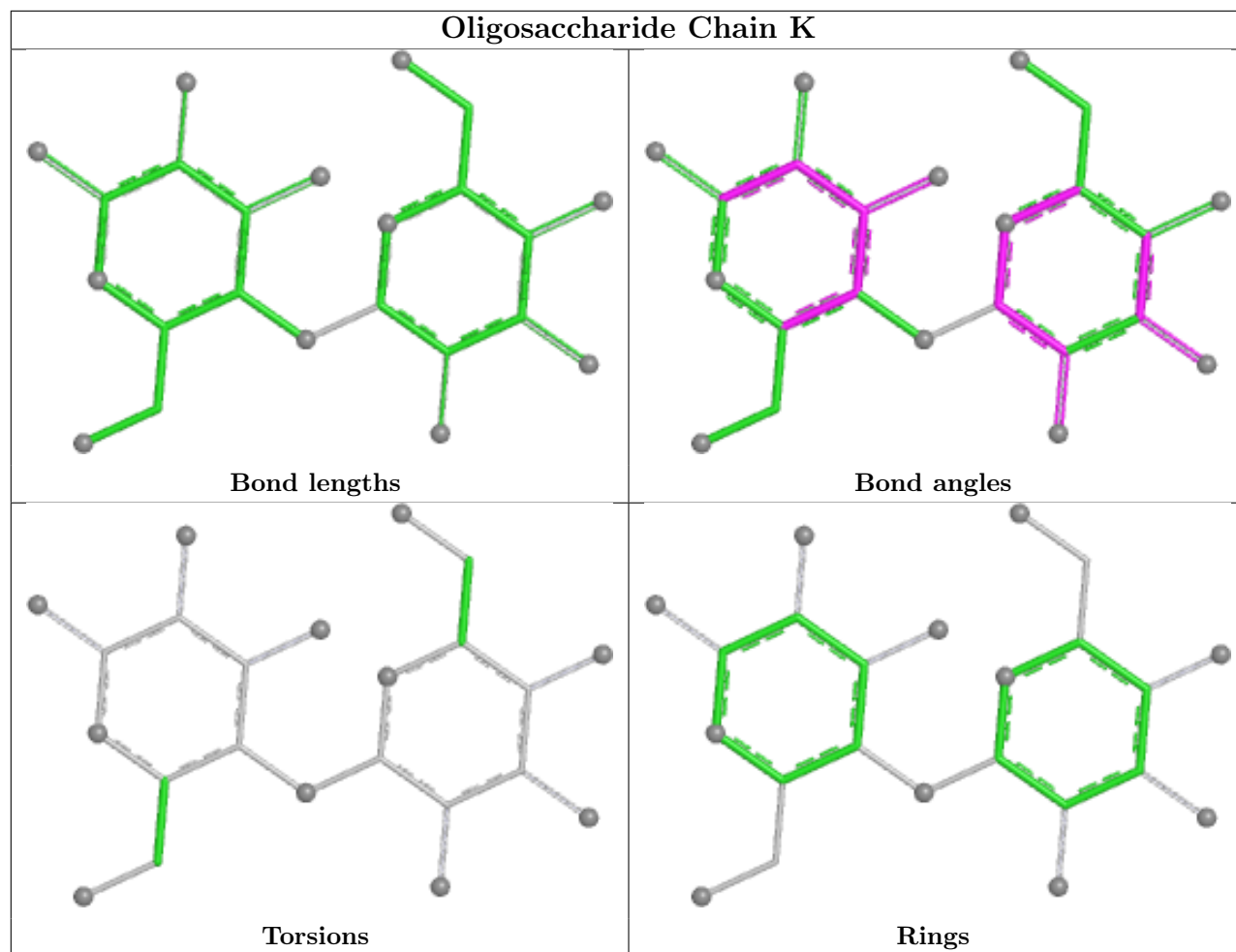
Mol	Chain	Res	Type	Atoms
2	T	1	GLC	C4-C5-C6-O6
2	L	2	GLC	O5-C5-C6-O6
2	M	1	GLC	C4-C5-C6-O6
2	T	1	GLC	O5-C5-C6-O6
2	M	1	GLC	O5-C5-C6-O6
2	Q	1	GLC	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	Q	2	GLC	C4-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6

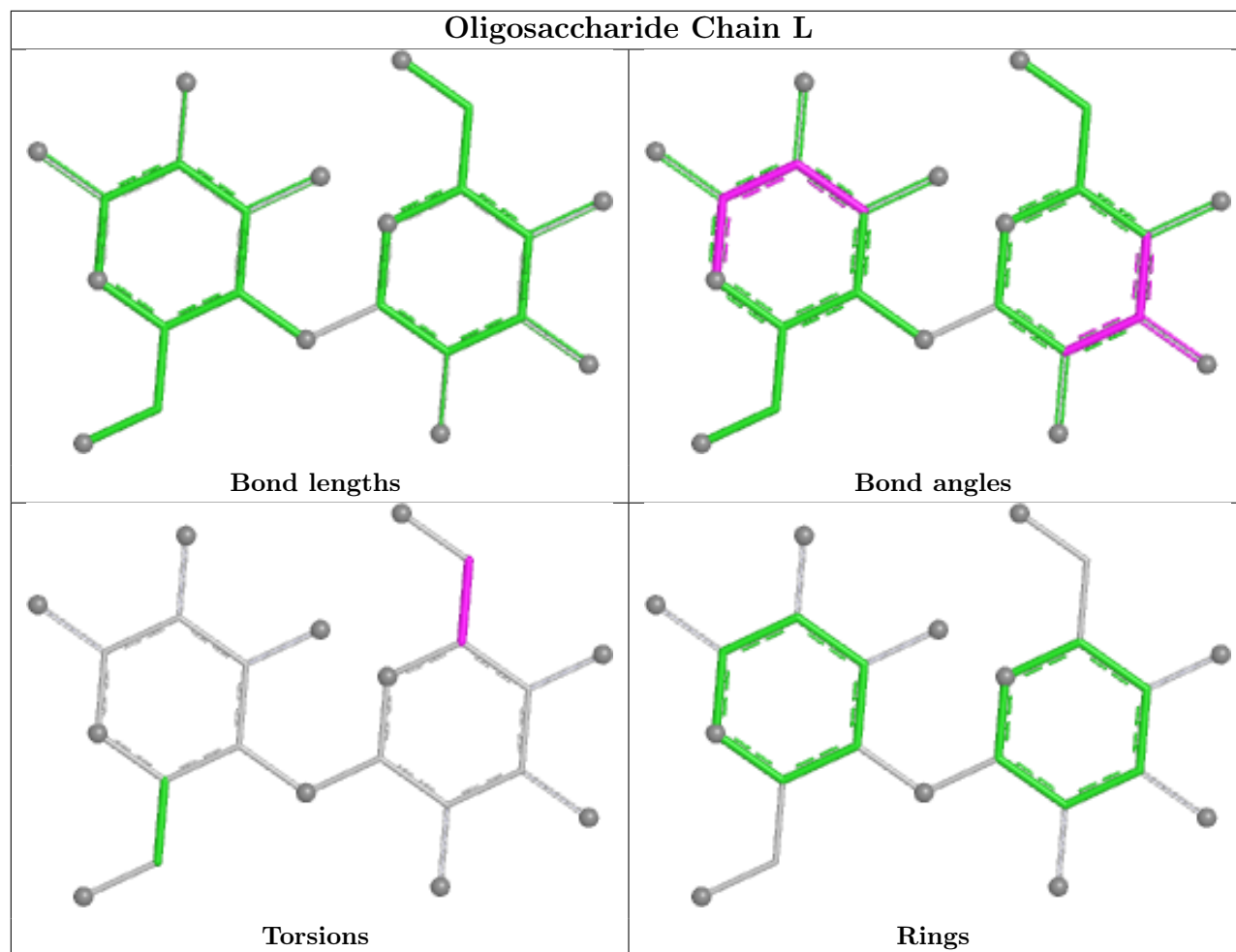
There are no ring outliers.

