



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:01 AM UTC

PDB ID : 4U33 / pdb_00004u33
Title : Structure of Mtb GlgE bound to maltose
Authors : Ronning, D.R.; Lindenberger, J.J.
Deposited on : 2014-07-18
Resolution : 3.29 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:

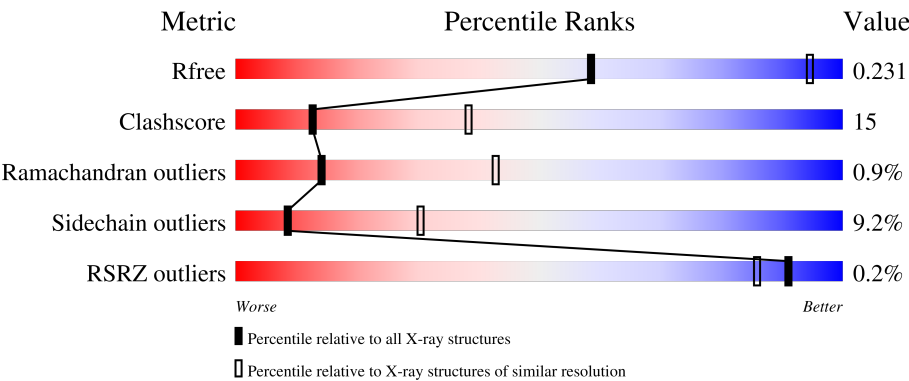
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	723	58%28%5%9%
1	B	723	59%27%6%9%
1	C	723	59%28%. .9%
1	D	723	60%27%. .9%
1	E	723	59%28%5%9%

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Mol	Chain	Length	Quality of chain
1	F	723	63% 24% • 9%
2	G	2	50% 50%
2	H	2	50% 50%
2	I	2	50% 50%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	B	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	C	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	D	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	E	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	F	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P9WQ16
A	-20	GLY	-	expression tag	UNP P9WQ16
A	-19	SER	-	expression tag	UNP P9WQ16
A	-18	SER	-	expression tag	UNP P9WQ16
A	-17	HIS	-	expression tag	UNP P9WQ16
A	-16	HIS	-	expression tag	UNP P9WQ16
A	-15	HIS	-	expression tag	UNP P9WQ16
A	-14	HIS	-	expression tag	UNP P9WQ16
A	-13	HIS	-	expression tag	UNP P9WQ16
A	-12	HIS	-	expression tag	UNP P9WQ16
A	-11	SER	-	expression tag	UNP P9WQ16
A	-10	SER	-	expression tag	UNP P9WQ16
A	-9	GLY	-	expression tag	UNP P9WQ16
A	-8	LEU	-	expression tag	UNP P9WQ16
A	-7	GLU	-	expression tag	UNP P9WQ16
A	-6	VAL	-	expression tag	UNP P9WQ16
A	-5	LEU	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PHE	-	expression tag	UNP P9WQ16
A	-3	GLN	-	expression tag	UNP P9WQ16
A	-2	GLY	-	expression tag	UNP P9WQ16
A	-1	PRO	-	expression tag	UNP P9WQ16
A	0	HIS	-	expression tag	UNP P9WQ16
B	-21	MET	-	expression tag	UNP P9WQ16
B	-20	GLY	-	expression tag	UNP P9WQ16
B	-19	SER	-	expression tag	UNP P9WQ16
B	-18	SER	-	expression tag	UNP P9WQ16
B	-17	HIS	-	expression tag	UNP P9WQ16
B	-16	HIS	-	expression tag	UNP P9WQ16
B	-15	HIS	-	expression tag	UNP P9WQ16
B	-14	HIS	-	expression tag	UNP P9WQ16
B	-13	HIS	-	expression tag	UNP P9WQ16
B	-12	HIS	-	expression tag	UNP P9WQ16
B	-11	SER	-	expression tag	UNP P9WQ16
B	-10	SER	-	expression tag	UNP P9WQ16
B	-9	GLY	-	expression tag	UNP P9WQ16
B	-8	LEU	-	expression tag	UNP P9WQ16
B	-7	GLU	-	expression tag	UNP P9WQ16
B	-6	VAL	-	expression tag	UNP P9WQ16
B	-5	LEU	-	expression tag	UNP P9WQ16
B	-4	PHE	-	expression tag	UNP P9WQ16
B	-3	GLN	-	expression tag	UNP P9WQ16
B	-2	GLY	-	expression tag	UNP P9WQ16
B	-1	PRO	-	expression tag	UNP P9WQ16
B	0	HIS	-	expression tag	UNP P9WQ16
C	-21	MET	-	expression tag	UNP P9WQ16
C	-20	GLY	-	expression tag	UNP P9WQ16
C	-19	SER	-	expression tag	UNP P9WQ16
C	-18	SER	-	expression tag	UNP P9WQ16
C	-17	HIS	-	expression tag	UNP P9WQ16
C	-16	HIS	-	expression tag	UNP P9WQ16
C	-15	HIS	-	expression tag	UNP P9WQ16
C	-14	HIS	-	expression tag	UNP P9WQ16
C	-13	HIS	-	expression tag	UNP P9WQ16
C	-12	HIS	-	expression tag	UNP P9WQ16
C	-11	SER	-	expression tag	UNP P9WQ16
C	-10	SER	-	expression tag	UNP P9WQ16
C	-9	GLY	-	expression tag	UNP P9WQ16
C	-8	LEU	-	expression tag	UNP P9WQ16
C	-7	GLU	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	expression tag	UNP P9WQ16
C	-5	LEU	-	expression tag	UNP P9WQ16
C	-4	PHE	-	expression tag	UNP P9WQ16
C	-3	GLN	-	expression tag	UNP P9WQ16
C	-2	GLY	-	expression tag	UNP P9WQ16
C	-1	PRO	-	expression tag	UNP P9WQ16
C	0	HIS	-	expression tag	UNP P9WQ16
D	-21	MET	-	expression tag	UNP P9WQ16
D	-20	GLY	-	expression tag	UNP P9WQ16
D	-19	SER	-	expression tag	UNP P9WQ16
D	-18	SER	-	expression tag	UNP P9WQ16
D	-17	HIS	-	expression tag	UNP P9WQ16
D	-16	HIS	-	expression tag	UNP P9WQ16
D	-15	HIS	-	expression tag	UNP P9WQ16
D	-14	HIS	-	expression tag	UNP P9WQ16
D	-13	HIS	-	expression tag	UNP P9WQ16
D	-12	HIS	-	expression tag	UNP P9WQ16
D	-11	SER	-	expression tag	UNP P9WQ16
D	-10	SER	-	expression tag	UNP P9WQ16
D	-9	GLY	-	expression tag	UNP P9WQ16
D	-8	LEU	-	expression tag	UNP P9WQ16
D	-7	GLU	-	expression tag	UNP P9WQ16
D	-6	VAL	-	expression tag	UNP P9WQ16
D	-5	LEU	-	expression tag	UNP P9WQ16
D	-4	PHE	-	expression tag	UNP P9WQ16
D	-3	GLN	-	expression tag	UNP P9WQ16
D	-2	GLY	-	expression tag	UNP P9WQ16
D	-1	PRO	-	expression tag	UNP P9WQ16
D	0	HIS	-	expression tag	UNP P9WQ16
E	-21	MET	-	expression tag	UNP P9WQ16
E	-20	GLY	-	expression tag	UNP P9WQ16
E	-19	SER	-	expression tag	UNP P9WQ16
E	-18	SER	-	expression tag	UNP P9WQ16
E	-17	HIS	-	expression tag	UNP P9WQ16
E	-16	HIS	-	expression tag	UNP P9WQ16
E	-15	HIS	-	expression tag	UNP P9WQ16
E	-14	HIS	-	expression tag	UNP P9WQ16
E	-13	HIS	-	expression tag	UNP P9WQ16
E	-12	HIS	-	expression tag	UNP P9WQ16
E	-11	SER	-	expression tag	UNP P9WQ16
E	-10	SER	-	expression tag	UNP P9WQ16
E	-9	GLY	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	LEU	-	expression tag	UNP P9WQ16
E	-7	GLU	-	expression tag	UNP P9WQ16
E	-6	VAL	-	expression tag	UNP P9WQ16
E	-5	LEU	-	expression tag	UNP P9WQ16
E	-4	PHE	-	expression tag	UNP P9WQ16
E	-3	GLN	-	expression tag	UNP P9WQ16
E	-2	GLY	-	expression tag	UNP P9WQ16
E	-1	PRO	-	expression tag	UNP P9WQ16
E	0	HIS	-	expression tag	UNP P9WQ16
F	-21	MET	-	expression tag	UNP P9WQ16
F	-20	GLY	-	expression tag	UNP P9WQ16
F	-19	SER	-	expression tag	UNP P9WQ16
F	-18	SER	-	expression tag	UNP P9WQ16
F	-17	HIS	-	expression tag	UNP P9WQ16
F	-16	HIS	-	expression tag	UNP P9WQ16
F	-15	HIS	-	expression tag	UNP P9WQ16
F	-14	HIS	-	expression tag	UNP P9WQ16
F	-13	HIS	-	expression tag	UNP P9WQ16
F	-12	HIS	-	expression tag	UNP P9WQ16
F	-11	SER	-	expression tag	UNP P9WQ16
F	-10	SER	-	expression tag	UNP P9WQ16
F	-9	GLY	-	expression tag	UNP P9WQ16
F	-8	LEU	-	expression tag	UNP P9WQ16
F	-7	GLU	-	expression tag	UNP P9WQ16
F	-6	VAL	-	expression tag	UNP P9WQ16
F	-5	LEU	-	expression tag	UNP P9WQ16
F	-4	PHE	-	expression tag	UNP P9WQ16
F	-3	GLN	-	expression tag	UNP P9WQ16
F	-2	GLY	-	expression tag	UNP P9WQ16
F	-1	PRO	-	expression tag	UNP P9WQ16
F	0	HIS	-	expression tag	UNP P9WQ16

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



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

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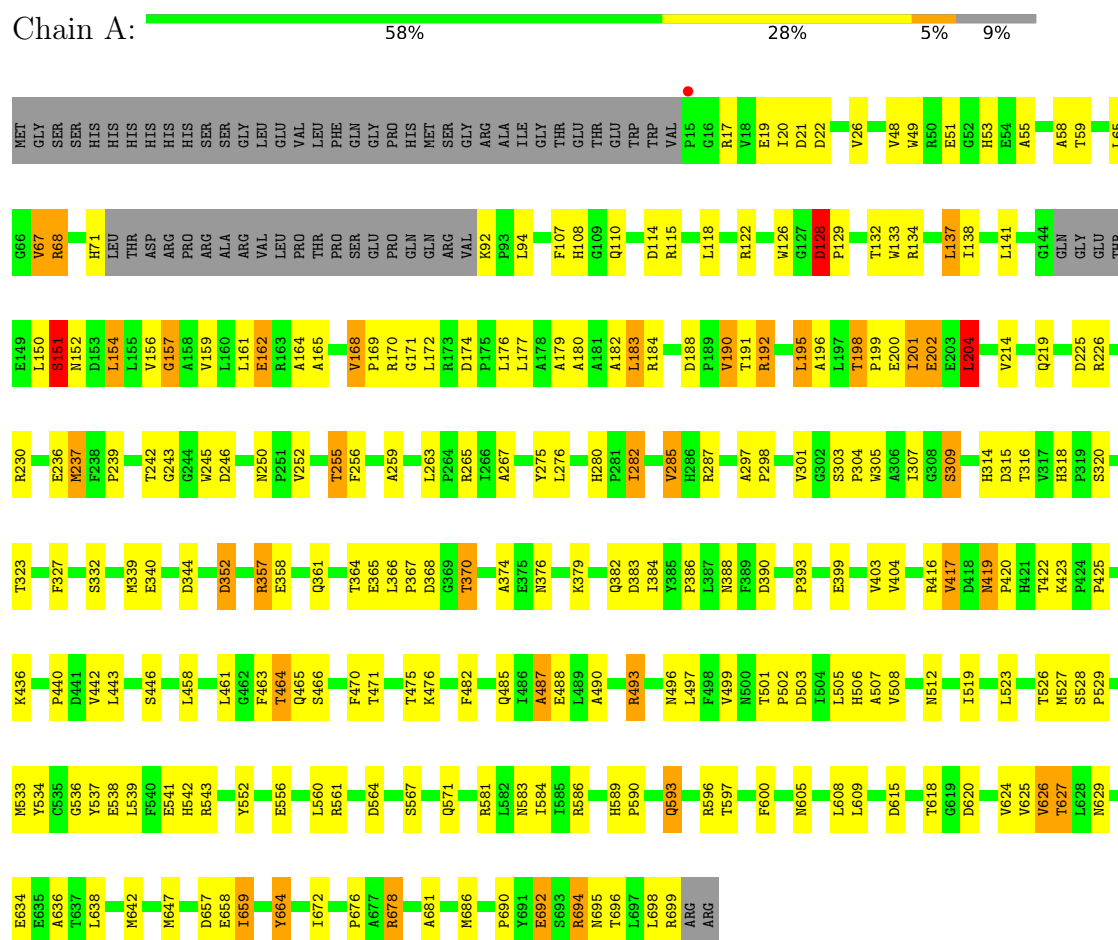
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	2	Total 23	C 12	O 11	0	0	0
2	I	2	Total 23	C 12	O 11	0	0	0
2	J	2	Total 23	C 12	O 11	0	0	0
2	K	2	Total 23	C 12	O 11	0	0	0
2	L	2	Total 23	C 12	O 11	0	0	0

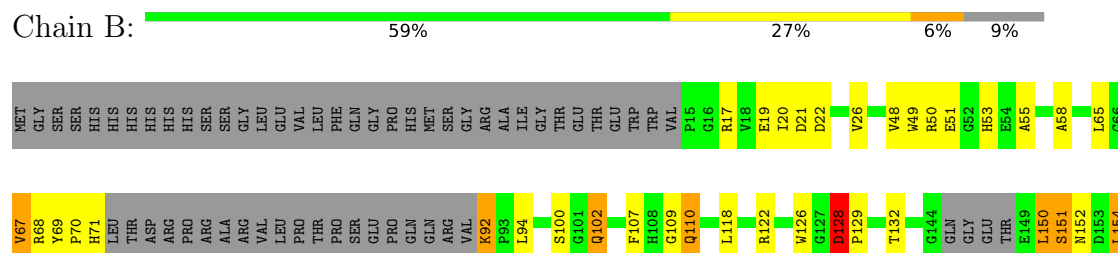
3 Residue-property plots

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: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

