Full wwPDB X-ray Structure Validation Report (i)

Mar 14, 2026 – 01:28 AM UTC

PDB ID	:	3MUU / pdb_00003muu
Title	:	Crystal structure of the Sindbis virus E2-E1 heterodimer at low pH
Authors	:	Li, L.; Jose, J.; Xiang, Y.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2010-05-03
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 (i) 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 (1)) were used in the production of this report:

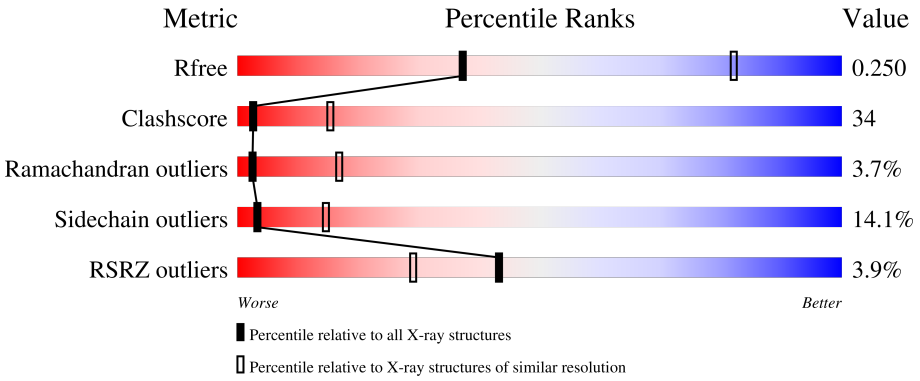
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 <=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	750	3% 38% 36% 9% • 17%
1	B	750	3% 37% 38% 8% • 17%
1	C	750	3% 37% 37% 8% • 17%
1	D	750	3% 38% 37% 8% • 17%
1	E	750	3% 39% 35% 9% • 17%

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Mol	Chain	Length	Quality of chain
1	F	750	3% 38% 35% 8% 18%
2	G	4	25% 75%
2	I	4	25% 75%
2	J	4	75% 25%
2	K	4	25% 75%
2	L	4	25% 75%
2	M	4	25% 50% 25%
2	O	4	50% 50%
2	Q	4	100%
3	H	5	20% 80%
3	P	5	20% 40% 40%
3	R	5	20% 20% 60%
4	N	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	1	X	-	-	-
2	NAG	Q	1	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29159 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 Structural polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	Se	0	0	0
			4767	3015	808	910	24	10			
1	B	622	Total	C	N	O	S	Se	0	0	0
			4761	3013	808	906	24	10			
1	C	622	Total	C	N	O	S	Se	0	0	0
			4761	3012	807	908	24	10			
1	D	622	Total	C	N	O	S	Se	0	0	0
			4760	3009	807	910	24	10			
1	E	623	Total	C	N	O	S	Se	0	0	0
			4761	3012	808	907	24	10			
1	F	618	Total	C	N	O	S	Se	0	0	0
			4727	2990	801	902	24	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	GLY	-	linker	UNP P03316
A	346	GLY	-	linker	UNP P03316
A	347	GLY	-	linker	UNP P03316
A	348	SER	-	linker	UNP P03316
A	349	TRP	-	linker	UNP P03316
A	350	SER	-	linker	UNP P03316
A	351	HIS	-	linker	UNP P03316
A	352	PRO	-	linker	UNP P03316
A	353	GLN	-	linker	UNP P03316
A	354	PHE	-	linker	UNP P03316
A	355	GLU	-	linker	UNP P03316
A	356	LYS	-	linker	UNP P03316
A	357	GLY	-	linker	UNP P03316
A	358	GLY	-	linker	UNP P03316
A	359	GLY	-	linker	UNP P03316
A	360	GLY	-	linker	UNP P03316
A	435	GLY	ASP	engineered mutation	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	GLY	-	linker	UNP P03316
B	346	GLY	-	linker	UNP P03316
B	347	GLY	-	linker	UNP P03316
B	348	SER	-	linker	UNP P03316
B	349	TRP	-	linker	UNP P03316
B	350	SER	-	linker	UNP P03316
B	351	HIS	-	linker	UNP P03316
B	352	PRO	-	linker	UNP P03316
B	353	GLN	-	linker	UNP P03316
B	354	PHE	-	linker	UNP P03316
B	355	GLU	-	linker	UNP P03316
B	356	LYS	-	linker	UNP P03316
B	357	GLY	-	linker	UNP P03316
B	358	GLY	-	linker	UNP P03316
B	359	GLY	-	linker	UNP P03316
B	360	GLY	-	linker	UNP P03316
B	435	GLY	ASP	engineered mutation	UNP P03316
C	345	GLY	-	linker	UNP P03316
C	346	GLY	-	linker	UNP P03316
C	347	GLY	-	linker	UNP P03316
C	348	SER	-	linker	UNP P03316
C	349	TRP	-	linker	UNP P03316
C	350	SER	-	linker	UNP P03316
C	351	HIS	-	linker	UNP P03316
C	352	PRO	-	linker	UNP P03316
C	353	GLN	-	linker	UNP P03316
C	354	PHE	-	linker	UNP P03316
C	355	GLU	-	linker	UNP P03316
C	356	LYS	-	linker	UNP P03316
C	357	GLY	-	linker	UNP P03316
C	358	GLY	-	linker	UNP P03316
C	359	GLY	-	linker	UNP P03316
C	360	GLY	-	linker	UNP P03316
C	435	GLY	ASP	engineered mutation	UNP P03316
D	345	GLY	-	linker	UNP P03316
D	346	GLY	-	linker	UNP P03316
D	347	GLY	-	linker	UNP P03316
D	348	SER	-	linker	UNP P03316
D	349	TRP	-	linker	UNP P03316
D	350	SER	-	linker	UNP P03316
D	351	HIS	-	linker	UNP P03316
D	352	PRO	-	linker	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
D	353	GLN	-	linker	UNP P03316
D	354	PHE	-	linker	UNP P03316
D	355	GLU	-	linker	UNP P03316
D	356	LYS	-	linker	UNP P03316
D	357	GLY	-	linker	UNP P03316
D	358	GLY	-	linker	UNP P03316
D	359	GLY	-	linker	UNP P03316
D	360	GLY	-	linker	UNP P03316
D	435	GLY	ASP	engineered mutation	UNP P03316
E	345	GLY	-	linker	UNP P03316
E	346	GLY	-	linker	UNP P03316
E	347	GLY	-	linker	UNP P03316
E	348	SER	-	linker	UNP P03316
E	349	TRP	-	linker	UNP P03316
E	350	SER	-	linker	UNP P03316
E	351	HIS	-	linker	UNP P03316
E	352	PRO	-	linker	UNP P03316
E	353	GLN	-	linker	UNP P03316
E	354	PHE	-	linker	UNP P03316
E	355	GLU	-	linker	UNP P03316
E	356	LYS	-	linker	UNP P03316
E	357	GLY	-	linker	UNP P03316
E	358	GLY	-	linker	UNP P03316
E	359	GLY	-	linker	UNP P03316
E	360	GLY	-	linker	UNP P03316
E	435	GLY	ASP	engineered mutation	UNP P03316
F	345	GLY	-	linker	UNP P03316
F	346	GLY	-	linker	UNP P03316
F	347	GLY	-	linker	UNP P03316
F	348	SER	-	linker	UNP P03316
F	349	TRP	-	linker	UNP P03316
F	350	SER	-	linker	UNP P03316
F	351	HIS	-	linker	UNP P03316
F	352	PRO	-	linker	UNP P03316
F	353	GLN	-	linker	UNP P03316
F	354	PHE	-	linker	UNP P03316
F	355	GLU	-	linker	UNP P03316
F	356	LYS	-	linker	UNP P03316
F	357	GLY	-	linker	UNP P03316
F	358	GLY	-	linker	UNP P03316
F	359	GLY	-	linker	UNP P03316
F	360	GLY	-	linker	UNP P03316

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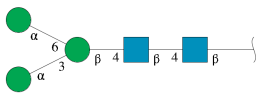
Chain	Residue	Modelled	Actual	Comment	Reference
F	435	GLY	ASP	engineered mutation	UNP P03316

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	4	Total C N O 50 28 2 20	0	0	0
2	I	4	Total C N O 50 28 2 20	0	0	0
2	J	4	Total C N O 50 28 2 20	0	0	0
2	K	4	Total C N O 50 28 2 20	0	0	0
2	L	4	Total C N O 50 28 2 20	0	0	0
2	M	4	Total C N O 50 28 2 20	0	0	0
2	O	4	Total C N O 50 28 2 20	0	0	0
2	Q	4	Total C N O 50 28 2 20	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	H	5	Total C N O 61 34 2 25	0	0	0
3	P	5	Total C N O 61 34 2 25	0	0	0

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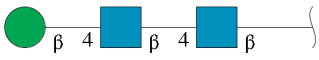
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	R	5	61	34	2	25	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

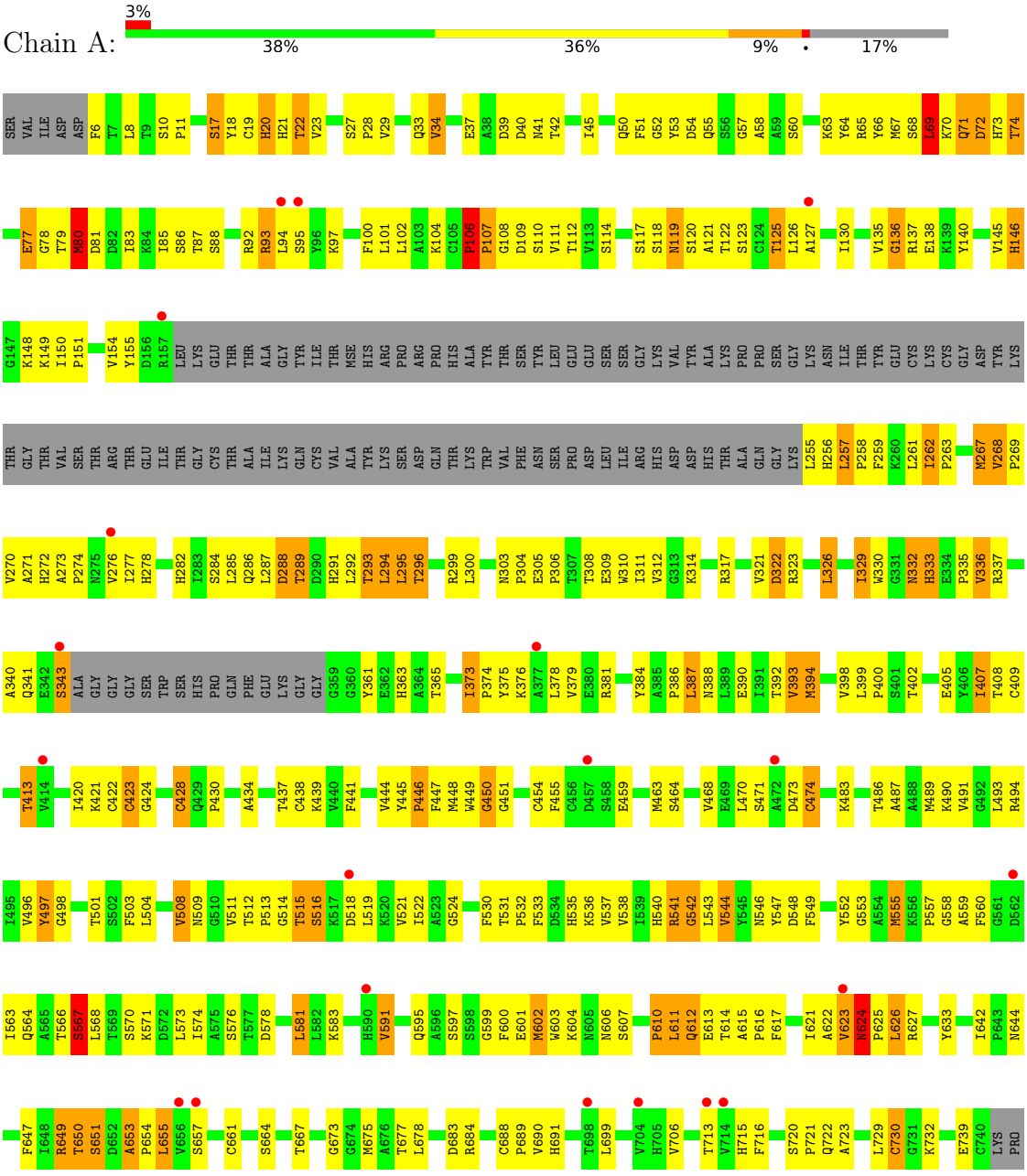


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	N	3	39	22	2	15	0	0	0

3 Residue-property plots (i)

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.

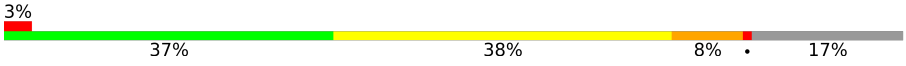
- Molecule 1: Structural polyprotein

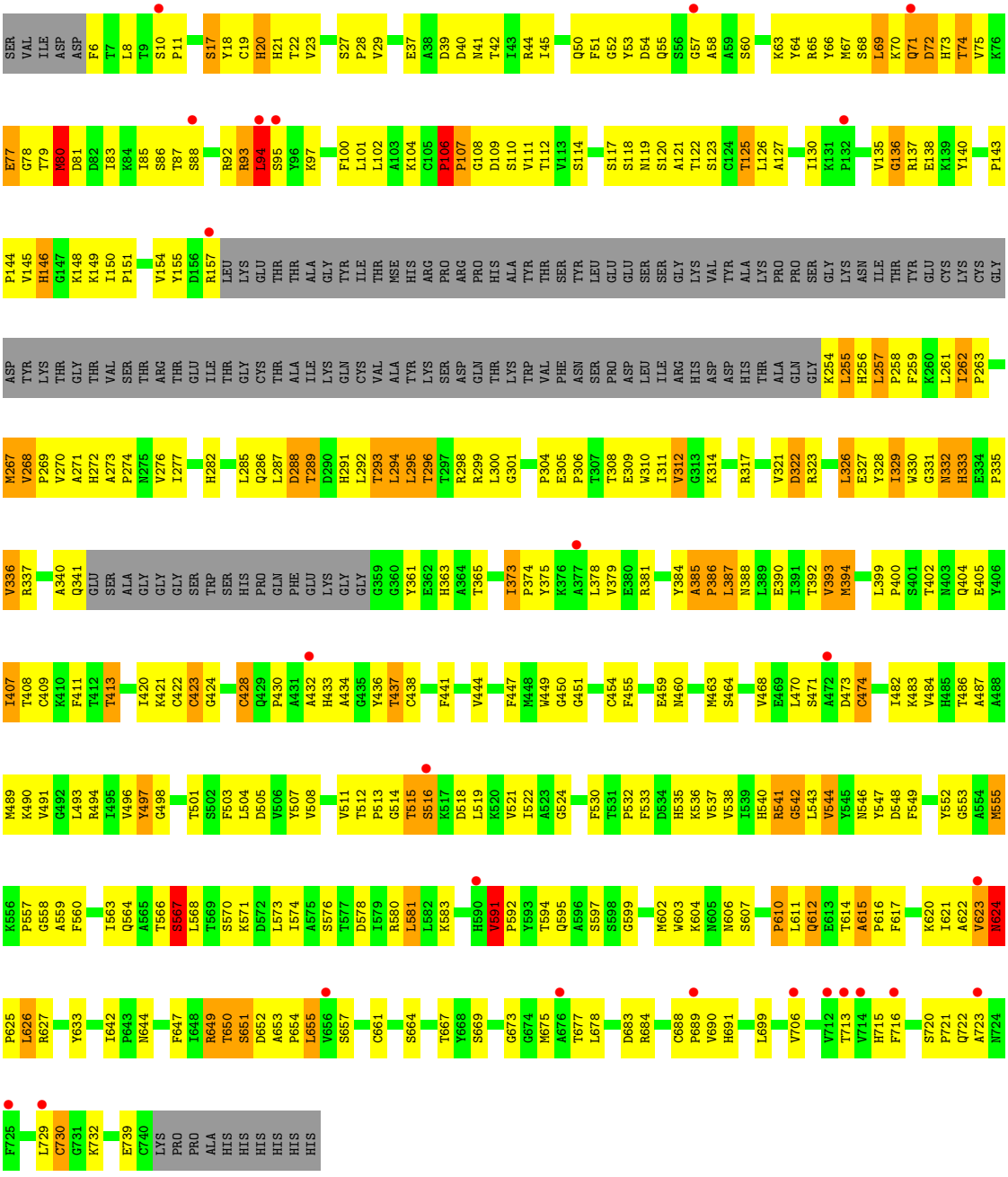




• Molecule 1: Structural polyprotein

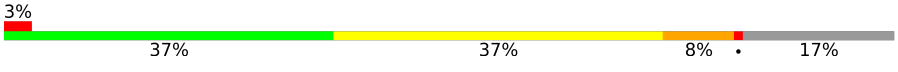
Chain B:

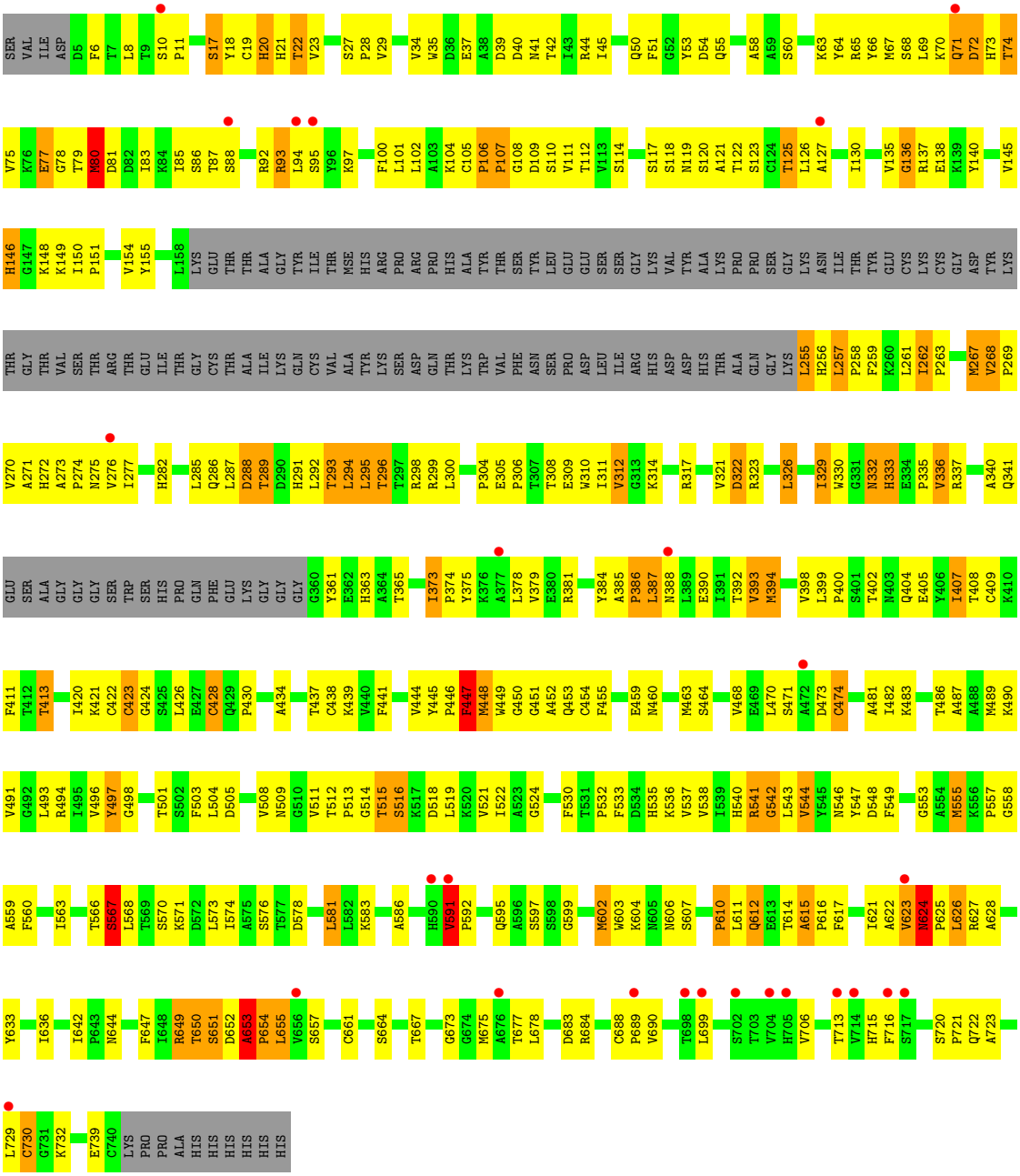




• Molecule 1: Structural polyprotein

Chain C:

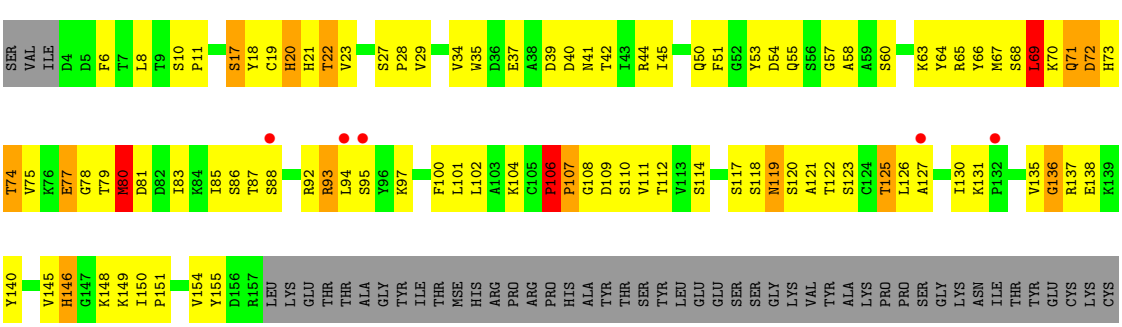


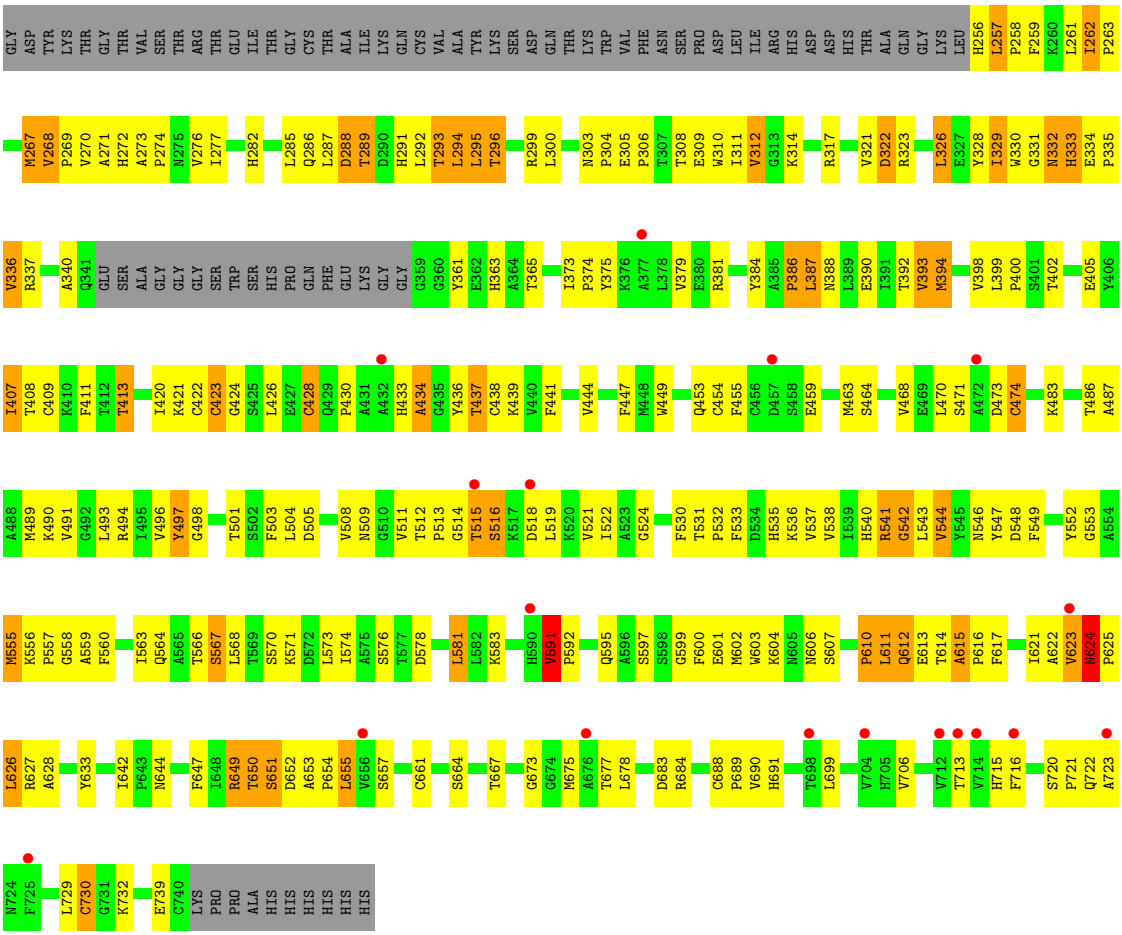


• Molecule 1: Structural polyprotein

Chain D:



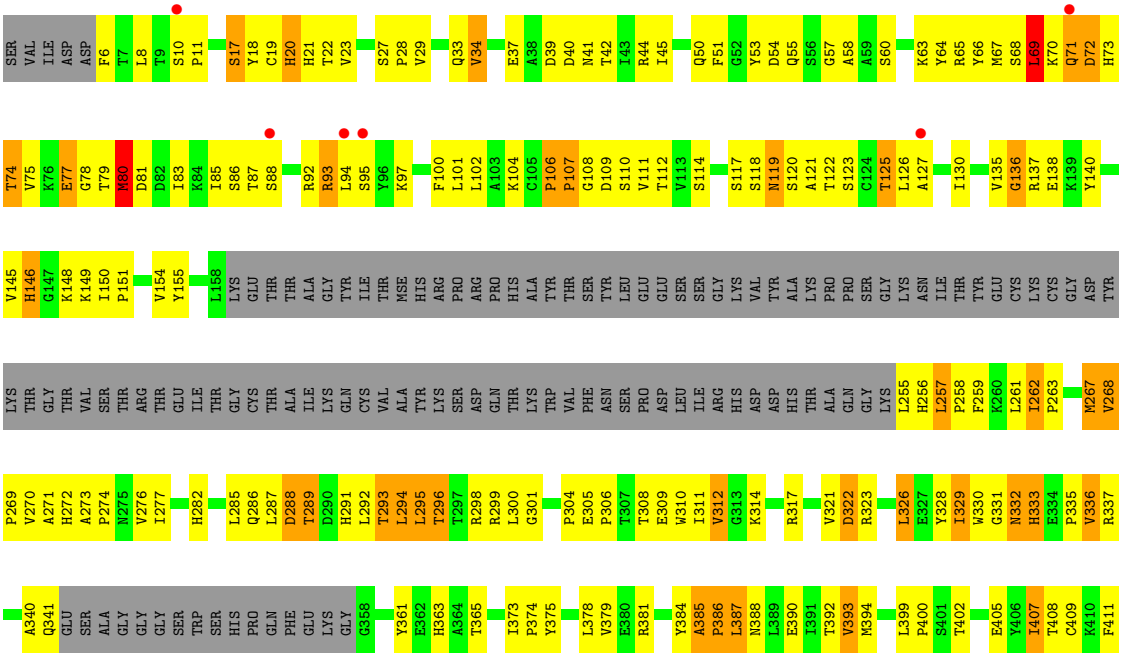


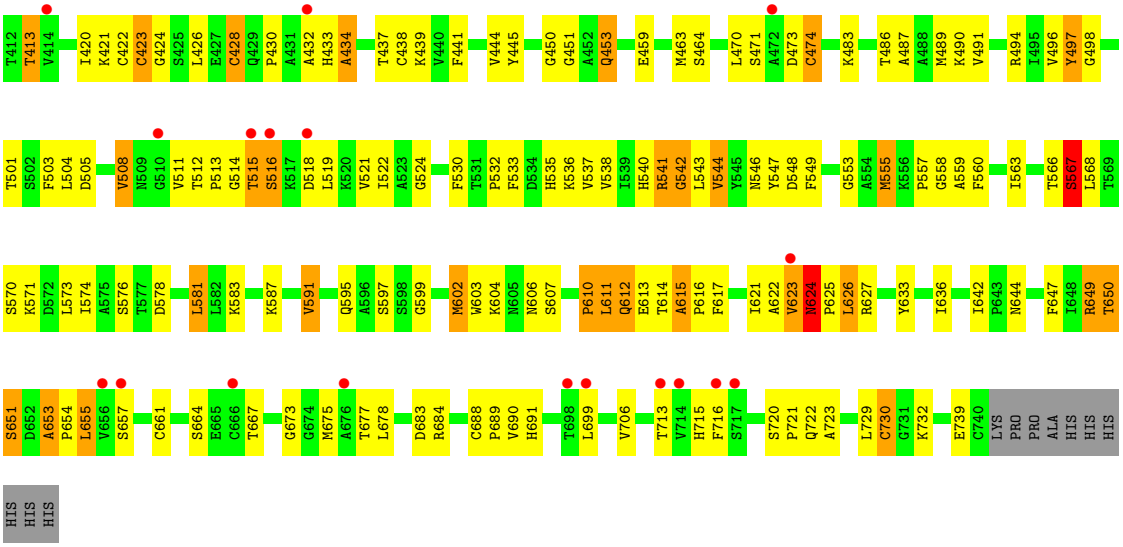


• Molecule 1: Structural polyprotein

Chain E:

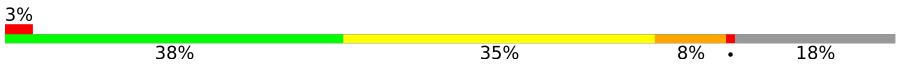


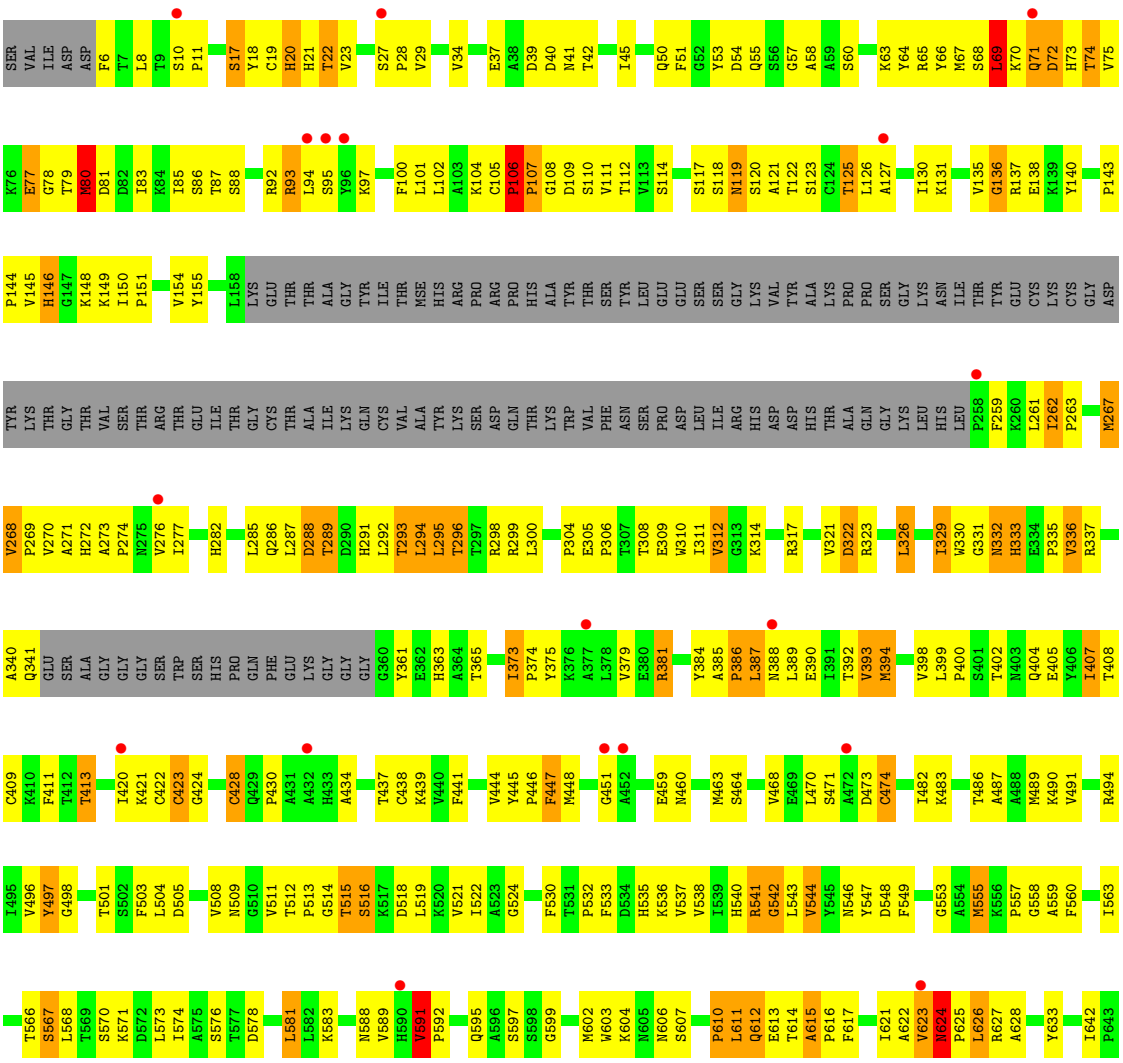


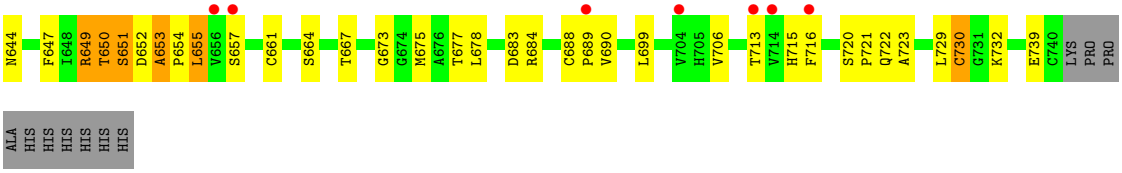


• Molecule 1: Structural polyprotein

Chain F:







• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

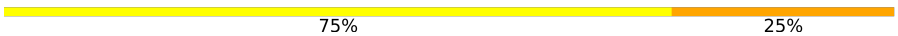
Chain I:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

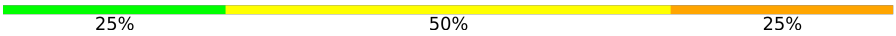
Chain L:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

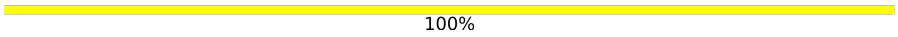
Chain O:





• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:





• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

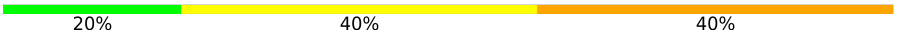
Chain H:





• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:





• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:





• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:




NAG1
NAG2
BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.48Å 158.43Å 160.68Å 60.42° 89.80° 89.65°	Depositor
Resolution (Å)	60.72 – 3.29 60.72 – 3.29	Depositor EDS
% Data completeness (in resolution range)	92.4 (60.72-3.29) 94.4 (60.72-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.239 , 0.252 0.238 , 0.250	Depositor DCC
R_{free} test set	4175 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	87.2	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 122.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,k-l,k 0.033 for h,l,-k+l 0.297 for h,-l,k-l 0.297 for h,-k+l,-k 0.037 for h,-k,-l 0.408 for -h,k,k-l 0.289 for -h,-l,-k 0.033 for -h,k-l,-l 0.309 for -h,-k+l,l 0.039 for -h,-k,-k+l 0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29159	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, BMA, NAG

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	0.44	0/4876	0.94	16/6624 (0.2%)
1	B	0.44	0/4870	0.93	14/6615 (0.2%)
1	C	0.48	3/4870 (0.1%)	0.95	16/6617 (0.2%)
1	D	0.43	0/4869	0.91	9/6615 (0.1%)
1	E	0.43	0/4870	0.93	15/6616 (0.2%)
1	F	0.44	0/4835	0.95	16/6568 (0.2%)
All	All	0.44	3/29190 (0.0%)	0.94	86/39655 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	653	ALA	CA-C	9.59	1.65	1.52
1	C	653	ALA	C-N	5.86	1.47	1.33
1	C	654	PRO	N-CA	5.35	1.54	1.47