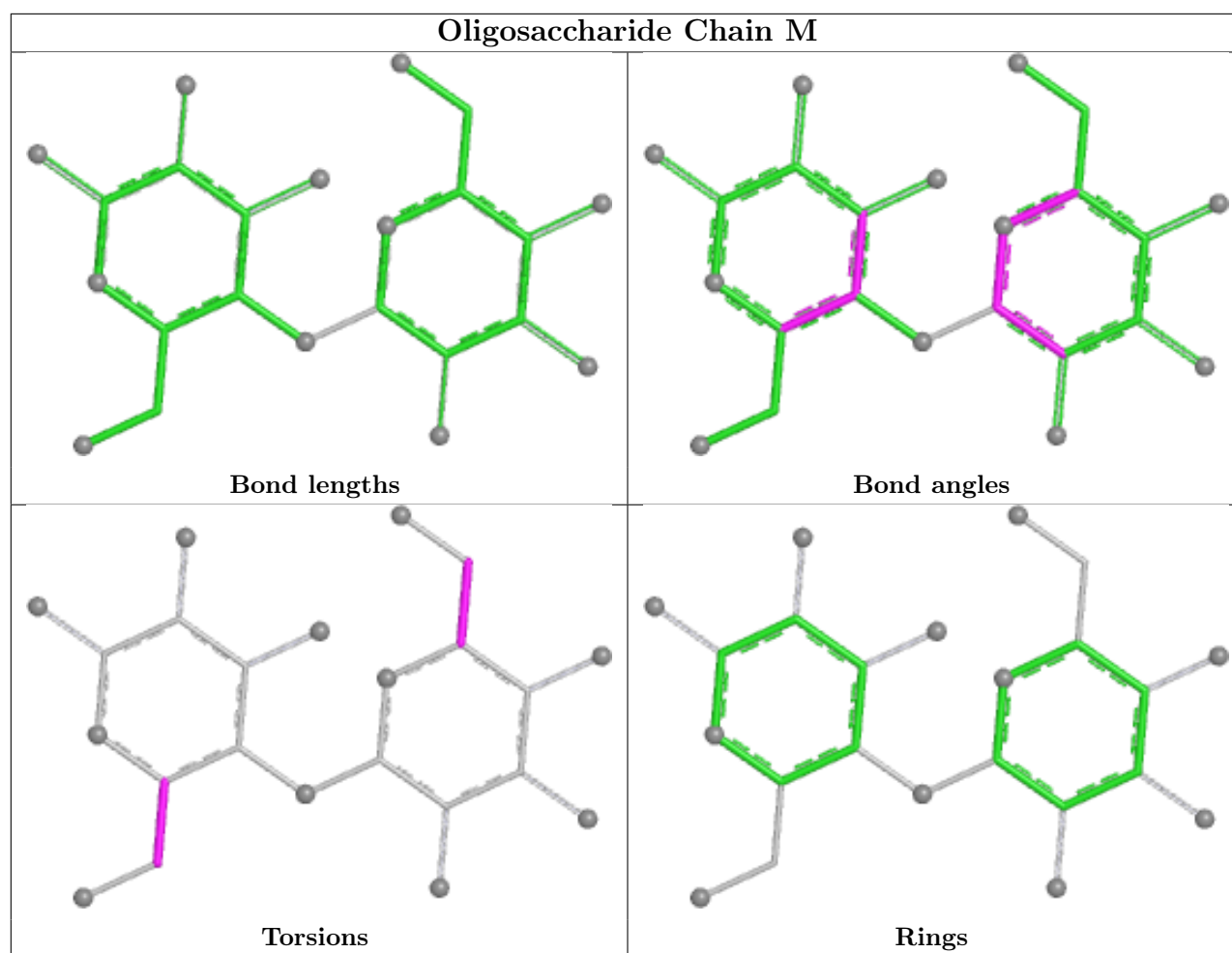
5 monomers are involved in 5 short contacts:

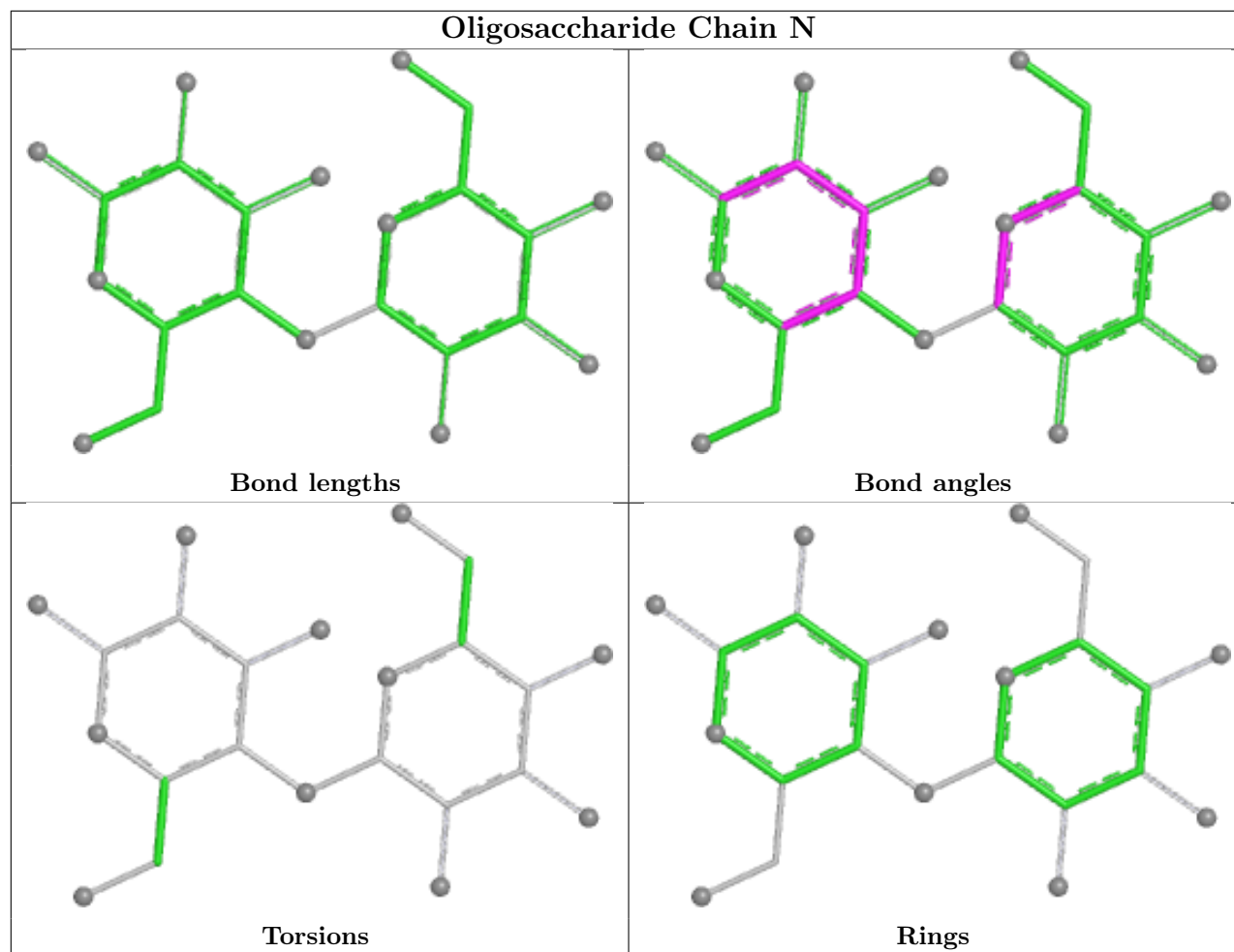
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	GLC	1	0
2	P	2	GLC	1	0
2	N	1	GLC	1	0
2	N	2	GLC	1	0
2	M	2	GLC	1	0