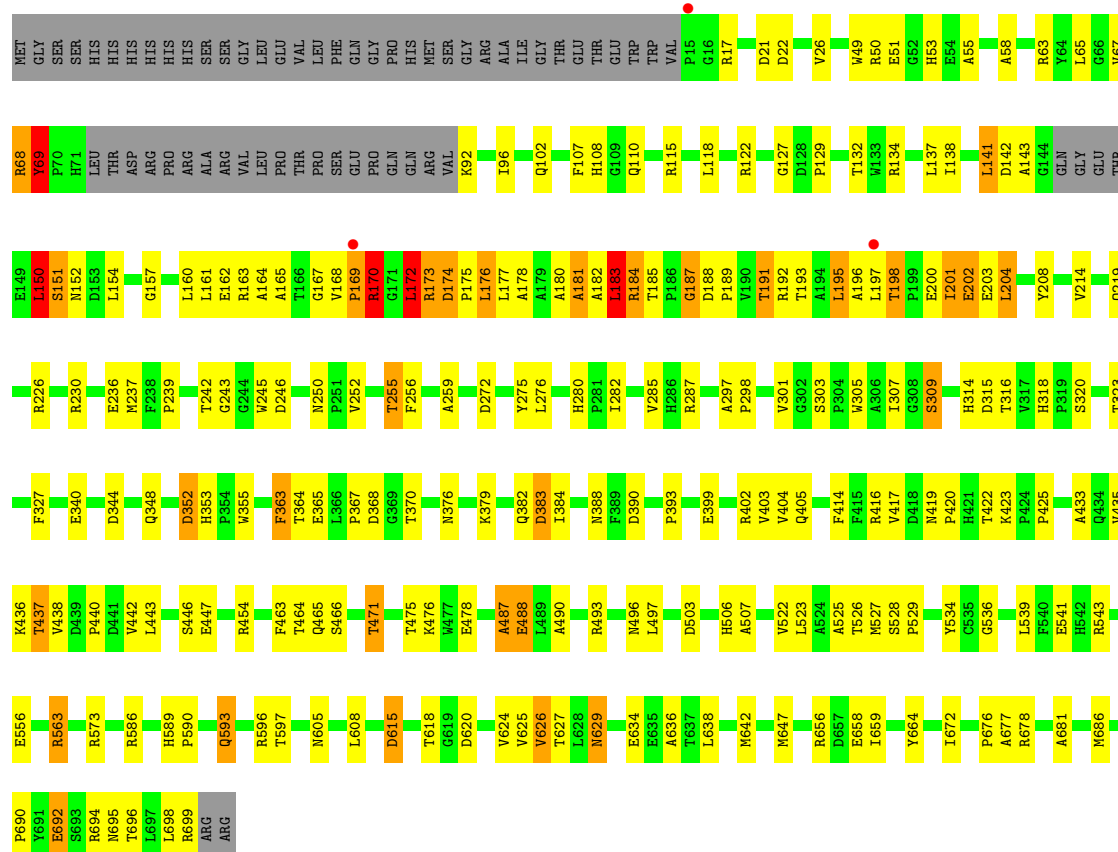


- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



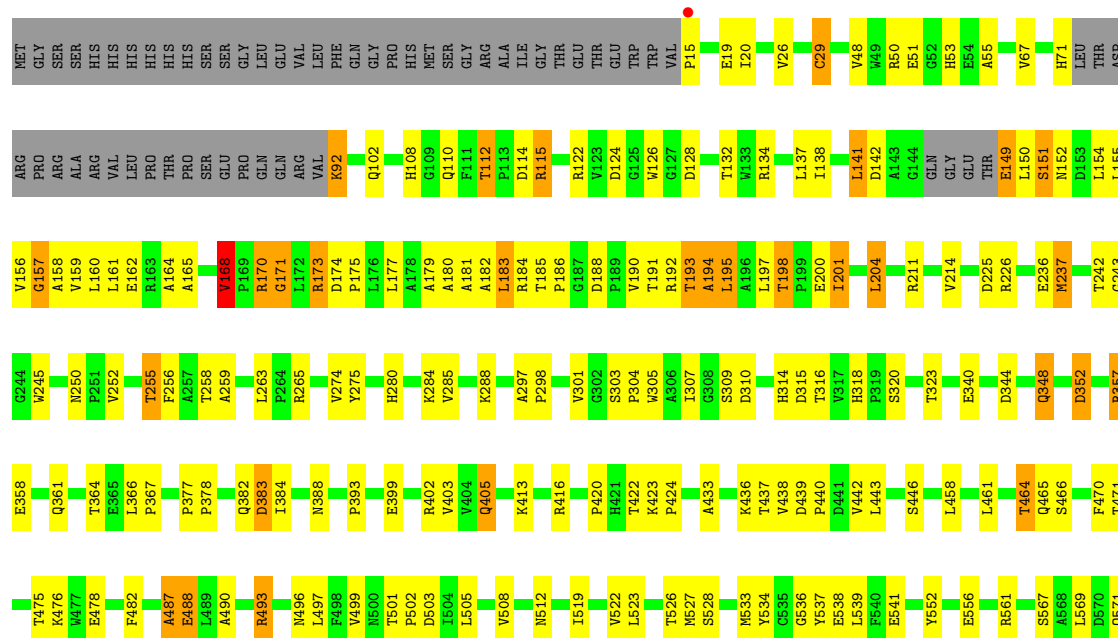


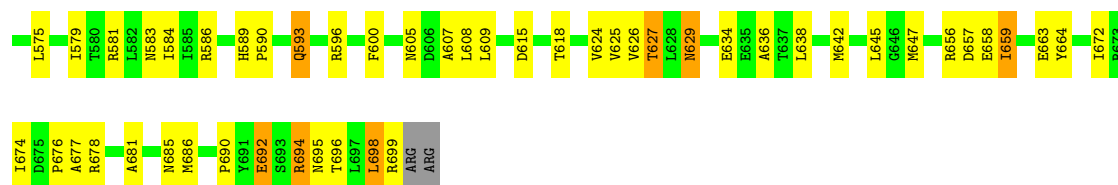
Chain D:  60% 27% 9%



• Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

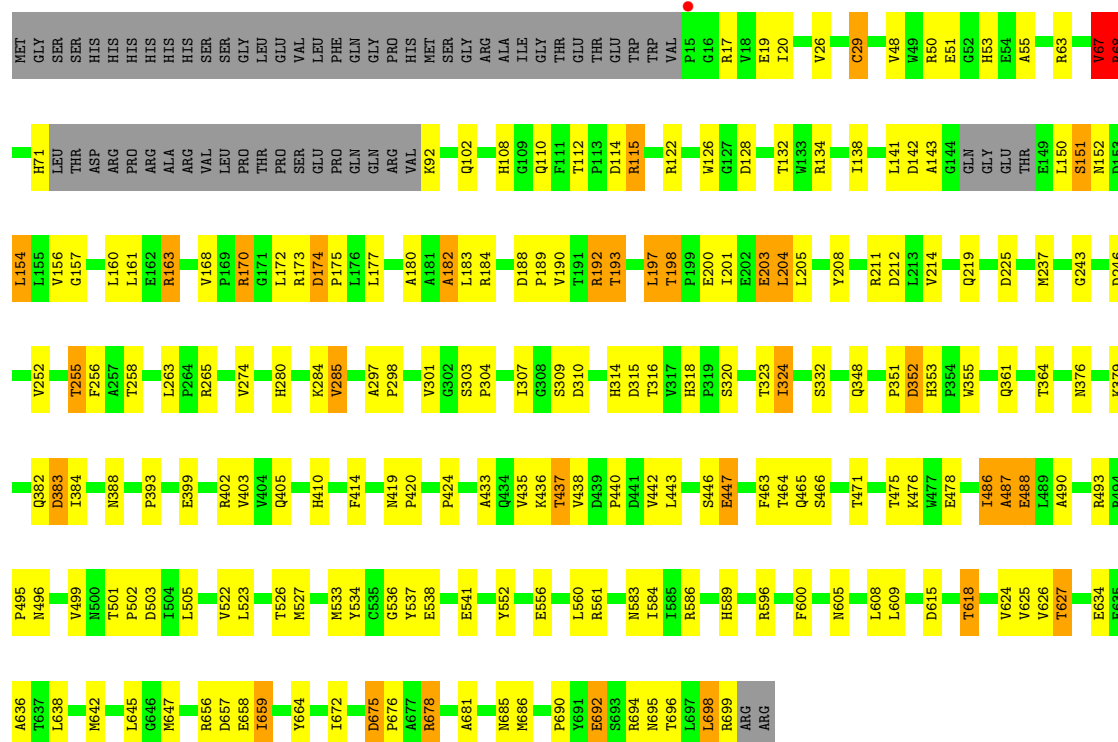
Chain E:  59% 28% 5% 9%





- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

Chain F: 63% 24% 9%



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

Chain G: 50% 50%



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

Chain H: 50% 50%



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

Chain I: 50% 50%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	343.23Å 242.60Å 243.67Å 90.00° 135.15° 90.00°	Depositor
Resolution (Å)	47.64 – 3.29 47.64 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.64-3.29) 90.4 (47.64-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.194 , 0.222 0.208 , 0.231	Depositor DCC
R_{free} test set	10542 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h-2*k,l,h+1 0.013 for -h-k-l,l,k 0.013 for -h+k-l,-l,-k 0.014 for -k+l,-h-l,-l 0.014 for k+l,h+l,-l 0.398 for k-l,h+l,-k 0.397 for h+k+l,-l,-h-l 0.397 for -k-l,-h-l,k 0.397 for h-k+l,l,-h-l 0.013 for h,-k,-h-l 0.457 for h+2*k,l,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31596	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: 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	1.02	4/5407 (0.1%)	0.99	16/7395 (0.2%)
1	B	1.02	2/5407 (0.0%)	1.00	22/7395 (0.3%)
1	C	1.01	2/5407 (0.0%)	0.99	26/7395 (0.4%)
1	D	1.02	4/5407 (0.1%)	1.01	26/7395 (0.4%)
1	E	1.00	1/5407 (0.0%)	1.00	21/7395 (0.3%)
1	F	1.02	3/5407 (0.1%)	0.96	17/7395 (0.2%)
All	All	1.01	16/32442 (0.0%)	0.99	128/44370 (0.3%)

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	C	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	487	ALA	CA-C	-6.79	1.44	1.52
1	F	487	ALA	CA-CB	-6.75	1.42	1.53
1	D	487	ALA	CA-C	-6.60	1.44	1.52
1	D	487	ALA	CA-CB	-6.46	1.43	1.53
1	A	487	ALA	CA-C	-6.42	1.45	1.52
1	F	487	ALA	CA-C	-6.34	1.45	1.52
1	B	487	ALA	CA-CB	-6.32	1.42	1.53
1	A	487	ALA	CA-CB	-6.21	1.42	1.53
1	D	96	ILE	CA-CB	-5.71	1.49	1.54
1	D	419	ASN	C-O	-5.57	1.21	1.23
1	C	419	ASN	C-O	-5.30	1.21	1.23
1	F	419	ASN	C-O	-5.23	1.21	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	487	ALA	CA-CB	-5.17	1.46	1.53
1	A	417	VAL	CA-CB	-5.11	1.49	1.54
1	A	419	ASN	C-O	-5.10	1.21	1.23
1	E	487	ALA	CA-CB	-5.09	1.46	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	ARG	N-CA-C	-11.14	99.22	111.36
1	A	184	ARG	N-CA-C	-9.66	100.75	111.28
1	C	196	ALA	N-CA-C	-9.19	100.46	112.68
1	B	92	LYS	CA-C-N	-8.68	111.20	120.66
1	B	92	LYS	C-N-CA	-8.68	111.20	120.66
1	D	202	GLU	N-CA-C	-8.54	101.91	111.14
1	B	184	ARG	N-CA-C	8.32	121.55	111.40
1	C	112	THR	CA-C-N	8.16	128.17	119.76
1	C	112	THR	C-N-CA	8.16	128.17	119.76
1	D	692	GLU	N-CA-C	-7.87	101.59	112.30
1	D	487	ALA	CA-C-N	7.61	135.40	121.70
1	D	487	ALA	C-N-CA	7.61	135.40	121.70
1	F	487	ALA	CA-C-N	7.59	135.36	121.70
1	F	487	ALA	C-N-CA	7.59	135.36	121.70
1	D	172	LEU	N-CA-C	-7.45	103.92	113.16
1	C	173	ARG	N-CA-C	-7.38	102.62	111.69
1	B	172	LEU	N-CA-C	-7.32	104.09	113.16
1	E	112	THR	CA-C-N	7.18	126.94	119.76
1	E	112	THR	C-N-CA	7.18	126.94	119.76
1	E	160	LEU	N-CA-C	7.17	120.49	111.24
1	A	692	GLU	N-CA-C	-7.16	102.56	112.30
1	C	692	GLU	N-CA-C	-7.06	102.70	112.30
1	A	263	LEU	CA-C-N	-7.04	111.65	118.97
1	A	263	LEU	C-N-CA	-7.04	111.65	118.97
1	F	174	ASP	CA-C-N	-7.02	112.47	119.56
1	F	174	ASP	C-N-CA	-7.02	112.47	119.56
1	D	69	TYR	CA-C-N	7.00	128.59	119.84
1	D	69	TYR	C-N-CA	7.00	128.59	119.84
1	B	487	ALA	CA-C-N	6.97	134.25	121.70
1	B	487	ALA	C-N-CA	6.97	134.25	121.70
1	C	169	PRO	N-CA-C	6.86	121.45	110.21
1	F	692	GLU	N-CA-C	-6.85	102.11	111.56
1	F	182	ALA	N-CA-C	-6.83	104.56	113.17
1	E	157	GLY	N-CA-C	-6.78	104.64	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	487	ALA	CA-C-N	6.70	133.76	121.70
1	A	487	ALA	C-N-CA	6.70	133.76	121.70
1	A	202	GLU	N-CA-C	-6.59	103.58	111.69
1	F	596	ARG	N-CA-C	6.53	118.47	111.36
1	C	182	ALA	N-CA-C	-6.49	104.93	112.92
1	E	92	LYS	CA-C-N	-6.49	111.72	119.84
1	E	92	LYS	C-N-CA	-6.49	111.72	119.84
1	C	168	VAL	N-CA-C	6.49	115.71	108.05
1	E	263	LEU	CA-C-N	-6.44	112.27	118.97
1	E	263	LEU	C-N-CA	-6.44	112.27	118.97
1	D	150	LEU	N-CA-C	-6.44	105.39	113.18
1	C	194	ALA	N-CA-C	6.42	120.23	111.17
1	B	128	ASP	CB-CA-C	6.35	116.15	110.44
1	B	67	VAL	N-CA-C	-6.21	106.94	112.90
1	B	263	LEU	CA-C-N	-6.19	112.53	118.97
1	B	263	LEU	C-N-CA	-6.19	112.53	118.97
1	A	92	LYS	CA-C-N	-6.17	112.13	119.84
1	A	92	LYS	C-N-CA	-6.17	112.13	119.84
1	D	187	GLY	N-CA-C	6.16	118.46	110.45
1	A	128	ASP	CB-CA-C	6.14	115.97	110.44
1	F	424	PRO	CA-C-N	6.14	125.35	118.97
1	F	424	PRO	C-N-CA	6.14	125.35	118.97
1	B	596	ARG	N-CA-C	6.13	118.93	111.82
1	C	150	LEU	N-CA-C	-6.11	105.79	113.18
1	B	69	TYR	CA-C-N	6.09	127.45	119.84
1	B	69	TYR	C-N-CA	6.09	127.45	119.84
1	A	157	GLY	N-CA-C	-6.08	105.44	112.50
1	A	596	ARG	N-CA-C	6.04	117.94	111.36
1	D	169	PRO	N-CA-C	6.01	120.07	110.21
1	C	263	LEU	CA-C-N	-5.99	112.74	118.97
1	C	263	LEU	C-N-CA	-5.99	112.74	118.97
1	C	184	ARG	N-CA-C	5.97	118.68	111.40
1	D	181	ALA	N-CA-C	-5.93	103.42	111.55
1	E	184	ARG	N-CA-C	5.86	118.55	111.40
1	E	692	GLU	N-CA-C	-5.84	104.35	112.30
1	C	174	ASP	C-N-CD	-5.84	107.76	120.60
1	E	596	ARG	N-CA-C	5.83	118.58	111.82
1	D	487	ALA	CA-C-O	-5.82	114.07	120.24
1	E	174	ASP	CA-C-N	-5.74	113.71	119.56
1	E	174	ASP	C-N-CA	-5.74	113.71	119.56
1	B	692	GLU	N-CA-C	-5.72	103.67	111.56
1	D	596	ARG	N-CA-C	5.68	118.40	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	LEU	N-CA-C	-5.66	106.42	113.38
1	A	384	ILE	N-CA-C	5.60	118.19	108.90
1	C	350	ALA	N-CA-C	-5.59	102.87	110.36
1	A	204	LEU	CA-CB-CG	5.55	135.71	116.30
1	E	168	VAL	CA-C-N	5.54	127.05	120.23
1	E	168	VAL	C-N-CA	5.54	127.05	120.23
1	C	597	THR	N-CA-C	5.54	119.67	113.02
1	E	384	ILE	N-CA-C	5.51	118.06	108.90
1	B	384	ILE	N-CA-C	5.50	118.03	108.90
1	C	615	ASP	CA-C-N	5.47	125.30	119.28
1	C	615	ASP	C-N-CA	5.47	125.30	119.28
1	D	615	ASP	CA-C-N	5.46	125.29	119.28
1	D	615	ASP	C-N-CA	5.46	125.29	119.28
1	F	263	LEU	CA-C-N	-5.46	113.30	118.97
1	F	263	LEU	C-N-CA	-5.46	113.30	118.97
1	E	424	PRO	CA-C-N	5.44	124.63	118.97
1	E	424	PRO	C-N-CA	5.44	124.63	118.97
1	A	597	THR	N-CA-C	5.44	119.55	113.02
1	E	181	ALA	N-CA-C	-5.41	106.26	112.92
1	D	597	THR	N-CA-C	5.40	119.50	113.02
1	C	181	ALA	N-CA-C	-5.39	106.29	112.92
1	D	68	ARG	CB-CA-C	-5.38	110.35	116.54
1	C	174	ASP	CA-C-N	5.36	139.86	127.00
1	C	174	ASP	C-N-CA	5.36	139.86	127.00
1	D	92	LYS	CA-C-N	-5.32	113.19	119.84
1	D	92	LYS	C-N-CA	-5.32	113.19	119.84
1	B	177	LEU	CA-CB-CG	5.30	134.84	116.30
1	C	168	VAL	CA-C-N	5.30	128.25	120.46
1	C	168	VAL	C-N-CA	5.30	128.25	120.46
1	B	150	LEU	N-CA-C	-5.26	106.12	112.54
1	F	67	VAL	N-CA-C	-5.25	98.42	109.34
1	C	424	PRO	CA-C-N	5.25	124.43	118.97
1	C	424	PRO	C-N-CA	5.25	124.43	118.97
1	B	181	ALA	N-CA-C	-5.23	106.14	112.88
1	D	203	GLU	N-CA-C	5.20	116.95	111.28
1	C	384	ILE	N-CA-C	5.20	117.53	108.90
1	F	112	THR	CA-C-N	5.14	125.30	119.90
1	F	112	THR	C-N-CA	5.14	125.30	119.90
1	F	487	ALA	CA-C-O	-5.12	113.95	120.20
1	F	384	ILE	N-CA-C	5.11	117.38	108.90
1	D	193	THR	N-CA-C	-5.09	106.33	112.54
1	F	488	GLU	N-CA-C	5.09	125.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	15	PRO	CA-C-N	5.08	130.84	121.70
1	E	15	PRO	C-N-CA	5.08	130.84	121.70
1	D	488	GLU	N-CA-C	5.07	125.21	111.00
1	B	631	PHE	N-CA-C	5.06	119.45	113.12
1	D	384	ILE	N-CA-C	5.05	117.28	108.90
1	B	248	ASP	N-CA-C	-5.04	103.03	110.48
1	B	488	GLU	N-CA-C	5.04	125.10	111.00
1	B	175	PRO	N-CA-C	-5.03	107.49	113.98
1	D	174	ASP	CA-C-N	-5.02	114.44	119.56
1	D	174	ASP	C-N-CA	-5.02	114.44	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	194	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5243	0	5051	170	0
1	B	5243	0	5051	168	0
1	C	5243	0	5051	161	0
1	D	5243	0	5051	168	0
1	E	5243	0	5052	159	1
1	F	5243	0	5052	141	1
2	G	23	0	21	1	0
2	H	23	0	21	1	0
2	I	23	0	21	1	0
2	J	23	0	21	1	0
2	K	23	0	21	2	0
2	L	23	0	21	2	0
All	All	31596	0	30434	945	2