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	381	ARG	NE-CZ-NH1	-11.15	110.35	121.50
1	F	381	ARG	NE-CZ-NH2	10.86	128.97	119.20
1	C	653	ALA	CA-C-N	10.23	132.63	119.84
1	C	653	ALA	C-N-CA	10.23	132.63	119.84
1	A	653	ALA	CA-C-N	-8.05	109.78	119.84
1	A	653	ALA	C-N-CA	-8.05	109.78	119.84
1	E	653	ALA	CA-C-N	-7.37	111.44	119.98
1	E	653	ALA	C-N-CA	-7.37	111.44	119.98
1	A	508	VAL	N-CA-C	7.12	113.83	106.21
1	C	615	ALA	CA-C-N	7.02	127.91	120.12
1	C	615	ALA	C-N-CA	7.02	127.91	120.12
1	D	615	ALA	CA-C-N	7.02	127.91	120.12
1	D	615	ALA	C-N-CA	7.02	127.91	120.12
1	E	508	VAL	N-CA-C	6.96	113.66	106.21
1	F	615	ALA	CA-C-N	6.89	127.77	120.12
1	F	615	ALA	C-N-CA	6.89	127.77	120.12
1	F	381	ARG	CD-NE-CZ	6.83	133.97	124.40
1	F	542	GLY	N-CA-C	-6.77	104.02	115.80
1	C	542	GLY	N-CA-C	-6.67	104.20	115.80
1	A	615	ALA	CA-C-N	6.65	127.50	120.12
1	A	615	ALA	C-N-CA	6.65	127.50	120.12
1	D	542	GLY	N-CA-C	-6.60	104.31	115.80
1	B	542	GLY	N-CA-C	-6.57	104.37	115.80
1	A	542	GLY	N-CA-C	-6.56	104.39	115.80
1	E	542	GLY	N-CA-C	-6.53	104.44	115.80
1	B	615	ALA	CA-C-N	6.48	127.31	120.12
1	B	615	ALA	C-N-CA	6.48	127.31	120.12
1	C	373	ILE	CA-C-N	6.29	126.05	119.76
1	C	373	ILE	C-N-CA	6.29	126.05	119.76
1	E	615	ALA	CA-C-N	6.21	127.01	120.12
1	E	615	ALA	C-N-CA	6.21	127.01	120.12
1	B	373	ILE	CA-C-N	6.09	125.85	119.76
1	B	373	ILE	C-N-CA	6.09	125.85	119.76
1	E	373	ILE	CA-C-N	6.06	125.82	119.76
1	E	373	ILE	C-N-CA	6.06	125.82	119.76
1	A	373	ILE	CA-C-N	5.99	125.75	119.76
1	A	373	ILE	C-N-CA	5.99	125.75	119.76
1	C	654	PRO	N-CA-C	5.96	124.75	112.47
1	D	373	ILE	CA-C-N	5.89	125.65	119.76
1	D	373	ILE	C-N-CA	5.89	125.65	119.76
1	F	653	ALA	CA-C-N	-5.89	112.98	120.23
1	F	653	ALA	C-N-CA	-5.89	112.98	120.23
1	F	373	ILE	CA-C-N	5.88	125.64	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	373	ILE	C-N-CA	5.88	125.64	119.76
1	C	653	ALA	N-CA-C	5.69	122.38	109.81
1	A	653	ALA	O-C-N	5.64	125.50	120.48
1	A	591	VAL	N-CA-C	5.61	112.67	107.56
1	B	591	VAL	N-CA-C	5.52	112.58	107.56
1	D	591	VAL	N-CA-C	5.51	112.58	107.56
1	F	591	VAL	N-CA-C	5.51	112.58	107.56
1	B	450	GLY	N-CA-C	-5.42	108.37	115.47
1	C	591	VAL	N-CA-C	5.39	112.47	107.56
1	A	624	ASN	CA-C-N	-5.37	114.26	119.90
1	A	624	ASN	C-N-CA	-5.37	114.26	119.90
1	E	591	VAL	N-CA-C	5.37	112.44	107.56
1	F	39	ASP	N-CA-C	-5.35	105.49	112.23
1	B	39	ASP	N-CA-C	-5.26	105.60	112.23
1	E	567	SER	N-CA-C	5.26	115.18	108.24
1	E	39	ASP	N-CA-C	-5.25	105.61	112.23
1	C	567	SER	N-CA-C	5.25	115.17	108.24
1	C	636	ILE	CB-CA-C	-5.25	104.81	110.85
1	B	94	LEU	CA-CB-CG	-5.24	97.95	116.30
1	A	39	ASP	N-CA-C	-5.24	105.63	112.23
1	C	624	ASN	CA-C-N	-5.23	114.41	119.90
1	C	624	ASN	C-N-CA	-5.23	114.41	119.90
1	C	39	ASP	N-CA-C	-5.21	105.66	112.23
1	A	69	LEU	N-CA-C	-5.21	105.68	111.36
1	D	69	LEU	N-CA-C	-5.19	105.80	111.82
1	D	106	PRO	N-CA-C	5.19	117.03	110.70
1	D	39	ASP	N-CA-C	-5.16	105.73	112.23
1	A	106	PRO	N-CA-C	5.14	116.97	110.70
1	B	69	LEU	N-CA-C	-5.14	105.85	111.82
1	A	567	SER	N-CA-C	5.13	115.02	108.24
1	F	624	ASN	CA-C-N	-5.10	114.54	119.90
1	F	624	ASN	C-N-CA	-5.10	114.54	119.90
1	E	69	LEU	N-CA-C	-5.08	105.93	111.82
1	F	69	LEU	N-CA-C	-5.08	105.93	111.82
1	E	636	ILE	CB-CA-C	-5.08	105.01	110.85
1	C	653	ALA	CA-C-O	-5.07	113.22	120.16
1	B	567	SER	N-CA-C	5.06	114.92	108.24
1	F	106	PRO	N-CA-C	5.03	116.83	110.70
1	B	106	PRO	N-CA-C	5.02	116.83	110.70
1	E	385	ALA	CA-C-N	5.01	126.11	119.84
1	E	385	ALA	C-N-CA	5.01	126.11	119.84
1	B	385	ALA	CA-C-N	5.01	126.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	385	ALA	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	VAL	Peptide
1	A	624	ASN	Peptide
1	B	254	LYS	Peptide
1	B	623	VAL	Peptide
1	B	624	ASN	Peptide
1	C	623	VAL	Peptide
1	C	624	ASN	Peptide
1	D	623	VAL	Peptide
1	D	624	ASN	Peptide
1	E	623	VAL	Peptide
1	E	624	ASN	Peptide
1	F	623	VAL	Peptide
1	F	624	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4767	0	4659	327	0
1	B	4761	0	4661	343	0
1	C	4761	0	4651	342	0
1	D	4760	0	4645	329	0
1	E	4761	0	4653	321	0
1	F	4727	0	4619	313	0
2	G	50	0	42	2	0
2	I	50	0	43	0	0
2	J	50	0	43	2	0
2	K	50	0	42	3	0
2	L	50	0	43	3	0
2	M	50	0	42	1	0
2	O	50	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	50	0	43	0	0
3	H	61	0	52	4	0
3	P	61	0	52	3	0
3	R	61	0	52	7	0
4	N	39	0	34	2	0
All	All	29159	0	28418	1966	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1966) 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:22:THR:HG21	1:E:104:LYS:HD2	1.29	1.14
1:B:507:TYR:CE1	1:D:625:PRO:HG2	1.88	1.09
1:D:88:SER:HB3	1:D:107:PRO:HG3	1.10	1.09
1:B:255:LEU:HG	1:B:256:HIS:H	1.14	1.08
1:B:88:SER:HB3	1:B:107:PRO:HG3	1.09	1.08
1:E:88:SER:HB3	1:E:107:PRO:HG3	1.09	1.06
1:C:88:SER:HB3	1:C:107:PRO:HG3	1.08	1.06
1:E:255:LEU:HG	1:E:256:HIS:H	1.14	1.05
1:B:311:ILE:HD11	1:B:330:TRP:HE1	1.20	1.05
1:A:255:LEU:HG	1:A:256:HIS:H	1.15	1.05
1:F:88:SER:HB3	1:F:107:PRO:HG3	1.08	1.05
1:A:145:VAL:HG22	1:C:17:SER:HB3	1.35	1.05
1:A:311:ILE:HD11	1:A:330:TRP:HE1	1.21	1.05
1:A:88:SER:HB3	1:A:107:PRO:HG3	1.09	1.05
1:B:22:THR:HG21	1:C:104:LYS:HD2	1.39	1.04
1:E:311:ILE:HD11	1:E:330:TRP:HE1	1.21	1.04
1:A:22:THR:HG21	1:B:104:LYS:HD2	1.38	1.02
1:D:311:ILE:HD11	1:D:330:TRP:HE1	1.22	1.02
1:F:311:ILE:HD11	1:F:330:TRP:HE1	1.20	1.02
1:B:93:ARG:HH11	1:B:93:ARG:H	1.06	1.01
1:B:304:PRO:HG3	1:B:616:PRO:HA	1.39	1.01
1:F:88:SER:HB3	1:F:107:PRO:CG	1.91	1.01
1:C:311:ILE:HD11	1:C:330:TRP:HE1	1.20	1.00
1:E:22:THR:HG21	1:F:104:LYS:HD2	1.41	1.00
1:E:88:SER:HB3	1:E:107:PRO:CG	1.92	1.00
1:B:136:GLY:HA3	1:B:268:VAL:HG21	1.44	1.00
1:C:88:SER:HB3	1:C:107:PRO:CG	1.91	1.00
1:F:93:ARG:HH11	1:F:93:ARG:H	1.08	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:SER:HB3	1:A:107:PRO:CG	1.92	0.99
1:B:257:LEU:H	1:B:258:PRO:HD3	1.27	0.99
1:C:93:ARG:HH11	1:C:93:ARG:H	1.09	0.99
1:D:88:SER:HB3	1:D:107:PRO:CG	1.93	0.99
1:B:88:SER:HB3	1:B:107:PRO:CG	1.92	0.99
1:D:93:ARG:HH11	1:D:93:ARG:H	1.07	0.98
1:A:257:LEU:H	1:A:258:PRO:HD3	1.27	0.98
1:F:136:GLY:HA3	1:F:268:VAL:HG21	1.45	0.98
1:A:93:ARG:H	1:A:93:ARG:HH11	1.10	0.97
1:B:289:THR:HG21	1:B:293:THR:HG21	1.47	0.97
1:C:289:THR:HG21	1:C:293:THR:HG21	1.45	0.97
1:A:289:THR:HG21	1:A:293:THR:HG21	1.45	0.97
1:C:136:GLY:HA3	1:C:268:VAL:HG21	1.44	0.97
1:C:257:LEU:H	1:C:258:PRO:HD3	1.27	0.97
1:E:257:LEU:H	1:E:258:PRO:HD3	1.27	0.97
1:D:104:LYS:HD2	1:F:22:THR:HG21	1.46	0.97
1:E:136:GLY:HA3	1:E:268:VAL:HG21	1.44	0.97
1:D:145:VAL:HG22	1:F:17:SER:HB3	1.43	0.96
1:D:257:LEU:H	1:D:258:PRO:HD3	1.28	0.96
1:A:136:GLY:HA3	1:A:268:VAL:HG21	1.46	0.96
1:D:136:GLY:HA3	1:D:268:VAL:HG21	1.45	0.96
1:A:104:LYS:HD2	1:C:22:THR:HG21	1.46	0.96
1:E:93:ARG:HH11	1:E:93:ARG:H	1.07	0.95
1:E:17:SER:HB3	1:F:145:VAL:HG22	1.47	0.95
1:E:304:PRO:HG3	1:E:616:PRO:HA	1.45	0.95
1:F:289:THR:HG21	1:F:293:THR:HG21	1.44	0.95
1:D:304:PRO:HG3	1:D:616:PRO:HA	1.49	0.95
1:D:289:THR:HG21	1:D:293:THR:HG21	1.46	0.95
1:E:289:THR:HG21	1:E:293:THR:HG21	1.46	0.94
1:B:17:SER:HB3	1:C:145:VAL:HG22	1.51	0.93
1:D:17:SER:HB3	1:E:145:VAL:HG22	1.53	0.90
1:C:428:CYS:HB2	1:C:463:MSE:SE	2.24	0.88
1:C:304:PRO:HG3	1:C:616:PRO:HA	1.54	0.87
1:E:428:CYS:HB2	1:E:463:MSE:SE	2.25	0.86
1:D:447:PHE:HD1	1:D:455:PHE:HA	1.40	0.85
1:B:428:CYS:HB2	1:B:463:MSE:SE	2.26	0.85
1:A:17:SER:HB3	1:B:145:VAL:HG22	1.58	0.85
1:A:304:PRO:HG3	1:A:616:PRO:HA	1.57	0.84
1:F:304:PRO:HG3	1:F:616:PRO:HA	1.57	0.84
1:B:507:TYR:HE1	1:D:625:PRO:HG2	1.43	0.84
1:A:255:LEU:HG	1:A:256:HIS:N	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HG	1:B:256:HIS:N	1.92	0.83
1:D:22:THR:HG21	1:E:104:LYS:CD	2.07	0.83
1:F:428:CYS:HB2	1:F:463:MSE:SE	2.29	0.83
1:C:677:THR:HG22	1:C:713:THR:HG22	1.60	0.83
1:E:677:THR:HG22	1:E:713:THR:HG22	1.61	0.83
1:F:677:THR:HG22	1:F:713:THR:HG22	1.61	0.82
1:B:677:THR:HG22	1:B:713:THR:HG22	1.61	0.82
1:A:677:THR:HG22	1:A:713:THR:HG22	1.60	0.82
1:D:677:THR:HG22	1:D:713:THR:HG22	1.60	0.82
1:A:428:CYS:HB2	1:A:463:MSE:SE	2.29	0.82
1:C:378:LEU:HD21	1:C:689:PRO:HB2	1.63	0.81
1:E:322:ASP:O	1:E:323:ARG:HB3	1.81	0.81
1:C:496:VAL:HG22	1:C:501:THR:HB	1.62	0.81
1:D:496:VAL:HG22	1:D:501:THR:HB	1.63	0.81
1:C:322:ASP:O	1:C:323:ARG:HB3	1.81	0.80
1:D:447:PHE:CD1	1:D:455:PHE:HA	2.17	0.80
1:A:496:VAL:HG22	1:A:501:THR:HB	1.64	0.80
1:C:257:LEU:N	1:C:258:PRO:HD3	1.95	0.80
1:D:322:ASP:O	1:D:323:ARG:HB3	1.81	0.80
1:C:445:TYR:HB3	1:C:451:GLY:HA3	1.62	0.80
1:D:428:CYS:HB2	1:D:463:MSE:SE	2.32	0.80
1:E:255:LEU:HG	1:E:256:HIS:N	1.90	0.80
1:A:257:LEU:N	1:A:258:PRO:HD3	1.95	0.80
1:B:257:LEU:N	1:B:258:PRO:HD3	1.96	0.80
1:E:257:LEU:N	1:E:258:PRO:HD3	1.96	0.80
1:B:94:LEU:HD22	1:B:157:ARG:HD3	1.64	0.79
1:C:653:ALA:HB1	1:C:684:ARG:HH11	1.47	0.79
1:D:257:LEU:N	1:D:258:PRO:HD3	1.96	0.79
1:F:322:ASP:O	1:F:323:ARG:HB3	1.82	0.79
1:A:322:ASP:O	1:A:323:ARG:HB3	1.82	0.79
1:E:114:SER:HB3	1:E:123:SER:CB	2.13	0.79
1:F:114:SER:HB3	1:F:123:SER:CB	2.11	0.79
1:C:114:SER:HB3	1:C:123:SER:CB	2.13	0.79
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.66	0.79
1:A:255:LEU:CG	1:A:256:HIS:H	1.96	0.79
1:A:114:SER:HB3	1:A:123:SER:CB	2.13	0.78
1:D:137:ARG:NH2	1:D:329:ILE:HB	1.98	0.78
1:F:137:ARG:NH2	1:F:329:ILE:HB	1.98	0.78
1:D:114:SER:HB3	1:D:123:SER:CB	2.12	0.78
1:B:322:ASP:O	1:B:323:ARG:HB3	1.81	0.78
1:B:106:PRO:HB2	1:B:107:PRO:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:VAL:HG22	1:E:501:THR:HB	1.65	0.78
1:E:137:ARG:NH2	1:E:329:ILE:HB	1.98	0.78
1:F:88:SER:CB	1:F:107:PRO:HG3	2.04	0.78
1:B:114:SER:HB3	1:B:123:SER:CB	2.12	0.78
1:C:106:PRO:HB2	1:C:107:PRO:HD3	1.66	0.78
1:F:496:VAL:HG22	1:F:501:THR:HB	1.64	0.78
1:A:137:ARG:NH2	1:A:329:ILE:HB	1.98	0.78
1:C:675:MSE:HE2	1:C:715:HIS:HE1	1.49	0.78
1:D:329:ILE:HD13	1:D:335:PRO:HB3	1.66	0.78
1:E:255:LEU:CG	1:E:256:HIS:H	1.95	0.78
1:B:496:VAL:HG22	1:B:501:THR:HB	1.65	0.77
1:A:544:VAL:H	1:A:612:GLN:NE2	1.83	0.77
1:B:544:VAL:H	1:B:612:GLN:NE2	1.83	0.77
1:D:544:VAL:H	1:D:612:GLN:NE2	1.83	0.77
3:R:1:NAG:H61	3:R:2:NAG:O7	1.85	0.77
1:D:543:LEU:HA	1:D:612:GLN:NE2	2.00	0.77
1:F:675:MSE:HE2	1:F:715:HIS:HE1	1.50	0.77
1:C:655:LEU:H	1:C:683:ASP:HB2	1.49	0.77
1:D:106:PRO:HB2	1:D:107:PRO:HD3	1.66	0.77
1:D:675:MSE:HE2	1:D:715:HIS:HE1	1.50	0.77
1:A:88:SER:CB	1:A:107:PRO:HG3	2.05	0.76
1:F:114:SER:HB3	1:F:123:SER:HB2	1.68	0.76
3:P:3:BMA:H3	3:R:5:MAN:O3	1.85	0.76
1:A:329:ILE:HD13	1:A:335:PRO:HB3	1.67	0.76
1:C:137:ARG:NH2	1:C:329:ILE:HB	2.00	0.76
1:F:543:LEU:HA	1:F:612:GLN:NE2	2.00	0.76
3:R:2:NAG:H83	3:R:5:MAN:H61	1.66	0.76
1:E:106:PRO:HB2	1:E:107:PRO:HD3	1.66	0.76
3:H:4:MAN:O3	2:L:3:BMA:H5	1.85	0.76
1:B:137:ARG:NH2	1:B:329:ILE:HB	2.01	0.75
1:E:544:VAL:H	1:E:612:GLN:NE2	1.84	0.75
1:F:106:PRO:HB2	1:F:107:PRO:HD3	1.66	0.75
1:B:255:LEU:CG	1:B:256:HIS:H	1.92	0.75
1:F:544:VAL:H	1:F:612:GLN:NE2	1.85	0.75
1:B:675:MSE:HE2	1:B:715:HIS:HE1	1.51	0.75
1:C:114:SER:HB3	1:C:123:SER:HB2	1.68	0.75
1:F:610:PRO:HB2	1:F:612:GLN:HG2	1.69	0.75
1:A:675:MSE:HE2	1:A:715:HIS:HE1	1.51	0.75
1:A:294:LEU:HG	1:A:310:TRP:CE2	2.22	0.75
1:B:22:THR:HG21	1:C:104:LYS:CD	2.15	0.75
1:E:22:THR:HG21	1:F:104:LYS:CD	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:C	1:A:81:ASP:H	1.94	0.75
1:A:543:LEU:HA	1:A:612:GLN:NE2	2.01	0.74
1:A:610:PRO:HB2	1:A:612:GLN:HG2	1.69	0.74
1:C:329:ILE:HD13	1:C:335:PRO:HB3	1.69	0.74
1:D:79:THR:C	1:D:81:ASP:H	1.94	0.74
1:E:536:LYS:HG2	1:E:549:PHE:CZ	2.23	0.74
1:A:104:LYS:CD	1:C:22:THR:HG21	2.17	0.74
1:F:294:LEU:HG	1:F:310:TRP:CE2	2.21	0.74
1:C:150:ILE:HG23	1:C:151:PRO:HD2	1.68	0.74
1:E:150:ILE:HG23	1:E:151:PRO:HD2	1.69	0.74
1:E:79:THR:C	1:E:81:ASP:H	1.95	0.74
1:F:655:LEU:H	1:F:683:ASP:HB2	1.53	0.74
1:E:675:MSE:HE2	1:E:715:HIS:HE1	1.50	0.74
1:B:543:LEU:HA	1:B:612:GLN:NE2	2.01	0.74
1:D:114:SER:HB3	1:D:123:SER:HB2	1.69	0.74
1:C:544:VAL:H	1:C:612:GLN:NE2	1.85	0.74
1:C:294:LEU:HG	1:C:310:TRP:CE2	2.23	0.73
1:D:88:SER:CB	1:D:107:PRO:HG3	2.05	0.73
1:C:79:THR:C	1:C:81:ASP:H	1.96	0.73
1:E:543:LEU:HA	1:E:612:GLN:NE2	2.02	0.73
1:E:610:PRO:HB2	1:E:612:GLN:HG2	1.70	0.73
1:F:329:ILE:HD13	1:F:335:PRO:HB3	1.68	0.73
1:A:137:ARG:HH22	1:A:329:ILE:HB	1.54	0.73
1:B:114:SER:HB3	1:B:123:SER:HB2	1.69	0.73
1:B:447:PHE:CD1	1:B:455:PHE:HA	2.23	0.73
1:B:329:ILE:HD13	1:B:335:PRO:HB3	1.69	0.73
1:C:543:LEU:HA	1:C:612:GLN:NE2	2.02	0.73
1:A:447:PHE:CD1	1:A:455:PHE:HA	2.23	0.73
1:B:294:LEU:HG	1:B:310:TRP:CE2	2.24	0.73
1:D:150:ILE:HG23	1:D:151:PRO:HD2	1.70	0.73
1:E:114:SER:HB3	1:E:123:SER:HB2	1.69	0.73
1:F:361:TYR:HB2	1:F:381:ARG:NH2	2.03	0.73
1:C:610:PRO:HB2	1:C:612:GLN:HG2	1.70	0.73