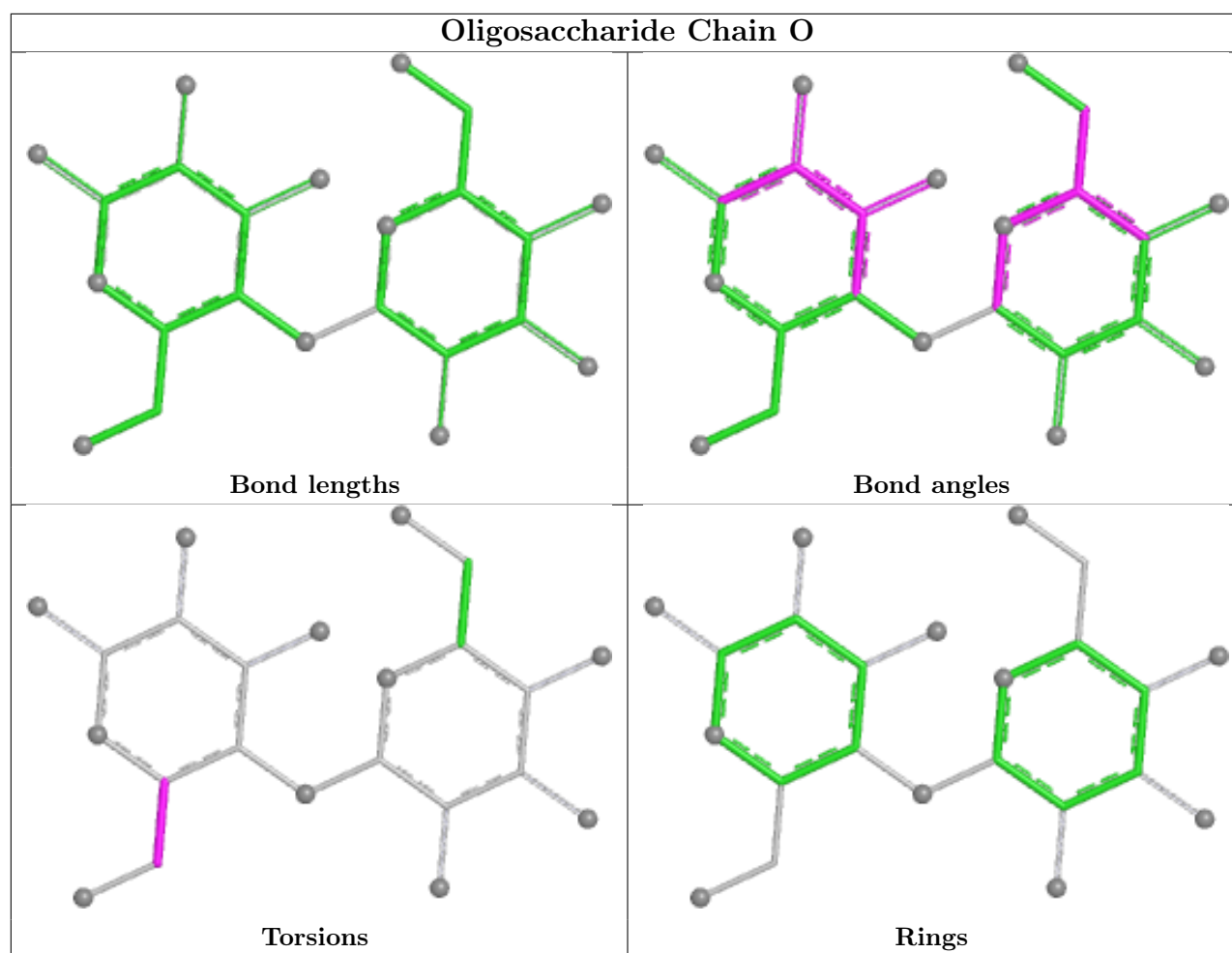
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