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 15.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:TYR:OH	1:D:416:ARG:NH1	1.98	0.96
1:E:275:TYR:OH	1:E:416:ARG:NH1	2.01	0.94
1:B:275:TYR:OH	1:B:416:ARG:NH1	2.03	0.91
1:C:275:TYR:OH	1:C:416:ARG:NH1	2.02	0.91
1:E:188:ASP:HB2	1:E:191:THR:HG23	1.55	0.89
1:D:589:HIS:NE2	1:D:658:GLU:OE2	2.08	0.87
1:C:589:HIS:NE2	1:C:658:GLU:OE2	2.09	0.86
1:B:589:HIS:NE2	1:B:658:GLU:OE2	2.08	0.85
1:D:184:ARG:H	1:D:192:ARG:HH11	1.22	0.85
1:B:195:LEU:HD22	1:B:201:ILE:HG23	1.59	0.84
1:F:589:HIS:NE2	1:F:658:GLU:OE2	2.08	0.84
1:E:110:GLN:HG2	1:E:694:ARG:HE	1.43	0.84
1:E:493:ARG:HG2	1:E:493:ARG:HH11	1.44	0.83
1:A:352:ASP:OD1	1:A:352:ASP:N	2.12	0.82
1:B:226:ARG:NH1	1:B:340:GLU:OE2	2.13	0.81
1:D:226:ARG:NH1	1:D:340:GLU:OE2	2.13	0.81
1:E:352:ASP:OD1	1:E:352:ASP:N	2.14	0.81
1:A:226:ARG:NH1	1:A:340:GLU:OE2	2.14	0.80
1:B:487:ALA:HB2	1:B:490:ALA:HB2	1.63	0.80
1:A:150:LEU:O	1:A:152:ASN:N	2.14	0.80
1:C:267:ALA:HB2	1:C:339:MET:HE2	1.64	0.80
1:A:267:ALA:HB2	1:A:339:MET:HE2	1.63	0.79
1:A:589:HIS:NE2	1:A:658:GLU:OE2	2.12	0.79
1:B:176:LEU:O	1:B:180:ALA:N	2.14	0.79
1:B:177:LEU:HA	1:B:180:ALA:HB3	1.64	0.79
1:F:352:ASP:OD1	1:F:352:ASP:N	2.15	0.79
1:B:656:ARG:NH1	1:B:658:GLU:OE1	2.16	0.78
1:F:656:ARG:NH1	1:F:658:GLU:OE1	2.16	0.78
1:B:55:ALA:H	1:B:132:THR:HG22	1.49	0.78
1:E:656:ARG:NH1	1:E:658:GLU:OE1	2.17	0.78
1:D:174:ASP:HA	1:D:177:LEU:HD13	1.65	0.78
1:F:675:ASP:HB3	1:F:678:ARG:HB2	1.65	0.78
1:E:154:LEU:HD12	1:E:154:LEU:H	1.49	0.78
1:F:695:ASN:HA	1:F:698:LEU:HD13	1.66	0.77
1:D:352:ASP:OD1	1:D:352:ASP:N	2.15	0.77
1:A:55:ALA:H	1:A:132:THR:HG22	1.49	0.77
1:E:149:GLU:OE1	1:E:149:GLU:N	2.18	0.77
1:E:150:LEU:HD12	1:E:154:LEU:HD11	1.66	0.77
1:E:465:GLN:OE1	1:E:496:ASN:ND2	2.17	0.77
1:C:656:ARG:NH1	1:C:658:GLU:OE1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:487:ALA:HB2	1:F:490:ALA:HB2	1.66	0.76
1:E:154:LEU:HB3	1:E:183:LEU:HD12	1.68	0.76
1:E:589:HIS:NE2	1:E:658:GLU:OE2	2.14	0.76
1:B:695:ASN:HA	1:B:698:LEU:HD13	1.68	0.75
1:C:55:ALA:H	1:C:132:THR:HG22	1.50	0.75
1:F:122:ARG:HB3	1:F:219:GLN:HG2	1.68	0.75
1:A:487:ALA:HB2	1:A:490:ALA:HB2	1.69	0.74
1:F:170:ARG:HA	1:F:173:ARG:HG2	1.69	0.74
1:F:55:ALA:H	1:F:132:THR:HG22	1.53	0.73
1:B:195:LEU:HD21	1:B:200:GLU:HB2	1.68	0.73
1:C:615:ASP:OD2	1:C:618:THR:HG22	1.88	0.73
1:E:183:LEU:HA	1:E:192:ARG:HD3	1.71	0.73
1:B:533:MET:HE2	1:B:537:TYR:HB3	1.69	0.73
1:D:487:ALA:HB2	1:D:490:ALA:HB2	1.70	0.73
1:E:126:TRP:HZ3	1:E:128:ASP:HB3	1.54	0.73
1:D:55:ALA:H	1:D:132:THR:HG22	1.52	0.73
1:A:615:ASP:OD2	1:A:618:THR:HG22	1.88	0.72
1:B:615:ASP:OD2	1:B:618:THR:HG22	1.87	0.72
1:C:352:ASP:OD1	1:C:352:ASP:N	2.19	0.72
1:B:352:ASP:OD1	1:B:352:ASP:N	2.22	0.72
1:A:122:ARG:HB3	1:A:219:GLN:HG2	1.71	0.72
1:C:150:LEU:HD12	1:C:154:LEU:HD11	1.71	0.71
1:F:676:PRO:O	1:F:678:ARG:NE	2.23	0.71
1:F:126:TRP:HZ3	1:F:128:ASP:HB3	1.55	0.71
1:B:284:LYS:N	1:B:352:ASP:OD2	2.20	0.71
1:D:184:ARG:N	1:D:192:ARG:HH11	1.88	0.71
1:C:368:ASP:OD1	1:C:368:ASP:N	2.20	0.71
1:C:188:ASP:O	1:C:192:ARG:HG3	1.90	0.70
1:A:275:TYR:CZ	1:A:416:ARG:HD3	2.26	0.70
1:E:55:ALA:H	1:E:132:THR:HG22	1.56	0.70
1:F:183:LEU:O	1:F:192:ARG:NH1	2.24	0.70
1:D:503:ASP:OD2	2:J:1:GLC:O2	2.10	0.70
1:C:465:GLN:OE1	1:C:496:ASN:ND2	2.23	0.69
1:D:615:ASP:OD2	1:D:618:THR:HG22	1.92	0.69
1:B:150:LEU:O	1:B:152:ASN:N	2.25	0.69
1:C:605:ASN:HD21	1:C:634:GLU:HG3	1.57	0.69
1:F:71:HIS:O	1:F:71:HIS:ND1	2.25	0.69
1:D:168:VAL:HG22	1:D:170:ARG:NH2	2.08	0.69
1:F:447:GLU:OE2	2:L:1:GLC:O1	2.11	0.69
1:C:309:SER:HA	1:C:352:ASP:HB2	1.74	0.69
1:C:365:GLU:OE1	1:C:365:GLU:N	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:SER:HA	1:F:154:LEU:HD23	1.75	0.69
1:B:556:GLU:HG3	1:B:561:ARG:HB2	1.74	0.69
1:B:122:ARG:HB3	1:B:219:GLN:HG2	1.76	0.68
1:B:169:PRO:HA	1:B:173:ARG:HE	1.56	0.68
1:B:275:TYR:CZ	1:B:416:ARG:HD2	2.28	0.68
1:C:134:ARG:NH2	1:C:202:GLU:OE1	2.26	0.68
1:B:503:ASP:OD2	2:H:1:GLC:O2	2.10	0.68
1:F:433:ALA:O	1:F:437:THR:OG1	2.10	0.68
1:A:154:LEU:HD13	1:A:154:LEU:H	1.59	0.68
1:D:420:PRO:HG2	1:D:446:SER:HB2	1.76	0.68
1:C:275:TYR:CZ	1:C:416:ARG:HD3	2.28	0.68
1:C:420:PRO:HG2	1:C:446:SER:HB2	1.75	0.68
1:C:174:ASP:OD1	1:C:178:ALA:N	2.21	0.68
1:F:50:ARG:NH2	1:F:51:GLU:OE1	2.25	0.67
1:B:174:ASP:OD1	1:B:174:ASP:N	2.28	0.67
1:C:154:LEU:H	1:C:154:LEU:HD12	1.59	0.67
1:D:541:GLU:OE1	1:D:563:ARG:NH1	2.26	0.67
1:D:414:PHE:CE1	1:D:443:LEU:HD12	2.30	0.67
1:D:465:GLN:OE1	1:D:496:ASN:ND2	2.23	0.67
1:C:318:HIS:CD2	1:C:320:SER:HB2	2.30	0.67
1:E:179:ALA:HB1	1:E:195:LEU:HG	1.77	0.67
1:A:67:VAL:HG11	1:A:440:PRO:HG3	1.77	0.67
1:D:154:LEU:HD12	1:D:154:LEU:H	1.60	0.66
1:D:168:VAL:HG22	1:D:170:ARG:CZ	2.23	0.66
1:D:318:HIS:CD2	1:D:320:SER:HB2	2.29	0.66
1:A:618:THR:HG23	1:A:620:ASP:H	1.60	0.66
1:C:170:ARG:HB2	1:C:173:ARG:HB2	1.77	0.66
1:E:50:ARG:NH2	1:E:51:GLU:OE1	2.24	0.66
1:B:501:THR:HG23	1:B:503:ASP:H	1.59	0.66
1:B:564:ASP:OD2	1:B:567:SER:OG	2.05	0.66
1:A:365:GLU:OE1	1:A:365:GLU:N	2.19	0.66
1:B:465:GLN:OE1	1:B:496:ASN:ND2	2.20	0.66
1:C:168:VAL:HG21	1:C:204:LEU:HD11	1.76	0.66
1:B:318:HIS:CD2	1:B:320:SER:HB2	2.32	0.65
1:C:503:ASP:OD2	2:I:1:GLC:O2	2.13	0.65
1:D:436:LYS:HE3	1:D:442:VAL:O	1.97	0.65
1:F:324:ILE:HD11	1:F:410:HIS:CD2	2.32	0.65
1:E:508:VAL:O	1:E:512:ASN:ND2	2.27	0.65
1:F:17:ARG:NH1	1:F:51:GLU:OE2	2.27	0.65
1:D:110:GLN:HB3	1:D:694:ARG:CZ	2.27	0.64
1:D:556:GLU:OE1	1:D:563:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASP:OD2	1:A:567:SER:OG	2.09	0.64
1:A:605:ASN:HD21	1:A:634:GLU:HG3	1.60	0.64
1:C:71:HIS:O	1:C:71:HIS:ND1	2.31	0.64
1:C:499:VAL:HG11	1:C:537:TYR:CZ	2.32	0.64
1:D:67:VAL:HG11	1:D:440:PRO:HG3	1.80	0.64
1:D:151:SER:HA	1:D:154:LEU:HD13	1.80	0.64
1:E:150:LEU:O	1:E:152:ASN:N	2.31	0.64
1:E:162:GLU:HG3	1:E:180:ALA:CB	2.28	0.64
1:A:368:ASP:OD2	1:A:370:THR:OG1	2.16	0.64
1:A:503:ASP:OD2	2:G:1:GLC:O2	2.15	0.64
1:F:399:GLU:OE1	1:F:402:ARG:NH1	2.31	0.64
1:E:503:ASP:OD2	2:K:1:GLC:O2	2.12	0.64
1:D:162:GLU:OE1	1:D:184:ARG:NH1	2.32	0.63
1:F:605:ASN:HD21	1:F:634:GLU:HG3	1.63	0.63
1:A:436:LYS:HE3	1:A:442:VAL:O	1.98	0.63
1:E:522:VAL:O	1:E:526:THR:OG1	2.16	0.63
1:D:188:ASP:O	1:D:191:THR:OG1	2.13	0.63
1:D:618:THR:HG23	1:D:620:ASP:H	1.63	0.63
1:B:17:ARG:NH1	1:B:51:GLU:OE2	2.29	0.63
1:F:556:GLU:HG3	1:F:561:ARG:HB2	1.81	0.63
1:B:618:THR:HG23	1:B:620:ASP:H	1.63	0.62
1:E:318:HIS:CD2	1:E:320:SER:HB2	2.34	0.62
1:B:309:SER:HA	1:B:352:ASP:HB2	1.81	0.62
1:B:170:ARG:O	1:B:173:ARG:HD2	2.00	0.62
1:E:265:ARG:NH2	1:E:538:GLU:OE1	2.33	0.62
1:C:436:LYS:HE3	1:C:442:VAL:O	1.99	0.62
1:C:556:GLU:HG3	1:C:561:ARG:HB2	1.81	0.62
1:A:275:TYR:OH	1:A:416:ARG:NH1	2.32	0.62
1:A:318:HIS:CD2	1:A:320:SER:HB2	2.34	0.62
1:B:605:ASN:HD21	1:B:634:GLU:HG3	1.64	0.62
1:C:122:ARG:HB3	1:C:219:GLN:HG2	1.80	0.62
1:C:194:ALA:N	1:C:195:LEU:HA	2.14	0.62
1:C:433:ALA:O	1:C:437:THR:OG1	2.18	0.62
1:F:465:GLN:OE1	1:F:496:ASN:ND2	2.28	0.62
1:D:50:ARG:NH2	1:D:51:GLU:OE1	2.22	0.61
1:F:163:ARG:NH2	1:F:212:ASP:OD1	2.34	0.61
1:D:365:GLU:OE1	1:D:365:GLU:N	2.20	0.61
1:D:605:ASN:HD21	1:D:634:GLU:HG3	1.65	0.61
1:B:151:SER:HA	1:B:154:LEU:HD23	1.83	0.61
1:E:126:TRP:CZ3	1:E:128:ASP:HB3	2.35	0.61
1:D:170:ARG:HH21	1:D:173:ARG:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:H	1:D:192:ARG:NH1	1.96	0.61
1:F:284:LYS:N	1:F:352:ASP:OD2	2.25	0.61
1:D:525:ALA:HB1	1:D:586:ARG:HD2	1.83	0.61
1:E:605:ASN:HD21	1:E:634:GLU:HG3	1.66	0.61
1:C:618:THR:HG23	1:C:620:ASP:H	1.63	0.60
1:D:188:ASP:OD1	1:D:191:THR:N	2.33	0.60
1:F:318:HIS:CD2	1:F:320:SER:HB2	2.35	0.60
1:F:382:GLN:OE1	1:F:382:GLN:N	2.31	0.60
1:C:584:ILE:HD13	1:E:664:TYR:HB3	1.83	0.60
1:A:465:GLN:OE1	1:A:496:ASN:ND2	2.25	0.60
1:D:200:GLU:O	1:D:204:LEU:HD13	2.01	0.60
1:E:383:ASP:OD1	1:E:383:ASP:N	2.26	0.60
1:A:605:ASN:ND2	1:A:634:GLU:HG3	2.17	0.60
1:D:383:ASP:OD1	1:D:383:ASP:N	2.30	0.60
1:F:168:VAL:HG12	1:F:208:TYR:HB2	1.82	0.60
1:A:309:SER:HA	1:A:352:ASP:HB2	1.84	0.60
1:D:168:VAL:O	1:D:170:ARG:NH2	2.34	0.60
1:F:503:ASP:OD2	2:L:1:GLC:O2	2.16	0.60
1:A:368:ASP:OD1	1:B:152:ASN:ND2	2.35	0.60
1:B:154:LEU:H	1:B:154:LEU:HD22	1.65	0.60
1:B:183:LEU:N	1:B:192:ARG:HH11	1.99	0.60
1:A:265:ARG:NH2	1:A:538:GLU:OE1	2.35	0.60
1:A:162:GLU:OE1	1:A:162:GLU:N	2.32	0.59
1:A:487:ALA:CB	1:A:490:ALA:HB2	2.32	0.59
1:D:150:LEU:O	1:D:152:ASN:N	2.35	0.59
1:D:168:VAL:HG23	1:D:208:TYR:CG	2.37	0.59
1:F:67:VAL:HG11	1:F:440:PRO:HG3	1.84	0.59
1:A:169:PRO:O	1:A:171:GLY:N	2.35	0.59
1:B:190:VAL:O	1:B:193:THR:HG22	2.02	0.59
1:F:110:GLN:OE1	1:F:694:ARG:HG3	2.02	0.59
1:A:583:ASN:HA	1:A:586:ARG:HD3	1.84	0.59
1:B:436:LYS:HE3	1:B:442:VAL:O	2.02	0.59
1:B:174:ASP:CG	1:B:177:LEU:HD22	2.28	0.59
1:C:170:ARG:CB	1:C:173:ARG:HB2	2.32	0.59
1:D:243:GLY:HA3	1:D:252:VAL:O	2.03	0.59
1:E:436:LYS:HE3	1:E:442:VAL:O	2.03	0.59
1:A:499:VAL:HG11	1:A:537:TYR:CZ	2.37	0.59
1:D:195:LEU:HA	1:D:198:THR:CG2	2.32	0.59
1:C:243:GLY:HA3	1:C:252:VAL:O	2.02	0.59
1:A:243:GLY:HA3	1:A:252:VAL:O	2.03	0.59
1:C:50:ARG:NH2	1:C:51:GLU:OE1	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PRO:HA	1:B:202:GLU:CD	2.28	0.58
1:B:382:GLN:OE1	1:B:382:GLN:N	2.32	0.58
1:C:150:LEU:O	1:C:152:ASN:N	2.36	0.58
1:D:433:ALA:O	1:D:437:THR:OG1	2.20	0.58
1:E:195:LEU:HA	1:E:201:ILE:HD11	1.85	0.58
1:F:499:VAL:HG11	1:F:537:TYR:CZ	2.37	0.58
1:C:169:PRO:HA	1:C:173:ARG:HD3	1.85	0.58
1:D:122:ARG:HB3	1:D:219:GLN:HG2	1.86	0.58
1:A:133:TRP:HH2	1:A:192:ARG:HH22	1.51	0.58
1:B:163:ARG:NH2	1:B:212:ASP:OD1	2.36	0.58
1:A:176:LEU:O	1:A:180:ALA:N	2.33	0.58
1:C:188:ASP:OD1	1:C:190:VAL:N	2.37	0.58
1:C:225:ASP:OD1	1:C:436:LYS:NZ	2.36	0.58
1:E:695:ASN:HA	1:E:698:LEU:HD13	1.84	0.58
1:F:126:TRP:CZ3	1:F:128:ASP:HB3	2.37	0.58
1:D:157:GLY:O	1:D:161:LEU:HD12	2.03	0.58
1:B:173:ARG:HG2	1:B:174:ASP:OD1	2.04	0.58
1:B:243:GLY:HA3	1:B:252:VAL:O	2.04	0.57
1:D:364:THR:OG1	1:D:388:ASN:ND2	2.27	0.57
1:A:183:LEU:HD12	1:A:192:ARG:HB3	1.85	0.57
1:E:194:ALA:O	1:E:198:THR:OG1	2.20	0.57
1:E:458:LEU:HA	1:E:461:LEU:HD13	1.85	0.57
1:A:382:GLN:OE1	1:A:382:GLN:N	2.32	0.57
1:C:122:ARG:HH11	1:C:219:GLN:HE21	1.53	0.57
1:A:122:ARG:HH11	1:A:219:GLN:HE21	1.51	0.57
1:A:458:LEU:HA	1:A:461:LEU:HD13	1.85	0.57
1:A:196:ALA:O	1:A:201:ILE:HD11	2.05	0.57
1:E:161:LEU:O	1:E:165:ALA:N	2.36	0.57
1:F:243:GLY:HA3	1:F:252:VAL:O	2.04	0.57
1:E:626:VAL:HG12	1:E:681:ALA:HB2	1.87	0.57
1:F:67:VAL:O	1:F:68:ARG:HG2	2.04	0.57
1:F:436:LYS:HE3	1:F:442:VAL:O	2.05	0.57
1:A:150:LEU:C	1:A:152:ASN:H	2.12	0.57
1:F:157:GLY:O	1:F:161:LEU:HD12	2.05	0.57
1:F:168:VAL:HG23	1:F:173:ARG:HB3	1.86	0.57
1:F:201:ILE:HA	1:F:204:LEU:HG	1.87	0.57
1:F:420:PRO:HG3	1:F:446:SER:HB2	1.86	0.56
1:C:127:GLY:O	1:C:129:PRO:HD3	2.05	0.56
1:C:169:PRO:HA	1:C:173:ARG:HH11	1.71	0.56
1:D:605:ASN:HB2	1:D:636:ALA:HB2	1.88	0.56
1:D:285:VAL:HG23	1:D:352:ASP:CG	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:HD12	1:E:177:LEU:H	1.70	0.56
1:E:193:THR:O	1:E:193:THR:OG1	2.24	0.56
1:E:605:ASN:ND2	1:E:634:GLU:HG3	2.21	0.56
1:D:605:ASN:ND2	1:D:634:GLU:HG3	2.21	0.56
1:A:200:GLU:O	1:A:204:LEU:HD13	2.06	0.56
1:A:526:THR:HG21	1:A:624:VAL:HG21	1.88	0.56
1:D:170:ARG:HG2	1:D:172:LEU:H	1.71	0.56
1:E:110:GLN:HG2	1:E:694:ARG:NE	2.18	0.56
1:B:605:ASN:ND2	1:B:634:GLU:HG3	2.20	0.55
1:C:605:ASN:ND2	1:C:634:GLU:HG3	2.19	0.55
1:D:167:GLY:O	1:D:169:PRO:HD3	2.07	0.55
1:E:243:GLY:HA3	1:E:252:VAL:O	2.05	0.55
1:E:590:PRO:O	1:E:593:GLN:HG3	2.06	0.55
1:E:200:GLU:O	1:E:204:LEU:HD13	2.06	0.55
1:F:180:ALA:O	1:F:184:ARG:HG3	2.07	0.55
1:F:605:ASN:ND2	1:F:634:GLU:HG3	2.20	0.55
1:A:188:ASP:OD2	1:A:190:VAL:N	2.40	0.55
1:C:284:LYS:N	1:C:352:ASP:OD2	2.30	0.55
1:D:58:ALA:HB3	1:D:107:PHE:HD2	1.70	0.55
1:D:275:TYR:HH	1:D:416:ARG:HH11	1.49	0.55
1:E:657:ASP:OD1	1:E:659:ILE:HG13	2.07	0.55
1:D:307:ILE:HG21	1:D:314:HIS:CD2	2.42	0.55
1:B:202:GLU:CD	1:B:202:GLU:H	2.14	0.55
1:C:605:ASN:HB2	1:C:636:ALA:HB2	1.89	0.55
1:D:187:GLY:HA3	1:D:191:THR:HG21	1.89	0.55
1:A:556:GLU:HG3	1:A:561:ARG:HB2	1.88	0.55
1:B:526:THR:HG21	1:B:624:VAL:HG21	1.89	0.55
1:C:157:GLY:O	1:C:161:LEU:HD12	2.07	0.55
1:C:318:HIS:CD2	1:C:320:SER:H	2.25	0.55
1:C:152:ASN:OD1	1:D:367:PRO:HD2	2.07	0.55
1:D:318:HIS:HD2	1:D:320:SER:H	1.55	0.55
1:E:382:GLN:OE1	1:E:382:GLN:N	2.32	0.55
1:A:183:LEU:HB2	1:A:192:ARG:HD3	1.89	0.54
1:D:165:ALA:HA	1:D:168:VAL:HG12	1.89	0.54
1:D:182:ALA:HB2	1:D:195:LEU:HD11	1.89	0.54
1:D:167:GLY:C	1:D:169:PRO:HD3	2.32	0.54
1:A:420:PRO:HG2	1:A:446:SER:HB2	1.88	0.54
1:C:526:THR:HG21	1:C:624:VAL:HG21	1.90	0.54
1:A:664:TYR:HB3	1:E:584:ILE:HD13	1.89	0.54
1:D:134:ARG:O	1:D:138:ILE:HG13	2.07	0.54
1:B:182:ALA:O	1:B:192:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:VAL:O	1:D:526:THR:OG1	2.20	0.54
1:A:285:VAL:HG23	1:A:352:ASP:CG	2.33	0.54
1:B:642:MET:HE3	1:B:647:MET:HB2	1.90	0.54
1:D:182:ALA:O	1:D:183:LEU:HB2	2.08	0.54
1:A:58:ALA:HB3	1:A:107:PHE:HD2	1.71	0.54
1:A:605:ASN:HB2	1:A:636:ALA:HB2	1.90	0.54
1:E:526:THR:HG21	1:E:624:VAL:HG21	1.90	0.54
1:F:204:LEU:HD12	1:F:205:LEU:N	2.22	0.54
1:F:297:ALA:HB1	1:F:298:PRO:HD2	1.90	0.54
1:F:307:ILE:HG21	1:F:314:HIS:ND1	2.22	0.54
1:A:156:VAL:O	1:A:159:VAL:HG12	2.08	0.54
1:B:420:PRO:HG2	1:B:446:SER:HB2	1.89	0.54
1:D:195:LEU:HA	1:D:198:THR:HG23	1.90	0.54
1:E:556:GLU:HG3	1:E:561:ARG:HB2	1.90	0.54
1:C:140:LYS:NZ	1:C:153:ASP:OD1	2.41	0.53
1:D:309:SER:HA	1:D:352:ASP:HB2	1.89	0.53
1:A:17:ARG:NH1	1:A:51:GLU:OE2	2.36	0.53
1:C:382:GLN:OE1	1:C:382:GLN:N	2.34	0.53
1:E:275:TYR:HH	1:E:416:ARG:HH11	1.48	0.53
1:B:58:ALA:HB3	1:B:107:PHE:HD2	1.73	0.53
1:E:110:GLN:CG	1:E:694:ARG:HE	2.19	0.53
1:F:188:ASP:O	1:F:192:ARG:HG2	2.09	0.53
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.90	0.53
1:D:176:LEU:O	1:D:180:ALA:N	2.42	0.53
1:A:182:ALA:HB3	1:A:192:ARG:HG3	1.89	0.53
1:B:664:TYR:HB3	1:F:584:ILE:HD13	1.90	0.53
1:C:522:VAL:O	1:C:526:THR:OG1	2.24	0.53
1:D:318:HIS:CD2	1:D:320:SER:H	2.26	0.53