1:D:610:PRO:HB2	1:D:612:GLN:HG2	1.69	0.73
1:B:79:THR:C	1:B:81:ASP:H	1.96	0.73
1:B:655:LEU:H	1:B:683:ASP:HB2	1.53	0.73
1:D:536:LYS:HG2	1:D:549:PHE:CZ	2.24	0.73
1:B:11:PRO:HD3	1:B:50:GLN:HE21	1.54	0.72
1:C:536:LYS:HG2	1:C:549:PHE:CZ	2.24	0.72
2:K:1:NAG:H4	2:K:2:NAG:N2	2.02	0.72
1:A:114:SER:HB3	1:A:123:SER:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:HG23	1:B:151:PRO:HD2	1.70	0.72
1:C:11:PRO:HD3	1:C:50:GLN:HE21	1.54	0.72
1:F:18:TYR:CE1	1:F:22:THR:HG22	2.25	0.72
1:F:536:LYS:HG2	1:F:549:PHE:CZ	2.25	0.72
1:A:18:TYR:CE1	1:A:22:THR:HG22	2.24	0.72
1:C:11:PRO:HD3	1:C:50:GLN:NE2	2.04	0.72
1:D:655:LEU:H	1:D:683:ASP:HB2	1.53	0.72
1:D:11:PRO:HD3	1:D:50:GLN:HE21	1.55	0.72
1:D:538:VAL:HG23	1:D:547:TYR:HB3	1.70	0.72
1:E:270:VAL:HG22	1:E:333:HIS:CE1	2.25	0.72
1:E:329:ILE:HD13	1:E:335:PRO:HB3	1.71	0.72
1:A:95:SER:OG	1:A:259:PHE:CE1	2.41	0.72
1:E:655:LEU:H	1:E:683:ASP:HB2	1.53	0.72
1:A:85:ILE:HD11	1:A:101:LEU:HD13	1.71	0.72
1:F:79:THR:C	1:F:81:ASP:H	1.95	0.72
1:B:538:VAL:HG23	1:B:547:TYR:HB3	1.71	0.71
1:C:85:ILE:HD11	1:C:101:LEU:HD13	1.72	0.71
1:F:11:PRO:HD3	1:F:50:GLN:HE21	1.53	0.71
1:A:655:LEU:H	1:A:683:ASP:HB2	1.54	0.71
1:D:18:TYR:CE1	1:D:22:THR:HG22	2.25	0.71
1:F:11:PRO:HD3	1:F:50:GLN:NE2	2.05	0.71
1:B:11:PRO:HD3	1:B:50:GLN:NE2	2.05	0.71
1:E:18:TYR:CE1	1:E:22:THR:HG22	2.25	0.71
1:F:150:ILE:HG23	1:F:151:PRO:HD2	1.71	0.71
1:A:11:PRO:HD3	1:A:50:GLN:HE21	1.55	0.71
1:C:18:TYR:CE1	1:C:22:THR:HG22	2.25	0.71
1:B:653:ALA:N	1:B:654:PRO:HD2	2.05	0.71
1:A:536:LYS:HG2	1:A:549:PHE:CZ	2.26	0.71
1:E:11:PRO:HD3	1:E:50:GLN:HE21	1.55	0.71
1:D:270:VAL:HG22	1:D:333:HIS:CE1	2.26	0.71
1:A:11:PRO:HD3	1:A:50:GLN:NE2	2.06	0.70
1:A:388:ASN:HB3	1:A:498:GLY:H	1.56	0.70
1:B:18:TYR:CE1	1:B:22:THR:HG22	2.25	0.70
1:B:287:LEU:HD22	1:B:330:TRP:NE1	2.07	0.70
1:E:294:LEU:HG	1:E:310:TRP:CE2	2.26	0.70
1:F:270:VAL:HG22	1:F:333:HIS:CE1	2.26	0.70
1:F:299:ARG:HH12	1:F:305:GLU:CD	1.99	0.70
1:A:270:VAL:HG22	1:A:333:HIS:CE1	2.27	0.70
1:E:137:ARG:HH22	1:E:329:ILE:HB	1.54	0.70
1:E:299:ARG:HH12	1:E:305:GLU:CD	2.00	0.70
1:D:11:PRO:HD3	1:D:50:GLN:NE2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HG21	1:B:104:LYS:CD	2.19	0.70
1:A:150:ILE:HG23	1:A:151:PRO:HD2	1.73	0.70
1:A:538:VAL:HG23	1:A:547:TYR:HB3	1.72	0.70
1:A:291:HIS:CD2	1:A:293:THR:HG22	2.27	0.70
1:A:511:VAL:HG23	1:A:512:THR:H	1.57	0.70
1:B:536:LYS:HG2	1:B:549:PHE:CZ	2.26	0.70
1:D:294:LEU:HG	1:D:310:TRP:CE2	2.27	0.70
1:E:85:ILE:HD11	1:E:101:LEU:HD13	1.73	0.70
1:F:538:VAL:HG23	1:F:547:TYR:HB3	1.72	0.70
1:B:85:ILE:HD11	1:B:101:LEU:HD13	1.73	0.70
1:D:137:ARG:HH22	1:D:329:ILE:HB	1.54	0.70
1:A:299:ARG:HB2	1:A:304:PRO:HA	1.74	0.70
1:A:299:ARG:HH12	1:A:305:GLU:CD	2.00	0.70
1:E:88:SER:CB	1:E:107:PRO:HG3	2.05	0.70
1:E:538:VAL:HG23	1:E:547:TYR:HB3	1.72	0.70
1:F:137:ARG:HH22	1:F:329:ILE:HB	1.54	0.70
1:A:446:PRO:HD2	1:A:450:GLY:O	1.90	0.70
1:A:447:PHE:HD1	1:A:454:CYS:O	1.75	0.70
1:D:299:ARG:HH12	1:D:305:GLU:CD	2.00	0.70
1:E:11:PRO:HD3	1:E:50:GLN:NE2	2.06	0.70
1:F:511:VAL:HG23	1:F:512:THR:H	1.56	0.70
1:D:85:ILE:HD11	1:D:101:LEU:HD13	1.73	0.69
1:F:85:ILE:HD11	1:F:101:LEU:HD13	1.73	0.69
1:A:447:PHE:CE1	1:A:455:PHE:HD1	2.11	0.69
1:B:270:VAL:HG22	1:B:333:HIS:CE1	2.26	0.69
1:C:299:ARG:HH12	1:C:305:GLU:CD	1.99	0.69
1:D:388:ASN:HB3	1:D:498:GLY:H	1.57	0.69
1:B:299:ARG:HH12	1:B:305:GLU:CD	2.00	0.69
1:C:88:SER:CB	1:C:107:PRO:HG3	2.04	0.69
1:D:653:ALA:N	1:D:654:PRO:HD2	2.08	0.69
1:D:291:HIS:CD2	1:D:293:THR:HG22	2.27	0.69
1:E:299:ARG:HB2	1:E:304:PRO:HA	1.73	0.69
1:E:287:LEU:HD22	1:E:330:TRP:NE1	2.06	0.69
1:B:610:PRO:HB2	1:B:612:GLN:HG2	1.72	0.69
1:C:95:SER:OG	1:C:259:PHE:CE1	2.42	0.69
1:C:538:VAL:HG23	1:C:547:TYR:HB3	1.73	0.69
1:D:108:GLY:HA3	1:D:130:ILE:HB	1.75	0.69
1:D:511:VAL:HG23	1:D:512:THR:H	1.57	0.69
1:D:650:THR:HG22	1:D:650:THR:O	1.93	0.69
1:B:624:ASN:HB3	1:B:625:PRO:CD	2.23	0.68
1:D:299:ARG:HB2	1:D:304:PRO:HA	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ARG:HB2	1:F:304:PRO:HA	1.75	0.68
1:C:311:ILE:HD11	1:C:330:TRP:NE1	2.04	0.68
1:D:107:PRO:HG2	1:D:108:GLY:H	1.58	0.68
1:A:650:THR:HG22	1:A:650:THR:O	1.92	0.68
1:C:291:HIS:CD2	1:C:293:THR:HG22	2.28	0.68
1:C:650:THR:HG22	1:C:650:THR:O	1.93	0.68
1:E:291:HIS:CD2	1:E:293:THR:HG22	2.28	0.68
1:A:287:LEU:HD22	1:A:330:TRP:NE1	2.08	0.68
1:C:446:PRO:HG2	1:C:450:GLY:C	2.19	0.68
1:B:511:VAL:HG23	1:B:512:THR:H	1.59	0.68
1:C:270:VAL:HG22	1:C:333:HIS:CE1	2.28	0.68
1:B:88:SER:CB	1:B:107:PRO:HG3	2.05	0.68
1:C:299:ARG:HB2	1:C:304:PRO:HA	1.75	0.68
1:F:650:THR:HG22	1:F:650:THR:O	1.92	0.68
1:A:445:TYR:HB3	1:A:451:GLY:HA3	1.76	0.68
1:F:388:ASN:HB3	1:F:498:GLY:H	1.58	0.68
1:B:137:ARG:HH22	1:B:329:ILE:HB	1.59	0.68
1:B:386:PRO:HB2	1:B:689:PRO:HG2	1.76	0.68
1:B:652:ASP:C	1:B:654:PRO:HD2	2.19	0.68
1:B:299:ARG:HB2	1:B:304:PRO:HA	1.75	0.67
1:C:108:GLY:HA3	1:C:130:ILE:HB	1.76	0.67
1:F:287:LEU:HD22	1:F:330:TRP:NE1	2.09	0.67
1:F:291:HIS:CD2	1:F:293:THR:HG22	2.29	0.67
1:C:107:PRO:HG2	1:C:108:GLY:H	1.59	0.67
1:E:95:SER:OG	1:E:259:PHE:CE1	2.42	0.67
1:C:287:LEU:HD22	1:C:330:TRP:NE1	2.10	0.67
1:D:530:PHE:HB3	1:D:633:TYR:CE1	2.29	0.67
1:C:511:VAL:HG23	1:C:512:THR:H	1.58	0.67
1:A:108:GLY:HA3	1:A:130:ILE:HB	1.76	0.67
1:B:291:HIS:CD2	1:B:293:THR:HG22	2.30	0.67
1:C:494:ARG:HB2	1:C:503:PHE:HD1	1.59	0.67
1:C:624:ASN:HB3	1:C:625:PRO:CD	2.25	0.67
1:C:388:ASN:HB3	1:C:498:GLY:H	1.59	0.67
1:E:108:GLY:HA3	1:E:130:ILE:HB	1.77	0.67
1:A:107:PRO:HG2	1:A:108:GLY:H	1.58	0.67
1:C:256:HIS:O	1:C:257:LEU:HD13	1.95	0.67
1:C:530:PHE:HB3	1:C:633:TYR:CE1	2.30	0.67
1:C:542:GLY:H	1:C:543:LEU:HD12	1.60	0.66
1:E:511:VAL:HG23	1:E:512:THR:H	1.59	0.66
1:F:108:GLY:HA3	1:F:130:ILE:HB	1.77	0.66
1:B:108:GLY:HA3	1:B:130:ILE:HB	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:HIS:O	1:B:257:LEU:HD13	1.95	0.66
1:E:388:ASN:HB3	1:E:498:GLY:H	1.60	0.66
1:B:388:ASN:HB3	1:B:498:GLY:H	1.59	0.66
1:F:624:ASN:HB3	1:F:625:PRO:CD	2.25	0.66
1:C:149:LYS:C	1:C:150:ILE:HD12	2.19	0.66
1:B:650:THR:O	1:B:650:THR:HG22	1.93	0.66
1:F:107:PRO:HG2	1:F:108:GLY:H	1.59	0.66
1:A:567:SER:HB2	1:A:571:LYS:HD2	1.78	0.66
1:B:97:LYS:HB2	1:B:259:PHE:CZ	2.31	0.66
1:B:107:PRO:HG2	1:B:108:GLY:H	1.60	0.66
1:B:494:ARG:HB2	1:B:503:PHE:HD1	1.61	0.66
1:D:494:ARG:HB2	1:D:503:PHE:HD1	1.61	0.66
1:E:107:PRO:HG2	1:E:108:GLY:H	1.59	0.66
1:C:136:GLY:HA3	1:C:268:VAL:CG2	2.25	0.66
1:A:256:HIS:O	1:A:257:LEU:HD13	1.96	0.66
1:D:104:LYS:CD	1:F:22:THR:HG21	2.22	0.66
1:F:530:PHE:HB3	1:F:633:TYR:CE1	2.31	0.66
1:C:137:ARG:HH22	1:C:329:ILE:HB	1.59	0.66
1:D:542:GLY:H	1:D:543:LEU:HD12	1.61	0.66
1:A:497:TYR:N	1:A:497:TYR:CD2	2.64	0.65
1:B:567:SER:HB2	1:B:571:LYS:HD2	1.78	0.65
1:E:624:ASN:HB3	1:E:625:PRO:CD	2.26	0.65
1:F:149:LYS:C	1:F:150:ILE:HD12	2.21	0.65
1:B:95:SER:OG	1:B:259:PHE:CE1	2.41	0.65
1:C:97:LYS:HB2	1:C:259:PHE:CZ	2.31	0.65
1:D:256:HIS:O	1:D:257:LEU:HD13	1.95	0.65
1:D:287:LEU:HD22	1:D:330:TRP:NE1	2.11	0.65
1:E:530:PHE:HB3	1:E:633:TYR:CE1	2.31	0.65
1:A:97:LYS:HB2	1:A:259:PHE:CZ	2.31	0.65
1:A:530:PHE:HB3	1:A:633:TYR:CE1	2.31	0.65
1:D:624:ASN:HB3	1:D:625:PRO:CD	2.27	0.65
1:A:624:ASN:HB3	1:A:625:PRO:CD	2.26	0.65
1:E:536:LYS:HG2	1:E:549:PHE:CE2	2.32	0.65
1:A:106:PRO:HB2	1:A:107:PRO:CD	2.27	0.65
1:D:497:TYR:N	1:D:497:TYR:CD2	2.63	0.65
1:F:97:LYS:HB2	1:F:259:PHE:CZ	2.32	0.65
1:E:256:HIS:O	1:E:257:LEU:HD13	1.96	0.65
1:F:494:ARG:HB2	1:F:503:PHE:HD1	1.62	0.65
1:A:494:ARG:HB2	1:A:503:PHE:HD1	1.62	0.64
1:B:37:GLU:OE1	1:B:473:ASP:OD2	2.15	0.64
1:D:108:GLY:HA2	1:D:130:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:TYR:HA	1:D:649:ARG:HA	1.79	0.64
1:A:542:GLY:H	1:A:543:LEU:HD12	1.62	0.64
1:B:530:PHE:HB3	1:B:633:TYR:CE1	2.31	0.64
1:D:567:SER:HB2	1:D:571:LYS:HD2	1.77	0.64
1:E:19:CYS:HA	1:E:123:SER:O	1.98	0.64
1:F:19:CYS:HA	1:F:123:SER:O	1.97	0.64
1:F:542:GLY:H	1:F:543:LEU:HD12	1.60	0.64
1:B:289:THR:HG21	1:B:293:THR:CG2	2.26	0.64
1:E:97:LYS:HB2	1:E:259:PHE:CZ	2.32	0.64
1:E:149:LYS:C	1:E:150:ILE:HD12	2.22	0.64
1:E:494:ARG:HB2	1:E:503:PHE:HD1	1.61	0.64
1:E:650:THR:O	1:E:650:THR:HG22	1.97	0.64
1:B:149:LYS:C	1:B:150:ILE:HD12	2.22	0.64
1:D:558:GLY:O	1:D:599:GLY:HA2	1.97	0.64
1:C:567:SER:HB2	1:C:571:LYS:HD2	1.80	0.64
1:D:97:LYS:HB2	1:D:259:PHE:CZ	2.31	0.64
1:B:108:GLY:HA2	1:B:130:ILE:HD12	1.80	0.64
1:E:567:SER:HB2	1:E:571:LYS:HD2	1.79	0.64
1:C:19:CYS:HA	1:C:123:SER:O	1.98	0.64
1:E:106:PRO:HB2	1:E:107:PRO:CD	2.27	0.64
1:E:542:GLY:H	1:E:543:LEU:HD12	1.62	0.64
1:D:19:CYS:HA	1:D:123:SER:O	1.98	0.64
1:F:311:ILE:HD11	1:F:330:TRP:NE1	2.04	0.64
1:D:624:ASN:HB3	1:D:625:PRO:HD3	1.80	0.64
1:A:558:GLY:O	1:A:599:GLY:HA2	1.97	0.63
1:B:19:CYS:HA	1:B:123:SER:O	1.97	0.63
1:B:558:GLY:O	1:B:599:GLY:HA2	1.98	0.63
1:D:106:PRO:HB2	1:D:107:PRO:CD	2.27	0.63
1:F:108:GLY:HA2	1:F:130:ILE:HD12	1.79	0.63
1:A:19:CYS:HA	1:A:123:SER:O	1.98	0.63
1:B:653:ALA:HB1	1:B:684:ARG:HD2	1.79	0.63
1:C:289:THR:HG21	1:C:293:THR:CG2	2.25	0.63
1:E:384:TYR:HA	1:E:649:ARG:HA	1.80	0.63
1:A:543:LEU:HD23	1:A:610:PRO:HG3	1.81	0.63
1:B:388:ASN:O	1:B:497:TYR:HA	1.99	0.63
1:B:542:GLY:H	1:B:543:LEU:HD12	1.62	0.63
1:B:384:TYR:HA	1:B:649:ARG:HA	1.80	0.63
1:C:108:GLY:HA2	1:C:130:ILE:HD12	1.79	0.63
1:C:448:MSE:HG3	1:C:454:CYS:H	1.63	0.63
1:C:553:GLY:HA2	1:C:574:ILE:HD12	1.81	0.63
1:D:19:CYS:C	1:D:21:HIS:H	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:CG2	1:C:17:SER:HB3	2.21	0.63
1:A:384:TYR:HA	1:A:649:ARG:HA	1.79	0.63
1:B:301:GLY:O	1:B:616:PRO:O	2.17	0.63
1:E:108:GLY:HA2	1:E:130:ILE:HD12	1.80	0.63
1:A:108:GLY:HA2	1:A:130:ILE:HD12	1.79	0.63
1:D:149:LYS:C	1:D:150:ILE:HD12	2.22	0.63
1:E:497:TYR:CD2	1:E:497:TYR:N	2.66	0.63
1:F:413:THR:CG2	1:F:595:GLN:HE22	2.11	0.63
1:C:384:TYR:HA	1:C:649:ARG:HA	1.80	0.63
1:E:553:GLY:HA2	1:E:574:ILE:HD12	1.81	0.63
1:F:497:TYR:N	1:F:497:TYR:CD2	2.66	0.63
1:B:93:ARG:HH11	1:B:93:ARG:N	1.88	0.63
1:C:321:VAL:HG12	1:C:340:ALA:HB2	1.80	0.63
1:E:388:ASN:O	1:E:497:TYR:HA	1.99	0.63
1:F:558:GLY:O	1:F:599:GLY:HA2	1.99	0.63
1:B:106:PRO:HB2	1:B:107:PRO:CD	2.27	0.62
1:D:557:PRO:HB3	1:D:576:SER:O	1.98	0.62
1:A:729:LEU:O	1:A:730:CYS:C	2.41	0.62
1:B:624:ASN:HB3	1:B:625:PRO:HD3	1.80	0.62
1:C:388:ASN:O	1:C:497:TYR:HA	1.99	0.62
1:E:729:LEU:O	1:E:730:CYS:C	2.42	0.62
1:E:653:ALA:N	1:E:654:PRO:HD2	2.14	0.62
1:C:497:TYR:N	1:C:497:TYR:CD2	2.67	0.62
1:C:729:LEU:O	1:C:730:CYS:C	2.42	0.62
1:D:413:THR:CG2	1:D:595:GLN:HE22	2.11	0.62
1:D:553:GLY:HA2	1:D:574:ILE:HD12	1.81	0.62
1:D:729:LEU:O	1:D:730:CYS:C	2.42	0.62
1:E:413:THR:CG2	1:E:595:GLN:HE22	2.13	0.62
1:F:388:ASN:O	1:F:497:TYR:HA	1.99	0.62
1:F:567:SER:HB2	1:F:571:LYS:HD2	1.79	0.62
1:A:19:CYS:C	1:A:21:HIS:H	2.07	0.62
1:A:511:VAL:HG23	1:A:512:THR:N	2.14	0.62
1:C:624:ASN:HB3	1:C:625:PRO:HD3	1.81	0.62
1:B:413:THR:CG2	1:B:595:GLN:HE22	2.12	0.62
1:B:553:GLY:HA2	1:B:574:ILE:HD12	1.82	0.62
1:C:19:CYS:C	1:C:21:HIS:H	2.07	0.62
1:C:255:LEU:HD22	1:C:256:HIS:H	1.64	0.62
1:C:447:PHE:CE1	1:C:455:PHE:HA	2.34	0.62
1:A:271:ALA:HB1	1:A:330:TRP:CH2	2.35	0.62
1:A:624:ASN:HB3	1:A:625:PRO:HD3	1.82	0.62
1:B:729:LEU:O	1:B:730:CYS:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:TYR:N	1:D:497:TYR:HD2	1.96	0.62
1:A:497:TYR:N	1:A:497:TYR:HD2	1.97	0.62
1:B:19:CYS:C	1:B:21:HIS:H	2.07	0.62
1:C:413:THR:CG2	1:C:595:GLN:HE22	2.12	0.62
1:D:289:THR:HG21	1:D:293:THR:CG2	2.27	0.62
1:F:11:PRO:HG3	1:F:50:GLN:HB2	1.82	0.62
1:F:289:THR:HG21	1:F:293:THR:CG2	2.24	0.62
1:F:384:TYR:HA	1:F:649:ARG:HA	1.80	0.62
1:D:311:ILE:HD11	1:D:330:TRP:NE1	2.05	0.62
1:E:19:CYS:C	1:E:21:HIS:H	2.07	0.62
1:E:136:GLY:HA3	1:E:268:VAL:CG2	2.26	0.62
1:A:388:ASN:O	1:A:497:TYR:HA	2.00	0.62
1:B:136:GLY:HA3	1:B:268:VAL:CG2	2.26	0.62
1:A:654:PRO:HB3	1:A:684:ARG:C	2.25	0.61
1:C:654:PRO:HB3	1:C:684:ARG:C	2.25	0.61
1:E:543:LEU:HD23	1:E:610:PRO:HG3	1.81	0.61
1:B:11:PRO:HG3	1:B:50:GLN:HB2	1.81	0.61
1:D:543:LEU:HD23	1:D:610:PRO:HG3	1.80	0.61
1:E:271:ALA:HB1	1:E:330:TRP:CH2	2.35	0.61
1:F:271:ALA:HB1	1:F:330:TRP:CH2	2.36	0.61
1:B:543:LEU:HD23	1:B:610:PRO:HG3	1.82	0.61
1:A:149:LYS:C	1:A:150:ILE:HD12	2.25	0.61
1:B:271:ALA:HB1	1:B:330:TRP:CH2	2.35	0.61
1:D:536:LYS:HG2	1:D:549:PHE:CE2	2.36	0.61
1:E:624:ASN:HB3	1:E:625:PRO:HD3	1.81	0.61
1:F:553:GLY:HA2	1:F:574:ILE:HD12	1.83	0.61
1:F:654:PRO:HB3	1:F:684:ARG:C	2.25	0.61
1:F:729:LEU:O	1:F:730:CYS:C	2.42	0.61
1:C:537:VAL:HG22	1:C:546:ASN:HD22	1.66	0.61
1:D:93:ARG:HH11	1:D:93:ARG:N	1.89	0.61
1:D:388:ASN:O	1:D:497:TYR:HA	2.00	0.61
1:A:321:VAL:HG12	1:A:340:ALA:HB2	1.83	0.61