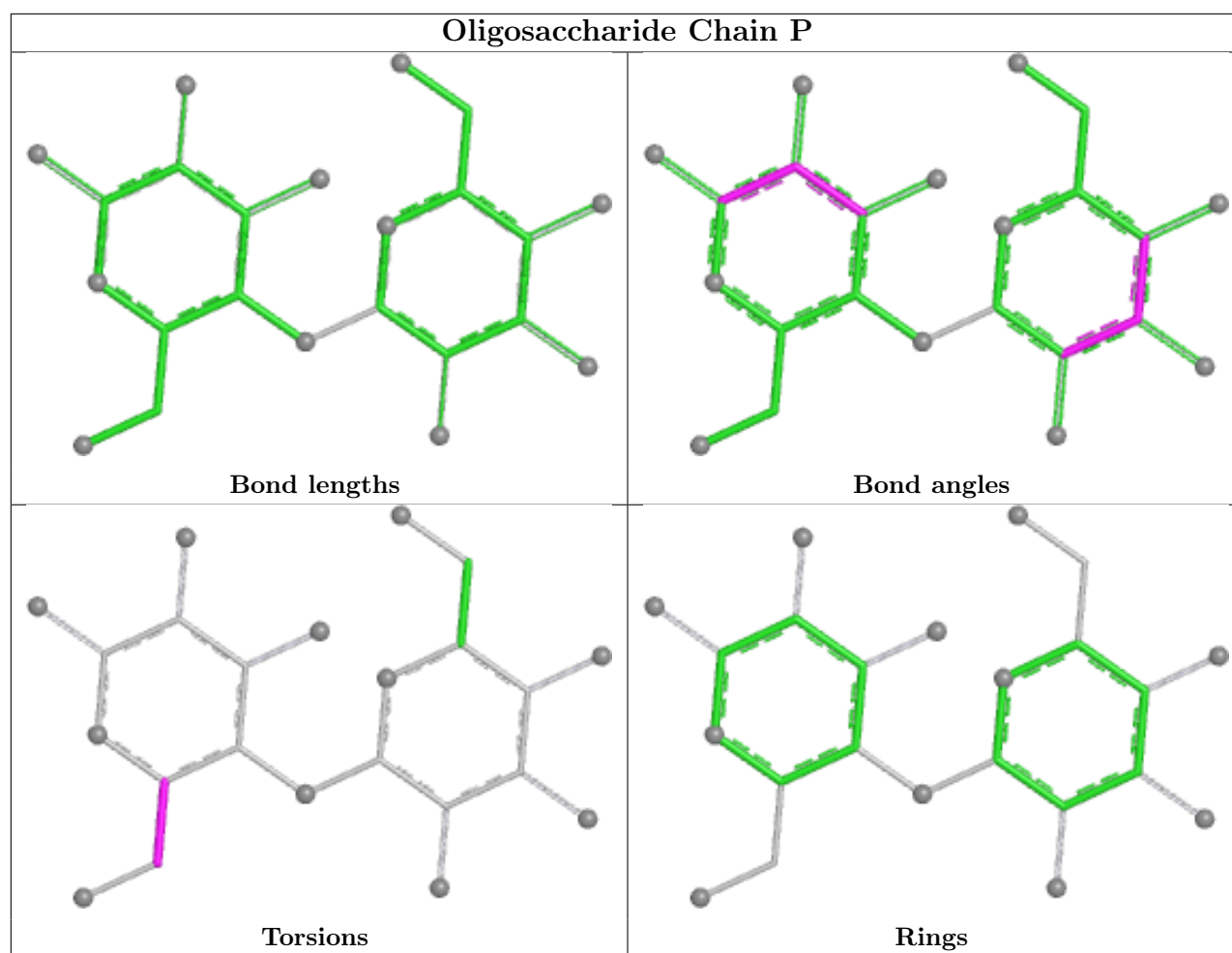


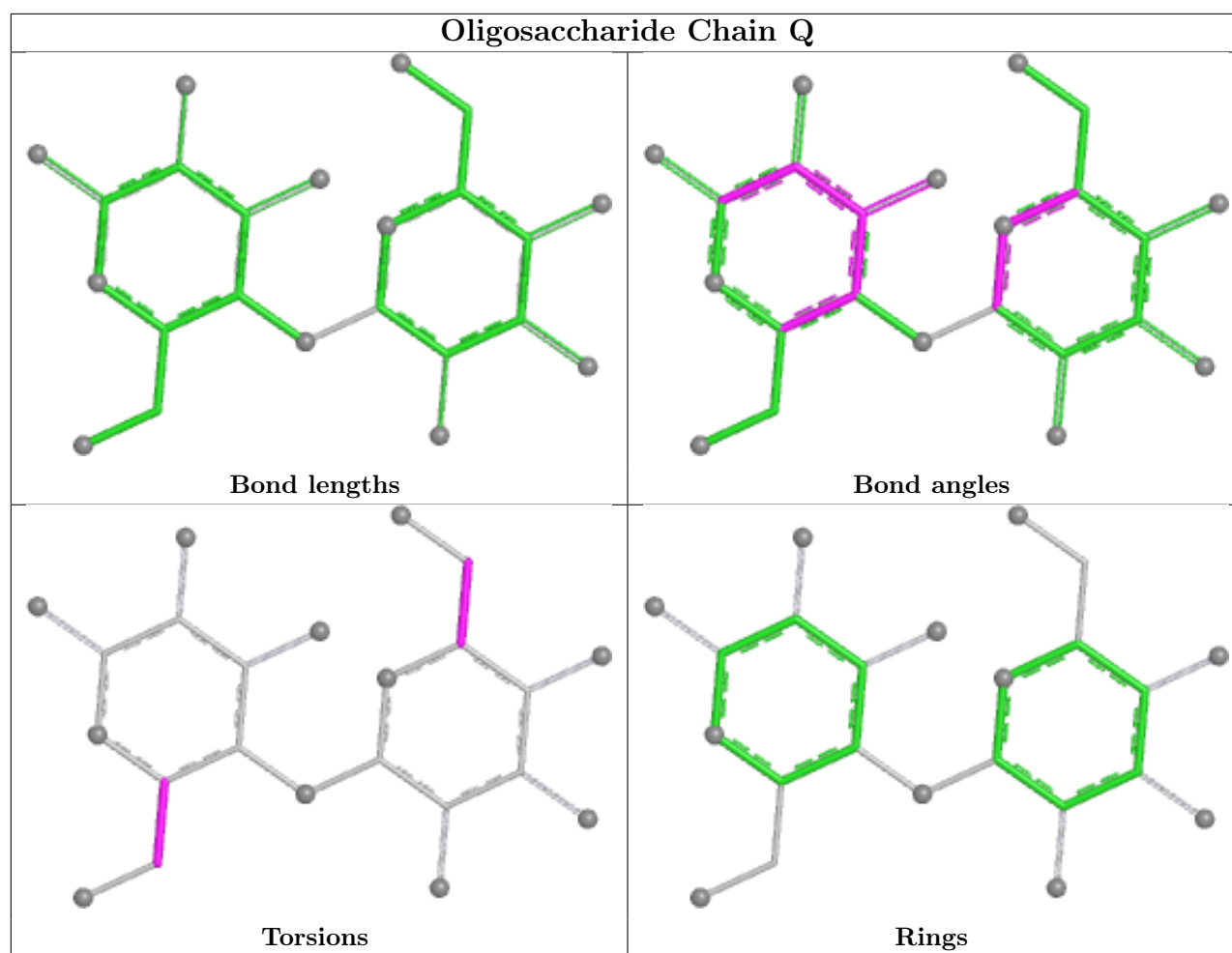


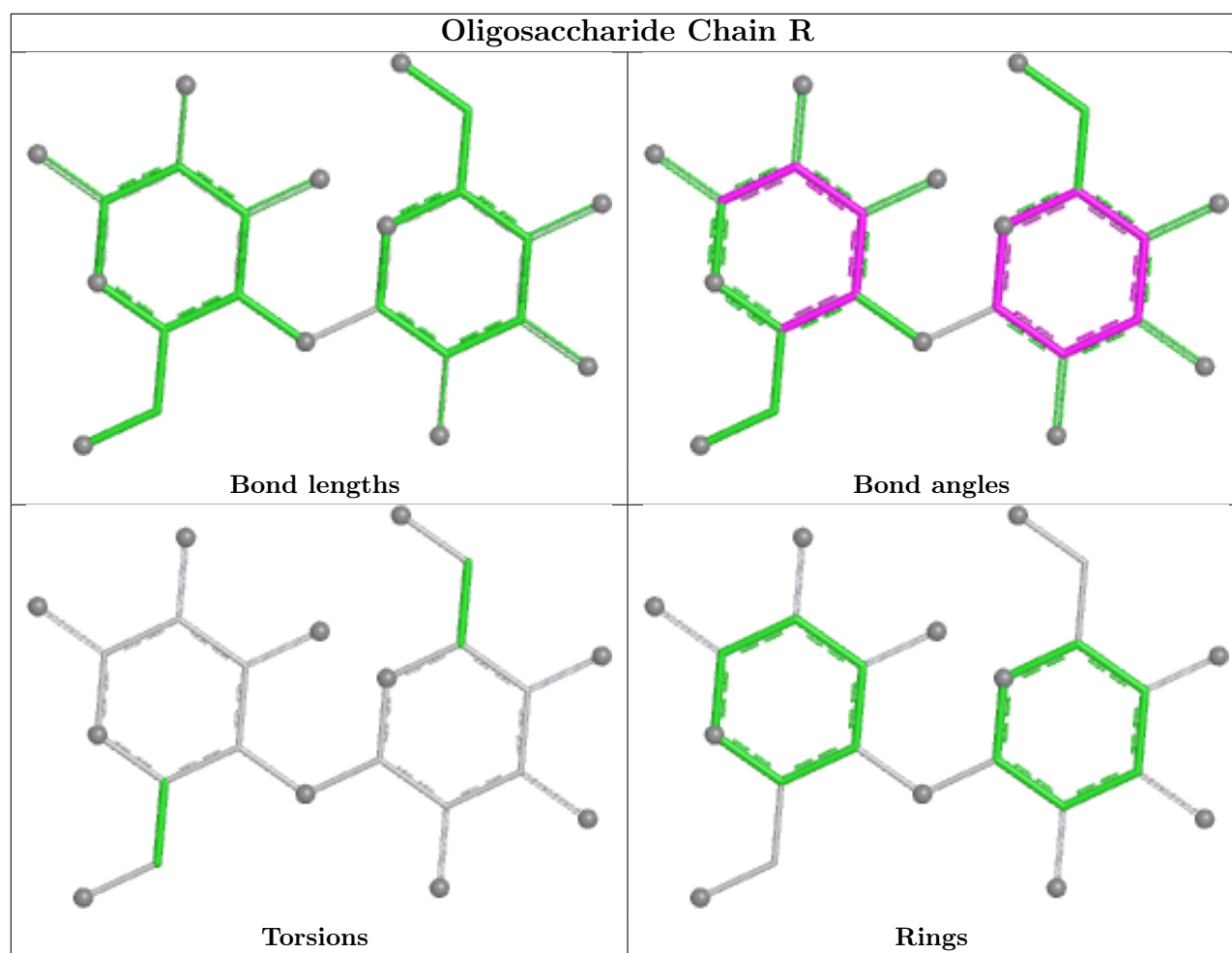


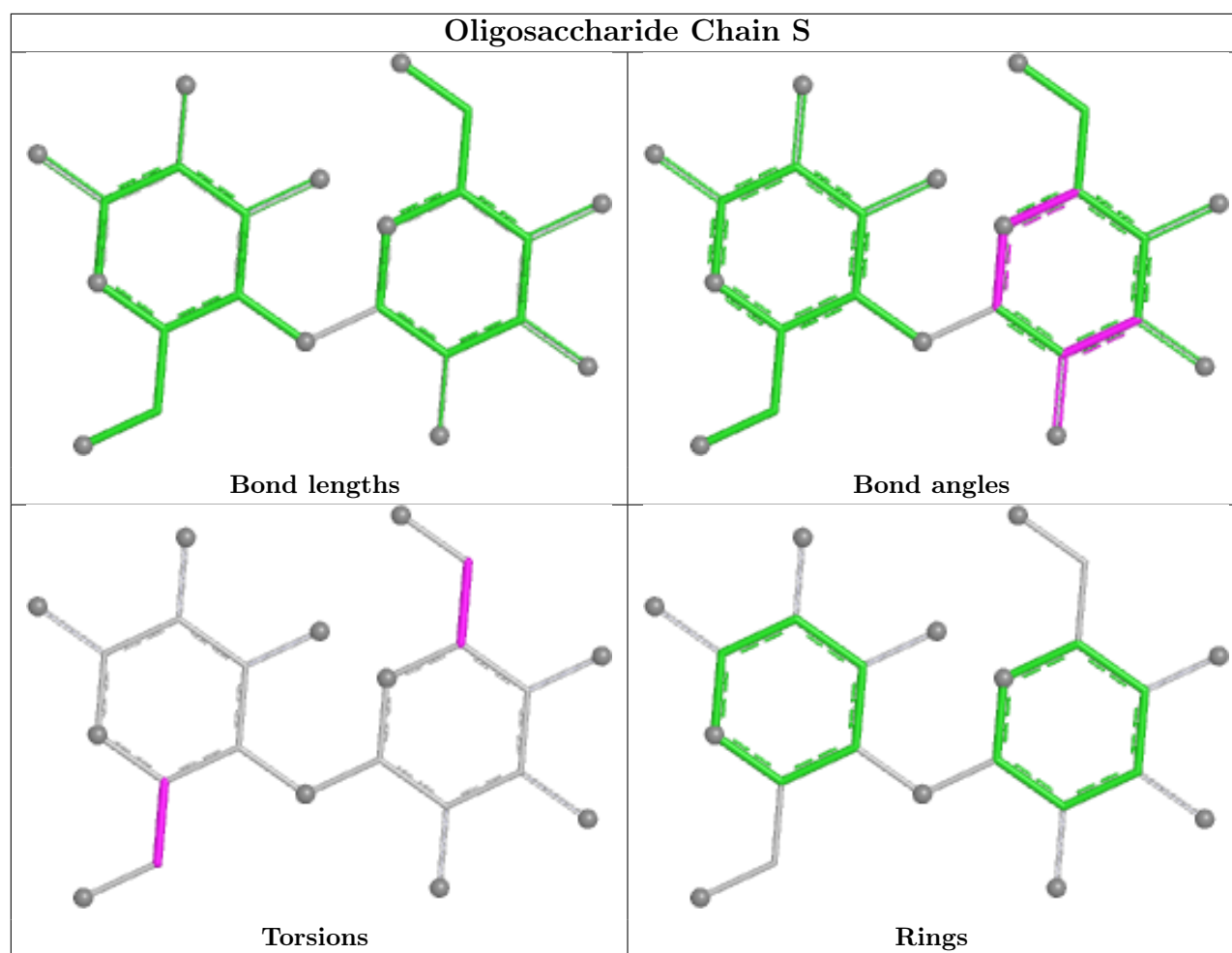


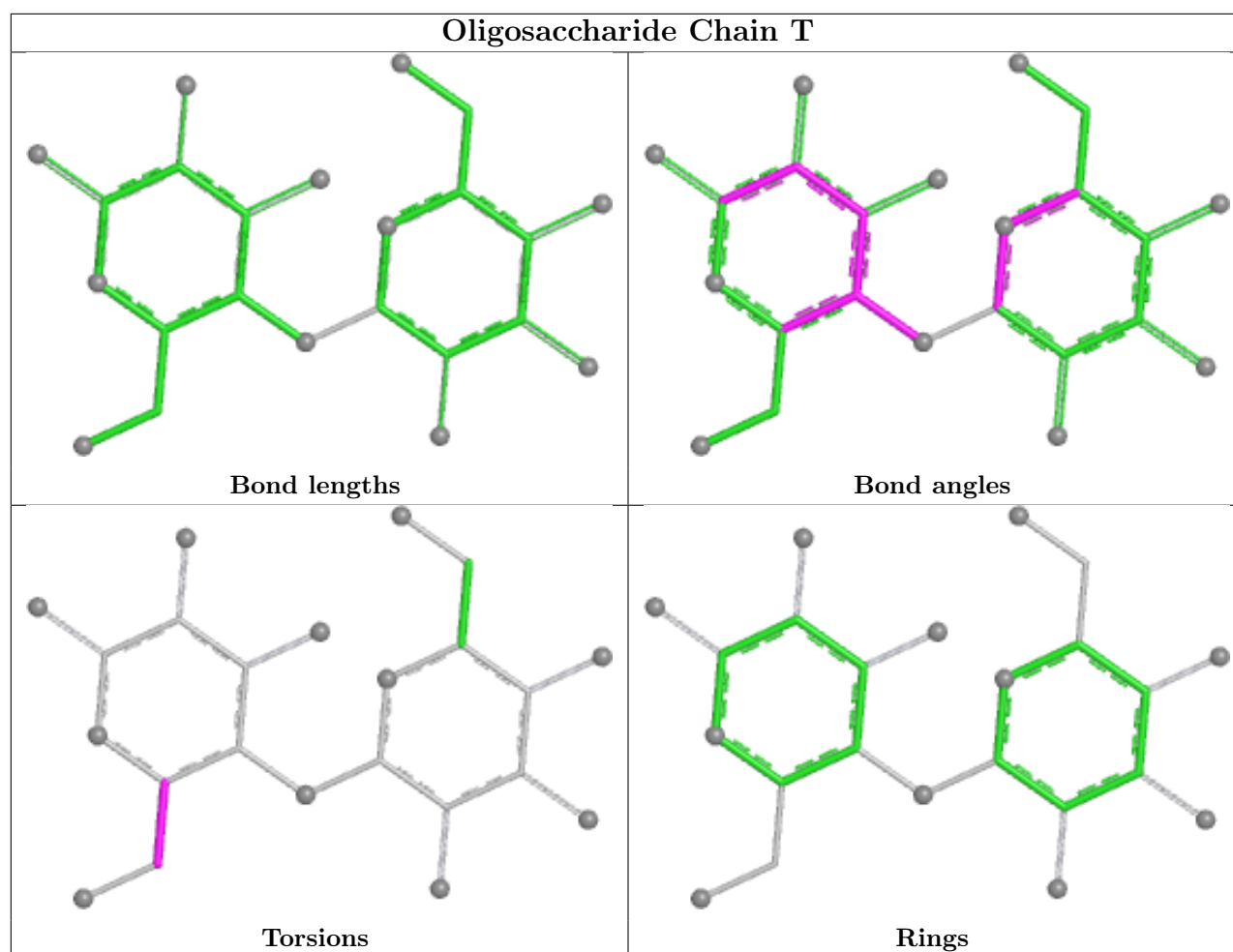












5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1405:GLY	C	1406:PRO	N	3.42

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	553/561 (98%)	-0.10	4 (0%) 84 63	36, 77, 141, 196	0
1	B	554/561 (98%)	-0.18	2 (0%) 88 72	38, 75, 128, 171	0
1	C	554/561 (98%)	0.00	3 (0%) 87 68	39, 82, 130, 181	0
1	D	541/561 (96%)	-0.12	5 (0%) 81 58	40, 79, 144, 200	0
1	E	556/561 (99%)	-0.17	4 (0%) 84 63	36, 76, 125, 175	0
1	F	541/561 (96%)	-0.16	1 (0%) 91 82	47, 86, 129, 193	0
1	G	543/561 (96%)	0.03	2 (0%) 88 72	55, 104, 146, 204	0
1	H	537/561 (95%)	0.07	3 (0%) 85 65	64, 112, 148, 184	0
1	I	535/561 (95%)	0.11	3 (0%) 85 65	68, 118, 161, 205	0
1	J	548/561 (97%)	0.20	11 (2%) 65 39	54, 120, 157, 202	0