1:D:382:GLN:OE1	1:D:382:GLN:N	2.31	0.53
1:E:149:GLU:HG2	1:E:150:LEU:H	1.73	0.53
1:E:420:PRO:HG3	1:E:446:SER:HB2	1.89	0.53
1:F:615:ASP:OD2	1:F:618:THR:OG1	2.25	0.53
1:A:364:THR:OG1	1:A:388:ASN:ND2	2.27	0.53
1:B:50:ARG:NH2	1:B:51:GLU:OE1	2.24	0.53
1:D:198:THR:OG1	1:D:201:ILE:HD13	2.08	0.53
1:F:315:ASP:OD1	1:F:316:THR:HG23	2.09	0.53
1:F:522:VAL:O	1:F:526:THR:OG1	2.22	0.53
1:A:476:LYS:HE3	1:A:608:LEU:O	2.08	0.53
1:B:157:GLY:O	1:B:161:LEU:HD12	2.09	0.53
1:D:134:ARG:NH2	1:D:202:GLU:OE2	2.41	0.53
1:E:307:ILE:HG21	1:E:314:HIS:ND1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ALA:HB1	1:D:298:PRO:HD2	1.91	0.53
1:E:190:VAL:O	1:E:193:THR:HG22	2.09	0.53
1:B:225:ASP:OD1	1:B:436:LYS:NZ	2.35	0.53
1:B:536:GLY:O	1:B:541:GLU:HG3	2.09	0.53
1:C:170:ARG:HG3	1:C:173:ARG:H	1.74	0.53
1:C:534:TYR:OH	1:C:556:GLU:OE1	2.14	0.53
1:F:314:HIS:HB3	1:F:403:VAL:HG11	1.90	0.53
1:A:192:ARG:O	1:A:192:ARG:HG2	2.07	0.53
1:D:529:PRO:O	1:D:586:ARG:NH2	2.42	0.53
1:B:405:GLN:O	1:B:409:ASN:ND2	2.41	0.52
1:C:297:ALA:HB1	1:C:298:PRO:HD2	1.91	0.52
1:E:642:MET:HE3	1:E:647:MET:HB2	1.90	0.52
1:B:201:ILE:HD13	1:B:201:ILE:H	1.75	0.52
1:D:170:ARG:HH21	1:D:173:ARG:CB	2.22	0.52
1:E:305:TRP:NE1	1:E:344:ASP:OD2	2.38	0.52
1:E:499:VAL:HG11	1:E:537:TYR:CZ	2.44	0.52
1:E:162:GLU:HG3	1:E:180:ALA:HB2	1.91	0.52
1:B:20:ILE:HG12	1:B:48:VAL:HG12	1.91	0.52
1:C:307:ILE:HG21	1:C:314:HIS:ND1	2.24	0.52
1:F:200:GLU:HG2	1:F:200:GLU:O	2.08	0.52
1:C:170:ARG:HA	1:C:171:GLY:C	2.35	0.52
1:C:405:GLN:OE1	1:C:438:VAL:HG21	2.09	0.52
1:D:110:GLN:HB3	1:D:694:ARG:NH1	2.24	0.52
1:F:20:ILE:HG12	1:F:48:VAL:HG12	1.91	0.52
1:B:413:LYS:NZ	1:B:439:ASP:OD1	2.32	0.52
1:D:476:LYS:HE3	1:D:608:LEU:O	2.10	0.52
1:E:173:ARG:HD2	1:E:177:LEU:HD11	1.92	0.52
1:E:280:HIS:C	1:E:318:HIS:HB2	2.35	0.52
1:C:487:ALA:O	1:C:488:GLU:HB2	2.10	0.52
1:F:526:THR:HG21	1:F:624:VAL:HG21	1.91	0.52
1:C:20:ILE:HG12	1:C:48:VAL:HG12	1.91	0.52
1:F:309:SER:HA	1:F:352:ASP:HB2	1.92	0.52
1:A:642:MET:HE3	1:A:647:MET:HB2	1.92	0.51
1:E:297:ALA:HB1	1:E:298:PRO:HD2	1.92	0.51
1:A:177:LEU:H	1:A:177:LEU:HD12	1.75	0.51
1:B:188:ASP:OD2	1:B:190:VAL:N	2.43	0.51
1:F:168:VAL:HG12	1:F:208:TYR:CB	2.40	0.51
1:F:318:HIS:CD2	1:F:320:SER:H	2.28	0.51
1:B:534:TYR:OH	1:B:556:GLU:OE1	2.13	0.51
1:C:695:ASN:O	1:C:698:LEU:HG	2.10	0.51
1:E:315:ASP:OD1	1:E:316:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:HZ3	1:A:128:ASP:HB2	1.76	0.51
1:B:184:ARG:N	1:B:192:ARG:NH1	2.58	0.51
1:C:590:PRO:O	1:C:593:GLN:HG3	2.10	0.51
1:E:307:ILE:HG21	1:E:314:HIS:CE1	2.45	0.51
1:F:642:MET:HE3	1:F:647:MET:HB2	1.92	0.51
1:B:417:VAL:HG12	1:B:420:PRO:HG3	1.92	0.51
1:B:533:MET:CE	1:B:537:TYR:HB3	2.41	0.51
1:C:625:VAL:HG11	1:C:672:ILE:HD13	1.91	0.51
1:D:526:THR:HG21	1:D:624:VAL:HG21	1.92	0.51
1:A:137:LEU:O	1:A:141:LEU:N	2.42	0.51
1:A:307:ILE:HG21	1:A:314:HIS:CE1	2.45	0.51
1:B:318:HIS:CD2	1:B:320:SER:H	2.28	0.51
1:D:102:GLN:HE22	1:D:698:LEU:HD12	1.75	0.51
1:E:155:LEU:HA	1:E:158:ALA:HB3	1.93	0.51
1:A:307:ILE:HG21	1:A:314:HIS:ND1	2.25	0.51
1:B:126:TRP:HZ3	1:B:128:ASP:HB2	1.76	0.51
1:B:476:LYS:HE3	1:B:608:LEU:O	2.11	0.51
1:C:134:ARG:HH21	1:C:197:LEU:HD23	1.76	0.51
1:E:476:LYS:HE3	1:E:608:LEU:O	2.11	0.51
1:A:318:HIS:NE2	1:A:320:SER:HB2	2.26	0.51
1:A:698:LEU:O	1:A:699:ARG:HB2	2.10	0.51
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.93	0.51
1:B:314:HIS:HB3	1:B:403:VAL:HG11	1.93	0.51
1:C:134:ARG:NH2	1:C:197:LEU:HD23	2.25	0.51
1:E:20:ILE:HG12	1:E:48:VAL:HG12	1.93	0.50
1:F:183:LEU:HD23	1:F:192:ARG:HB2	1.93	0.50
1:A:285:VAL:HG23	1:A:352:ASP:OD1	2.11	0.50
1:B:109:GLY:C	1:B:110:GLN:HG3	2.36	0.50
1:C:367:PRO:HD2	1:D:152:ASN:OD1	2.11	0.50
1:E:157:GLY:O	1:E:161:LEU:HD12	2.12	0.50
1:C:425:PRO:HG3	1:D:49:TRP:CZ3	2.47	0.50
1:D:142:ASP:OD1	1:D:143:ALA:N	2.45	0.50
1:D:363:PHE:CD1	1:D:363:PHE:N	2.80	0.50
1:E:487:ALA:O	1:E:488:GLU:HB2	2.09	0.50
1:A:110:GLN:NE2	1:A:694:ARG:HG3	2.27	0.50
1:A:198:THR:O	1:A:201:ILE:HD13	2.11	0.50
1:B:170:ARG:HB2	1:B:172:LEU:HG	1.94	0.50
1:E:275:TYR:CZ	1:E:416:ARG:HD3	2.47	0.50
1:E:284:LYS:N	1:E:352:ASP:OD2	2.29	0.50
1:F:122:ARG:HH11	1:F:219:GLN:HE21	1.58	0.50
1:A:417:VAL:HG12	1:A:420:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ASN:O	1:A:698:LEU:HG	2.11	0.50
1:A:110:GLN:HB3	1:A:694:ARG:CZ	2.42	0.50
1:B:175:PRO:O	1:B:178:ALA:HB3	2.11	0.50
1:B:443:LEU:HD22	1:B:464:THR:HG21	1.92	0.50
1:A:162:GLU:H	1:A:162:GLU:CD	2.18	0.49
1:D:127:GLY:O	1:D:129:PRO:HD3	2.11	0.49
1:A:151:SER:C	1:A:154:LEU:HD21	2.37	0.49
1:E:605:ASN:HB2	1:E:636:ALA:HB2	1.94	0.49
1:F:134:ARG:O	1:F:138:ILE:HG13	2.12	0.49
1:A:183:LEU:HB2	1:A:192:ARG:CD	2.42	0.49
1:B:315:ASP:OD1	1:B:316:THR:HG23	2.11	0.49
1:C:226:ARG:HH12	1:C:340:GLU:CD	2.19	0.49
1:C:170:ARG:H	1:C:173:ARG:CZ	2.26	0.49
1:C:307:ILE:HG21	1:C:314:HIS:CE1	2.47	0.49
1:E:185:THR:OG1	1:E:192:ARG:NH2	2.45	0.49
1:E:493:ARG:HG2	1:E:493:ARG:NH1	2.21	0.49
1:A:157:GLY:O	1:A:161:LEU:HD12	2.12	0.49
1:D:185:THR:H	1:D:192:ARG:NH1	2.10	0.49
1:D:305:TRP:NE1	1:D:344:ASP:OD2	2.37	0.49
1:E:182:ALA:HB3	1:E:195:LEU:HD21	1.93	0.49
1:C:170:ARG:H	1:C:173:ARG:CD	2.26	0.49
1:E:443:LEU:HD22	1:E:464:THR:HG21	1.94	0.49
1:A:188:ASP:HB3	1:A:191:THR:HG23	1.95	0.49
1:A:20:ILE:HG12	1:A:48:VAL:HG12	1.95	0.49
1:A:305:TRP:NE1	1:A:344:ASP:OD2	2.42	0.49
1:D:169:PRO:O	1:D:170:ARG:HB3	2.13	0.49
1:F:626:VAL:HG12	1:F:681:ALA:HB2	1.95	0.49
1:D:364:THR:HG1	1:D:388:ASN:HD22	1.58	0.49
1:D:698:LEU:O	1:D:699:ARG:HB2	2.13	0.49
1:A:134:ARG:O	1:A:138:ILE:HG13	2.13	0.49
1:A:366:LEU:HB3	1:A:367:PRO:HD2	1.95	0.49
1:C:151:SER:HA	1:C:154:LEU:HD13	1.94	0.49
1:C:170:ARG:HA	1:C:172:LEU:N	2.27	0.49
1:C:170:ARG:H	1:C:173:ARG:NE	2.11	0.49
1:C:642:MET:HE3	1:C:647:MET:HB2	1.95	0.49
1:D:183:LEU:HD23	1:D:192:ARG:HB2	1.95	0.49
1:D:272:ASP:OD2	1:D:272:ASP:N	2.46	0.49
1:E:161:LEU:HD12	1:E:161:LEU:H	1.78	0.49
1:F:656:ARG:NH2	1:F:685:ASN:HD22	2.10	0.49
1:A:508:VAL:O	1:A:512:ASN:ND2	2.37	0.48
1:E:318:HIS:CD2	1:E:320:SER:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:583:ASN:HA	1:F:586:ARG:HD3	1.94	0.48
1:C:318:HIS:HD2	1:C:320:SER:H	1.60	0.48
1:E:625:VAL:HG11	1:E:672:ILE:HD13	1.95	0.48
1:F:625:VAL:HG11	1:F:672:ILE:HD13	1.95	0.48
1:A:314:HIS:HB3	1:A:403:VAL:HG11	1.96	0.48
1:B:65:LEU:HD12	1:B:118:LEU:HD23	1.95	0.48
1:A:318:HIS:CD2	1:A:320:SER:H	2.32	0.48
1:B:366:LEU:HB3	1:B:367:PRO:HD2	1.94	0.48
1:C:390:ASP:CG	1:D:17:ARG:HH21	2.21	0.48
1:D:417:VAL:HG12	1:D:420:PRO:HG3	1.96	0.48
1:E:285:VAL:HG23	1:E:352:ASP:CG	2.39	0.48
1:E:422:THR:OG1	1:E:423:LYS:HE3	2.14	0.48
1:A:67:VAL:HG12	1:A:68:ARG:N	2.28	0.48
1:B:202:GLU:O	1:B:206:ALA:N	2.42	0.48
1:B:242:THR:HG21	1:B:259:ALA:HA	1.96	0.48
1:D:590:PRO:O	1:D:593:GLN:HG3	2.12	0.48
1:E:108:HIS:CG	1:E:698:LEU:HG	2.49	0.48
1:E:318:HIS:NE2	1:E:320:SER:HB2	2.29	0.48
1:E:698:LEU:O	1:E:699:ARG:HB2	2.13	0.48
1:F:364:THR:OG1	1:F:388:ASN:ND2	2.33	0.48
1:A:161:LEU:HD12	1:A:161:LEU:H	1.77	0.48
1:A:425:PRO:HG3	1:B:49:TRP:CZ3	2.49	0.48
1:A:533:MET:HE2	1:A:533:MET:HB3	1.71	0.48
1:A:536:GLY:O	1:A:541:GLU:HG3	2.14	0.48
1:C:265:ARG:NH2	1:C:538:GLU:OE1	2.45	0.48
1:C:583:ASN:HA	1:C:586:ARG:HD3	1.96	0.48
1:E:198:THR:HB	1:E:201:ILE:HD11	1.95	0.48
1:A:200:GLU:OE1	1:A:200:GLU:N	2.47	0.48
1:D:182:ALA:O	1:D:192:ARG:HB2	2.13	0.48
1:D:275:TYR:CZ	1:D:416:ARG:HD3	2.48	0.48
1:E:170:ARG:O	1:E:173:ARG:HG2	2.14	0.48
1:A:534:TYR:OH	1:A:556:GLU:OE1	2.18	0.48
1:C:67:VAL:CG1	1:C:440:PRO:HG3	2.44	0.48
1:A:493:ARG:HG2	1:A:493:ARG:HH11	1.78	0.48
1:B:475:THR:OG1	1:B:478:GLU:HG3	2.14	0.48
1:C:536:GLY:O	1:C:541:GLU:HG3	2.14	0.48
1:C:698:LEU:O	1:C:699:ARG:HB2	2.13	0.48
1:D:399:GLU:O	1:D:403:VAL:HG23	2.14	0.48
1:A:49:TRP:CZ3	1:B:425:PRO:HG3	2.49	0.48
1:A:390:ASP:CG	1:B:17:ARG:HH21	2.22	0.48
1:A:657:ASP:OD1	1:A:659:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:NH2	1:B:538:GLU:OE1	2.47	0.48
1:B:318:HIS:HD2	1:B:320:SER:H	1.61	0.48
1:D:68:ARG:O	1:D:69:TYR:HB2	2.14	0.48
1:F:280:HIS:C	1:F:318:HIS:HB2	2.39	0.48
1:F:307:ILE:HG21	1:F:314:HIS:CE1	2.49	0.48
1:B:493:ARG:HG2	1:B:493:ARG:HH11	1.79	0.47
1:C:364:THR:OG1	1:C:388:ASN:ND2	2.31	0.47
1:D:493:ARG:HG2	1:D:493:ARG:HH11	1.79	0.47
1:F:285:VAL:HG22	1:F:352:ASP:OD1	2.14	0.47
1:A:177:LEU:HA	1:A:180:ALA:HB3	1.96	0.47
1:A:230:ARG:O	1:A:529:PRO:HB2	2.14	0.47
1:A:237:MET:HE3	1:A:237:MET:HB2	1.77	0.47
1:C:17:ARG:HH21	1:D:390:ASP:CG	2.22	0.47
1:C:255:THR:OG1	1:C:256:PHE:N	2.47	0.47
1:D:315:ASP:OD1	1:D:316:THR:HG23	2.14	0.47
1:E:645:LEU:HD13	1:E:686:MET:HE2	1.95	0.47
1:E:188:ASP:HB2	1:E:191:THR:CG2	2.37	0.47
1:F:285:VAL:HG21	1:F:351:PRO:HB2	1.97	0.47
1:A:315:ASP:OD1	1:A:316:THR:HG23	2.14	0.47
1:B:656:ARG:NH2	1:B:685:ASN:HD22	2.12	0.47
1:C:275:TYR:OH	1:C:416:ARG:HD3	2.14	0.47
1:D:656:ARG:NH1	1:D:658:GLU:OE1	2.44	0.47
1:E:357:ARG:HG2	1:E:358:GLU:N	2.29	0.47
1:A:110:GLN:OE1	1:A:694:ARG:NE	2.46	0.47
1:C:497:LEU:HD22	1:C:528:SER:HB3	1.95	0.47
1:D:694:ARG:HD2	1:D:694:ARG:HA	1.59	0.47
1:E:141:LEU:HD13	1:E:142:ASP:N	2.30	0.47
1:F:114:ASP:OD1	1:F:115:ARG:NH1	2.48	0.47
1:E:194:ALA:HB3	1:E:195:LEU:HD22	1.97	0.47
1:F:255:THR:OG1	1:F:256:PHE:N	2.48	0.47
1:F:605:ASN:HB2	1:F:636:ALA:HB2	1.96	0.47
1:F:657:ASP:OD1	1:F:659:ILE:HG13	2.15	0.47
1:A:201:ILE:HA	1:A:204:LEU:HD13	1.96	0.47
1:B:102:GLN:CD	1:B:102:GLN:H	2.21	0.47
1:C:170:ARG:H	1:C:173:ARG:HD3	1.79	0.47
1:D:168:VAL:HG22	1:D:170:ARG:NH1	2.29	0.47
1:D:183:LEU:HD22	1:D:183:LEU:HA	1.75	0.47
1:C:493:ARG:HH11	1:C:493:ARG:HG2	1.80	0.47
1:F:201:ILE:HG23	1:F:204:LEU:HD11	1.95	0.47
1:C:318:HIS:NE2	1:C:320:SER:HB2	2.29	0.47
1:D:122:ARG:HH11	1:D:219:GLN:HE21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:THR:OG1	1:E:256:PHE:N	2.47	0.47
1:E:615:ASP:OD2	1:E:618:THR:HG23	2.14	0.47
1:A:225:ASP:OD1	1:A:436:LYS:NZ	2.38	0.47
1:A:383:ASP:OD1	1:A:383:ASP:N	2.26	0.47
1:B:102:GLN:H	1:B:102:GLN:NE2	2.12	0.47
1:C:280:HIS:C	1:C:318:HIS:HB2	2.40	0.47
1:F:676:PRO:C	1:F:678:ARG:H	2.21	0.47
1:E:134:ARG:O	1:E:138:ILE:HG12	2.15	0.46
1:E:656:ARG:NH2	1:E:685:ASN:HD22	2.13	0.46
1:F:154:LEU:HD12	1:F:183:LEU:HD22	1.96	0.46
1:A:590:PRO:O	1:A:593:GLN:HG3	2.16	0.46
1:B:185:THR:OG1	1:B:192:ARG:NH2	2.48	0.46
1:A:506:HIS:ND1	1:A:507:ALA:N	2.64	0.46
1:B:110:GLN:OE1	1:B:694:ARG:HD2	2.15	0.46
1:C:150:LEU:CD1	1:C:154:LEU:HD11	2.42	0.46
1:C:245:TRP:HA	1:C:250:ASN:O	2.16	0.46
1:D:363:PHE:N	1:D:363:PHE:HD1	2.14	0.46
1:E:686:MET:HE3	1:E:686:MET:HB3	1.73	0.46
1:A:110:GLN:O	1:A:110:GLN:HG2	2.15	0.46
1:D:376:ASN:O	1:D:379:LYS:N	2.48	0.46
1:D:399:GLU:OE2	1:D:402:ARG:NH1	2.48	0.46
1:D:642:MET:HE3	1:D:647:MET:HB2	1.97	0.46
1:E:314:HIS:HB3	1:E:403:VAL:HG11	1.96	0.46
1:E:413:LYS:NZ	1:E:439:ASP:OD1	2.38	0.46
1:F:318:HIS:HD2	1:F:320:SER:H	1.61	0.46
1:A:280:HIS:C	1:A:318:HIS:HB2	2.41	0.46
1:A:584:ILE:HD13	1:C:664:TYR:HB3	1.96	0.46
1:B:188:ASP:O	1:B:191:THR:OG1	2.33	0.46
1:B:497:LEU:HD22	1:B:528:SER:HB3	1.97	0.46
1:C:357:ARG:HG2	1:C:358:GLU:N	2.29	0.46
1:D:497:LEU:HD22	1:D:528:SER:HB3	1.98	0.46
1:B:499:VAL:HG11	1:B:537:TYR:CZ	2.50	0.46
1:B:583:ASN:HA	1:B:586:ARG:HD3	1.98	0.46
1:F:200:GLU:HA	1:F:203:GLU:OE2	2.16	0.46
1:A:71:HIS:O	1:A:71:HIS:ND1	2.49	0.46
1:B:522:VAL:O	1:B:526:THR:OG1	2.25	0.46
1:C:108:HIS:CG	1:C:698:LEU:HD22	2.51	0.46
1:C:314:HIS:HB3	1:C:403:VAL:HG11	1.98	0.46
1:E:173:ARG:CD	1:E:177:LEU:HD11	2.45	0.46
1:E:288:LYS:HE3	2:K:2:GLC:O4	2.15	0.46
1:E:676:PRO:C	1:E:678:ARG:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ASP:OD1	1:C:316:THR:HG23	2.15	0.46
1:B:501:THR:HG22	1:B:504:ILE:HG13	1.97	0.46
1:E:161:LEU:O	1:E:164:ALA:HB3	2.16	0.46
1:E:583:ASN:HA	1:E:586:ARG:HD3	1.97	0.46
1:F:152:ASN:O	1:F:156:VAL:HG23	2.15	0.46
1:A:626:VAL:HG12	1:A:681:ALA:HB2	1.98	0.46
1:C:49:TRP:CZ3	1:D:425:PRO:HG3	2.51	0.46
1:D:65:LEU:HD12	1:D:118:LEU:HD23	1.97	0.46
1:E:237:MET:HE3	1:E:237:MET:HB2	1.75	0.46
1:E:475:THR:OG1	1:E:478:GLU:HG3	2.15	0.46
1:F:318:HIS:NE2	1:F:320:SER:HB2	2.30	0.46
1:F:534:TYR:OH	1:F:556:GLU:OE1	2.13	0.46
1:A:255:THR:OG1	1:A:256:PHE:N	2.48	0.45
1:C:68:ARG:O	1:C:69:TYR:HB2	2.16	0.45
1:C:188:ASP:O	1:C:192:ARG:CG	2.63	0.45
1:F:142:ASP:OD1	1:F:143:ALA:N	2.49	0.45
1:F:193:THR:O	1:F:197:LEU:HD22	2.16	0.45
1:F:686:MET:HE3	1:F:686:MET:HB3	1.75	0.45
1:A:600:PHE:CE1	1:A:609:LEU:HD11	2.51	0.45
1:F:182:ALA:O	1:F:192:ARG:HA	2.15	0.45
1:F:446:SER:HB3	1:F:463:PHE:CD1	2.51	0.45
1:C:15:PRO:HA	1:C:16:GLY:HA2	1.83	0.45
1:C:256:PHE:CE2	1:C:327:PHE:HB2	2.51	0.45
1:D:475:THR:OG1	1:D:478:GLU:HG3	2.16	0.45
1:E:533:MET:HE1	1:E:579:ILE:CD1	2.46	0.45
1:B:659:ILE:H	1:B:659:ILE:HG13	1.38	0.45
1:A:183:LEU:HB2	1:A:192:ARG:CB	2.47	0.45
1:A:501:THR:HB	1:A:502:PRO:HD2	1.99	0.45
1:F:173:ARG:O	1:F:177:LEU:HD12	2.16	0.45
1:F:174:ASP:N	1:F:175:PRO:CD	2.80	0.45
1:B:486:ILE:HD13	1:B:495:PRO:HG3	1.98	0.45
1:C:475:THR:OG1	1:C:478:GLU:HG3	2.16	0.45
1:E:115:ARG:HG3	1:E:115:ARG:HH11	1.82	0.45
1:E:364:THR:OG1	1:E:388:ASN:ND2	2.35	0.45
1:E:536:GLY:O	1:E:541:GLU:HG3	2.17	0.45
1:F:265:ARG:NH2	1:F:538:GLU:OE1	2.49	0.45
1:F:536:GLY:O	1:F:541:GLU:HG3	2.16	0.45
1:B:487:ALA:CB	1:B:490:ALA:HB2	2.40	0.45
1:C:186:PRO:HA	1:C:192:ARG:NH2	2.32	0.45
1:F:177:LEU:HD12	1:F:177:LEU:H	1.82	0.45
1:A:202:GLU:OE1	1:A:202:GLU:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:O	1:C:138:ILE:HG13	2.16	0.45
1:C:156:VAL:O	1:C:160:LEU:HD23	2.17	0.45
1:C:163:ARG:NH2	1:C:212:ASP:OD1	2.50	0.45
1:C:290:ARG:HH11	1:C:559:GLU:CD	2.25	0.45
1:C:443:LEU:HD22	1:C:464:THR:HG21	1.97	0.45
1:C:476:LYS:HE3	1:C:608:LEU:O	2.16	0.45
1:D:690:PRO:C	1:D:692:GLU:H	2.24	0.45
1:F:383:ASP:OD1	1:F:383:ASP:N	2.29	0.45
1:A:161:LEU:O	1:A:164:ALA:HB3	2.17	0.45
1:A:443:LEU:HD22	1:A:464:THR:HG21	1.98	0.45
1:C:446:SER:HB3	1:C:463:PHE:CD1	2.52	0.45
1:C:686:MET:HB3	1:C:686:MET:HE3	1.63	0.45
1:E:183:LEU:C	1:E:192:ARG:HH11	2.24	0.45
1:E:405:GLN:OE1	1:E:438:VAL:HG21	2.16	0.45