1:A:421:LYS:HE2	1:A:424:GLY:HA3	1.83	0.61
1:D:271:ALA:HB1	1:D:330:TRP:CH2	2.36	0.61
1:D:610:PRO:O	1:D:614:THR:HG23	2.01	0.61
1:E:289:THR:HG21	1:E:293:THR:CG2	2.25	0.61
1:F:497:TYR:N	1:F:497:TYR:HD2	1.99	0.61
1:F:511:VAL:HG23	1:F:512:THR:N	2.15	0.61
1:A:413:THR:CG2	1:A:595:GLN:HE22	2.14	0.61
1:B:497:TYR:CD2	1:B:497:TYR:N	2.67	0.61
1:C:257:LEU:N	1:C:258:PRO:CD	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:PRO:HB3	1:D:684:ARG:C	2.25	0.61
1:A:514:GLY:O	1:A:516:SER:N	2.31	0.61
1:C:536:LYS:HG2	1:C:549:PHE:CE2	2.36	0.61
1:D:421:LYS:HE2	1:D:424:GLY:HA3	1.83	0.61
1:D:511:VAL:HG23	1:D:512:THR:N	2.15	0.61
1:E:497:TYR:N	1:E:497:TYR:HD2	1.99	0.61
1:F:536:LYS:HG2	1:F:549:PHE:CE2	2.36	0.61
1:F:557:PRO:HB3	1:F:576:SER:O	2.01	0.61
1:A:553:GLY:HA2	1:A:574:ILE:HD12	1.82	0.60
1:E:654:PRO:HB3	1:E:684:ARG:C	2.25	0.60
1:C:274:PRO:HD3	1:C:330:TRP:CE3	2.36	0.60
1:A:257:LEU:N	1:A:258:PRO:CD	2.64	0.60
1:E:257:LEU:N	1:E:258:PRO:CD	2.64	0.60
1:B:654:PRO:HB3	1:B:684:ARG:C	2.26	0.60
1:E:93:ARG:HH11	1:E:93:ARG:N	1.89	0.60
1:C:11:PRO:HG3	1:C:50:GLN:HB2	1.83	0.60
1:A:378:LEU:HG	1:A:691:HIS:CD2	2.37	0.60
1:F:19:CYS:C	1:F:21:HIS:H	2.08	0.60
1:A:447:PHE:HD1	1:A:455:PHE:HA	1.67	0.60
1:B:126:LEU:HD12	1:B:127:ALA:H	1.67	0.60
1:B:300:LEU:HG	1:B:326:LEU:HA	1.84	0.60
1:B:537:VAL:HG22	1:B:546:ASN:HD22	1.67	0.60
1:A:289:THR:HG21	1:A:293:THR:CG2	2.26	0.60
1:D:11:PRO:HG3	1:D:50:GLN:HB2	1.83	0.60
1:D:496:VAL:HG22	1:D:501:THR:CB	2.32	0.60
1:F:624:ASN:HB3	1:F:625:PRO:HD3	1.84	0.60
1:A:536:LYS:HG2	1:A:549:PHE:CE2	2.37	0.60
1:E:298:ARG:HH12	1:E:615:ALA:HB3	1.66	0.60
1:F:423:CYS:HA	1:F:459:GLU:O	2.02	0.60
1:D:566:THR:OG1	1:D:571:LYS:HB2	2.02	0.59
1:E:11:PRO:HG3	1:E:50:GLN:HB2	1.83	0.59
1:E:511:VAL:HG23	1:E:512:THR:N	2.17	0.59
1:E:537:VAL:HG22	1:E:546:ASN:HD22	1.67	0.59
1:C:557:PRO:HB3	1:C:576:SER:O	2.02	0.59
1:D:257:LEU:N	1:D:258:PRO:CD	2.64	0.59
1:E:566:THR:OG1	1:E:571:LYS:HB2	2.02	0.59
1:F:451:GLY:O	1:F:589:VAL:HG23	2.02	0.59
1:A:496:VAL:HG22	1:A:501:THR:CB	2.33	0.59
1:A:537:VAL:HG22	1:A:546:ASN:HD22	1.67	0.59
1:C:511:VAL:HG23	1:C:512:THR:N	2.17	0.59
1:D:50:GLN:HE22	1:D:65:ARG:NH2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:VAL:HG12	1:B:340:ALA:HB2	1.85	0.59
1:C:271:ALA:HB1	1:C:330:TRP:CH2	2.38	0.59
1:F:106:PRO:HB2	1:F:107:PRO:CD	2.28	0.59
1:A:126:LEU:HD12	1:A:127:ALA:H	1.67	0.59
1:B:470:LEU:HB3	1:B:474:CYS:SG	2.42	0.59
1:E:470:LEU:HB3	1:E:474:CYS:SG	2.43	0.59
1:B:257:LEU:H	1:B:258:PRO:CD	2.10	0.59
1:B:311:ILE:HD11	1:B:330:TRP:NE1	2.04	0.59
1:C:257:LEU:H	1:C:258:PRO:CD	2.09	0.59
1:C:497:TYR:N	1:C:497:TYR:HD2	2.00	0.59
1:D:136:GLY:HA3	1:D:268:VAL:CG2	2.27	0.59
1:F:496:VAL:HG22	1:F:501:THR:CB	2.33	0.59
1:F:537:VAL:HG22	1:F:546:ASN:HD22	1.68	0.59
1:A:557:PRO:HB3	1:A:576:SER:O	2.03	0.59
1:C:423:CYS:HA	1:C:459:GLU:O	2.02	0.59
1:F:136:GLY:HA3	1:F:268:VAL:CG2	2.27	0.59
1:B:257:LEU:N	1:B:258:PRO:CD	2.64	0.59
1:B:566:THR:OG1	1:B:571:LYS:HB2	2.03	0.59
1:C:50:GLN:HE22	1:C:65:ARG:NH2	2.01	0.59
1:D:126:LEU:HD12	1:D:127:ALA:H	1.68	0.59
1:D:387:LEU:HD12	1:D:647:PHE:CE1	2.38	0.59
1:E:558:GLY:O	1:E:599:GLY:HA2	2.03	0.59
1:F:566:THR:OG1	1:F:571:LYS:HB2	2.02	0.59
1:C:514:GLY:O	1:C:516:SER:N	2.30	0.59
1:E:574:ILE:O	1:E:574:ILE:HG13	2.01	0.59
1:C:543:LEU:HD23	1:C:610:PRO:HG3	1.84	0.58
1:D:95:SER:OG	1:D:259:PHE:CE1	2.42	0.58
1:F:470:LEU:HB3	1:F:474:CYS:SG	2.43	0.58
1:A:18:TYR:HE1	1:A:22:THR:HG22	1.68	0.58
1:A:79:THR:C	1:A:81:ASP:N	2.60	0.58
1:B:497:TYR:N	1:B:497:TYR:HD2	2.00	0.58
1:B:511:VAL:HG23	1:B:512:THR:N	2.17	0.58
1:F:79:THR:C	1:F:81:ASP:N	2.61	0.58
1:F:321:VAL:HG12	1:F:340:ALA:HB2	1.86	0.58
1:B:361:TYR:HB2	1:B:381:ARG:NH2	2.18	0.58
1:C:106:PRO:HB2	1:C:107:PRO:CD	2.28	0.58
1:C:386:PRO:HB2	1:C:689:PRO:HG2	1.85	0.58
1:C:496:VAL:HG22	1:C:501:THR:CB	2.30	0.58
1:F:274:PRO:HD3	1:F:330:TRP:CE3	2.38	0.58
1:F:610:PRO:O	1:F:614:THR:HG23	2.03	0.58
2:L:1:NAG:H62	2:L:2:NAG:O7	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:1:NAG:H61	3:R:2:NAG:C7	2.32	0.58
1:A:566:THR:OG1	1:A:571:LYS:HB2	2.03	0.58
1:D:514:GLY:O	1:D:516:SER:N	2.31	0.58
1:C:300:LEU:HG	1:C:326:LEU:HA	1.85	0.58
1:E:421:LYS:HE2	1:E:424:GLY:HA3	1.85	0.58
3:P:3:BMA:H3	3:R:5:MAN:HO3	1.68	0.58
1:A:447:PHE:CD1	1:A:448:MSE:N	2.69	0.58
1:A:610:PRO:O	1:A:614:THR:HG23	2.03	0.58
1:D:361:TYR:HB2	1:D:381:ARG:NH2	2.19	0.58
1:D:543:LEU:HA	1:D:612:GLN:HE22	1.69	0.58
1:E:423:CYS:HA	1:E:459:GLU:O	2.04	0.58
1:A:423:CYS:HA	1:A:459:GLU:O	2.04	0.58
1:E:675:MSE:HE2	1:E:715:HIS:CE1	2.36	0.58
1:F:50:GLN:HE22	1:F:65:ARG:NH2	2.02	0.58
1:B:653:ALA:N	1:B:654:PRO:CD	2.67	0.58
1:D:537:VAL:HG22	1:D:546:ASN:HD22	1.68	0.58
1:A:11:PRO:HG3	1:A:50:GLN:HB2	1.84	0.58
1:A:50:GLN:HE22	1:A:65:ARG:NH2	2.02	0.58
1:B:421:LYS:HE2	1:B:424:GLY:HA3	1.85	0.58
1:C:79:THR:C	1:C:81:ASP:N	2.61	0.58
1:C:566:THR:OG1	1:C:571:LYS:HB2	2.02	0.58
1:C:652:ASP:C	1:C:654:PRO:HD2	2.29	0.58
1:E:300:LEU:HG	1:E:326:LEU:HA	1.85	0.58
1:F:126:LEU:HD12	1:F:127:ALA:H	1.69	0.58
1:C:544:VAL:H	1:C:612:GLN:HE22	1.51	0.57
1:D:497:TYR:HD2	1:D:497:TYR:H	1.52	0.57
1:F:544:VAL:H	1:F:612:GLN:HE22	1.50	0.57
1:B:274:PRO:HD3	1:B:330:TRP:CE3	2.39	0.57
1:B:423:CYS:HA	1:B:459:GLU:O	2.03	0.57
1:D:321:VAL:HG12	1:D:340:ALA:HB2	1.85	0.57
1:E:50:GLN:HE22	1:E:65:ARG:NH2	2.03	0.57
1:E:450:GLY:HA3	1:E:587:LYS:HA	1.85	0.57
1:E:514:GLY:O	1:E:516:SER:N	2.31	0.57
1:A:387:LEU:HD12	1:A:647:PHE:CE1	2.38	0.57
1:B:390:GLU:HG2	1:B:496:VAL:HB	1.87	0.57
1:E:361:TYR:HB2	1:E:381:ARG:NH2	2.20	0.57
1:E:450:GLY:HA2	1:E:587:LYS:O	2.04	0.57
1:A:288:ASP:OD1	1:A:314:LYS:HB2	2.05	0.57
1:A:300:LEU:HG	1:A:326:LEU:HA	1.86	0.57
1:D:399:LEU:O	1:D:487:ALA:HB1	2.03	0.57
1:E:387:LEU:HD12	1:E:647:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:SER:HB2	1:F:28:PRO:HD2	1.87	0.57
1:F:675:MSE:HE2	1:F:715:HIS:CE1	2.37	0.57
1:A:399:LEU:O	1:A:487:ALA:HB1	2.04	0.57
1:B:536:LYS:HG2	1:B:549:PHE:CE2	2.39	0.57
1:C:361:TYR:HB2	1:C:381:ARG:NH2	2.18	0.57
1:C:667:THR:OG1	1:C:673:GLY:HA3	2.05	0.57
1:D:50:GLN:HE22	1:D:65:ARG:HH21	1.51	0.57
1:D:300:LEU:HG	1:D:326:LEU:HA	1.85	0.57
1:D:544:VAL:H	1:D:612:GLN:HE22	1.52	0.57
1:E:311:ILE:HD11	1:E:330:TRP:NE1	2.05	0.57
1:F:300:LEU:HG	1:F:326:LEU:HA	1.85	0.57
1:A:27:SER:HB2	1:A:28:PRO:HD2	1.87	0.57
1:B:544:VAL:H	1:B:612:GLN:HE22	1.50	0.57
1:B:675:MSE:HE2	1:B:715:HIS:CE1	2.38	0.57
1:C:690:VAL:HG12	1:C:699:LEU:HD13	1.87	0.57
1:F:18:TYR:HE1	1:F:22:THR:HG22	1.69	0.57
1:F:653:ALA:HB1	1:F:684:ARG:HD2	1.87	0.57
1:A:544:VAL:H	1:A:612:GLN:HE22	1.52	0.57
1:B:387:LEU:HD12	1:B:647:PHE:CE1	2.39	0.57
1:F:421:LYS:HE2	1:F:424:GLY:HA3	1.85	0.57
1:F:543:LEU:HD23	1:F:610:PRO:HG3	1.86	0.57
1:F:653:ALA:N	1:F:654:PRO:HD2	2.19	0.57
1:A:92:ARG:HA	1:A:93:ARG:NH1	2.20	0.57
1:A:268:VAL:HG22	1:A:269:PRO:HD2	1.87	0.57
1:C:399:LEU:O	1:C:487:ALA:HB1	2.05	0.57
1:C:558:GLY:O	1:C:599:GLY:HA2	2.04	0.57
1:F:514:GLY:O	1:F:516:SER:N	2.30	0.57
1:A:361:TYR:HB2	1:A:381:ARG:NH2	2.19	0.57
1:A:622:ALA:HB3	1:A:627:ARG:HG3	1.87	0.57
1:B:543:LEU:HA	1:B:612:GLN:HE22	1.70	0.57
1:D:274:PRO:HD3	1:D:330:TRP:CE3	2.40	0.57
1:D:423:CYS:HA	1:D:459:GLU:O	2.04	0.57
1:A:274:PRO:HD3	1:A:330:TRP:CE3	2.39	0.57
1:B:298:ARG:HH12	1:B:615:ALA:HB3	1.70	0.57
1:D:390:GLU:HG2	1:D:496:VAL:HB	1.87	0.57
1:E:544:VAL:H	1:E:612:GLN:HE22	1.51	0.57
1:E:557:PRO:HB3	1:E:576:SER:O	2.05	0.57
1:E:690:VAL:HG12	1:E:699:LEU:HD13	1.86	0.57
1:F:387:LEU:HD12	1:F:647:PHE:CE1	2.40	0.57
1:A:278:HIS:HB3	1:A:343:SER:HB3	1.87	0.56
1:B:496:VAL:HG22	1:B:501:THR:CB	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ARG:HH11	1:C:93:ARG:N	1.91	0.56
1:D:667:THR:OG1	1:D:673:GLY:HA3	2.05	0.56
1:E:390:GLU:HG2	1:E:496:VAL:HB	1.86	0.56
1:F:399:LEU:O	1:F:487:ALA:HB1	2.05	0.56
1:F:667:THR:OG1	1:F:673:GLY:HA3	2.05	0.56
1:B:530:PHE:CZ	1:B:617:PHE:HD1	2.23	0.56
1:C:288:ASP:OD1	1:C:314:LYS:HB2	2.04	0.56
1:D:454:CYS:SG	1:D:455:PHE:N	2.75	0.56
1:B:557:PRO:HB3	1:B:576:SER:O	2.05	0.56
1:B:690:VAL:HG12	1:B:699:LEU:HD13	1.86	0.56
1:C:27:SER:HB2	1:C:28:PRO:HD2	1.87	0.56
1:D:118:SER:O	1:D:119:ASN:HB2	2.05	0.56
1:D:470:LEU:HB3	1:D:474:CYS:SG	2.46	0.56
1:D:622:ALA:HB3	1:D:627:ARG:HG3	1.87	0.56
1:E:18:TYR:HE1	1:E:22:THR:HG22	1.69	0.56
1:A:390:GLU:HG2	1:A:496:VAL:HB	1.86	0.56
1:B:50:GLN:HE22	1:B:65:ARG:NH2	2.02	0.56
1:C:470:LEU:HB3	1:C:474:CYS:SG	2.46	0.56
1:E:37:GLU:OE1	1:E:473:ASP:OD2	2.24	0.56
1:E:441:PHE:CD1	1:E:583:LYS:HG2	2.41	0.56
1:C:421:LYS:HE2	1:C:424:GLY:HA3	1.87	0.56
1:C:448:MSE:C	1:C:450:GLY:H	2.13	0.56
1:E:622:ALA:HB3	1:E:627:ARG:HG3	1.87	0.56
1:A:138:GLU:OE2	1:A:271:ALA:HB2	2.05	0.56
1:B:374:PRO:HA	1:B:392:THR:HG22	1.88	0.56
1:B:574:ILE:HG13	1:B:574:ILE:O	2.06	0.56
1:C:51:PHE:HB3	1:C:80:MSE:SE	2.55	0.56
1:D:675:MSE:HE2	1:D:715:HIS:CE1	2.37	0.56
1:E:50:GLN:HE22	1:E:65:ARG:HH21	1.52	0.56
1:E:321:VAL:HG12	1:E:340:ALA:HB2	1.86	0.56
1:E:496:VAL:HG22	1:E:501:THR:CB	2.33	0.56
1:E:667:THR:OG1	1:E:673:GLY:HA3	2.05	0.56
2:J:3:BMA:C2	2:J:4:MAN:O5	2.53	0.56
1:A:470:LEU:HB3	1:A:474:CYS:SG	2.46	0.56
1:A:690:VAL:HG12	1:A:699:LEU:HD13	1.87	0.56
1:D:321:VAL:HG22	1:D:326:LEU:HD23	1.87	0.56
1:F:66:TYR:CD2	1:F:67:MSE:O	2.59	0.56
1:F:288:ASP:OD1	1:F:314:LYS:HB2	2.05	0.56
1:A:574:ILE:HG13	1:A:574:ILE:O	2.06	0.56
1:B:27:SER:HB2	1:B:28:PRO:HD2	1.86	0.56
1:C:66:TYR:CD2	1:C:67:MSE:O	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LEU:H	1:D:258:PRO:CD	2.10	0.56
1:E:655:LEU:HB2	1:E:683:ASP:OD2	2.06	0.56
1:F:50:GLN:HE22	1:F:65:ARG:HH21	1.52	0.56
1:F:93:ARG:HH11	1:F:93:ARG:N	1.90	0.56
1:B:87:THR:OG1	1:B:107:PRO:HD2	2.06	0.56
1:C:622:ALA:HB3	1:C:627:ARG:HG3	1.88	0.56
1:E:274:PRO:HD3	1:E:330:TRP:CE3	2.41	0.56
1:A:50:GLN:HE22	1:A:65:ARG:HH21	1.52	0.56
1:A:93:ARG:HH11	1:A:93:ARG:N	1.91	0.56
1:A:311:ILE:HD11	1:A:330:TRP:NE1	2.05	0.56
1:B:50:GLN:HE22	1:B:65:ARG:HH21	1.52	0.56
1:C:387:LEU:HD12	1:C:647:PHE:CE1	2.41	0.56
1:D:690:VAL:HG12	1:D:699:LEU:HD13	1.87	0.56
1:E:27:SER:HB2	1:E:28:PRO:HD2	1.88	0.56
1:E:288:ASP:OD1	1:E:314:LYS:HB2	2.06	0.56
1:A:87:THR:OG1	1:A:107:PRO:HD2	2.06	0.55
1:C:18:TYR:HE1	1:C:22:THR:HG22	1.68	0.55
1:E:87:THR:OG1	1:E:107:PRO:HD2	2.06	0.55
1:B:138:GLU:OE2	1:B:271:ALA:HB2	2.07	0.55
1:B:514:GLY:O	1:B:516:SER:N	2.31	0.55
1:C:50:GLN:HE22	1:C:65:ARG:HH21	1.52	0.55
1:C:441:PHE:CD1	1:C:583:LYS:HG2	2.42	0.55
1:F:135:VAL:HG12	1:F:140:TYR:OH	2.06	0.55
1:F:390:GLU:HG2	1:F:496:VAL:HB	1.86	0.55
1:C:126:LEU:HD12	1:C:127:ALA:H	1.71	0.55
1:D:393:VAL:HG23	1:D:491:VAL:HG13	1.89	0.55
1:E:126:LEU:HD12	1:E:127:ALA:H	1.71	0.55
1:A:135:VAL:HG12	1:A:140:TYR:OH	2.07	0.55
1:B:288:ASP:OD1	1:B:314:LYS:HB2	2.07	0.55
1:D:27:SER:HB2	1:D:28:PRO:HD2	1.88	0.55
1:D:574:ILE:HG13	1:D:574:ILE:O	2.06	0.55
1:F:451:GLY:HA2	1:F:588:ASN:HA	1.88	0.55
1:B:51:PHE:HB3	1:B:80:MSE:SE	2.55	0.55
1:B:667:THR:OG1	1:B:673:GLY:HA3	2.06	0.55
1:D:79:THR:C	1:D:81:ASP:N	2.60	0.55
1:D:92:ARG:HA	1:D:93:ARG:NH1	2.21	0.55
1:E:79:THR:C	1:E:81:ASP:N	2.61	0.55
1:E:374:PRO:HA	1:E:392:THR:HG22	1.88	0.55
1:F:441:PHE:CD1	1:F:583:LYS:HG2	2.42	0.55
1:A:114:SER:HB3	1:A:123:SER:HB3	1.88	0.55
1:A:292:LEU:HD22	1:A:310:TRP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:LEU:HB2	1:C:683:ASP:OD2	2.06	0.55
1:E:530:PHE:CZ	1:E:617:PHE:HD1	2.25	0.55
1:B:610:PRO:O	1:B:614:THR:HG23	2.06	0.55
1:C:390:GLU:HG2	1:C:496:VAL:HB	1.87	0.55
1:C:675:MSE:HE2	1:C:715:HIS:CE1	2.35	0.55
1:D:135:VAL:HG12	1:D:140:TYR:OH	2.07	0.55
1:D:288:ASP:OD1	1:D:314:LYS:HB2	2.05	0.55
1:D:655:LEU:HB2	1:D:683:ASP:OD2	2.06	0.55
1:F:51:PHE:HB3	1:F:80:MSE:SE	2.57	0.55
1:C:135:VAL:HG12	1:C:140:TYR:OH	2.06	0.55
1:D:87:THR:OG1	1:D:107:PRO:HD2	2.07	0.55
1:E:66:TYR:CD2	1:E:67:MSE:O	2.60	0.55
1:A:497:TYR:HD2	1:A:497:TYR:H	1.54	0.55
1:B:298:ARG:NH1	1:B:615:ALA:HB3	2.22	0.55
1:D:18:TYR:HE1	1:D:22:THR:HG22	1.70	0.55
1:D:268:VAL:HG22	1:D:269:PRO:HD2	1.88	0.55
1:F:655:LEU:HB2	1:F:683:ASP:OD2	2.07	0.55
1:B:114:SER:HB3	1:B:123:SER:HB3	1.88	0.55
1:F:118:SER:O	1:F:119:ASN:HB2	2.07	0.55
1:F:690:VAL:HG12	1:F:699:LEU:HD13	1.87	0.55
1:A:257:LEU:H	1:A:258:PRO:CD	2.09	0.54
1:A:667:THR:OG1	1:A:673:GLY:HA3	2.05	0.54
1:C:393:VAL:HG23	1:C:491:VAL:HG13	1.90	0.54
1:D:138:GLU:OE2	1:D:271:ALA:HB2	2.07	0.54
1:E:63:LYS:C	1:E:80:MSE:HG2	2.32	0.54
1:E:114:SER:HB3	1:E:123:SER:HB3	1.88	0.54
1:F:92:ARG:HA	1:F:93:ARG:NH1	2.22	0.54
1:A:118:SER:O	1:A:119:ASN:HB2	2.07	0.54
1:A:393:VAL:HG23	1:A:491:VAL:HG13	1.88	0.54
1:B:441:PHE:CD1	1:B:583:LYS:HG2	2.42	0.54
1:E:298:ARG:NH1	1:E:615:ALA:HB3	2.22	0.54