All	All	5462/5610 (97%)	-0.03	38 (0%) 84 63	36, 93, 147, 205	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1299	GLY	3.6
1	C	1317	ALA	3.3
1	J	1293	SER	3.1
1	E	1231	LYS	2.9
1	J	1382	TYR	2.8
1	J	1307	ASP	2.7
1	C	173	ALA	2.7
1	J	164	ASP	2.6
1	J	172	ALA	2.6
1	D	1311	LEU	2.5
1	C	174	GLY	2.5
1	I	232	TRP	2.5
1	A	1381	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	225	THR	2.4
1	I	254	PRO	2.4
1	D	1309	PRO	2.3
1	G	173	ALA	2.3
1	A	1302	HIS	2.3
1	J	236	ASP	2.3
1	E	1232	THR	2.3
1	A	1378	PRO	2.3
1	H	1354	THR	2.2
1	J	232	TRP	2.2
1	J	1405	GLY	2.2
1	B	1384	PRO	2.2
1	I	4	GLU	2.2
1	G	236	ASP	2.2
1	D	5	GLY	2.2
1	D	1318	ALA	2.1
1	E	1229	ARG	2.1
1	J	1296	LEU	2.1
1	D	237	THR	2.1
1	E	1234	SER	2.1
1	B	1318	ALA	2.0
1	H	112	ALA	2.0
1	J	1319	GLY	2.0
1	A	1403	ALA	2.0
1	H	1365	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	T	1	12/12	0.92	0.10	93,97,115,116	0
2	GLC	S	1	12/12	0.93	0.09	63,67,76,81	0
2	GLC	R	2	11/12	0.93	0.08	69,78,88,90	0