1:F:475:THR:OG1	1:F:478:GLU:HG3	2.17	0.45
1:A:304:PRO:O	1:A:307:ILE:HD13	2.17	0.45
1:A:625:VAL:HG11	1:A:672:ILE:HD13	1.99	0.45
1:B:184:ARG:N	1:B:192:ARG:HH11	2.14	0.45
1:C:67:VAL:O	1:C:68:ARG:C	2.60	0.45
1:D:242:THR:HG21	1:D:259:ALA:HA	1.98	0.45
1:D:318:HIS:HD2	1:D:320:SER:N	2.14	0.45
1:A:152:ASN:HD21	1:B:368:ASP:CG	2.25	0.44
1:A:676:PRO:C	1:A:678:ARG:H	2.25	0.44
1:B:698:LEU:O	1:B:699:ARG:HB2	2.18	0.44
1:E:150:LEU:CD1	1:E:154:LEU:HD11	2.43	0.44
1:E:225:ASP:OD1	1:E:436:LYS:NZ	2.47	0.44
1:F:19:GLU:O	1:F:48:VAL:HA	2.17	0.44
1:F:493:ARG:HG2	1:F:493:ARG:HH11	1.83	0.44
1:A:150:LEU:H	1:A:150:LEU:HD23	1.81	0.44
1:C:193:THR:C	1:C:195:LEU:HA	2.42	0.44
1:C:417:VAL:HG12	1:C:420:PRO:HG3	1.98	0.44
1:E:67:VAL:CG1	1:E:440:PRO:HG3	2.47	0.44
1:F:698:LEU:O	1:F:699:ARG:HB2	2.17	0.44
1:A:275:TYR:CE1	1:A:416:ARG:HD3	2.52	0.44
1:B:170:ARG:O	1:B:172:LEU:N	2.51	0.44
1:B:567:SER:O	1:B:571:GLN:HG3	2.17	0.44
1:E:399:GLU:OE2	1:E:402:ARG:NH1	2.50	0.44
1:F:246:ASP:OD1	1:F:246:ASP:N	2.50	0.44
1:A:256:PHE:CE2	1:A:327:PHE:HB2	2.53	0.44
1:B:676:PRO:C	1:B:678:ARG:H	2.24	0.44
1:C:197:LEU:O	1:C:199:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ASP:OD1	1:C:383:ASP:N	2.31	0.44
1:E:19:GLU:O	1:E:48:VAL:HA	2.17	0.44
1:A:108:HIS:HB3	1:A:698:LEU:HD22	2.00	0.44
1:B:174:ASP:HB2	1:B:176:LEU:HB2	1.99	0.44
1:B:178:ALA:O	1:B:182:ALA:HB2	2.17	0.44
1:B:422:THR:C	1:B:423:LYS:HD2	2.43	0.44
1:E:533:MET:HE1	1:E:579:ILE:HD13	2.00	0.44
1:A:245:TRP:HA	1:A:250:ASN:O	2.17	0.44
1:A:357:ARG:HG2	1:A:358:GLU:N	2.32	0.44
1:B:174:ASP:HB2	1:B:176:LEU:H	1.83	0.44
1:D:168:VAL:O	1:D:168:VAL:HG13	2.17	0.44
1:D:416:ARG:HH21	1:D:447:GLU:CG	2.31	0.44
1:D:695:ASN:O	1:D:698:LEU:HG	2.18	0.44
1:F:102:GLN:CD	1:F:102:GLN:H	2.25	0.44
1:F:188:ASP:OD2	1:F:190:VAL:N	2.51	0.44
1:F:675:ASP:OD1	1:F:678:ARG:NH2	2.50	0.44
1:A:17:ARG:HH21	1:B:390:ASP:CG	2.25	0.44
1:B:280:HIS:C	1:B:318:HIS:HB2	2.43	0.44
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.84	0.44
1:E:156:VAL:O	1:E:159:VAL:HG12	2.18	0.44
1:E:366:LEU:HB3	1:E:367:PRO:HD2	2.00	0.44
1:F:201:ILE:N	1:F:201:ILE:HD12	2.32	0.44
1:A:126:TRP:CZ3	1:A:128:ASP:HB2	2.52	0.44
1:A:246:ASP:OD2	1:A:246:ASP:N	2.50	0.44
1:A:446:SER:HB3	1:A:463:PHE:CD1	2.53	0.44
1:B:600:PHE:CD1	1:B:611:TYR:HB3	2.53	0.44
1:A:179:ALA:HA	1:A:195:LEU:HB3	2.00	0.44
1:A:600:PHE:HE1	1:A:609:LEU:HD11	1.81	0.44
1:B:282:ILE:O	1:B:287:ARG:NH2	2.51	0.44
1:C:170:ARG:HB2	1:C:173:ARG:NE	2.33	0.44
1:C:171:GLY:O	1:C:172:LEU:HB2	2.17	0.44
1:C:454:ARG:HG3	1:D:49:TRP:CE3	2.53	0.44
1:D:174:ASP:O	1:D:177:LEU:N	2.51	0.44
1:D:280:HIS:C	1:D:318:HIS:HB2	2.42	0.44
1:E:156:VAL:HA	1:E:159:VAL:HG12	2.00	0.44
1:F:476:LYS:HE3	1:F:608:LEU:O	2.18	0.44
1:B:21:ASP:OD1	1:B:22:ASP:N	2.48	0.43
1:B:383:ASP:OD1	1:B:383:ASP:N	2.28	0.43
1:C:237:MET:HE3	1:C:237:MET:HB2	1.76	0.43
1:D:182:ALA:HA	1:D:192:ARG:HB3	2.00	0.43
1:E:114:ASP:OD1	1:E:115:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:THR:HG21	1:E:259:ALA:HA	2.00	0.43
1:A:165:ALA:HA	1:A:168:VAL:HG23	2.00	0.43
1:A:686:MET:HE3	1:A:686:MET:HB3	1.73	0.43
1:C:68:ARG:HB3	1:C:69:TYR:H	1.47	0.43
1:D:198:THR:C	1:D:200:GLU:H	2.26	0.43
1:D:686:MET:HB3	1:D:686:MET:HE3	1.65	0.43
1:F:486:ILE:HD13	1:F:495:PRO:HG3	1.99	0.43
1:A:608:LEU:HD23	1:A:627:THR:HA	1.99	0.43
1:C:239:PRO:HD3	1:C:276:LEU:HD22	2.00	0.43
1:C:694:ARG:HD2	1:C:694:ARG:HA	1.84	0.43
1:D:625:VAL:HG11	1:D:672:ILE:HD13	2.01	0.43
1:F:225:ASP:OD1	1:F:436:LYS:NZ	2.42	0.43
1:F:659:ILE:HG13	1:F:659:ILE:H	1.42	0.43
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.81	0.43
1:B:256:PHE:CE2	1:B:327:PHE:HB2	2.53	0.43
1:C:114:ASP:OD1	1:C:115:ARG:HG3	2.17	0.43
1:D:196:ALA:O	1:D:201:ILE:HD11	2.18	0.43
1:D:256:PHE:CE2	1:D:327:PHE:HB2	2.53	0.43
1:E:690:PRO:C	1:E:692:GLU:H	2.26	0.43
1:F:189:PRO:O	1:F:193:THR:HG22	2.18	0.43
1:A:49:TRP:CE3	1:B:454:ARG:HG3	2.53	0.43
1:C:285:VAL:HG13	1:C:352:ASP:OD1	2.19	0.43
1:D:138:ILE:HA	1:D:141:LEU:HD23	2.00	0.43
1:D:442:VAL:C	1:D:443:LEU:HD23	2.43	0.43
1:E:182:ALA:O	1:E:192:ARG:HB3	2.17	0.43
1:E:226:ARG:HH12	1:E:340:GLU:CD	2.26	0.43
1:F:353:HIS:CE1	1:F:355:TRP:CG	3.07	0.43
1:A:150:LEU:HD12	1:A:154:LEU:HD12	2.00	0.43
1:B:181:ALA:O	1:B:192:ARG:NH1	2.51	0.43
1:F:108:HIS:CG	1:F:698:LEU:HG	2.54	0.43
1:F:304:PRO:O	1:F:307:ILE:HD13	2.18	0.43
1:A:282:ILE:O	1:A:287:ARG:NH2	2.50	0.43
1:B:645:LEU:HD13	1:B:686:MET:HE2	2.00	0.43
1:C:156:VAL:O	1:C:159:VAL:HG12	2.19	0.43
1:C:399:GLU:O	1:C:403:VAL:HG23	2.18	0.43
1:D:175:PRO:O	1:D:178:ALA:HB3	2.18	0.43
1:D:230:ARG:O	1:D:529:PRO:HB2	2.19	0.43
1:D:282:ILE:O	1:D:287:ARG:NH2	2.51	0.43
1:E:162:GLU:CG	1:E:180:ALA:CB	2.96	0.43
1:E:179:ALA:CB	1:E:195:LEU:HG	2.46	0.43
1:F:505:LEU:HD13	1:F:552:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:SER:O	1:A:571:GLN:HG3	2.18	0.43
1:B:150:LEU:C	1:B:152:ASN:H	2.26	0.43
1:B:173:ARG:HA	1:B:174:ASP:HA	1.48	0.43
1:B:374:ALA:HA	1:B:386:PRO:HG3	2.00	0.43
1:C:318:HIS:HD2	1:C:320:SER:N	2.17	0.43
1:C:435:VAL:O	1:C:438:VAL:HG22	2.18	0.43
1:D:506:HIS:ND1	1:D:507:ALA:N	2.66	0.43
1:F:114:ASP:OD1	1:F:115:ARG:HG3	2.19	0.43
1:A:199:PRO:HA	1:A:202:GLU:OE2	2.19	0.43
1:B:126:TRP:CZ3	1:B:128:ASP:HB2	2.53	0.43
1:C:506:HIS:ND1	1:C:507:ALA:N	2.67	0.43
1:D:539:LEU:HA	1:D:539:LEU:HD23	1.74	0.43
1:E:567:SER:O	1:E:571:GLN:HG3	2.19	0.43
1:F:645:LEU:HD13	1:F:686:MET:HE2	2.00	0.43
1:A:165:ALA:O	1:A:168:VAL:HG23	2.19	0.43
1:B:230:ARG:O	1:B:529:PRO:HB2	2.19	0.43
1:C:177:LEU:HD12	1:C:177:LEU:H	1.84	0.43
1:E:115:ARG:HG3	1:E:115:ARG:NH1	2.34	0.43
1:B:19:GLU:O	1:B:48:VAL:HA	2.18	0.42
1:B:168:VAL:HG12	1:B:208:TYR:CD1	2.54	0.42
1:B:183:LEU:HA	1:B:192:ARG:HD2	2.01	0.42
1:B:318:HIS:NE2	1:B:320:SER:HB2	2.33	0.42
1:C:19:GLU:O	1:C:48:VAL:HA	2.18	0.42
1:E:305:TRP:O	1:E:348:GLN:NE2	2.51	0.42
1:E:470:PHE:HD1	1:E:482:PHE:CE2	2.36	0.42
1:F:63:ARG:HH22	1:F:92:LYS:HE2	1.84	0.42
1:F:690:PRO:C	1:F:692:GLU:H	2.27	0.42
1:A:422:THR:C	1:A:423:LYS:HD2	2.43	0.42
1:A:505:LEU:HD13	1:A:552:TYR:CZ	2.54	0.42
1:B:183:LEU:N	1:B:192:ARG:NH1	2.67	0.42
1:B:353:HIS:CE1	1:B:355:TRP:CG	3.06	0.42
1:B:608:LEU:HD23	1:B:627:THR:HA	2.00	0.42
1:C:676:PRO:C	1:C:678:ARG:H	2.27	0.42
1:A:128:ASP:HA	1:A:129:PRO:HD2	1.93	0.42
1:A:242:THR:HG21	1:A:259:ALA:HA	2.01	0.42
1:D:188:ASP:HB2	1:D:189:PRO:HD2	2.01	0.42
1:E:122:ARG:NH1	1:E:124:ASP:OD1	2.52	0.42
1:E:309:SER:OG	1:E:310:ASP:N	2.52	0.42
1:F:600:PHE:CE1	1:F:609:LEU:HD11	2.55	0.42
1:B:600:PHE:CE1	1:B:609:LEU:HD11	2.54	0.42
1:D:21:ASP:OD1	1:D:22:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:HIS:NE2	1:D:320:SER:HB2	2.34	0.42
1:E:165:ALA:HA	1:E:168:VAL:HG23	1.99	0.42
1:E:501:THR:HB	1:E:502:PRO:HD2	2.00	0.42
1:A:374:ALA:HA	1:A:386:PRO:HG3	2.00	0.42
1:C:49:TRP:CE3	1:D:454:ARG:HG3	2.54	0.42
1:C:246:ASP:OD1	1:C:246:ASP:N	2.51	0.42
1:C:600:PHE:CD1	1:C:611:TYR:HB3	2.55	0.42
1:D:17:ARG:NH1	1:D:51:GLU:OE2	2.38	0.42
1:D:138:ILE:HG23	1:D:141:LEU:HD23	2.02	0.42
1:D:435:VAL:O	1:D:438:VAL:HG22	2.19	0.42
1:D:446:SER:HB3	1:D:463:PHE:CD1	2.53	0.42
1:D:676:PRO:C	1:D:678:ARG:H	2.26	0.42
1:F:192:ARG:HG2	1:F:192:ARG:H	1.66	0.42
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.81	0.42
1:A:390:ASP:OD2	1:B:17:ARG:NH2	2.53	0.42
1:B:197:LEU:HD13	1:B:198:THR:HG23	2.01	0.42
1:B:405:GLN:OE1	1:B:438:VAL:HG21	2.19	0.42
1:B:676:PRO:O	1:B:677:ALA:HB3	2.20	0.42
1:D:523:LEU:O	1:D:527:MET:HG3	2.20	0.42
1:E:497:LEU:HD22	1:E:528:SER:HB3	2.01	0.42
1:F:141:LEU:HD11	1:F:193:THR:HG21	2.01	0.42
1:F:160:LEU:HD23	1:F:160:LEU:HA	1.95	0.42
1:F:255:THR:HG23	1:F:258:THR:H	1.85	0.42
1:B:154:LEU:HD22	1:B:154:LEU:N	2.34	0.42
1:B:376:ASN:O	1:B:379:LYS:N	2.53	0.42
1:C:438:VAL:HG23	1:C:439:ASP:N	2.34	0.42
1:D:629:ASN:ND2	1:D:629:ASN:O	2.52	0.42
1:E:607:ALA:HB3	1:E:634:GLU:HG2	2.01	0.42
1:B:246:ASP:OD1	1:B:246:ASP:N	2.51	0.42
1:B:435:VAL:O	1:B:438:VAL:HG22	2.20	0.42
1:C:390:ASP:OD2	1:D:17:ARG:NH2	2.50	0.42
1:C:515:GLY:O	1:C:519:ILE:HG13	2.20	0.42
1:D:422:THR:C	1:D:423:LYS:HD2	2.45	0.42
1:F:414:PHE:CE1	1:F:443:LEU:HD12	2.55	0.42
1:F:435:VAL:O	1:F:438:VAL:HG22	2.20	0.42
1:F:608:LEU:HD23	1:F:627:THR:HA	2.01	0.42
1:B:198:THR:HA	1:B:199:PRO:HD3	1.94	0.42
1:B:285:VAL:HG21	1:B:351:PRO:HB2	2.01	0.42
1:B:605:ASN:HB2	1:B:636:ALA:HB2	2.02	0.42
1:C:161:LEU:O	1:C:165:ALA:N	2.50	0.42
1:C:573:ARG:HG3	1:C:573:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:THR:OG1	1:D:256:PHE:N	2.52	0.42
1:E:236:GLU:HB3	1:E:534:TYR:HA	2.02	0.42
1:F:204:LEU:HD12	1:F:205:LEU:HG	2.02	0.42
1:F:533:MET:HE2	1:F:533:MET:HB3	1.81	0.42
1:A:497:LEU:HD22	1:A:528:SER:HB3	2.02	0.42
1:A:659:ILE:HG13	1:A:659:ILE:H	1.43	0.42
1:B:128:ASP:HA	1:B:129:PRO:HD2	1.91	0.42
1:B:185:THR:HG23	1:B:192:ARG:NH2	2.34	0.42
1:F:183:LEU:HD23	1:F:192:ARG:CB	2.50	0.42
1:F:318:HIS:HD2	1:F:320:SER:N	2.17	0.42
1:B:168:VAL:HG12	1:B:208:TYR:CG	2.55	0.41
1:B:170:ARG:C	1:B:172:LEU:H	2.28	0.41
1:B:198:THR:O	1:B:200:GLU:N	2.47	0.41
1:C:21:ASP:OD1	1:C:22:ASP:N	2.50	0.41
1:E:170:ARG:HB2	1:E:171:GLY:H	1.44	0.41
1:F:560:LEU:HD23	1:F:560:LEU:HA	1.75	0.41
1:F:676:PRO:HD2	1:F:678:ARG:HH21	1.85	0.41
1:A:114:ASP:OD1	1:A:115:ARG:HG3	2.21	0.41
1:A:239:PRO:HD3	1:A:276:LEU:HD22	2.02	0.41
1:C:170:ARG:HG2	1:C:171:GLY:HA2	2.01	0.41
1:C:533:MET:HB3	1:C:533:MET:HE2	1.77	0.41
1:C:582:LEU:HD23	1:C:582:LEU:HA	1.90	0.41
1:D:536:GLY:O	1:D:541:GLU:HG3	2.19	0.41
1:E:519:ILE:HD13	1:E:627:THR:O	2.20	0.41
1:E:523:LEU:O	1:E:527:MET:HG3	2.20	0.41
1:F:376:ASN:O	1:F:379:LYS:N	2.52	0.41
1:A:65:LEU:HD12	1:A:118:LEU:HD23	2.03	0.41
1:B:686:MET:HB3	1:B:686:MET:HE3	1.71	0.41
1:D:198:THR:C	1:D:200:GLU:N	2.78	0.41
1:E:114:ASP:OD1	1:E:115:ARG:NH1	2.54	0.41
1:E:151:SER:HA	1:E:154:LEU:HD13	2.02	0.41
1:E:255:THR:HG23	1:E:258:THR:H	1.85	0.41
1:E:629:ASN:O	1:E:629:ASN:ND2	2.54	0.41
1:F:523:LEU:O	1:F:527:MET:HG3	2.19	0.41
1:A:19:GLU:O	1:A:48:VAL:HA	2.21	0.41
1:A:236:GLU:HB3	1:A:534:TYR:HA	2.03	0.41
1:A:318:HIS:HD2	1:A:320:SER:H	1.67	0.41
1:A:376:ASN:O	1:A:379:LYS:N	2.53	0.41
1:A:417:VAL:CG1	1:A:420:PRO:HG3	2.50	0.41
1:A:539:LEU:HA	1:A:539:LEU:HD23	1.79	0.41
1:C:228:LEU:HD23	1:C:340:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:TRP:HA	1:D:250:ASN:O	2.20	0.41
1:E:488:GLU:C	1:E:490:ALA:H	2.28	0.41
1:B:67:VAL:HG12	1:B:67:VAL:O	2.21	0.41
1:B:184:ARG:H	1:B:192:ARG:NH1	2.19	0.41
1:B:199:PRO:HA	1:B:202:GLU:OE2	2.21	0.41
1:B:377:PRO:HA	1:B:378:PRO:HA	1.76	0.41
1:B:505:LEU:HD12	1:B:552:TYR:CD1	2.56	0.41
1:C:112:THR:HA	1:C:113:PRO:HD3	1.74	0.41
1:C:280:HIS:HB2	1:C:307:ILE:HG23	2.02	0.41
1:D:108:HIS:HB3	1:D:698:LEU:HD22	2.02	0.41
1:F:309:SER:OG	1:F:310:ASP:N	2.54	0.41
1:A:399:GLU:O	1:A:403:VAL:HG23	2.20	0.41
1:B:183:LEU:HA	1:B:192:ARG:HB3	2.01	0.41
1:C:508:VAL:HG21	1:C:516:MET:HE2	2.03	0.41
1:D:416:ARG:HH21	1:D:447:GLU:HG3	1.84	0.41
1:E:150:LEU:C	1:E:152:ASN:H	2.28	0.41
1:F:675:ASP:CG	1:F:678:ARG:CZ	2.94	0.41
1:B:168:VAL:O	1:B:170:ARG:N	2.48	0.41
1:C:353:HIS:CE1	1:C:355:TRP:CG	3.09	0.41
1:D:160:LEU:O	1:D:164:ALA:N	2.44	0.41
1:D:315:ASP:OD2	1:D:402:ARG:NH2	2.54	0.41
1:D:353:HIS:CE1	1:D:355:TRP:CG	3.09	0.41
1:E:198:THR:HB	1:E:201:ILE:CD1	2.50	0.41
1:F:626:VAL:HG12	1:F:681:ALA:CB	2.51	0.41
1:A:470:PHE:HD1	1:A:482:PHE:CE2	2.39	0.41
1:B:236:GLU:CD	1:B:275:TYR:CE2	2.99	0.41
1:B:318:HIS:HD2	1:B:320:SER:N	2.18	0.41
1:E:377:PRO:HA	1:E:378:PRO:HA	1.75	0.41
1:E:505:LEU:HD13	1:E:552:TYR:CZ	2.56	0.41
1:F:324:ILE:HD11	1:F:410:HIS:NE2	2.36	0.41
1:A:21:ASP:OD1	1:A:22:ASP:N	2.53	0.41
1:A:519:ILE:HD13	1:A:627:THR:O	2.21	0.41
1:A:690:PRO:C	1:A:692:GLU:H	2.29	0.41
1:B:185:THR:H	1:B:192:ARG:CZ	2.34	0.41
1:B:446:SER:HB3	1:B:463:PHE:CD1	2.56	0.41
1:B:625:VAL:HG11	1:B:672:ILE:HD13	2.02	0.41
1:C:152:ASN:HD21	1:D:368:ASP:CG	2.28	0.41
1:C:377:PRO:HA	1:C:378:PRO:HA	1.81	0.41
1:D:534:TYR:OH	1:D:556:GLU:OE1	2.14	0.41
1:D:626:VAL:HG12	1:D:681:ALA:HB2	2.03	0.41
1:E:175:PRO:O	1:E:179:ALA:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:THR:HA	1:E:186:PRO:HD3	1.95	0.41
1:E:676:PRO:C	1:E:678:ARG:N	2.79	0.41
1:F:115:ARG:NH1	1:F:115:ARG:HG3	2.36	0.41
1:F:501:THR:HB	1:F:502:PRO:HD2	2.03	0.41
1:B:399:GLU:OE2	1:B:402:ARG:NH1	2.54	0.41
1:C:188:ASP:O	1:C:191:THR:HG22	2.21	0.41
1:C:523:LEU:O	1:C:527:MET:HG3	2.21	0.41
1:D:676:PRO:O	1:D:677:ALA:HB3	2.21	0.41
1:E:600:PHE:CE1	1:E:609:LEU:HD11	2.56	0.41
1:F:115:ARG:HG3	1:F:115:ARG:HH11	1.86	0.41
1:B:357:ARG:HH11	1:B:357:ARG:HB2	1.85	0.40
1:D:573:ARG:HH11	1:D:573:ARG:HG3	1.86	0.40
1:E:245:TRP:HA	1:E:250:ASN:O	2.20	0.40
1:E:304:PRO:O	1:E:307:ILE:HD13	2.21	0.40
1:E:433:ALA:O	1:E:437:THR:HG22	2.21	0.40
1:F:197:LEU:HD23	1:F:198:THR:N	2.36	0.40
1:A:419:ASN:N	1:A:420:PRO:HD3	2.36	0.40
1:B:174:ASP:OD2	1:B:177:LEU:HD22	2.22	0.40
1:B:690:PRO:C	1:B:692:GLU:H	2.29	0.40
1:C:676:PRO:O	1:C:677:ALA:HB3	2.21	0.40
1:D:150:LEU:HG	1:D:154:LEU:HD11	2.02	0.40
1:D:471:THR:O	1:D:506:HIS:CD2	2.74	0.40
1:E:236:GLU:CD	1:E:275:TYR:CE2	3.00	0.40
1:C:150:LEU:C	1:C:152:ASN:H	2.29	0.40
1:C:615:ASP:HA	1:C:616:PRO:HD2	1.82	0.40
1:D:150:LEU:C	1:D:152:ASN:H	2.29	0.40
1:D:246:ASP:OD1	1:D:246:ASP:N	2.54	0.40
1:D:314:HIS:CD2	1:D:353:HIS:HE2	2.40	0.40
1:F:446:SER:O	1:F:446:SER:OG	2.37	0.40
1:F:676:PRO:C	1:F:678:ARG:N	2.79	0.40
1:A:133:TRP:CE2	1:A:157:GLY:HA3	2.57	0.40
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.89	0.40
1:B:357:ARG:HG3	1:B:358:GLU:N	2.37	0.40
1:B:523:LEU:O	1:B:527:MET:HG3	2.21	0.40
1:C:580:THR:O	1:C:584:ILE:HG13	2.21	0.40
1:D:236:GLU:HB3	1:D:534:TYR:HA	2.02	0.40
1:E:539:LEU:HA	1:E:539:LEU:HD23	1.83	0.40
1:E:575:LEU:O	1:E:579:ILE:HG13	2.21	0.40
1:E:676:PRO:O	1:E:677:ALA:HB3	2.21	0.40
1:A:318:HIS:HE2	1:A:320:SER:HB2	1.86	0.40
1:A:523:LEU:O	1:A:527:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:181:ALA:N	2.44	0.40
1:D:181:ALA:HB1	1:D:192:ARG:HH22	1.86	0.40
1:D:239:PRO:HD3	1:D:276:LEU:HD22	2.02	0.40