1:E:610:PRO:O	1:E:614:THR:HG23	2.06	0.54
1:B:92:ARG:HA	1:B:93:ARG:NH1	2.22	0.54
1:C:610:PRO:O	1:C:614:THR:HG23	2.08	0.54
1:D:51:PHE:HB3	1:D:80:MSE:SE	2.58	0.54
1:E:292:LEU:HD22	1:E:310:TRP:HB3	1.88	0.54
1:B:655:LEU:HB2	1:B:683:ASP:OD2	2.06	0.54
1:C:92:ARG:HA	1:C:93:ARG:NH1	2.22	0.54
1:D:66:TYR:CD2	1:D:67:MSE:O	2.60	0.54
1:D:622:ALA:HB3	1:D:627:ARG:CG	2.38	0.54
1:F:268:VAL:HG11	1:F:332:ASN:ND2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:CD1	1:A:583:LYS:HG2	2.42	0.54
1:C:87:THR:OG1	1:C:107:PRO:HD2	2.07	0.54
1:D:374:PRO:HA	1:D:392:THR:HG22	1.89	0.54
1:E:399:LEU:O	1:E:487:ALA:HB1	2.07	0.54
1:F:374:PRO:HA	1:F:392:THR:HG22	1.89	0.54
1:A:321:VAL:HG22	1:A:326:LEU:HD23	1.88	0.54
1:B:135:VAL:HG12	1:B:140:TYR:OH	2.07	0.54
1:B:399:LEU:O	1:B:487:ALA:HB1	2.07	0.54
1:C:114:SER:HB3	1:C:123:SER:HB3	1.90	0.54
1:F:295:LEU:HG	1:F:330:TRP:HD1	1.73	0.54
1:A:655:LEU:HB2	1:A:683:ASP:OD2	2.07	0.54
1:B:292:LEU:HD22	1:B:310:TRP:HB3	1.88	0.54
1:C:136:GLY:CA	1:C:268:VAL:HG21	2.29	0.54
1:C:374:PRO:HA	1:C:392:THR:HG22	1.90	0.54
1:C:445:TYR:CD2	1:C:452:ALA:HB3	2.43	0.54
1:C:574:ILE:O	1:C:574:ILE:HG13	2.07	0.54
1:D:63:LYS:C	1:D:80:MSE:HG2	2.33	0.54
1:E:92:ARG:HA	1:E:93:ARG:NH1	2.22	0.54
1:E:268:VAL:HG22	1:E:269:PRO:HD2	1.90	0.54
1:E:295:LEU:HG	1:E:330:TRP:HD1	1.72	0.54
1:F:87:THR:OG1	1:F:107:PRO:HD2	2.07	0.54
1:C:63:LYS:C	1:C:80:MSE:HG2	2.33	0.54
1:C:445:TYR:HB3	1:C:451:GLY:CA	2.33	0.54
1:D:79:THR:HG23	1:D:81:ASP:HB3	1.90	0.54
1:F:508:VAL:HG13	1:F:524:GLY:O	2.08	0.54
1:A:543:LEU:HA	1:A:612:GLN:HE22	1.72	0.54
1:E:20:HIS:NE2	1:E:121:ALA:HB1	2.23	0.54
1:E:138:GLU:OE2	1:E:271:ALA:HB2	2.07	0.54
1:F:114:SER:HB3	1:F:123:SER:HB3	1.87	0.54
1:E:622:ALA:HB3	1:E:627:ARG:CG	2.38	0.54
1:F:530:PHE:CZ	1:F:617:PHE:HD1	2.26	0.54
1:A:63:LYS:C	1:A:80:MSE:HG2	2.33	0.53
1:A:374:PRO:HA	1:A:392:THR:HG22	1.88	0.53
1:B:66:TYR:CD2	1:B:67:MSE:O	2.61	0.53
1:F:393:VAL:HG23	1:F:491:VAL:HG13	1.90	0.53
1:A:295:LEU:HG	1:A:330:TRP:HD1	1.73	0.53
1:C:445:TYR:HB3	1:C:452:ALA:N	2.23	0.53
1:D:114:SER:HB3	1:D:123:SER:HB3	1.88	0.53
1:E:257:LEU:H	1:E:258:PRO:CD	2.10	0.53
1:E:393:VAL:HG23	1:E:491:VAL:HG13	1.90	0.53
1:F:287:LEU:HD13	1:F:311:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LEU:HD11	1:D:337:ARG:HD3	1.90	0.53
1:E:51:PHE:HB3	1:E:80:MSE:SE	2.58	0.53
1:E:53:TYR:HD2	1:E:58:ALA:O	1.91	0.53
1:F:543:LEU:HA	1:F:612:GLN:HE22	1.69	0.53
1:A:66:TYR:CD2	1:A:67:MSE:O	2.61	0.53
1:C:262:ILE:HG13	1:C:263:PRO:N	2.23	0.53
1:F:29:VAL:O	1:F:29:VAL:HG12	2.08	0.53
1:B:20:HIS:NE2	1:B:121:ALA:HB1	2.24	0.53
1:C:42:THR:HG22	1:C:104:LYS:HG3	1.91	0.53
1:C:454:CYS:SG	1:C:455:PHE:N	2.81	0.53
1:D:441:PHE:CD1	1:D:583:LYS:HG2	2.43	0.53
1:D:652:ASP:C	1:D:654:PRO:HD2	2.34	0.53
1:E:532:PRO:HD2	1:E:533:PHE:CD1	2.43	0.53
1:F:95:SER:OG	1:F:259:PHE:CE1	2.42	0.53
1:A:136:GLY:HA3	1:A:268:VAL:CG2	2.27	0.53
1:B:532:PRO:HD2	1:B:533:PHE:CD1	2.44	0.53
1:C:508:VAL:HG13	1:C:524:GLY:O	2.08	0.53
1:D:532:PRO:HD2	1:D:533:PHE:CD1	2.44	0.53
1:A:272:HIS:O	1:A:273:ALA:C	2.51	0.53
1:C:497:TYR:HD2	1:C:497:TYR:H	1.57	0.53
1:D:508:VAL:HG13	1:D:524:GLY:O	2.09	0.53
1:E:29:VAL:O	1:E:29:VAL:HG12	2.09	0.53
1:A:20:HIS:NE2	1:A:121:ALA:HB1	2.23	0.53
1:A:29:VAL:O	1:A:29:VAL:HG12	2.09	0.53
1:A:622:ALA:HB3	1:A:627:ARG:CG	2.38	0.53
1:D:292:LEU:HD22	1:D:310:TRP:HB3	1.90	0.53
1:D:447:PHE:HB2	1:D:455:PHE:O	2.09	0.53
1:E:301:GLY:O	1:E:616:PRO:O	2.27	0.53
1:B:18:TYR:HE1	1:B:22:THR:HG22	1.70	0.53
1:C:20:HIS:NE2	1:C:121:ALA:HB1	2.23	0.53
1:C:29:VAL:HG12	1:C:29:VAL:O	2.09	0.53
1:D:131:LYS:NZ	4:N:1:NAG:H81	2.24	0.53
1:B:29:VAL:O	1:B:29:VAL:HG12	2.09	0.53
1:B:93:ARG:H	1:B:93:ARG:NH1	1.90	0.53
1:C:292:LEU:HD22	1:C:310:TRP:HB3	1.90	0.53
1:D:20:HIS:NE2	1:D:121:ALA:HB1	2.23	0.53
1:F:63:LYS:C	1:F:80:MSE:HG2	2.33	0.53
1:F:268:VAL:HG22	1:F:269:PRO:HD2	1.91	0.53
1:F:361:TYR:HB2	1:F:381:ARG:HH21	1.74	0.53
1:B:118:SER:O	1:B:119:ASN:HB2	2.10	0.52
1:B:295:LEU:HG	1:B:330:TRP:HD1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:VAL:HG22	1:B:326:LEU:HD23	1.91	0.52
1:B:393:VAL:HG23	1:B:491:VAL:HG13	1.91	0.52
1:C:53:TYR:HD2	1:C:58:ALA:O	1.91	0.52
1:E:508:VAL:HG13	1:E:524:GLY:O	2.09	0.52
1:F:53:TYR:HD2	1:F:58:ALA:O	1.92	0.52
1:A:530:PHE:CZ	1:A:617:PHE:HD1	2.27	0.52
1:D:107:PRO:CG	1:D:108:GLY:H	2.22	0.52
1:E:135:VAL:HG12	1:E:140:TYR:OH	2.08	0.52
1:E:603:TRP:O	1:E:607:SER:N	2.43	0.52
1:F:497:TYR:HD2	1:F:497:TYR:H	1.55	0.52
1:B:137:ARG:NH1	1:B:296:THR:OG1	2.42	0.52
1:C:150:ILE:HG23	1:C:151:PRO:CD	2.39	0.52
1:C:447:PHE:HE1	1:C:455:PHE:HA	1.72	0.52
1:D:42:THR:HG22	1:D:104:LYS:HG3	1.91	0.52
1:F:138:GLU:OE2	1:F:271:ALA:HB2	2.10	0.52
1:A:287:LEU:HD13	1:A:311:ILE:HD13	1.92	0.52
1:C:530:PHE:CZ	1:C:617:PHE:HD1	2.27	0.52
1:D:295:LEU:HG	1:D:330:TRP:HD1	1.74	0.52
1:F:292:LEU:HD22	1:F:310:TRP:HB3	1.90	0.52
1:F:544:VAL:HG12	1:F:623:VAL:HG21	1.92	0.52
1:E:321:VAL:HG22	1:E:326:LEU:HD23	1.91	0.52
1:F:37:GLU:OE1	1:F:473:ASP:OD2	2.27	0.52
1:F:413:THR:HG23	1:F:595:GLN:HE22	1.75	0.52
1:F:532:PRO:HD2	1:F:533:PHE:CD1	2.44	0.52
1:A:51:PHE:HB3	1:A:80:MSE:SE	2.60	0.52
1:A:483:LYS:HD3	1:A:535:HIS:NE2	2.25	0.52
1:B:413:THR:HG23	1:B:595:GLN:HE22	1.75	0.52
1:B:438:CYS:HA	1:B:464:SER:O	2.10	0.52
1:B:622:ALA:HB3	1:B:627:ARG:HG3	1.91	0.52
1:D:93:ARG:H	1:D:93:ARG:NH1	1.91	0.52
1:D:438:CYS:HA	1:D:464:SER:O	2.09	0.52
1:F:20:HIS:NE2	1:F:121:ALA:HB1	2.23	0.52
1:A:53:TYR:HD2	1:A:58:ALA:O	1.93	0.52
1:A:79:THR:HG23	1:A:81:ASP:HB3	1.91	0.52
1:A:555:MSE:H	1:A:555:MSE:HE2	1.74	0.52
1:B:85:ILE:HG22	1:B:86:SER:N	2.25	0.52
1:B:268:VAL:HG22	1:B:269:PRO:HD2	1.92	0.52
1:D:287:LEU:HD13	1:D:311:ILE:HD13	1.92	0.52
1:D:689:PRO:HD2	1:D:730:CYS:HA	1.92	0.52
1:E:79:THR:HG23	1:E:81:ASP:HB3	1.91	0.52
1:E:112:THR:OG1	1:E:125:THR:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:321:VAL:HG22	1:F:326:LEU:HD23	1.91	0.52
1:A:112:THR:OG1	1:A:125:THR:HB	2.10	0.52
1:B:341:GLN:O	1:B:669:SER:O	2.27	0.52
1:C:294:LEU:HD23	1:C:309:GLU:O	2.10	0.52
1:D:29:VAL:O	1:D:29:VAL:HG12	2.09	0.52
1:D:72:ASP:HB2	1:D:74:THR:OG1	2.10	0.52
1:F:272:HIS:O	1:F:273:ALA:C	2.53	0.52
1:F:294:LEU:HG	1:F:310:TRP:NE1	2.25	0.52
1:F:438:CYS:HA	1:F:464:SER:O	2.10	0.52
1:A:137:ARG:NH1	1:A:296:THR:OG1	2.43	0.52
1:B:63:LYS:C	1:B:80:MSE:HG2	2.35	0.52
1:B:79:THR:HG23	1:B:81:ASP:HB3	1.92	0.52
1:B:544:VAL:HG12	1:B:623:VAL:HG21	1.92	0.52
1:C:295:LEU:HG	1:C:330:TRP:HD1	1.75	0.52
1:A:496:VAL:HG13	1:A:501:THR:HG22	1.92	0.52
1:B:496:VAL:HG13	1:B:501:THR:HG22	1.92	0.52
1:E:496:VAL:HG13	1:E:501:THR:HG22	1.92	0.52
1:A:508:VAL:HG13	1:A:524:GLY:O	2.10	0.51
1:C:438:CYS:HA	1:C:464:SER:O	2.10	0.51
1:E:118:SER:O	1:E:119:ASN:HB2	2.09	0.51
1:F:262:ILE:HG13	1:F:263:PRO:O	2.10	0.51
1:C:543:LEU:HA	1:C:612:GLN:HE22	1.71	0.51
1:E:45:ILE:HB	1:E:101:LEU:HB2	1.93	0.51
1:E:85:ILE:HG22	1:E:86:SER:N	2.25	0.51
1:A:72:ASP:HB2	1:A:74:THR:OG1	2.10	0.51
1:A:79:THR:O	1:A:81:ASP:N	2.43	0.51
1:A:540:HIS:HD2	1:A:541:ARG:HB2	1.76	0.51
1:A:675:MSE:HE2	1:A:715:HIS:CE1	2.38	0.51
1:C:272:HIS:O	1:C:273:ALA:C	2.53	0.51
1:D:54:ASP:CG	1:D:55:GLN:H	2.18	0.51
1:D:79:THR:O	1:D:81:ASP:N	2.43	0.51
1:D:603:TRP:O	1:D:607:SER:N	2.44	0.51
1:E:136:GLY:CA	1:E:268:VAL:HG21	2.30	0.51
1:F:79:THR:HG23	1:F:81:ASP:HB3	1.92	0.51
1:F:276:VAL:HG22	1:F:285:LEU:HD23	1.91	0.51
1:B:483:LYS:HD3	1:B:535:HIS:CE1	2.45	0.51
1:B:497:TYR:HD2	1:B:497:TYR:H	1.58	0.51
1:C:390:GLU:HG3	1:C:390:GLU:O	2.10	0.51
1:C:483:LYS:HD3	1:C:535:HIS:CE1	2.45	0.51
1:C:544:VAL:HG12	1:C:623:VAL:HG21	1.92	0.51
1:D:496:VAL:HG13	1:D:501:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:483:LYS:HD3	1:E:535:HIS:CE1	2.44	0.51
1:E:544:VAL:HG12	1:E:623:VAL:HG21	1.91	0.51
1:F:483:LYS:HD3	1:F:535:HIS:CE1	2.45	0.51
1:A:689:PRO:HD2	1:A:730:CYS:HA	1.92	0.51
1:B:483:LYS:HD3	1:B:535:HIS:NE2	2.26	0.51
1:C:85:ILE:HG22	1:C:86:SER:N	2.24	0.51
1:F:262:ILE:HG13	1:F:263:PRO:N	2.24	0.51
1:F:603:TRP:O	1:F:607:SER:N	2.44	0.51
1:A:438:CYS:HA	1:A:464:SER:O	2.10	0.51
1:B:53:TYR:HD2	1:B:58:ALA:O	1.92	0.51
1:C:413:THR:HG23	1:C:595:GLN:HE22	1.76	0.51
1:C:496:VAL:HG13	1:C:501:THR:HG22	1.93	0.51
1:D:483:LYS:HD3	1:D:535:HIS:CE1	2.46	0.51
1:E:262:ILE:HG13	1:E:263:PRO:O	2.10	0.51
1:E:413:THR:HG23	1:E:595:GLN:HE22	1.75	0.51
1:F:85:ILE:HG22	1:F:86:SER:N	2.26	0.51
1:F:622:ALA:HB3	1:F:627:ARG:CG	2.40	0.51
1:A:42:THR:HG22	1:A:104:LYS:HG3	1.92	0.51
1:B:42:THR:HG22	1:B:104:LYS:HG3	1.93	0.51
1:B:508:VAL:HG13	1:B:524:GLY:O	2.10	0.51
1:B:540:HIS:HD2	1:B:541:ARG:HB2	1.76	0.51
1:B:689:PRO:HD2	1:B:730:CYS:HA	1.92	0.51
1:D:85:ILE:HG22	1:D:86:SER:N	2.25	0.51
1:D:530:PHE:CZ	1:D:617:PHE:HD1	2.27	0.51
1:D:544:VAL:HG12	1:D:623:VAL:HG21	1.93	0.51
1:E:137:ARG:NH1	1:E:296:THR:OG1	2.43	0.51
1:F:483:LYS:HD3	1:F:535:HIS:NE2	2.26	0.51
1:A:390:GLU:HG3	1:A:390:GLU:O	2.10	0.51
1:C:287:LEU:HD13	1:C:311:ILE:HD13	1.93	0.51
1:C:603:TRP:O	1:C:607:SER:N	2.44	0.51
1:C:649:ARG:O	1:C:651:SER:N	2.44	0.51
1:A:399:LEU:C	1:A:487:ALA:HB1	2.36	0.51
1:B:94:LEU:HD22	1:B:157:ARG:CD	2.38	0.51
1:B:603:TRP:O	1:B:607:SER:N	2.43	0.51
1:C:274:PRO:HD3	1:C:330:TRP:CZ3	2.46	0.51
1:C:483:LYS:HD3	1:C:535:HIS:NE2	2.26	0.51
1:C:581:LEU:HD22	1:C:581:LEU:N	2.26	0.51
1:D:483:LYS:HD3	1:D:535:HIS:NE2	2.25	0.51
1:D:540:HIS:HD2	1:D:541:ARG:HB2	1.76	0.51
1:E:287:LEU:HD13	1:E:311:ILE:HD13	1.93	0.51
1:E:294:LEU:HD23	1:E:309:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:MSE:H	1:E:555:MSE:HE2	1.75	0.51
1:E:689:PRO:HD2	1:E:730:CYS:HA	1.92	0.51
1:F:649:ARG:O	1:F:651:SER:N	2.44	0.51
1:A:54:ASP:CG	1:A:55:GLN:H	2.19	0.51
1:B:45:ILE:HB	1:B:101:LEU:HB2	1.93	0.51
1:B:287:LEU:HD13	1:B:311:ILE:HD13	1.93	0.51
1:C:137:ARG:NH1	1:C:296:THR:OG1	2.42	0.51
1:E:42:THR:HG22	1:E:104:LYS:HG3	1.92	0.51
1:F:390:GLU:O	1:F:390:GLU:HG3	2.10	0.51
1:F:622:ALA:HB3	1:F:627:ARG:HG3	1.92	0.51
1:A:447:PHE:CZ	1:A:448:MSE:HG2	2.46	0.50
1:B:262:ILE:HG13	1:B:263:PRO:O	2.11	0.50
1:B:449:TRP:C	1:B:451:GLY:H	2.19	0.50
1:C:268:VAL:HG22	1:C:269:PRO:HD2	1.92	0.50
1:E:107:PRO:CG	1:E:108:GLY:H	2.23	0.50
1:E:438:CYS:HA	1:E:464:SER:O	2.11	0.50
1:E:483:LYS:HD3	1:E:535:HIS:NE2	2.26	0.50
1:F:496:VAL:HG13	1:F:501:THR:HG22	1.93	0.50
1:A:504:LEU:HD21	1:A:521:VAL:HB	1.93	0.50
1:B:94:LEU:CD2	1:B:157:ARG:HD3	2.38	0.50
1:C:321:VAL:HG22	1:C:326:LEU:HD23	1.94	0.50
1:C:653:ALA:O	1:C:684:ARG:HD2	2.11	0.50
1:D:413:THR:HG23	1:D:595:GLN:HE22	1.75	0.50
1:E:79:THR:O	1:E:81:ASP:N	2.44	0.50
1:F:54:ASP:CG	1:F:55:GLN:H	2.19	0.50
1:A:85:ILE:HG22	1:A:86:SER:N	2.27	0.50
1:A:400:PRO:CA	1:A:487:ALA:HB2	2.41	0.50
1:B:79:THR:C	1:B:81:ASP:N	2.61	0.50
1:D:262:ILE:HG13	1:D:263:PRO:N	2.25	0.50
1:D:390:GLU:HG3	1:D:390:GLU:O	2.11	0.50
1:E:54:ASP:CG	1:E:55:GLN:H	2.19	0.50
1:E:80:MSE:CA	1:E:80:MSE:HE3	2.41	0.50
1:A:262:ILE:HG13	1:A:263:PRO:N	2.25	0.50
1:A:262:ILE:HG13	1:A:263:PRO:O	2.11	0.50
1:C:79:THR:HG23	1:C:81:ASP:HB3	1.92	0.50
1:C:689:PRO:HD2	1:C:730:CYS:HA	1.92	0.50
1:D:262:ILE:HG13	1:D:263:PRO:O	2.11	0.50
1:E:504:LEU:HD21	1:E:521:VAL:HB	1.94	0.50
1:F:79:THR:O	1:F:81:ASP:N	2.44	0.50
1:A:447:PHE:CD1	1:A:454:CYS:O	2.61	0.50
1:A:278:HIS:CB	1:A:343:SER:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PRO:HD2	1:A:626:LEU:O	2.12	0.50
1:C:138:GLU:OE2	1:C:271:ALA:HB2	2.12	0.50
1:C:622:ALA:HB3	1:C:627:ARG:CG	2.42	0.50
1:D:581:LEU:HD22	1:D:581:LEU:N	2.26	0.50
1:F:42:THR:HG22	1:F:104:LYS:HG3	1.92	0.50
1:F:80:MSE:HA	1:F:80:MSE:HE3	1.94	0.50
1:A:483:LYS:HD3	1:A:535:HIS:CE1	2.47	0.50
1:A:544:VAL:HG12	1:A:623:VAL:HG21	1.93	0.50
1:B:294:LEU:HG	1:B:310:TRP:NE1	2.26	0.50
1:B:722:GLN:HG2	1:B:739:GLU:HG2	1.94	0.50
1:C:118:SER:O	1:C:119:ASN:HB2	2.10	0.50
1:C:262:ILE:HG13	1:C:263:PRO:O	2.11	0.50
1:C:277:ILE:HD12	1:C:286:GLN:NE2	2.27	0.50
1:C:420:ILE:O	1:C:420:ILE:HD12	2.12	0.50
1:F:689:PRO:HD2	1:F:730:CYS:HA	1.92	0.50
1:A:276:VAL:HG12	1:A:277:ILE:N	2.26	0.50
1:A:300:LEU:HD11	1:A:337:ARG:HD3	1.93	0.50
1:A:581:LEU:N	1:A:581:LEU:HD22	2.26	0.50
1:A:690:VAL:HG12	1:A:699:LEU:CD1	2.42	0.50
1:B:374:PRO:CA	1:B:392:THR:HG22	2.42	0.50
1:B:622:ALA:HB3	1:B:627:ARG:CG	2.41	0.50
1:B:690:VAL:HG12	1:B:699:LEU:CD1	2.42	0.50
1:C:532:PRO:HD2	1:C:533:PHE:CD1	2.47	0.50
1:D:399:LEU:C	1:D:487:ALA:HB1	2.37	0.50
1:D:400:PRO:HD2	1:D:626:LEU:O	2.12	0.50
1:E:276:VAL:HG22	1:E:285:LEU:HD23	1.94	0.50
1:E:400:PRO:HD2	1:E:626:LEU:O	2.12	0.50
1:F:112:THR:OG1	1:F:125:THR:HB	2.12	0.50
1:F:568:LEU:C	1:F:570:SER:H	2.20	0.50
1:A:45:ILE:HB	1:A:101:LEU:HB2	1.94	0.50
1:D:504:LEU:HD21	1:D:521:VAL:HB	1.94	0.50
1:E:540:HIS:HD2	1:E:541:ARG:HB2	1.77	0.50