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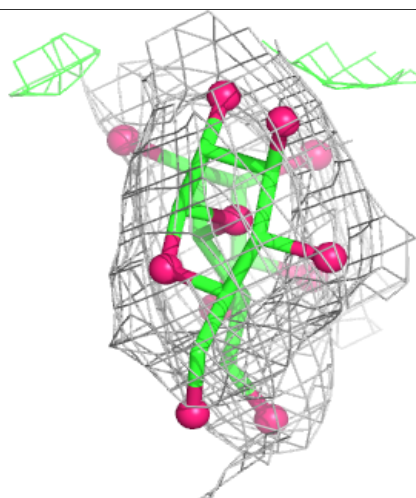
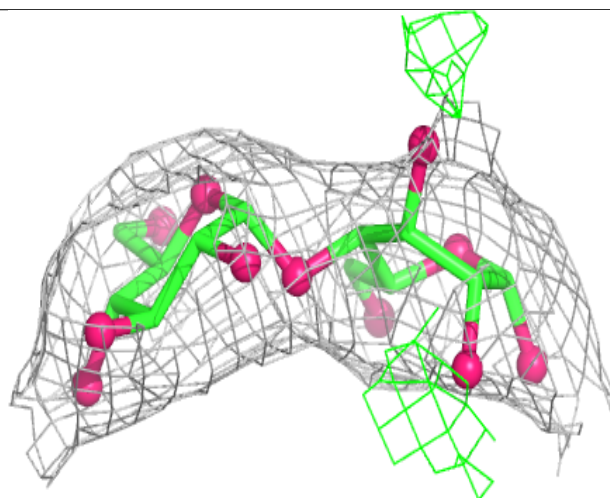
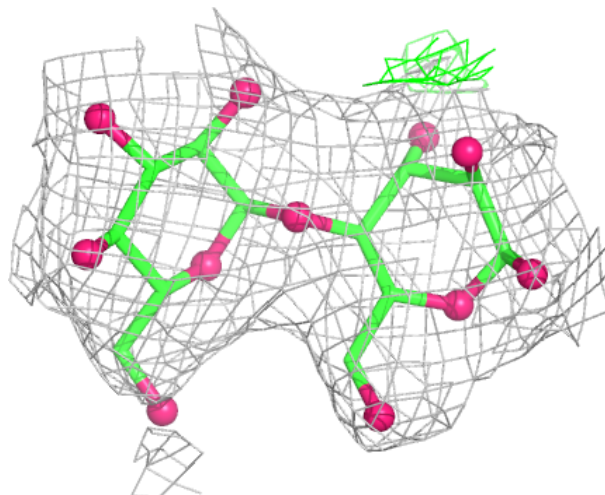
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	Q	1	12/12	0.94	0.08	57,64,72,84	0
2	GLC	S	2	11/12	0.95	0.06	58,67,69,69	0
2	GLC	R	1	12/12	0.95	0.10	76,87,106,114	0
2	GLC	M	2	11/12	0.96	0.08	51,63,77,80	0
2	GLC	K	1	12/12	0.96	0.09	42,46,54,67	0
2	GLC	Q	2	11/12	0.96	0.06	53,59,62,63	0
2	GLC	M	1	12/12	0.96	0.10	62,72,82,88	0
2	GLC	T	2	11/12	0.96	0.06	76,87,94,97	0
2	GLC	L	1	12/12	0.97	0.08	50,56,64,66	0
2	GLC	L	2	11/12	0.97	0.07	46,50,53,56	0
2	GLC	N	1	12/12	0.97	0.07	48,59,70,76	0
2	GLC	P	1	12/12	0.97	0.06	46,53,63,70	0
2	GLC	N	2	11/12	0.98	0.06	39,44,48,48	0
2	GLC	O	1	12/12	0.98	0.07	59,68,72,80	0
2	GLC	O	2	11/12	0.98	0.06	45,47,50,55	0
2	GLC	K	2	11/12	0.98	0.07	41,48,66,72	0
2	GLC	P	2	11/12	0.99	0.04	36,39,42,43	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.

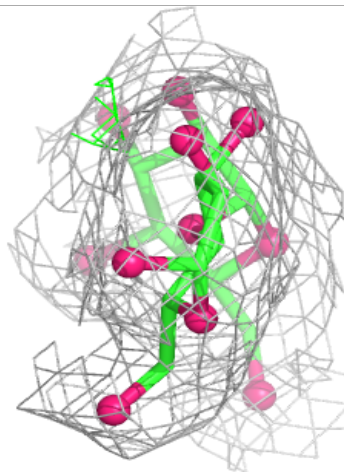
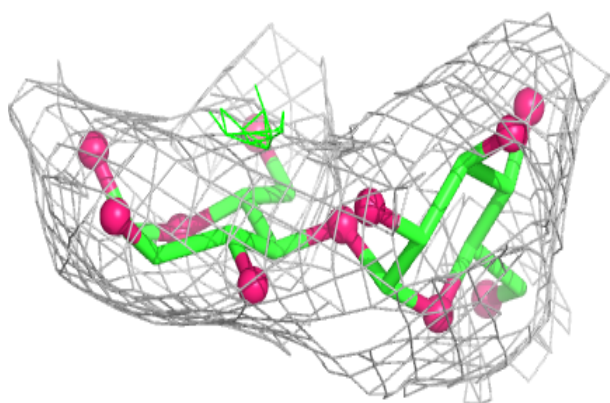
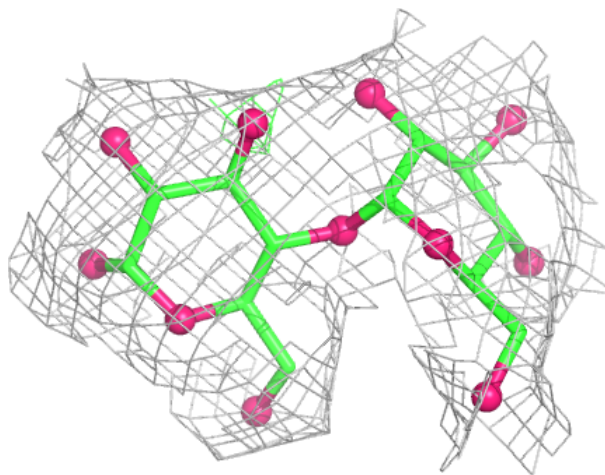
Electron density around Chain K:

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



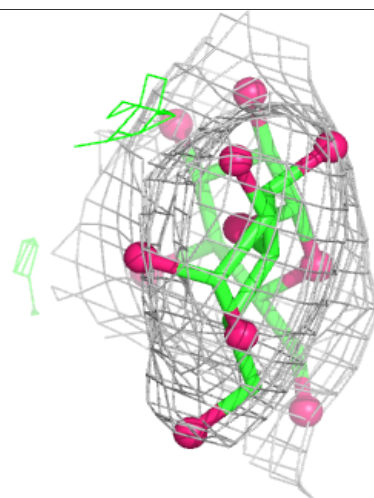
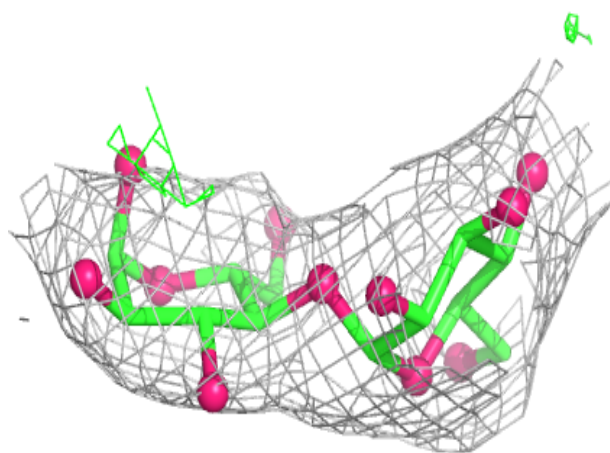
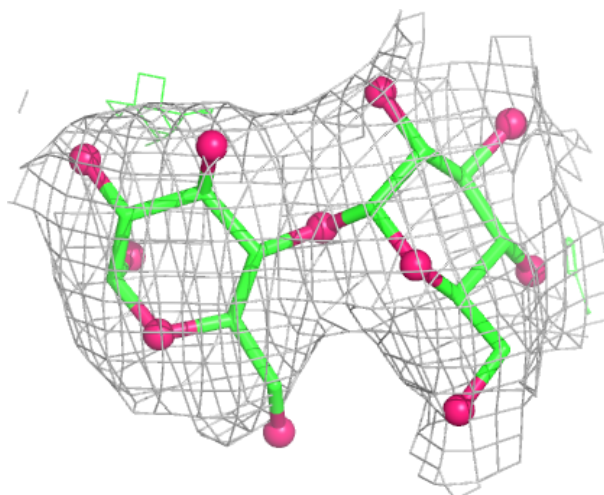
Electron density around Chain L:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



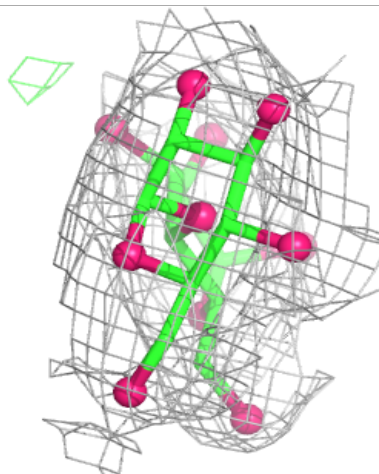
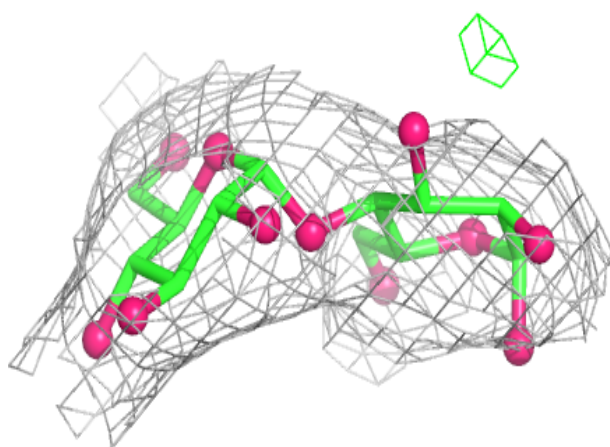
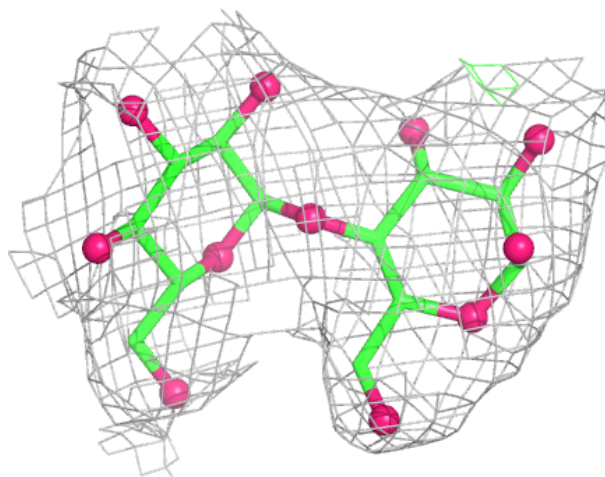
Electron density around Chain M:

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



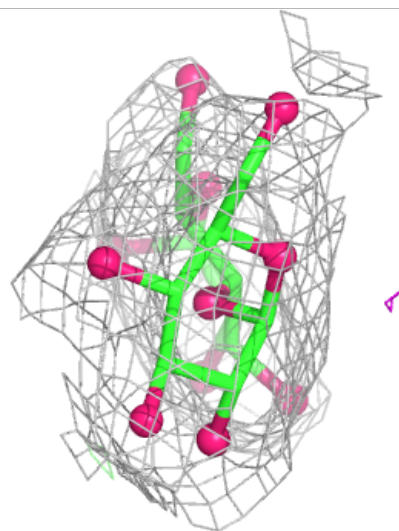
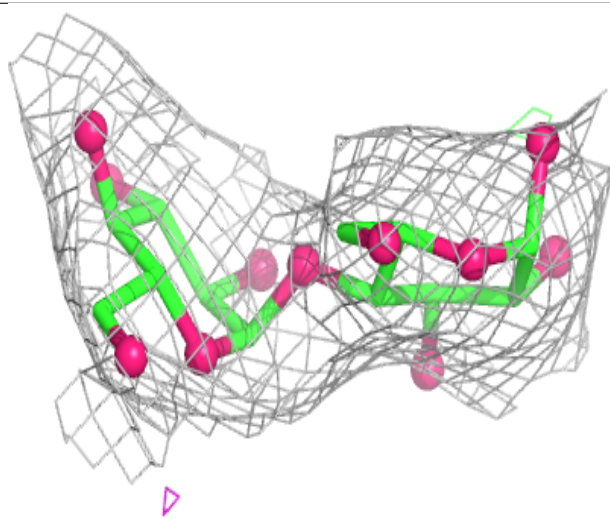
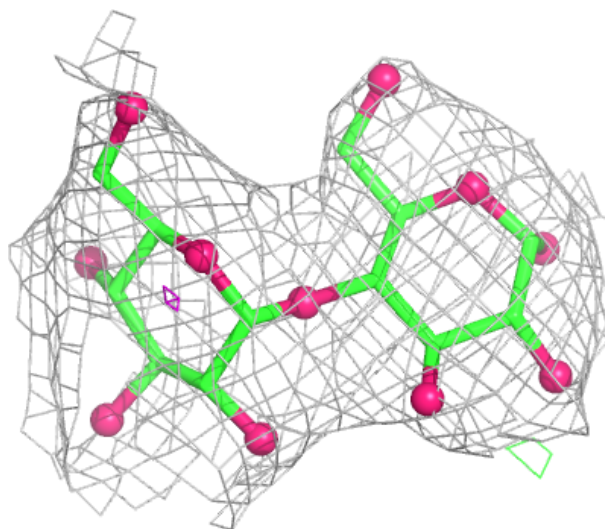
Electron density around Chain N:

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



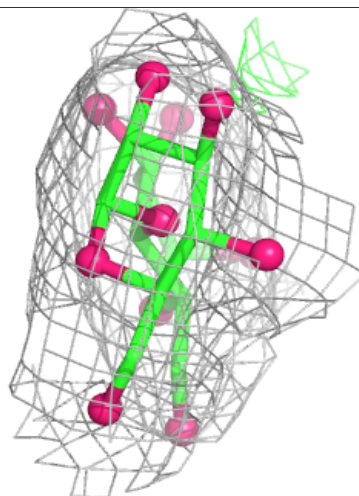
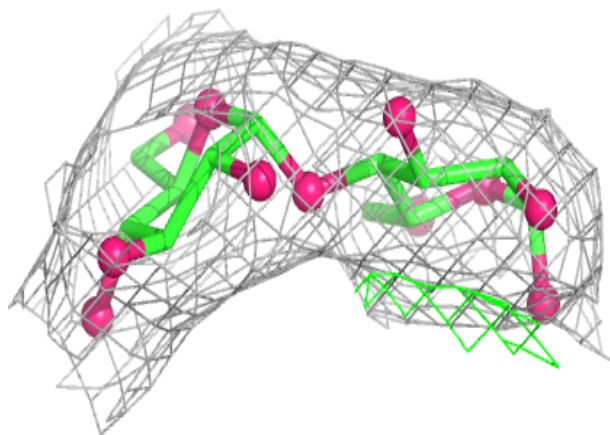
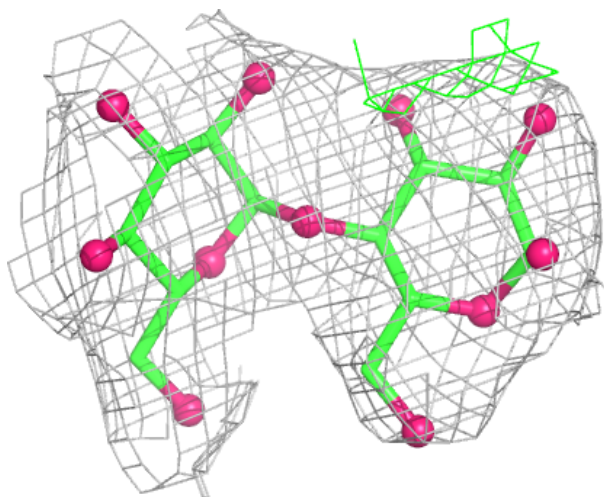
Electron density around Chain O:

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



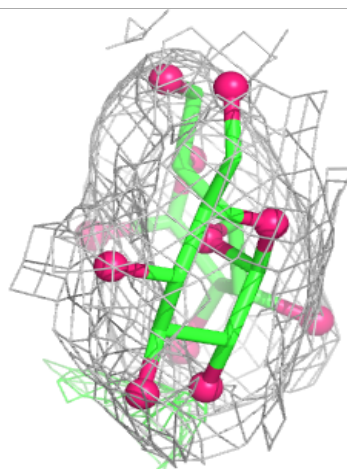
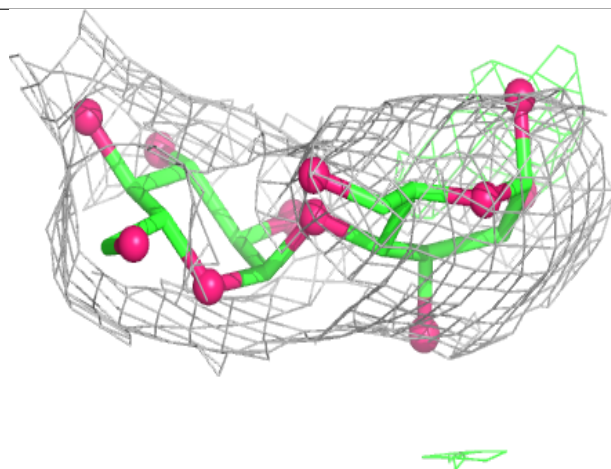
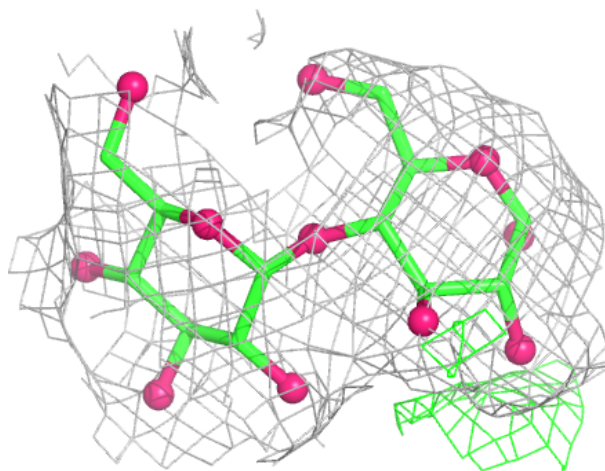
Electron density around Chain P:

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



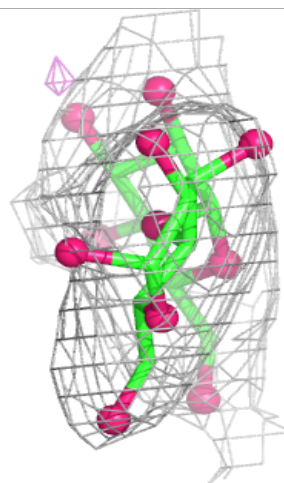
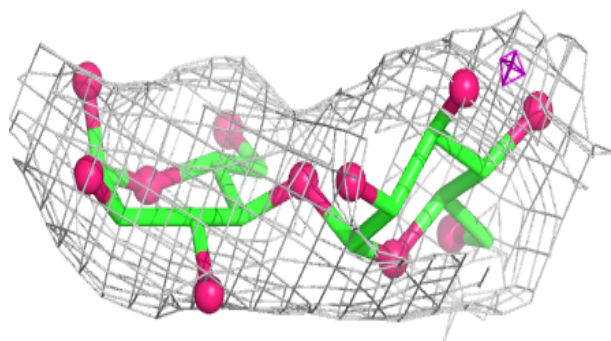
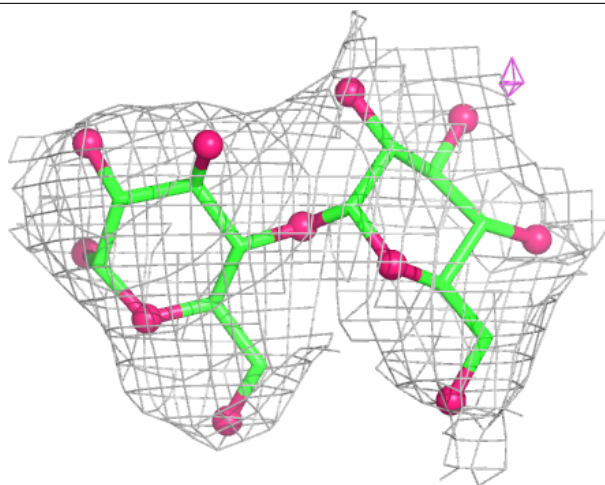
Electron density around Chain Q:

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



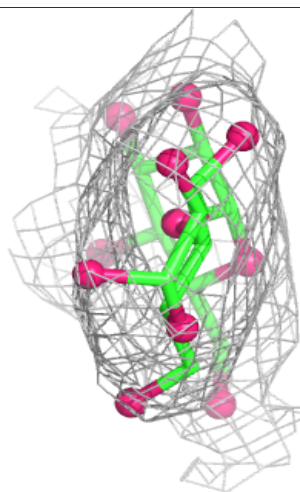
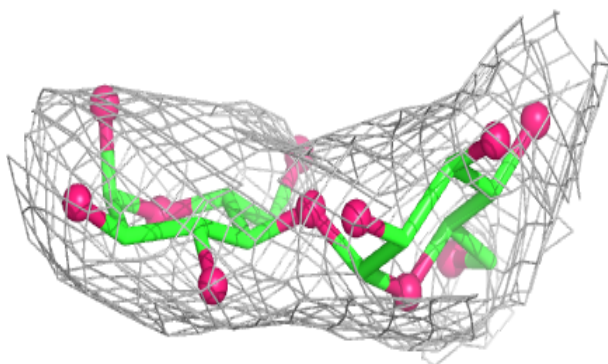
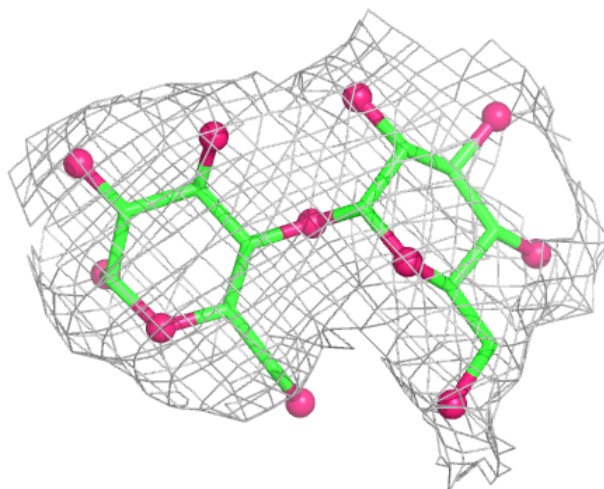
Electron density around Chain R:

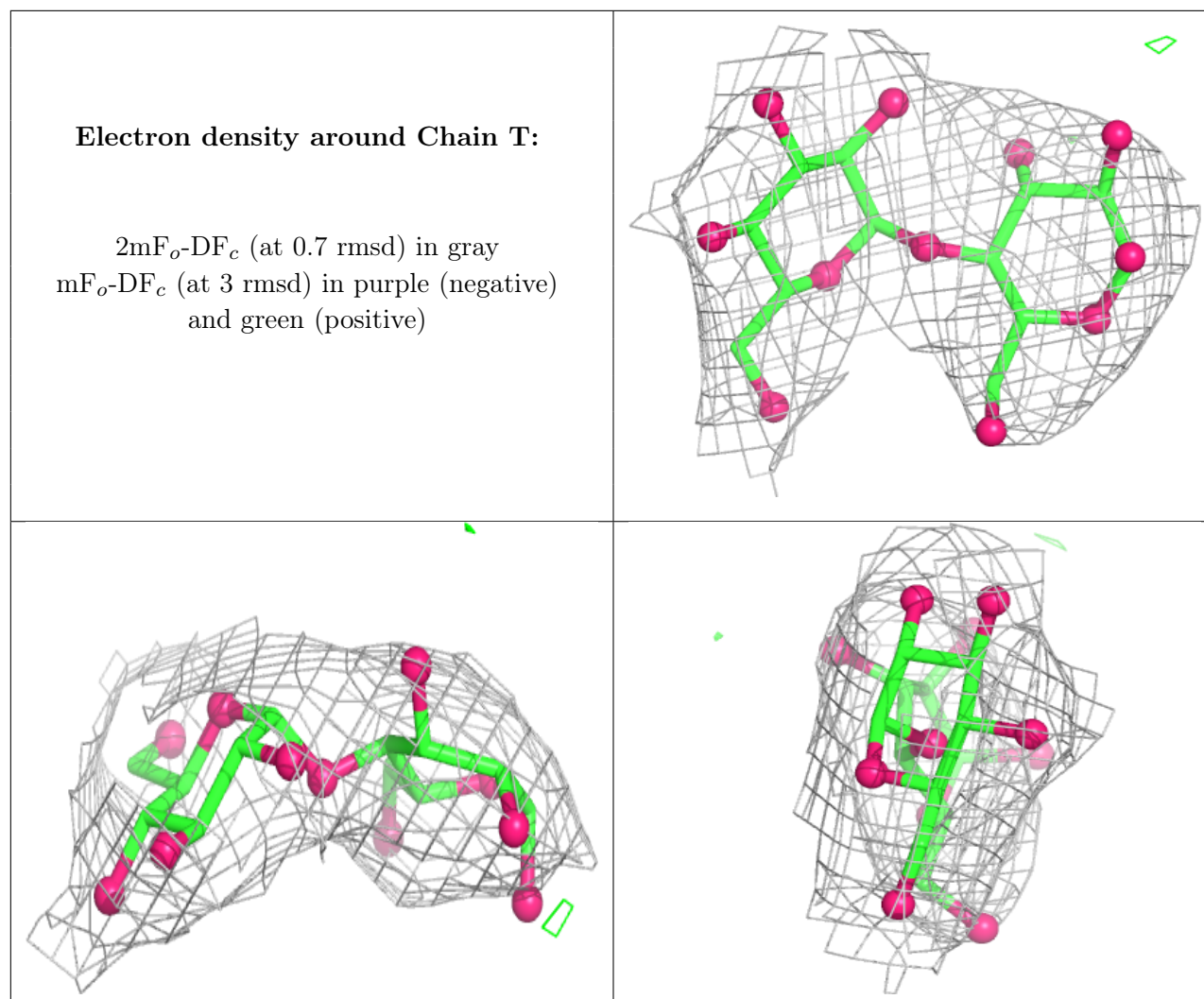
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain S:

$2mF_o-DF_c$ (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	NA	E	1502	1/1	0.97	0.08	59,59,59,59	0
3	NA	B	1502	1/1	0.98	0.04	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.