All (2) 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:E:29:CYS:CB	1:E:29:CYS:SG[2_656]	1.82	0.38
1:F:29:CYS:CB	1:F:29:CYS:SG[2_555]	1.84	0.36

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	655/723 (91%)	632 (96%)	18 (3%)	5 (1%)	16	45
1	B	655/723 (91%)	630 (96%)	16 (2%)	9 (1%)	9	33
1	C	655/723 (91%)	632 (96%)	17 (3%)	6 (1%)	14	43
1	D	655/723 (91%)	624 (95%)	25 (4%)	6 (1%)	14	43
1	E	655/723 (91%)	632 (96%)	18 (3%)	5 (1%)	16	45
1	F	655/723 (91%)	631 (96%)	18 (3%)	6 (1%)	14	43
All	All	3930/4338 (91%)	3781 (96%)	112 (3%)	37 (1%)	14	43

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	SER
1	A	170	ARG
1	B	151	SER
1	B	488	GLU

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Mol	Chain	Res	Type
1	C	68	ARG
1	C	69	TYR
1	C	151	SER
1	C	172	LEU
1	C	488	GLU
1	D	69	TYR
1	D	151	SER
1	D	170	ARG
1	D	183	LEU
1	D	488	GLU
1	E	151	SER
1	E	488	GLU
1	F	488	GLU
1	A	67	VAL
1	A	488	GLU
1	B	171	GLY
1	B	194	ALA
1	F	150	LEU
1	B	100	SER
1	E	194	ALA
1	F	68	ARG
1	F	193	THR
1	B	70	PRO
1	B	199	PRO
1	E	171	GLY
1	F	67	VAL
1	A	393	PRO
1	B	168	VAL
1	B	393	PRO
1	E	393	PRO
1	F	393	PRO
1	C	393	PRO
1	D	393	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	543/597 (91%)	490 (90%)	53 (10%)	7	28
1	B	543/597 (91%)	485 (89%)	58 (11%)	6	24
1	C	543/597 (91%)	498 (92%)	45 (8%)	10	34
1	D	543/597 (91%)	496 (91%)	47 (9%)	9	32
1	E	543/597 (91%)	492 (91%)	51 (9%)	8	30
1	F	543/597 (91%)	497 (92%)	46 (8%)	10	33
All	All	3258/3582 (91%)	2958 (91%)	300 (9%)	8	30

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	53	HIS
1	A	59	THR
1	A	68	ARG
1	A	94	LEU
1	A	128	ASP
1	A	137	LEU
1	A	151	SER
1	A	154	LEU
1	A	162	GLU
1	A	168	VAL
1	A	172	LEU
1	A	174	ASP
1	A	183	LEU
1	A	190	VAL
1	A	192	ARG
1	A	198	THR
1	A	201	ILE
1	A	204	LEU
1	A	214	VAL
1	A	237	MET
1	A	255	THR
1	A	282	ILE
1	A	285	VAL
1	A	301	VAL
1	A	303	SER
1	A	309	SER
1	A	323	THR
1	A	332	SER
1	A	352	ASP

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Mol	Chain	Res	Type
1	A	357	ARG
1	A	361	GLN
1	A	370	THR
1	A	404	VAL
1	A	464	THR
1	A	466	SER
1	A	471	THR
1	A	475	THR
1	A	485	GLN
1	A	493	ARG
1	A	542	HIS
1	A	543	ARG
1	A	581	ARG
1	A	593	GLN
1	A	626	VAL
1	A	627	THR
1	A	629	ASN
1	A	638	LEU
1	A	659	ILE
1	A	664	TYR
1	A	678	ARG
1	A	694	ARG
1	A	696	THR
1	B	26	VAL
1	B	53	HIS
1	B	68	ARG
1	B	71	HIS
1	B	92	LYS
1	B	94	LEU
1	B	102	GLN
1	B	110	GLN
1	B	128	ASP
1	B	154	LEU
1	B	170	ARG
1	B	173	ARG
1	B	174	ASP
1	B	176	LEU
1	B	177	LEU
1	B	183	LEU
1	B	195	LEU
1	B	197	LEU
1	B	198	THR

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Mol	Chain	Res	Type
1	B	201	ILE
1	B	204	LEU
1	B	207	ASP
1	B	214	VAL
1	B	237	MET
1	B	240	ARG
1	B	255	THR
1	B	274	VAL
1	B	282	ILE
1	B	285	VAL
1	B	301	VAL
1	B	303	SER
1	B	323	THR
1	B	332	SER
1	B	348	GLN
1	B	352	ASP
1	B	357	ARG
1	B	370	THR
1	B	404	VAL
1	B	405	GLN
1	B	416	ARG
1	B	464	THR
1	B	466	SER
1	B	471	THR
1	B	485	GLN
1	B	486	ILE
1	B	493	ARG
1	B	501	THR
1	B	505	LEU
1	B	581	ARG
1	B	626	VAL
1	B	627	THR
1	B	638	LEU
1	B	659	ILE
1	B	664	TYR
1	B	678	ARG
1	B	695	ASN
1	B	696	THR
1	B	698	LEU
1	C	26	VAL
1	C	53	HIS
1	C	71	HIS

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Mol	Chain	Res	Type
1	C	92	LYS
1	C	102	GLN
1	C	110	GLN
1	C	112	THR
1	C	141	LEU
1	C	163	ARG
1	C	170	ARG
1	C	173	ARG
1	C	174	ASP
1	C	198	THR
1	C	211	ARG
1	C	214	VAL
1	C	237	MET
1	C	255	THR
1	C	274	VAL
1	C	285	VAL
1	C	287	ARG
1	C	301	VAL
1	C	303	SER
1	C	309	SER
1	C	323	THR
1	C	332	SER
1	C	348	GLN
1	C	352	ASP
1	C	357	ARG
1	C	361	GLN
1	C	368	ASP
1	C	404	VAL
1	C	405	GLN
1	C	464	THR
1	C	466	SER
1	C	543	ARG
1	C	581	ARG
1	C	593	GLN
1	C	627	THR
1	C	629	ASN
1	C	638	LEU
1	C	659	ILE
1	C	664	TYR
1	C	678	ARG
1	C	695	ASN
1	C	696	THR

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Mol	Chain	Res	Type
1	D	26	VAL
1	D	53	HIS
1	D	63	ARG
1	D	115	ARG
1	D	137	LEU
1	D	141	LEU
1	D	150	LEU
1	D	163	ARG
1	D	170	ARG
1	D	172	LEU
1	D	173	ARG
1	D	176	LEU
1	D	183	LEU
1	D	191	THR
1	D	195	LEU
1	D	197	LEU
1	D	198	THR
1	D	201	ILE
1	D	204	LEU
1	D	214	VAL
1	D	237	MET
1	D	255	THR
1	D	301	VAL
1	D	303	SER
1	D	309	SER
1	D	323	THR
1	D	348	GLN
1	D	352	ASP
1	D	363	PHE
1	D	370	THR
1	D	383	ASP
1	D	404	VAL
1	D	405	GLN
1	D	437	THR
1	D	464	THR
1	D	466	SER
1	D	471	THR
1	D	543	ARG
1	D	563	ARG
1	D	593	GLN
1	D	626	VAL
1	D	627	THR

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Mol	Chain	Res	Type
1	D	629	ASN
1	D	638	LEU
1	D	659	ILE
1	D	664	TYR
1	D	696	THR
1	E	26	VAL
1	E	29	CYS
1	E	53	HIS
1	E	71	HIS
1	E	92	LYS
1	E	102	GLN
1	E	112	THR
1	E	115	ARG
1	E	137	LEU
1	E	141	LEU
1	E	149	GLU
1	E	168	VAL
1	E	170	ARG
1	E	173	ARG
1	E	183	LEU
1	E	193	THR
1	E	195	LEU
1	E	197	LEU
1	E	198	THR
1	E	201	ILE
1	E	204	LEU
1	E	211	ARG
1	E	214	VAL
1	E	237	MET
1	E	255	THR
1	E	274	VAL
1	E	301	VAL
1	E	303	SER
1	E	323	THR
1	E	348	GLN
1	E	352	ASP
1	E	357	ARG
1	E	361	GLN
1	E	383	ASP
1	E	405	GLN
1	E	464	THR
1	E	466	SER

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Mol	Chain	Res	Type
1	E	471	THR
1	E	493	ARG
1	E	569	LEU
1	E	581	ARG
1	E	593	GLN
1	E	627	THR
1	E	629	ASN
1	E	638	LEU
1	E	659	ILE
1	E	663	GLU
1	E	674	ILE
1	E	694	ARG
1	E	696	THR
1	E	698	LEU
1	F	26	VAL
1	F	29	CYS
1	F	53	HIS
1	F	68	ARG
1	F	115	ARG
1	F	151	SER
1	F	154	LEU
1	F	163	ARG
1	F	170	ARG
1	F	172	LEU
1	F	192	ARG
1	F	197	LEU
1	F	198	THR
1	F	203	GLU
1	F	204	LEU
1	F	211	ARG
1	F	214	VAL
1	F	237	MET
1	F	255	THR
1	F	274	VAL
1	F	285	VAL
1	F	301	VAL
1	F	303	SER
1	F	323	THR
1	F	324	ILE
1	F	332	SER
1	F	348	GLN
1	F	352	ASP

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Mol	Chain	Res	Type
1	F	361	GLN
1	F	383	ASP
1	F	405	GLN
1	F	437	THR
1	F	447	GLU
1	F	464	THR
1	F	466	SER
1	F	471	THR
1	F	486	ILE
1	F	618	THR
1	F	627	THR
1	F	638	LEU
1	F	659	ILE
1	F	664	TYR
1	F	675	ASP
1	F	678	ARG
1	F	696	THR
1	F	698	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	485	GLN
1	B	318	HIS
1	B	348	GLN
1	B	359	HIS
1	B	593	GLN
1	B	685	ASN
1	C	318	HIS
1	C	359	HIS
1	C	406	HIS
1	C	455	GLN
1	D	314	HIS
1	D	318	HIS
1	D	406	HIS
1	E	318	HIS
1	E	406	HIS
1	E	455	GLN
1	E	485	GLN
1	F	318	HIS
1	F	359	HIS