1:F:555:MSE:H	1:F:555:MSE:HE2	1.76	0.50
1:A:722:GLN:HG2	1:A:739:GLU:HG2	1.94	0.49
1:B:272:HIS:O	1:B:273:ALA:C	2.55	0.49
1:B:604:LYS:C	1:B:606:ASN:H	2.19	0.49
1:C:112:THR:OG1	1:C:125:THR:HB	2.11	0.49
1:C:722:GLN:HG2	1:C:739:GLU:HG2	1.94	0.49
1:F:45:ILE:HB	1:F:101:LEU:HB2	1.93	0.49
1:F:106:PRO:CB	1:F:107:PRO:HD3	2.41	0.49
1:A:80:MSE:CA	1:A:80:MSE:HE3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:TRP:O	1:A:607:SER:N	2.45	0.49
1:C:45:ILE:HB	1:C:101:LEU:HB2	1.93	0.49
1:C:255:LEU:HD22	1:C:256:HIS:CD2	2.47	0.49
1:C:568:LEU:C	1:C:570:SER:H	2.20	0.49
1:C:604:LYS:C	1:C:606:ASN:H	2.20	0.49
1:C:652:ASP:HB3	1:C:654:PRO:HD2	1.95	0.49
1:D:654:PRO:HB3	1:D:684:ARG:O	2.12	0.49
1:E:262:ILE:HG13	1:E:263:PRO:N	2.25	0.49
1:E:497:TYR:HD2	1:E:497:TYR:H	1.56	0.49
1:F:574:ILE:O	1:F:574:ILE:HG13	2.11	0.49
1:B:79:THR:O	1:B:81:ASP:N	2.45	0.49
1:B:504:LEU:HD21	1:B:521:VAL:HB	1.94	0.49
1:D:649:ARG:O	1:D:651:SER:N	2.45	0.49
1:F:581:LEU:HD22	1:F:581:LEU:N	2.27	0.49
1:A:532:PRO:HD2	1:A:533:PHE:CD1	2.48	0.49
1:B:138:GLU:OE2	1:B:271:ALA:N	2.46	0.49
1:B:262:ILE:HG13	1:B:263:PRO:N	2.27	0.49
1:D:272:HIS:O	1:D:273:ALA:C	2.56	0.49
1:E:399:LEU:C	1:E:487:ALA:HB1	2.37	0.49
1:A:154:VAL:HG22	1:A:155:TYR:N	2.28	0.49
1:C:72:ASP:HB2	1:C:74:THR:OG1	2.12	0.49
1:C:79:THR:O	1:C:81:ASP:N	2.45	0.49
1:C:276:VAL:HG22	1:C:285:LEU:HD23	1.93	0.49
1:D:112:THR:OG1	1:D:125:THR:HB	2.12	0.49
1:D:374:PRO:CA	1:D:392:THR:HG22	2.42	0.49
1:E:72:ASP:HB2	1:E:74:THR:OG1	2.13	0.49
1:E:374:PRO:CA	1:E:392:THR:HG22	2.42	0.49
1:E:690:VAL:HG12	1:E:699:LEU:CD1	2.42	0.49
1:A:276:VAL:HG22	1:A:285:LEU:HD23	1.94	0.49
1:A:336:VAL:CG2	1:A:337:ARG:N	2.76	0.49
1:A:374:PRO:CA	1:A:392:THR:HG22	2.42	0.49
1:B:568:LEU:C	1:B:570:SER:H	2.21	0.49
1:C:399:LEU:C	1:C:487:ALA:HB1	2.37	0.49
1:C:400:PRO:HD2	1:C:626:LEU:O	2.13	0.49
1:C:644:ASN:HA	1:C:647:PHE:CD2	2.48	0.49
1:D:45:ILE:HB	1:D:101:LEU:HB2	1.94	0.49
1:D:625:PRO:HD2	1:D:627:ARG:HH12	1.78	0.49
1:E:654:PRO:HB3	1:E:684:ARG:O	2.12	0.49
1:F:399:LEU:C	1:F:487:ALA:HB1	2.38	0.49
1:A:294:LEU:HG	1:A:310:TRP:NE1	2.26	0.49
1:A:400:PRO:HA	1:A:487:ALA:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ARG:O	1:B:651:SER:N	2.45	0.49
1:B:654:PRO:HB3	1:B:684:ARG:O	2.13	0.49
1:D:80:MSE:HA	1:D:80:MSE:HE3	1.94	0.49
1:D:268:VAL:HG11	1:D:332:ASN:ND2	2.27	0.49
1:E:276:VAL:HG12	1:E:277:ILE:N	2.28	0.49
1:E:543:LEU:HA	1:E:612:GLN:HE22	1.72	0.49
1:E:604:LYS:C	1:E:606:ASN:H	2.20	0.49
1:F:504:LEU:HD21	1:F:521:VAL:HB	1.95	0.49
1:B:112:THR:OG1	1:B:125:THR:HB	2.12	0.49
1:C:54:ASP:CG	1:C:55:GLN:H	2.19	0.49
1:C:504:LEU:HD21	1:C:521:VAL:HB	1.95	0.49
1:C:508:VAL:O	1:C:508:VAL:HG12	2.13	0.49
1:C:80:MSE:HE3	1:C:80:MSE:HA	1.95	0.49
1:E:138:GLU:OE2	1:E:271:ALA:N	2.46	0.49
1:E:300:LEU:HD11	1:E:337:ARG:HD3	1.95	0.49
1:E:649:ARG:O	1:E:651:SER:N	2.46	0.49
1:E:722:GLN:HG2	1:E:739:GLU:HG2	1.94	0.49
1:F:276:VAL:HG12	1:F:277:ILE:N	2.28	0.49
1:B:54:ASP:CG	1:B:55:GLN:H	2.21	0.49
1:B:390:GLU:HG3	1:B:390:GLU:O	2.13	0.49
1:B:555:MSE:H	1:B:555:MSE:HE2	1.77	0.49
1:C:80:MSE:HE3	1:C:80:MSE:CA	2.43	0.49
1:D:276:VAL:HG22	1:D:285:LEU:HD23	1.95	0.49
1:D:400:PRO:CA	1:D:487:ALA:HB2	2.42	0.49
1:E:77:GLU:HG2	1:E:78:GLY:N	2.28	0.49
1:E:568:LEU:C	1:E:570:SER:H	2.21	0.49
1:F:407:ILE:HG21	1:F:568:LEU:HD13	1.95	0.49
1:F:508:VAL:O	1:F:508:VAL:HG12	2.12	0.49
1:F:604:LYS:C	1:F:606:ASN:H	2.21	0.49
1:D:137:ARG:NH1	1:D:296:THR:OG1	2.46	0.48
1:D:653:ALA:N	1:D:654:PRO:CD	2.74	0.48
1:D:722:GLN:HG2	1:D:739:GLU:HG2	1.94	0.48
1:F:722:GLN:HG2	1:F:739:GLU:HG2	1.94	0.48
1:B:72:ASP:HB2	1:B:74:THR:OG1	2.12	0.48
1:B:92:ARG:HA	1:B:93:ARG:HH12	1.79	0.48
1:B:268:VAL:HG11	1:B:332:ASN:ND2	2.28	0.48
1:E:644:ASN:HA	1:E:647:PHE:CD2	2.49	0.48
1:F:77:GLU:HG2	1:F:78:GLY:N	2.28	0.48
1:F:93:ARG:H	1:F:93:ARG:NH1	1.92	0.48
1:F:644:ASN:HA	1:F:647:PHE:CD2	2.48	0.48
1:B:136:GLY:CA	1:B:268:VAL:HG21	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:CYS:SG	1:B:706:VAL:HG21	2.53	0.48
1:D:604:LYS:C	1:D:606:ASN:H	2.22	0.48
1:E:688:CYS:SG	1:E:706:VAL:HG21	2.53	0.48
1:F:80:MSE:HE3	1:F:80:MSE:CA	2.43	0.48
1:F:446:PRO:O	1:F:447:PHE:CB	2.61	0.48
1:A:649:ARG:O	1:A:651:SER:N	2.45	0.48
1:A:653:ALA:N	1:A:654:PRO:HD2	2.28	0.48
1:C:690:VAL:HG12	1:C:699:LEU:CD1	2.42	0.48
1:D:80:MSE:HE3	1:D:80:MSE:CA	2.43	0.48
1:D:154:VAL:HG22	1:D:155:TYR:N	2.28	0.48
1:D:644:ASN:HA	1:D:647:PHE:CD2	2.48	0.48
1:E:537:VAL:HG22	1:E:546:ASN:ND2	2.28	0.48
1:F:274:PRO:HD3	1:F:330:TRP:CZ3	2.48	0.48
1:F:690:VAL:HG12	1:F:699:LEU:CD1	2.43	0.48
1:B:399:LEU:C	1:B:487:ALA:HB1	2.38	0.48
1:B:399:LEU:HD12	1:B:399:LEU:N	2.28	0.48
1:B:420:ILE:HD12	1:B:420:ILE:O	2.14	0.48
1:C:321:VAL:CG1	1:C:340:ALA:HB2	2.44	0.48
1:D:92:ARG:HA	1:D:93:ARG:HH12	1.78	0.48
1:F:420:ILE:HD12	1:F:420:ILE:O	2.13	0.48
1:F:688:CYS:SG	1:F:706:VAL:HG21	2.54	0.48
1:A:64:TYR:CG	1:A:83:ILE:HD11	2.49	0.48
1:A:644:ASN:HA	1:A:647:PHE:CD2	2.48	0.48
1:A:653:ALA:O	1:A:654:PRO:C	2.56	0.48
1:B:644:ASN:HA	1:B:647:PHE:CD2	2.48	0.48
1:C:537:VAL:HG22	1:C:546:ASN:ND2	2.27	0.48
1:D:53:TYR:HD2	1:D:58:ALA:O	1.97	0.48
1:D:276:VAL:HG12	1:D:277:ILE:N	2.27	0.48
1:D:277:ILE:HD12	1:D:286:GLN:NE2	2.28	0.48
1:F:92:ARG:HA	1:F:93:ARG:HH12	1.79	0.48
1:F:150:ILE:HG23	1:F:151:PRO:CD	2.42	0.48
1:A:106:PRO:CB	1:A:107:PRO:HD3	2.40	0.48
1:A:537:VAL:HG22	1:A:546:ASN:ND2	2.28	0.48
1:C:336:VAL:CG2	1:C:337:ARG:N	2.76	0.48
1:D:400:PRO:HA	1:D:487:ALA:CB	2.44	0.48
1:E:92:ARG:HA	1:E:93:ARG:HH12	1.79	0.48
1:E:272:HIS:O	1:E:273:ALA:C	2.57	0.48
1:E:420:ILE:HD12	1:E:420:ILE:O	2.13	0.48
1:F:72:ASP:HB2	1:F:74:THR:OG1	2.13	0.48
1:F:154:VAL:HG22	1:F:155:TYR:N	2.28	0.48
1:F:336:VAL:CG2	1:F:337:ARG:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:PRO:HD2	1:F:626:LEU:O	2.13	0.48
1:F:649:ARG:O	1:F:650:THR:C	2.56	0.48
1:A:107:PRO:CG	1:A:108:GLY:H	2.22	0.48
1:A:413:THR:HG23	1:A:595:GLN:HE22	1.77	0.48
1:B:594:THR:HG21	1:C:272:HIS:HA	1.95	0.48
1:C:445:TYR:CB	1:C:451:GLY:HA3	2.37	0.48
1:E:19:CYS:C	1:E:21:HIS:N	2.72	0.48
1:E:400:PRO:CA	1:E:487:ALA:HB2	2.44	0.48
1:F:374:PRO:CA	1:F:392:THR:HG22	2.44	0.48
1:A:262:ILE:HD12	1:A:263:PRO:HD2	1.96	0.48
1:B:274:PRO:HD3	1:B:330:TRP:CZ3	2.49	0.48
1:D:568:LEU:C	1:D:570:SER:H	2.21	0.48
1:E:504:LEU:O	1:E:504:LEU:HD12	2.14	0.48
1:A:449:TRP:O	1:A:451:GLY:N	2.46	0.48
1:B:394:MSE:HE2	1:B:394:MSE:HB3	1.91	0.48
1:C:688:CYS:SG	1:C:706:VAL:HG21	2.53	0.48
1:D:106:PRO:CB	1:D:107:PRO:HD3	2.40	0.48
1:D:555:MSE:HE2	1:D:555:MSE:H	1.78	0.48
1:E:80:MSE:HE3	1:E:80:MSE:HA	1.94	0.48
1:E:93:ARG:H	1:E:93:ARG:NH1	1.91	0.48
1:E:329:ILE:H	1:E:329:ILE:HG12	1.49	0.48
1:F:137:ARG:NH1	1:F:296:THR:OG1	2.45	0.48
1:F:400:PRO:CA	1:F:487:ALA:HB2	2.44	0.48
1:B:336:VAL:CG2	1:B:337:ARG:N	2.77	0.47
1:D:690:VAL:HG12	1:D:699:LEU:CD1	2.43	0.47
1:E:400:PRO:HA	1:E:487:ALA:CB	2.44	0.47
1:E:503:PHE:CD2	1:E:503:PHE:C	2.92	0.47
1:F:329:ILE:H	1:F:329:ILE:HG12	1.50	0.47
1:A:80:MSE:HE3	1:A:80:MSE:HA	1.95	0.47
1:A:294:LEU:HD23	1:A:309:GLU:O	2.14	0.47
1:B:340:ALA:C	1:B:341:GLN:HG2	2.39	0.47
1:B:537:VAL:HG22	1:B:546:ASN:ND2	2.28	0.47
1:C:92:ARG:HA	1:C:93:ARG:HH12	1.80	0.47
1:C:300:LEU:HD11	1:C:337:ARG:HD3	1.95	0.47
1:C:374:PRO:CA	1:C:392:THR:HG22	2.43	0.47
1:D:106:PRO:CB	1:D:107:PRO:CD	2.92	0.47
1:F:64:TYR:CG	1:F:83:ILE:HD11	2.49	0.47
1:F:138:GLU:OE2	1:F:271:ALA:N	2.47	0.47
1:F:148:LYS:O	1:F:267:MSE:HA	2.15	0.47
1:B:106:PRO:CB	1:B:107:PRO:CD	2.92	0.47
1:B:400:PRO:HD2	1:B:626:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:VAL:O	1:B:508:VAL:HG12	2.15	0.47
1:C:540:HIS:HD2	1:C:541:ARG:HB2	1.79	0.47
1:D:77:GLU:HG2	1:D:78:GLY:N	2.29	0.47
1:D:145:VAL:CG2	1:F:17:SER:HB3	2.30	0.47
1:D:336:VAL:CG2	1:D:337:ARG:N	2.78	0.47
1:E:106:PRO:CB	1:E:107:PRO:CD	2.92	0.47
1:F:277:ILE:HD12	1:F:286:GLN:NE2	2.30	0.47
1:F:540:HIS:HD2	1:F:541:ARG:HB2	1.79	0.47
1:F:654:PRO:HB3	1:F:684:ARG:O	2.14	0.47
1:A:568:LEU:C	1:A:570:SER:H	2.22	0.47
1:B:80:MSE:HA	1:B:80:MSE:HE3	1.95	0.47
1:B:106:PRO:CB	1:B:107:PRO:HD3	2.40	0.47
1:B:400:PRO:HA	1:B:487:ALA:CB	2.44	0.47
1:C:294:LEU:HG	1:C:310:TRP:NE1	2.28	0.47
1:D:615:ALA:HA	1:D:616:PRO:HD3	1.55	0.47
1:D:661:CYS:HA	1:D:678:LEU:HD23	1.97	0.47
1:E:154:VAL:HG22	1:E:155:TYR:N	2.29	0.47
1:E:390:GLU:HG3	1:E:390:GLU:O	2.13	0.47
1:A:420:ILE:HD12	1:A:420:ILE:O	2.13	0.47
1:B:148:LYS:O	1:B:267:MSE:HA	2.14	0.47
1:B:276:VAL:HG22	1:B:285:LEU:HD23	1.95	0.47
1:E:137:ARG:H	1:E:332:ASN:HD22	1.63	0.47
1:F:400:PRO:HA	1:F:487:ALA:CB	2.45	0.47
1:F:503:PHE:C	1:F:503:PHE:CD2	2.91	0.47
1:B:80:MSE:HE3	1:B:80:MSE:CA	2.45	0.47
1:B:294:LEU:HD23	1:B:309:GLU:O	2.14	0.47
1:D:493:LEU:HD23	1:D:493:LEU:HA	1.61	0.47
1:E:148:LYS:O	1:E:267:MSE:HA	2.15	0.47
1:A:268:VAL:HG22	1:A:269:PRO:CD	2.44	0.47
1:B:300:LEU:HD11	1:B:337:ARG:HD3	1.96	0.47
1:B:504:LEU:O	1:B:504:LEU:HD12	2.13	0.47
1:B:505:ASP:OD1	1:D:505:ASP:OD1	2.32	0.47
1:C:106:PRO:CB	1:C:107:PRO:CD	2.93	0.47
1:C:268:VAL:HG11	1:C:332:ASN:ND2	2.29	0.47
1:C:375:TYR:O	1:C:390:GLU:HA	2.14	0.47
1:C:452:ALA:O	1:C:453:GLN:C	2.58	0.47
1:D:262:ILE:HD12	1:D:263:PRO:HD2	1.97	0.47
1:D:375:TYR:O	1:D:390:GLU:HA	2.15	0.47
1:D:508:VAL:O	1:D:508:VAL:HG12	2.15	0.47
1:E:305:GLU:N	1:E:306:PRO:HD3	2.30	0.47
1:E:336:VAL:CG2	1:E:337:ARG:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:LEU:HG	1:E:691:HIS:CG	2.49	0.47
1:F:375:TYR:O	1:F:390:GLU:HA	2.14	0.47
1:F:394:MSE:HE2	1:F:394:MSE:HB3	1.92	0.47
1:F:621:ILE:CD1	1:F:621:ILE:H	2.27	0.47
1:A:19:CYS:C	1:A:21:HIS:N	2.72	0.47
1:A:268:VAL:HG11	1:A:332:ASN:ND2	2.29	0.47
1:B:77:GLU:HG2	1:B:78:GLY:N	2.29	0.47
1:B:375:TYR:O	1:B:390:GLU:HA	2.15	0.47
1:B:661:CYS:HA	1:B:678:LEU:HD23	1.97	0.47
1:D:294:LEU:HD23	1:D:309:GLU:O	2.15	0.47
1:A:407:ILE:HG21	1:A:568:LEU:HD13	1.96	0.47
1:A:688:CYS:SG	1:A:706:VAL:HG21	2.55	0.47
1:B:154:VAL:HG22	1:B:155:TYR:N	2.29	0.47
1:B:400:PRO:CA	1:B:487:ALA:HB2	2.45	0.47
1:C:148:LYS:O	1:C:267:MSE:HA	2.14	0.47
1:C:720:SER:OG	1:C:723:ALA:HB2	2.15	0.47
1:D:537:VAL:HG22	1:D:546:ASN:ND2	2.29	0.47
1:D:688:CYS:SG	1:D:706:VAL:HG21	2.54	0.47
1:F:19:CYS:C	1:F:21:HIS:N	2.73	0.47
1:A:60:SER:HB2	1:A:63:LYS:HB2	1.97	0.47
1:A:305:GLU:N	1:A:306:PRO:HD3	2.30	0.47
1:A:445:TYR:CG	1:A:451:GLY:HA3	2.51	0.47
1:A:504:LEU:HD21	1:A:521:VAL:CG2	2.45	0.47
1:A:604:LYS:C	1:A:606:ASN:H	2.22	0.47
1:A:661:CYS:HA	1:A:678:LEU:HD23	1.97	0.47
1:B:305:GLU:N	1:B:306:PRO:HD3	2.30	0.47
1:C:154:VAL:HG22	1:C:155:TYR:N	2.30	0.47
1:C:400:PRO:CA	1:C:487:ALA:HB2	2.45	0.47
1:C:451:GLY:HA2	1:C:586:ALA:HB1	1.95	0.47
1:D:504:LEU:HD21	1:D:521:VAL:CG2	2.45	0.47
1:F:262:ILE:HD12	1:F:263:PRO:HD2	1.96	0.47
1:A:277:ILE:HD12	1:A:286:GLN:NE2	2.29	0.46
1:A:375:TYR:O	1:A:390:GLU:HA	2.15	0.46
1:A:503:PHE:C	1:A:503:PHE:CD2	2.93	0.46
1:D:449:TRP:HD1	1:D:453:GLN:HG3	1.80	0.46
1:E:375:TYR:O	1:E:390:GLU:HA	2.15	0.46
1:F:471:SER:C	1:F:473:ASP:H	2.23	0.46
1:F:471:SER:C	1:F:473:ASP:N	2.72	0.46
1:F:504:LEU:HD21	1:F:521:VAL:CG2	2.45	0.46
1:F:720:SER:OG	1:F:723:ALA:HB2	2.15	0.46
1:A:97:LYS:HB3	1:A:100:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG22	1:C:17:SER:CB	2.25	0.46
1:A:321:VAL:CG1	1:A:340:ALA:HB2	2.45	0.46
1:A:471:SER:C	1:A:473:ASP:N	2.72	0.46
1:A:621:ILE:CD1	1:A:621:ILE:H	2.28	0.46
1:B:150:ILE:HG23	1:B:151:PRO:CD	2.41	0.46
1:B:503:PHE:C	1:B:503:PHE:CD2	2.92	0.46
1:C:64:TYR:CG	1:C:83:ILE:HD11	2.50	0.46
1:C:107:PRO:CG	1:C:108:GLY:H	2.23	0.46
1:C:621:ILE:CD1	1:C:621:ILE:H	2.28	0.46
1:D:399:LEU:HD12	1:D:399:LEU:N	2.30	0.46
1:D:471:SER:C	1:D:473:ASP:H	2.23	0.46
1:D:503:PHE:C	1:D:503:PHE:CD2	2.94	0.46
1:E:294:LEU:HG	1:E:310:TRP:NE1	2.30	0.46
1:B:471:SER:C	1:B:473:ASP:H	2.23	0.46
1:C:262:ILE:HD12	1:C:263:PRO:HD2	1.97	0.46
1:C:305:GLU:N	1:C:306:PRO:HD3	2.30	0.46
1:D:407:ILE:HG21	1:D:568:LEU:HD13	1.96	0.46
1:D:422:CYS:SG	1:D:455:PHE:N	2.88	0.46
1:F:294:LEU:HD23	1:F:309:GLU:O	2.16	0.46
1:F:652:ASP:C	1:F:654:PRO:HD2	2.40	0.46
1:A:77:GLU:HG2	1:A:78:GLY:N	2.28	0.46
1:A:274:PRO:HD3	1:A:330:TRP:CZ3	2.51	0.46
1:A:399:LEU:N	1:A:399:LEU:HD12	2.30	0.46
1:C:503:PHE:C	1:C:503:PHE:CD2	2.94	0.46
1:D:64:TYR:CG	1:D:83:ILE:HD11	2.51	0.46
1:D:400:PRO:HA	1:D:487:ALA:HB2	1.98	0.46
1:E:60:SER:HB2	1:E:63:LYS:HB2	1.98	0.46
1:E:64:TYR:CG	1:E:83:ILE:HD11	2.50	0.46
1:E:268:VAL:HG11	1:E:332:ASN:ND2	2.30	0.46
1:E:378:LEU:HG	1:E:691:HIS:CD2	2.51	0.46
1:F:106:PRO:CB	1:F:107:PRO:CD	2.93	0.46
1:F:655:LEU:N	1:F:683:ASP:HB2	2.27	0.46
1:A:400:PRO:HA	1:A:487:ALA:HB2	1.97	0.46
1:B:486:THR:HG22	1:B:487:ALA:H	1.81	0.46
1:C:37:GLU:OE1	1:C:473:ASP:OD2	2.33	0.46