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Mol	Chain	Res	Type
1	F	685	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	G	1	2	12,12,12	0.58	0	17,17,17	0.86	0
2	GLC	G	2	2	11,11,12	0.96	0	15,15,17	0.72	0
2	GLC	H	1	2	12,12,12	0.56	0	17,17,17	1.05	1 (5%)
2	GLC	H	2	2	11,11,12	1.02	0	15,15,17	0.82	0
2	GLC	I	1	2	12,12,12	0.56	0	17,17,17	0.91	0
2	GLC	I	2	2	11,11,12	0.92	0	15,15,17	0.76	0
2	GLC	J	1	2	12,12,12	0.52	0	17,17,17	1.04	1 (5%)
2	GLC	J	2	2	11,11,12	0.91	0	15,15,17	0.73	0
2	GLC	K	1	2	12,12,12	0.51	0	17,17,17	1.04	1 (5%)
2	GLC	K	2	2	11,11,12	1.00	0	15,15,17	0.86	0
2	GLC	L	1	2	12,12,12	0.53	0	17,17,17	1.00	1 (5%)
2	GLC	L	2	2	11,11,12	0.97	0	15,15,17	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	1	2	-	1/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	1/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	GLC	C4-C3-C2	-2.45	106.53	110.83
2	K	1	GLC	C4-C3-C2	-2.19	106.99	110.83
2	J	1	GLC	C1-O5-C5	2.08	117.68	113.65
2	L	1	GLC	C4-C3-C2	-2.02	107.29	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	GLC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	J	2	GLC	O5-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

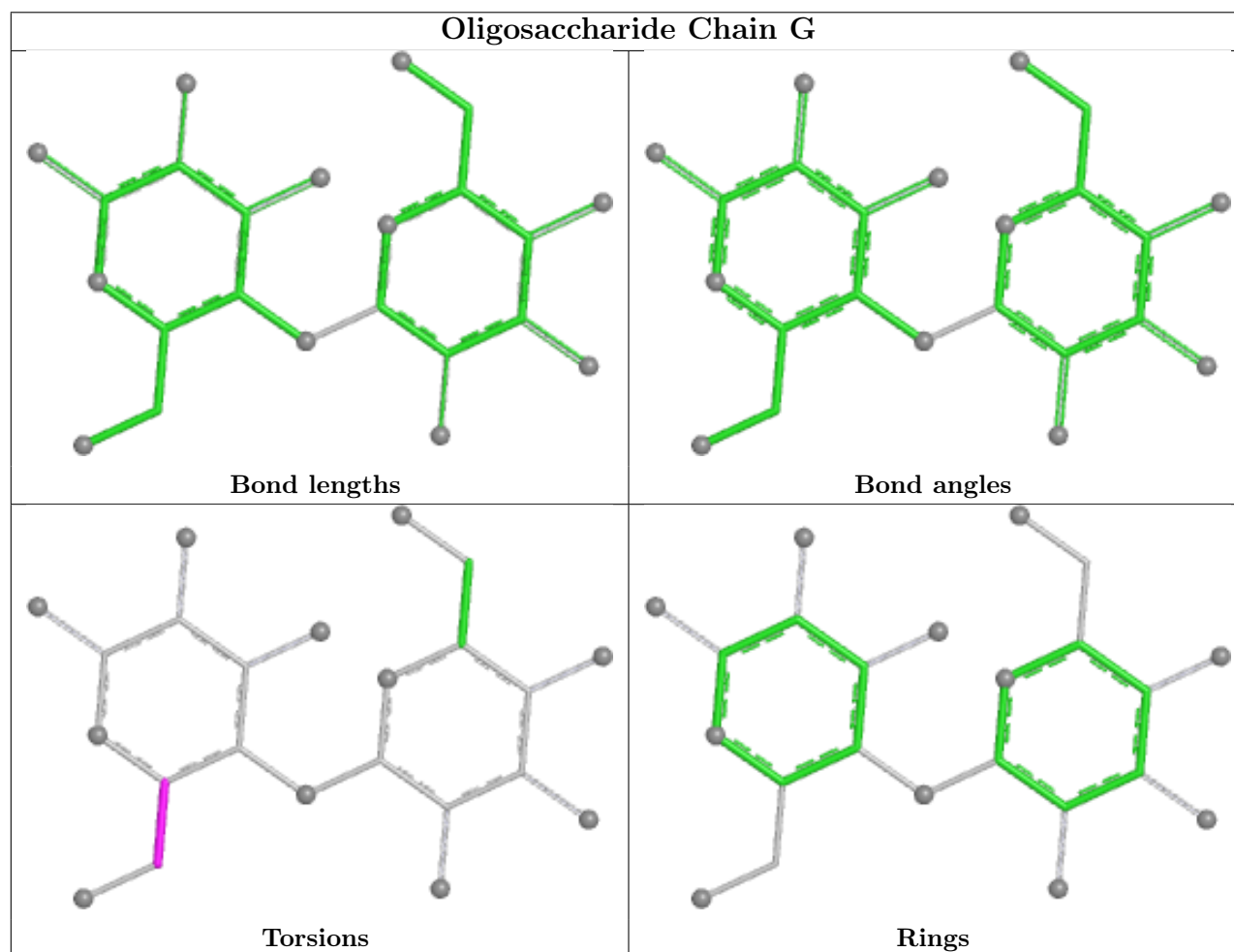
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	GLC	1	0
2	H	1	GLC	1	0

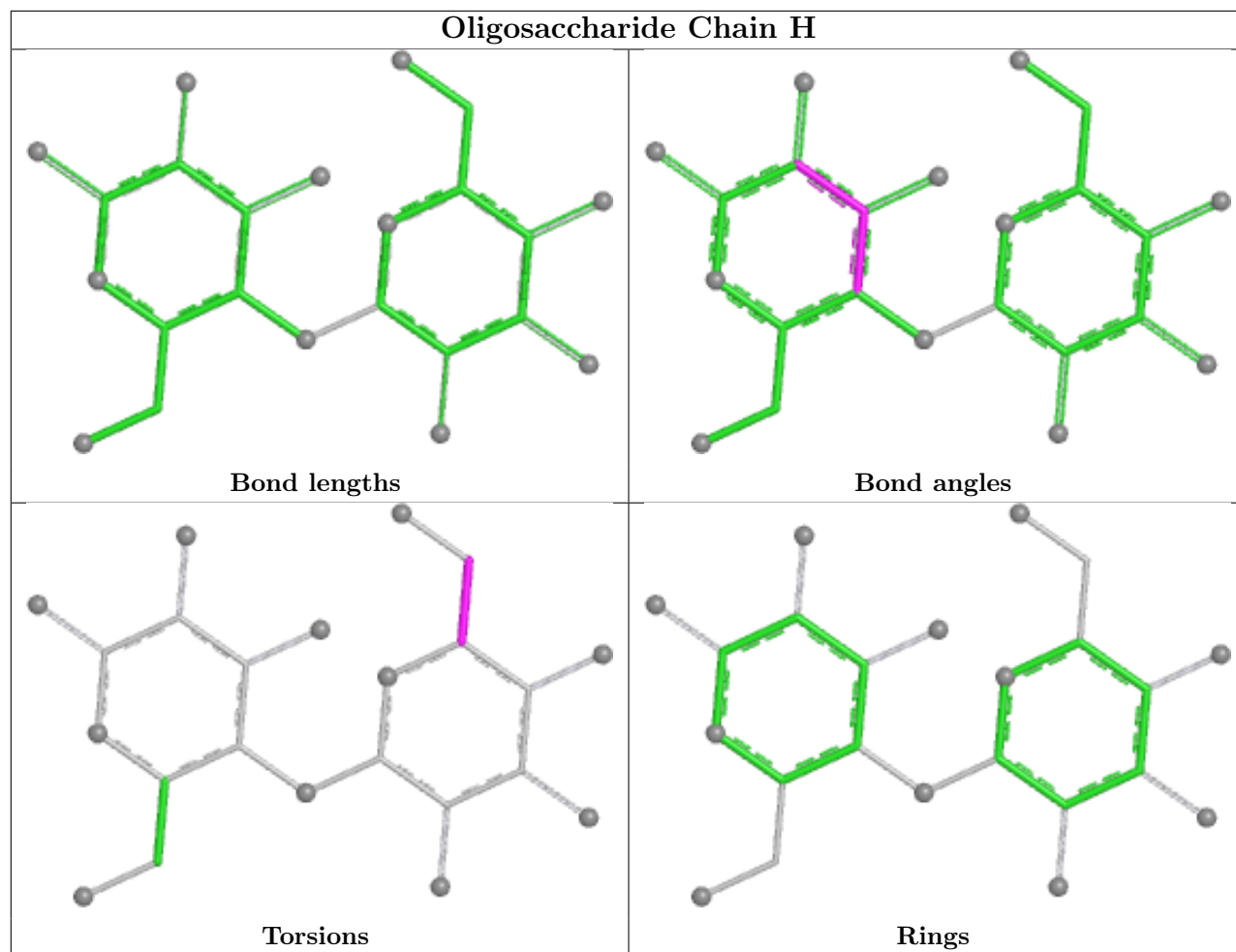
Continued on next page...

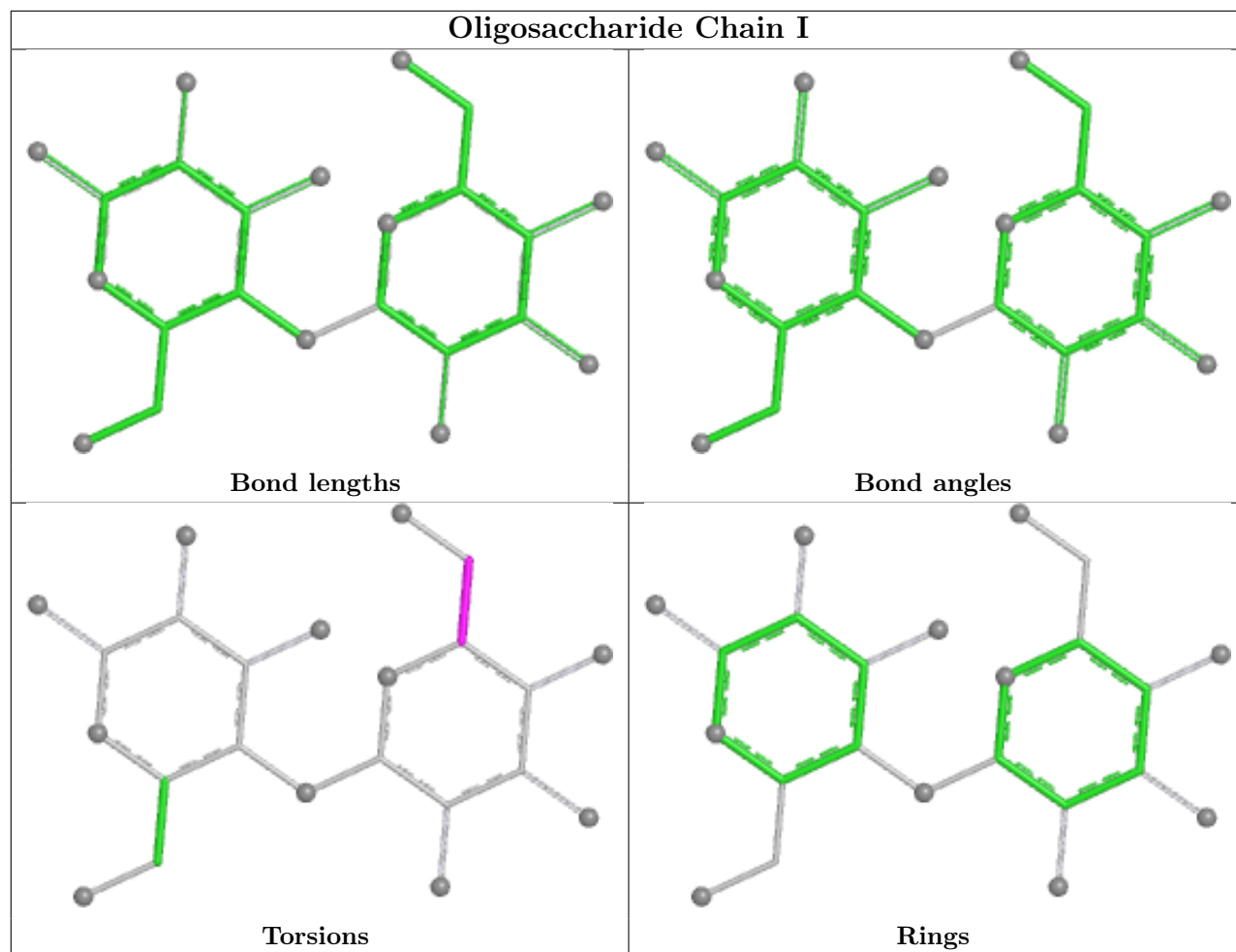
Continued from previous page...

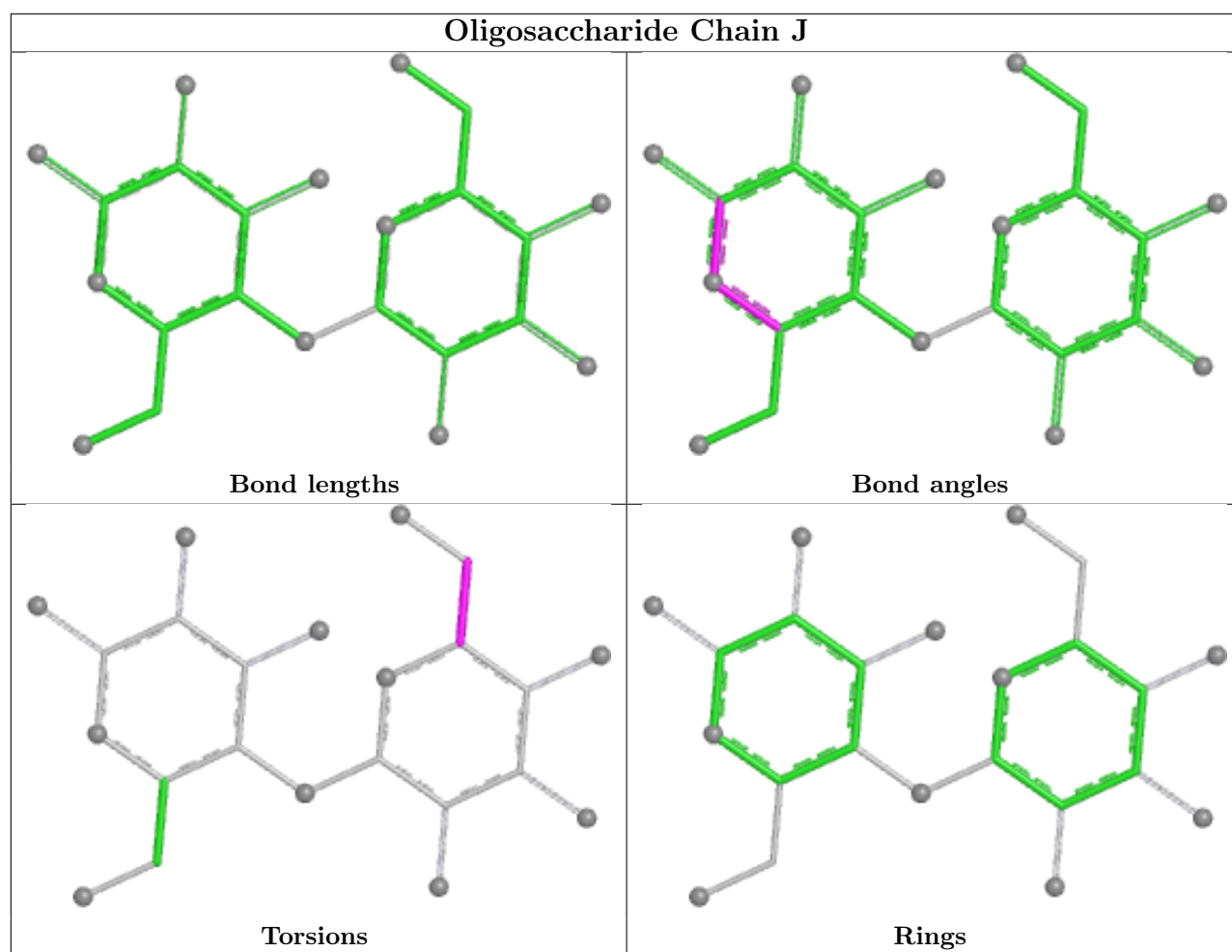
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	GLC	1	0
2	K	2	GLC	1	0
2	L	1	GLC	2	0
2	K	1	GLC	1	0
2	G	1	GLC	1	0

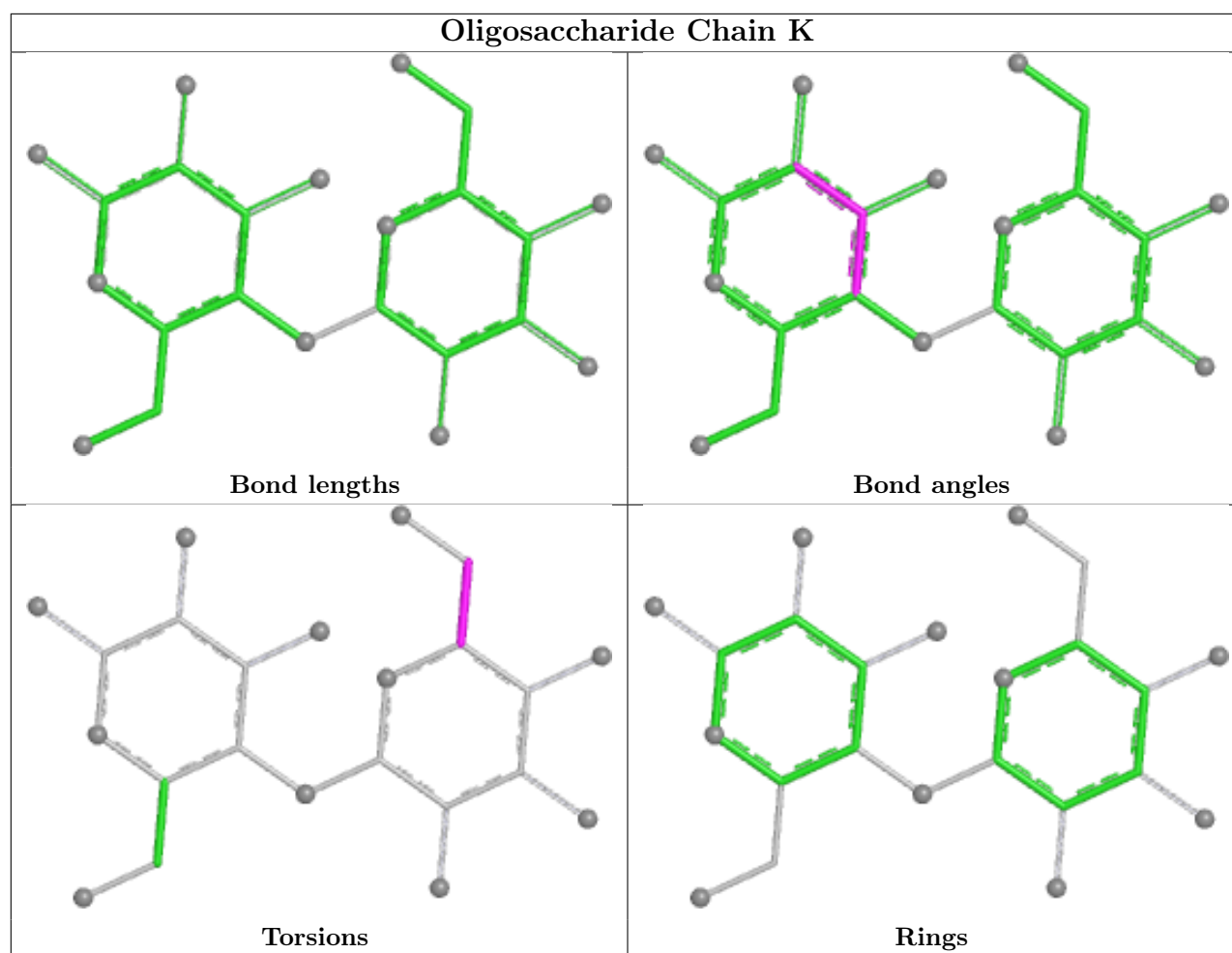
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

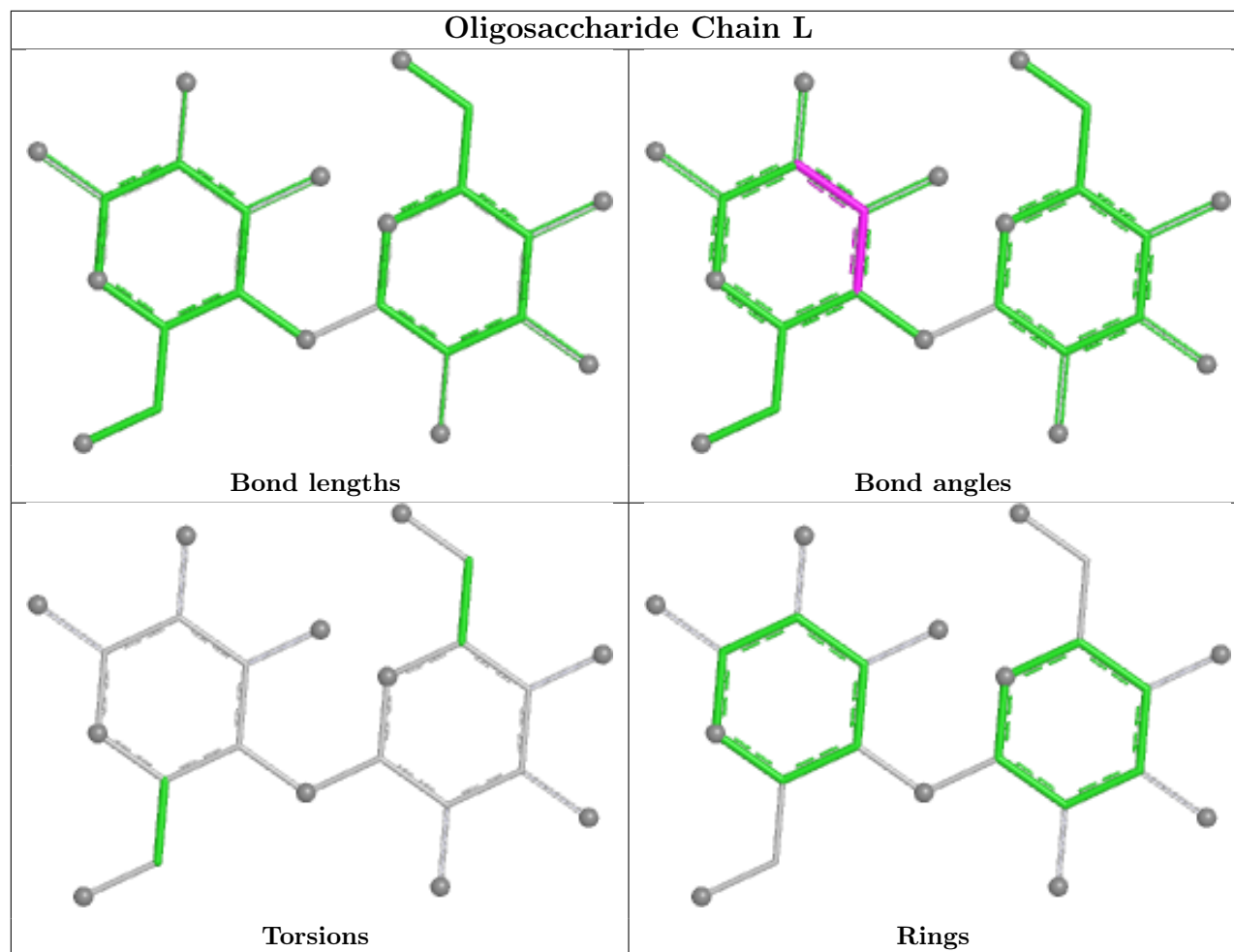












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	661/723 (91%)	-1.36	1 (0%) 91 86	47, 65, 120, 146	0
1	B	661/723 (91%)	-1.38	1 (0%) 91 86	46, 66, 124, 148	0
1	C	661/723 (91%)	-1.35	2 (0%) 90 82	46, 65, 119, 137	0
1	D	661/723 (91%)	-1.37	3 (0%) 87 76	45, 65, 123, 144	0
1	E	661/723 (91%)	-1.37	1 (0%) 91 86	47, 65, 119, 148	0
1	F	661/723 (91%)	-1.41	1 (0%) 91 86	47, 65, 114, 136	0
All	All	3966/4338 (91%)	-1.37	9 (0%) 91 86	45, 65, 120, 148	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	PRO	3.1
1	A	15	PRO	3.1
1	D	15	PRO	2.8
1	B	169	PRO	2.7
1	D	197	LEU	2.6
1	D	169	PRO	2.6
1	F	15	PRO	2.3
1	E	15	PRO	2.2
1	C	71	HIS	2.1

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

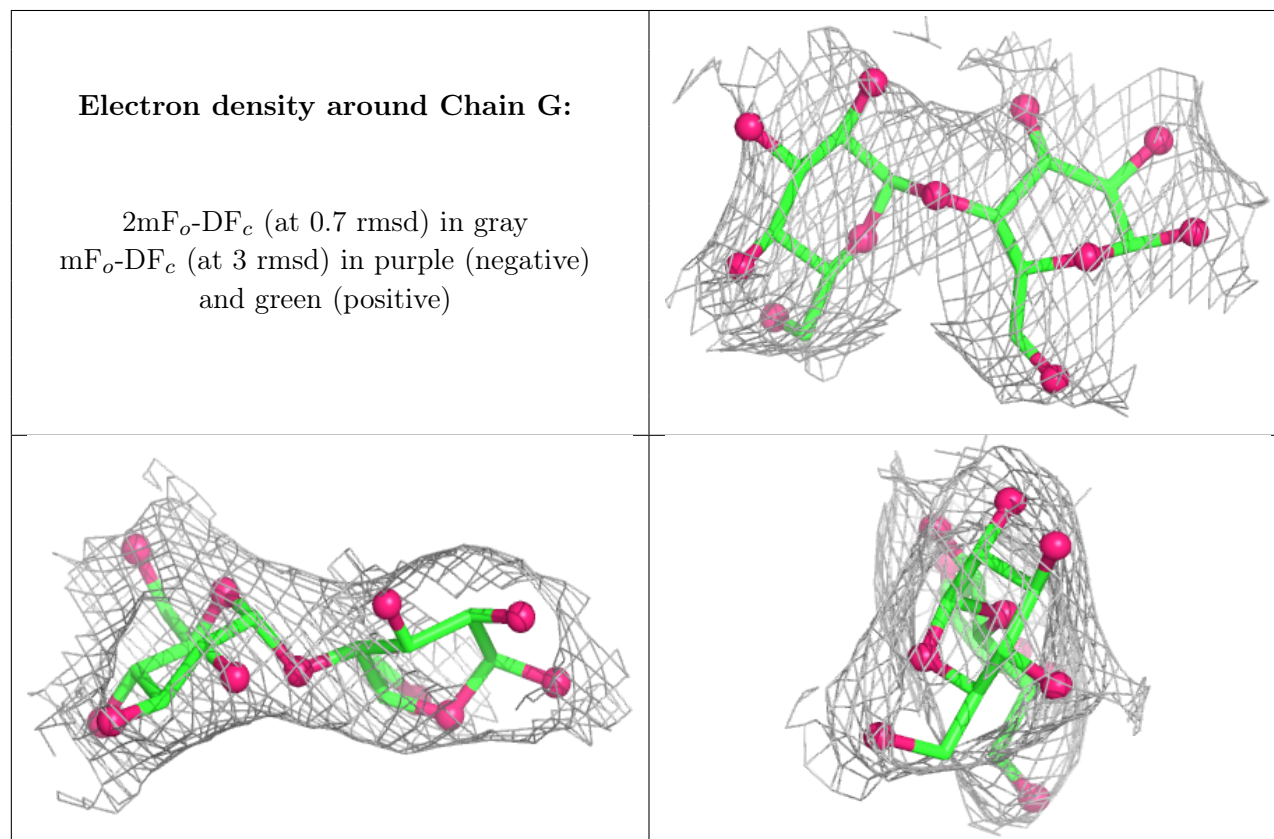
There are no non-standard protein/DNA/RNA residues in this entry.

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.

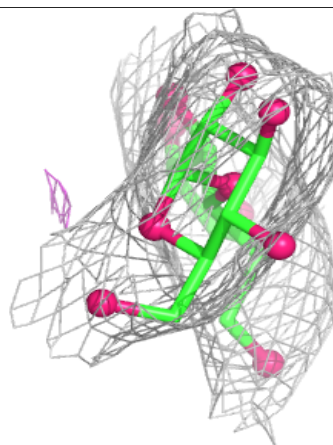
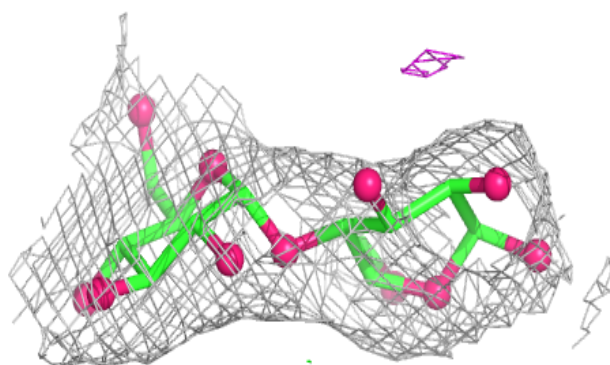
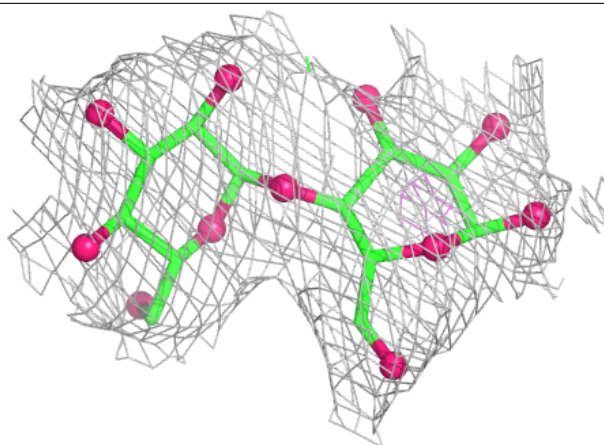
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	H	1	12/12	0.99	0.04	76,83,87,89	0
2	GLC	I	2	11/12	0.99	0.03	76,80,81,82	0
2	GLC	L	1	12/12	0.99	0.03	74,80,88,88	0
2	GLC	L	2	11/12	0.99	0.04	74,79,82,82	0
2	GLC	I	1	12/12	1.00	0.03	78,83,87,89	0
2	GLC	G	2	11/12	1.00	0.04	77,83,84,85	0
2	GLC	J	1	12/12	1.00	0.03	76,82,87,87	0
2	GLC	J	2	11/12	1.00	0.03	77,81,83,84	0
2	GLC	K	1	12/12	1.00	0.03	79,85,90,92	0
2	GLC	K	2	11/12	1.00	0.04	76,81,83,83	0
2	GLC	G	1	12/12	1.00	0.03	75,83,87,89	0
2	GLC	H	2	11/12	1.00	0.03	75,80,82,82	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.

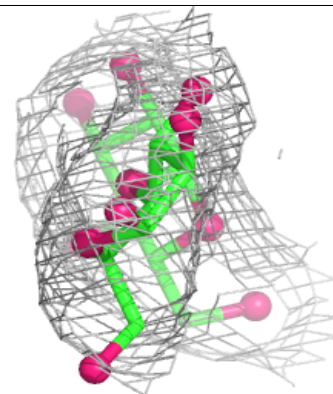
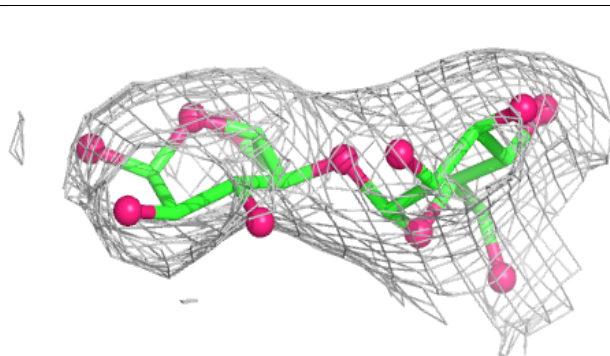
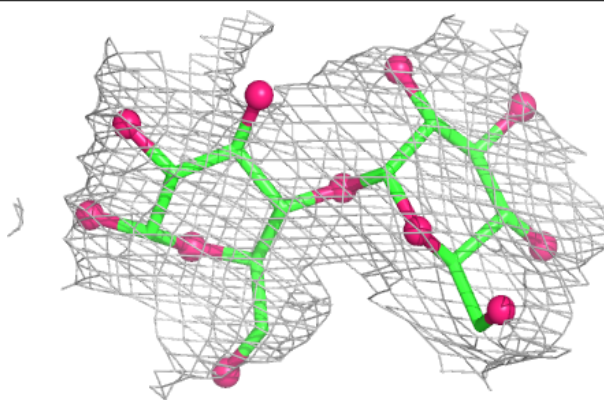


Electron density around Chain H:

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

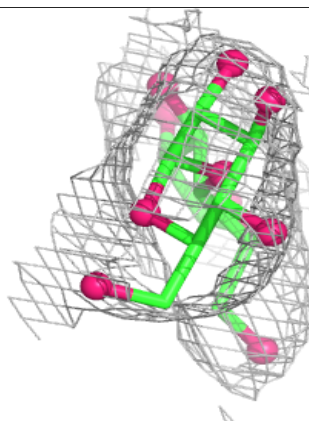
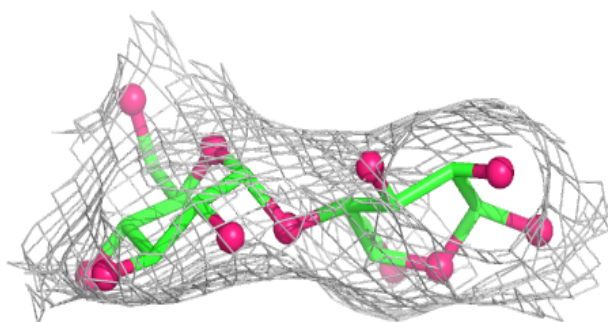
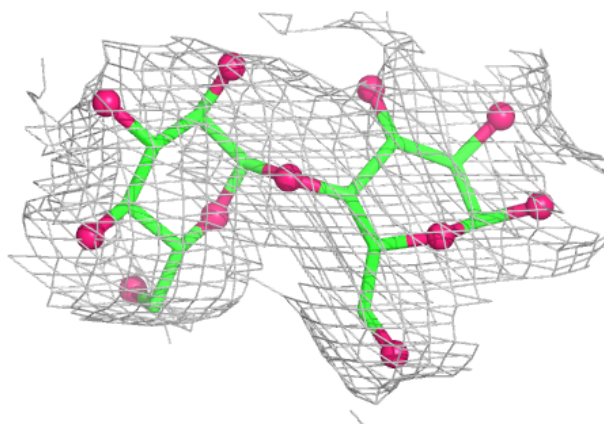
**Electron density around Chain I:**

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

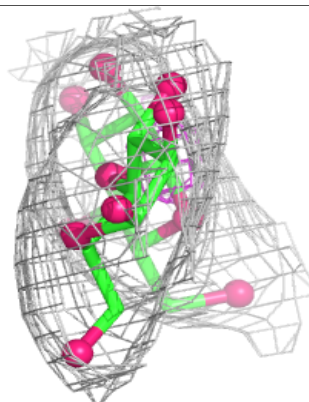
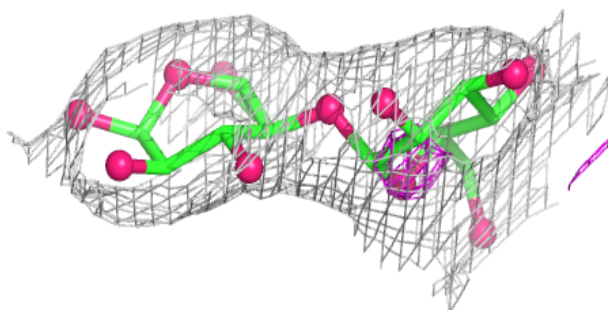
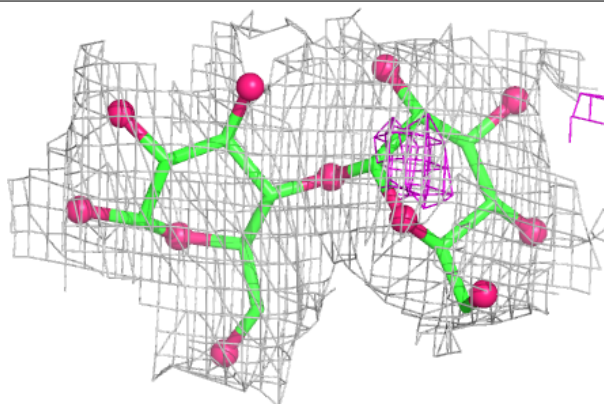


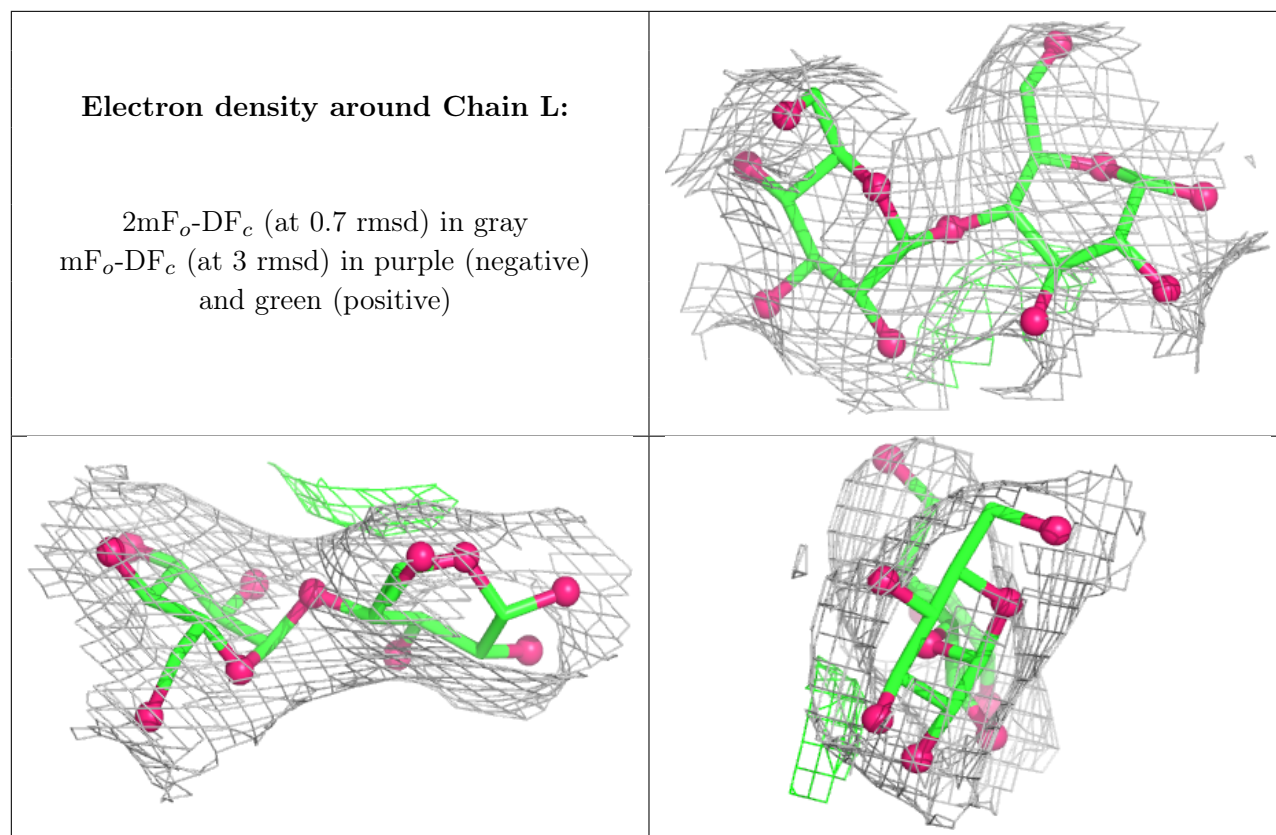
Electron density around Chain J:

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

**Electron density around Chain K:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.