1:D:97:LYS:HB3	1:D:100:PHE:HB2	1.98	0.46
1:D:720:SER:OG	1:D:723:ALA:HB2	2.15	0.46
1:E:399:LEU:HD12	1:E:399:LEU:N	2.31	0.46
1:A:148:LYS:O	1:A:267:MSE:HA	2.16	0.46
1:A:489:MSE:HG3	1:A:508:VAL:HB	1.98	0.46
1:F:504:LEU:HD12	1:F:504:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:661:CYS:HA	1:F:678:LEU:HD23	1.97	0.46
2:K:1:NAG:C4	2:K:2:NAG:N2	2.74	0.46
1:A:363:HIS:NE2	1:A:365:THR:HG23	2.30	0.46
1:B:64:TYR:CG	1:B:83:ILE:HD11	2.50	0.46
1:B:97:LYS:HB3	1:B:100:PHE:HB2	1.98	0.46
1:B:146:HIS:CD2	1:B:146:HIS:H	2.34	0.46
1:B:276:VAL:HG12	1:B:277:ILE:N	2.29	0.46
1:C:106:PRO:CB	1:C:107:PRO:HD3	2.41	0.46
1:C:299:ARG:NH1	1:C:305:GLU:CD	2.73	0.46
1:C:407:ILE:HG21	1:C:568:LEU:HD13	1.95	0.46
1:C:555:MSE:HB2	1:C:555:MSE:HE3	1.70	0.46
1:C:661:CYS:HA	1:C:678:LEU:HD23	1.97	0.46
1:D:150:ILE:HG23	1:D:151:PRO:CD	2.41	0.46
1:D:268:VAL:HG22	1:D:269:PRO:CD	2.45	0.46
1:E:494:ARG:HB2	1:E:503:PHE:CD1	2.47	0.46
1:E:555:MSE:HE3	1:E:555:MSE:HB2	1.75	0.46
1:E:720:SER:OG	1:E:723:ALA:HB2	2.16	0.46
1:F:513:PRO:HA	1:F:522:ILE:HG12	1.98	0.46
1:A:295:LEU:HG	1:A:330:TRP:CD1	2.51	0.46
1:C:40:ASP:OD1	1:C:41:ASN:N	2.48	0.46
1:C:504:LEU:HD21	1:C:521:VAL:CG2	2.46	0.46
1:F:559:ALA:O	1:F:599:GLY:HA3	2.16	0.46
1:A:654:PRO:HB3	1:A:684:ARG:O	2.16	0.46
1:B:60:SER:HB2	1:B:63:LYS:HB2	1.98	0.46
1:B:277:ILE:HD12	1:B:286:GLN:NE2	2.31	0.46
1:B:720:SER:OG	1:B:723:ALA:HB2	2.16	0.46
1:C:53:TYR:CD2	1:C:58:ALA:O	2.69	0.46
1:E:150:ILE:HG23	1:E:151:PRO:CD	2.40	0.46
1:F:581:LEU:HD22	1:F:581:LEU:H	1.81	0.46
1:C:400:PRO:HA	1:C:487:ALA:CB	2.46	0.46
1:C:494:ARG:HB2	1:C:503:PHE:CD1	2.45	0.46
1:D:295:LEU:HG	1:D:330:TRP:CD1	2.51	0.46
1:E:97:LYS:HB3	1:E:100:PHE:HB2	1.98	0.46
1:E:453:GLN:CD	1:E:453:GLN:H	2.23	0.46
1:F:494:ARG:HB2	1:F:503:PHE:CD1	2.47	0.46
1:A:37:GLU:OE1	1:A:473:ASP:OD2	2.33	0.45
1:A:146:HIS:H	1:A:146:HIS:CD2	2.34	0.45
1:C:63:LYS:HD3	1:C:79:THR:HA	1.98	0.45
1:E:262:ILE:HD12	1:E:263:PRO:HD2	1.98	0.45
1:E:363:HIS:NE2	1:E:365:THR:HG23	2.32	0.45
1:E:655:LEU:N	1:E:683:ASP:HB2	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:413:THR:HG21	1:F:595:GLN:NE2	2.31	0.45
1:A:92:ARG:HA	1:A:93:ARG:HH12	1.79	0.45
1:A:138:GLU:OE2	1:A:271:ALA:N	2.48	0.45
1:A:650:THR:O	1:A:650:THR:CG2	2.64	0.45
1:B:262:ILE:HD12	1:B:263:PRO:HD2	1.97	0.45
1:B:268:VAL:HG22	1:B:269:PRO:CD	2.46	0.45
1:B:411:PHE:CD1	1:B:411:PHE:C	2.93	0.45
1:C:10:SER:HA	1:C:50:GLN:NE2	2.32	0.45
3:R:1:NAG:H61	3:R:2:NAG:N2	2.30	0.45
1:A:40:ASP:OD1	1:A:41:ASN:N	2.50	0.45
1:A:508:VAL:O	1:A:508:VAL:HG12	2.15	0.45
1:B:63:LYS:HD3	1:B:79:THR:HA	1.98	0.45
1:C:45:ILE:HD12	1:C:85:ILE:HD13	1.99	0.45
1:C:60:SER:HB2	1:C:63:LYS:HB2	1.99	0.45
1:C:446:PRO:O	1:C:447:PHE:O	2.34	0.45
1:C:471:SER:C	1:C:473:ASP:N	2.73	0.45
1:C:497:TYR:CD1	1:C:642:ILE:HG23	2.51	0.45
1:E:106:PRO:CB	1:E:107:PRO:HD3	2.41	0.45
1:E:471:SER:C	1:E:473:ASP:H	2.24	0.45
1:A:110:SER:HB2	1:A:126:LEU:O	2.16	0.45
1:A:471:SER:C	1:A:473:ASP:H	2.24	0.45
1:A:581:LEU:HD22	1:A:581:LEU:H	1.81	0.45
1:C:97:LYS:HB3	1:C:100:PHE:HB2	1.98	0.45
1:C:399:LEU:N	1:C:399:LEU:HD12	2.32	0.45
1:C:413:THR:HG21	1:C:595:GLN:NE2	2.32	0.45
1:D:45:ILE:HD12	1:D:85:ILE:HD13	1.99	0.45
1:D:363:HIS:NE2	1:D:365:THR:HG23	2.31	0.45
1:D:581:LEU:HD22	1:D:581:LEU:H	1.80	0.45
1:E:268:VAL:HG22	1:E:269:PRO:CD	2.46	0.45
1:E:508:VAL:O	1:E:508:VAL:HG12	2.15	0.45
1:E:581:LEU:HD22	1:E:581:LEU:N	2.31	0.45
1:F:537:VAL:HG22	1:F:546:ASN:ND2	2.29	0.45
1:F:621:ILE:HD12	1:F:621:ILE:N	2.31	0.45
1:F:653:ALA:N	1:F:654:PRO:CD	2.79	0.45
1:A:497:TYR:CD1	1:A:642:ILE:HG23	2.51	0.45
1:C:77:GLU:HG2	1:C:78:GLY:N	2.28	0.45
1:C:504:LEU:HD12	1:C:504:LEU:O	2.17	0.45
1:D:136:GLY:CA	1:D:268:VAL:HG21	2.33	0.45
1:E:274:PRO:HD3	1:E:330:TRP:CZ3	2.52	0.45
1:E:277:ILE:HD12	1:E:286:GLN:NE2	2.31	0.45
1:F:40:ASP:OD1	1:F:41:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:TYR:CD1	1:B:642:ILE:HG23	2.52	0.45
1:C:137:ARG:H	1:C:332:ASN:HD22	1.64	0.45
1:D:110:SER:HB2	1:D:126:LEU:O	2.17	0.45
1:D:321:VAL:HG12	1:D:321:VAL:O	2.16	0.45
1:D:413:THR:HG21	1:D:595:GLN:NE2	2.31	0.45
1:E:299:ARG:NH1	1:E:305:GLU:CD	2.73	0.45
1:F:97:LYS:HB3	1:F:100:PHE:HB2	1.99	0.45
1:F:400:PRO:HA	1:F:487:ALA:HB2	1.99	0.45
1:A:625:PRO:HD2	1:A:627:ARG:HH12	1.81	0.45
1:A:720:SER:OG	1:A:723:ALA:HB2	2.16	0.45
1:B:45:ILE:HD12	1:B:85:ILE:HD13	1.98	0.45
1:B:110:SER:HB2	1:B:126:LEU:O	2.17	0.45
1:B:581:LEU:HD22	1:B:581:LEU:N	2.32	0.45
1:C:71:GLN:C	1:C:73:HIS:H	2.25	0.45
1:C:321:VAL:HG12	1:C:321:VAL:O	2.16	0.45
1:C:363:HIS:NE2	1:C:365:THR:HG23	2.32	0.45
1:C:513:PRO:HA	1:C:522:ILE:HG12	1.99	0.45
1:C:591:VAL:HA	1:C:592:PRO:HD3	1.79	0.45
1:D:148:LYS:O	1:D:267:MSE:HA	2.16	0.45
1:D:274:PRO:HD3	1:D:330:TRP:CZ3	2.51	0.45
1:D:292:LEU:HD23	1:D:312:VAL:HG22	1.99	0.45
1:D:471:SER:C	1:D:473:ASP:N	2.72	0.45
1:D:486:THR:HG22	1:D:487:ALA:H	1.81	0.45
1:F:107:PRO:CG	1:F:108:GLY:H	2.23	0.45
1:F:305:GLU:N	1:F:306:PRO:HD3	2.32	0.45
1:F:363:HIS:NE2	1:F:365:THR:HG23	2.32	0.45
1:B:295:LEU:HG	1:B:330:TRP:CD1	2.52	0.45
1:B:321:VAL:HG12	1:B:321:VAL:O	2.16	0.45
1:B:407:ILE:HG21	1:B:568:LEU:HD13	1.97	0.45
1:B:642:ILE:HB	1:B:647:PHE:HZ	1.82	0.45
1:C:655:LEU:N	1:C:683:ASP:HB2	2.25	0.45
1:D:71:GLN:C	1:D:73:HIS:H	2.24	0.45
1:D:138:GLU:OE2	1:D:271:ALA:N	2.50	0.45
1:D:294:LEU:HG	1:D:310:TRP:NE1	2.32	0.45
1:E:321:VAL:HG12	1:E:321:VAL:O	2.17	0.45
1:E:661:CYS:HA	1:E:678:LEU:HD23	1.97	0.45
1:F:321:VAL:HG12	1:F:321:VAL:O	2.17	0.45
1:F:497:TYR:CD1	1:F:642:ILE:HG23	2.52	0.45
1:A:53:TYR:CD2	1:A:58:ALA:O	2.70	0.45
1:A:445:TYR:CB	1:A:451:GLY:HA3	2.47	0.45
1:A:602:MSE:HE3	1:A:602:MSE:HB3	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LEU:HB2	1:B:683:ASP:CG	2.42	0.45
1:C:268:VAL:HG22	1:C:269:PRO:CD	2.47	0.45
1:C:471:SER:C	1:C:473:ASP:H	2.24	0.45
1:C:621:ILE:N	1:C:621:ILE:HD12	2.32	0.45
1:D:420:ILE:HD12	1:D:420:ILE:O	2.16	0.45
1:D:497:TYR:CD1	1:D:642:ILE:HG23	2.51	0.45
1:E:53:TYR:CD2	1:E:58:ALA:O	2.69	0.45
1:E:63:LYS:HD3	1:E:79:THR:HA	1.98	0.45
1:E:486:THR:HG22	1:E:487:ALA:H	1.82	0.45
1:A:45:ILE:HD12	1:A:85:ILE:HD13	1.99	0.45
1:A:87:THR:OG1	1:A:106:PRO:HD2	2.17	0.45
1:A:150:ILE:HG23	1:A:151:PRO:CD	2.45	0.45
1:B:642:ILE:HB	1:B:647:PHE:CZ	2.52	0.45
1:E:45:ILE:HD12	1:E:85:ILE:HD13	1.98	0.45
1:E:400:PRO:HA	1:E:487:ALA:HB2	1.99	0.45
1:E:504:LEU:HD21	1:E:521:VAL:CG2	2.47	0.45
1:A:63:LYS:HD3	1:A:79:THR:HA	1.99	0.44
1:A:284:SER:HB3	2:G:1:NAG:O5	2.17	0.44
1:B:559:ALA:O	1:B:599:GLY:HA3	2.17	0.44
1:B:580:ARG:NH2	1:C:275:ASN:HB2	2.32	0.44
1:B:621:ILE:CD1	1:B:621:ILE:H	2.30	0.44
1:C:448:MSE:C	1:C:450:GLY:N	2.74	0.44
1:C:581:LEU:HD22	1:C:581:LEU:H	1.81	0.44
1:D:63:LYS:HD3	1:D:79:THR:HA	1.99	0.44
1:D:305:GLU:N	1:D:306:PRO:HD3	2.33	0.44
1:D:489:MSE:HG3	1:D:508:VAL:HB	1.99	0.44
1:D:494:ARG:HB2	1:D:503:PHE:CD1	2.47	0.44
1:E:497:TYR:CD1	1:E:642:ILE:HG23	2.52	0.44
1:F:110:SER:HB2	1:F:126:LEU:O	2.18	0.44
1:F:298:ARG:HH12	1:F:615:ALA:HB3	1.81	0.44
1:A:321:VAL:HG12	1:A:321:VAL:O	2.16	0.44
1:A:486:THR:HG22	1:A:487:ALA:H	1.82	0.44
1:B:287:LEU:CD2	1:B:330:TRP:NE1	2.80	0.44
1:B:649:ARG:H	1:B:649:ARG:HG3	1.51	0.44
1:C:446:PRO:HG2	1:C:450:GLY:O	2.16	0.44
1:D:19:CYS:C	1:D:21:HIS:N	2.72	0.44
1:F:10:SER:HA	1:F:50:GLN:NE2	2.32	0.44
1:F:53:TYR:CD2	1:F:58:ALA:O	2.70	0.44
1:F:300:LEU:HD11	1:F:337:ARG:HD3	1.98	0.44
1:F:486:THR:HG22	1:F:487:ALA:H	1.82	0.44
1:A:642:ILE:HB	1:A:647:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ARG:H	1:C:93:ARG:NH1	1.93	0.44
1:C:138:GLU:OE2	1:C:271:ALA:N	2.50	0.44
1:C:486:THR:HG22	1:C:487:ALA:H	1.81	0.44
1:E:407:ILE:HG22	1:E:408:THR:N	2.32	0.44
1:F:399:LEU:N	1:F:399:LEU:HD12	2.32	0.44
1:A:71:GLN:C	1:A:73:HIS:H	2.25	0.44
1:A:106:PRO:CB	1:A:107:PRO:CD	2.92	0.44
1:B:454:CYS:SG	1:B:460:ASN:OD1	2.76	0.44
1:B:504:LEU:HD21	1:B:521:VAL:CG2	2.46	0.44
1:D:40:ASP:OD1	1:D:41:ASN:N	2.49	0.44
1:D:642:ILE:HB	1:D:647:PHE:HZ	1.83	0.44
1:D:699:LEU:HD23	1:D:716:PHE:HB3	2.00	0.44
1:E:271:ALA:CB	1:E:330:TRP:CZ3	3.00	0.44
1:E:655:LEU:HB2	1:E:683:ASP:CG	2.42	0.44
1:F:21:HIS:O	1:F:23:VAL:N	2.51	0.44
1:F:45:ILE:HD12	1:F:85:ILE:HD13	1.99	0.44
1:F:655:LEU:HB2	1:F:683:ASP:CG	2.43	0.44
1:B:71:GLN:C	1:B:73:HIS:H	2.25	0.44
1:B:108:GLY:CA	1:B:130:ILE:HB	2.47	0.44
1:E:21:HIS:O	1:E:23:VAL:N	2.51	0.44
1:E:471:SER:C	1:E:473:ASP:N	2.73	0.44
1:F:268:VAL:HG22	1:F:269:PRO:CD	2.47	0.44
1:F:295:LEU:HG	1:F:330:TRP:CD1	2.51	0.44
1:A:394:MSE:HE2	1:A:394:MSE:HB3	1.92	0.44
1:A:621:ILE:HD12	1:A:621:ILE:N	2.33	0.44
1:A:642:ILE:HB	1:A:647:PHE:CZ	2.52	0.44
1:D:60:SER:HB2	1:D:63:LYS:HB2	2.00	0.44
1:D:112:THR:HG23	1:D:125:THR:HG22	1.99	0.44
1:D:394:MSE:HE2	1:D:394:MSE:HB3	1.91	0.44
1:D:642:ILE:HB	1:D:647:PHE:CZ	2.52	0.44
1:E:146:HIS:CD2	1:E:146:HIS:H	2.34	0.44
1:E:287:LEU:CD2	1:E:330:TRP:NE1	2.77	0.44
1:E:407:ILE:HG21	1:E:568:LEU:HD13	1.99	0.44
1:E:642:ILE:HB	1:E:647:PHE:CZ	2.52	0.44
1:A:299:ARG:NH1	1:A:305:GLU:CD	2.73	0.44
1:B:40:ASP:OD1	1:B:41:ASN:N	2.50	0.44
1:C:19:CYS:C	1:C:21:HIS:N	2.73	0.44
1:E:40:ASP:OD1	1:E:41:ASN:N	2.49	0.44
1:E:270:VAL:HG22	1:E:333:HIS:HE1	1.80	0.44
1:F:385:ALA:HA	1:F:386:PRO:HD2	1.79	0.44
1:A:102:LEU:HD11	1:A:155:TYR:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG23	1:A:125:THR:HG22	2.00	0.44
1:A:494:ARG:HB2	1:A:503:PHE:CD1	2.47	0.44
1:B:363:HIS:NE2	1:B:365:THR:HG23	2.32	0.44
1:C:21:HIS:O	1:C:23:VAL:N	2.50	0.44
1:D:146:HIS:H	1:D:146:HIS:CD2	2.35	0.44
1:E:137:ARG:HH21	1:E:331:GLY:H	1.66	0.44
1:E:621:ILE:N	1:E:621:ILE:HD12	2.33	0.44
1:A:72:ASP:O	1:A:73:HIS:HB2	2.17	0.44
1:A:108:GLY:CA	1:A:130:ILE:HB	2.47	0.44
1:A:513:PRO:HA	1:A:522:ILE:HG12	2.00	0.44
1:B:513:PRO:HA	1:B:522:ILE:HG12	1.99	0.44
1:C:655:LEU:HB2	1:C:683:ASP:CG	2.43	0.44
1:D:10:SER:HA	1:D:50:GLN:NE2	2.32	0.44
1:E:295:LEU:HG	1:E:330:TRP:CD1	2.51	0.44
1:E:559:ALA:O	1:E:599:GLY:HA3	2.18	0.44
1:F:72:ASP:O	1:F:73:HIS:HB2	2.18	0.44
1:F:131:LYS:NZ	3:R:1:NAG:H81	2.33	0.44
1:F:512:THR:HA	1:F:513:PRO:HD3	1.75	0.44
1:A:102:LEU:HD11	1:A:155:TYR:HB3	2.00	0.43
1:A:504:LEU:HD12	1:A:504:LEU:O	2.17	0.43
1:C:411:PHE:CD1	1:C:411:PHE:C	2.95	0.43
1:E:385:ALA:HA	1:E:386:PRO:HD2	1.78	0.43
1:E:386:PRO:HG3	1:E:730:CYS:O	2.18	0.43
1:E:407:ILE:CG2	1:E:408:THR:N	2.81	0.43
1:E:653:ALA:N	1:E:654:PRO:CD	2.79	0.43
1:F:63:LYS:HD3	1:F:79:THR:HA	1.99	0.43
1:F:87:THR:OG1	1:F:106:PRO:HD2	2.18	0.43
2:J:3:BMA:O2	2:J:4:MAN:O5	2.32	0.43
1:A:559:ALA:O	1:A:599:GLY:HA3	2.18	0.43
1:A:699:LEU:HD23	1:A:716:PHE:HB3	2.00	0.43
1:B:112:THR:HG23	1:B:125:THR:HG22	2.00	0.43
1:C:559:ALA:O	1:C:599:GLY:HA3	2.18	0.43
1:E:489:MSE:HG3	1:E:508:VAL:HB	2.00	0.43
1:F:60:SER:HB2	1:F:63:LYS:HB2	1.99	0.43
1:F:112:THR:HG23	1:F:125:THR:HG22	2.01	0.43
1:F:642:ILE:HB	1:F:647:PHE:CZ	2.53	0.43
1:A:21:HIS:O	1:A:23:VAL:N	2.51	0.43
1:A:287:LEU:CD2	1:A:330:TRP:NE1	2.80	0.43
1:B:493:LEU:HA	1:B:493:LEU:HD23	1.60	0.43
1:B:530:PHE:CE2	1:B:617:PHE:HD1	2.36	0.43
1:D:504:LEU:HD12	1:D:504:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:625:PRO:HD2	1:E:627:ARG:HH12	1.82	0.43
1:E:642:ILE:HB	1:E:647:PHE:HZ	1.83	0.43
1:A:271:ALA:CB	1:A:330:TRP:CZ3	3.02	0.43
1:B:107:PRO:CG	1:B:108:GLY:H	2.23	0.43
1:B:400:PRO:HA	1:B:487:ALA:HB2	1.99	0.43
1:B:494:ARG:HB2	1:B:503:PHE:CD1	2.47	0.43
1:B:621:ILE:HD12	1:B:621:ILE:N	2.33	0.43
1:C:445:TYR:O	1:C:460:ASN:ND2	2.51	0.43
1:D:69:LEU:HD22	1:D:69:LEU:HA	1.84	0.43
1:D:87:THR:OG1	1:D:106:PRO:HD2	2.18	0.43
1:D:411:PHE:C	1:D:411:PHE:CD1	2.96	0.43
1:E:18:TYR:C	1:E:18:TYR:CD2	2.97	0.43
1:E:621:ILE:H	1:E:621:ILE:CD1	2.31	0.43
1:F:321:VAL:CG1	1:F:340:ALA:HB2	2.48	0.43
1:A:445:TYR:CD1	1:A:451:GLY:HA3	2.53	0.43
1:B:10:SER:HA	1:B:50:GLN:NE2	2.33	0.43
1:B:53:TYR:CD2	1:B:58:ALA:O	2.70	0.43
1:B:471:SER:C	1:B:473:ASP:N	2.72	0.43
1:C:447:PHE:CD1	1:C:455:PHE:HA	2.53	0.43
1:C:664:SER:OG	1:C:675:MSE:HB3	2.19	0.43
1:E:6:PHE:HA	1:E:57:GLY:O	2.18	0.43
1:E:71:GLN:C	1:E:73:HIS:H	2.25	0.43
1:E:292:LEU:HD23	1:E:312:VAL:HG22	2.00	0.43
1:E:411:PHE:CD1	1:E:411:PHE:C	2.96	0.43
1:E:602:MSE:HE3	1:E:602:MSE:HB3	1.68	0.43
1:E:612:GLN:HG2	1:E:612:GLN:H	1.53	0.43
1:F:146:HIS:H	1:F:146:HIS:CD2	2.35	0.43
1:F:398:VAL:HB	1:F:628:ALA:HB3	1.99	0.43
1:F:555:MSE:HE3	1:F:555:MSE:HB2	1.69	0.43
1:A:447:PHE:CG	1:A:448:MSE:N	2.86	0.43
1:C:146:HIS:H	1:C:146:HIS:CD2	2.36	0.43
1:C:446:PRO:O	1:C:447:PHE:C	2.61	0.43
1:C:642:ILE:HB	1:C:647:PHE:CZ	2.53	0.43
1:D:21:HIS:O	1:D:23:VAL:N	2.52	0.43
1:D:72:ASP:O	1:D:73:HIS:HB2	2.19	0.43
1:D:102:LEU:HD11	1:D:155:TYR:HB3	2.01	0.43
1:E:102:LEU:HD11	1:E:155:TYR:CB	2.49	0.43
1:E:615:ALA:HA	1:E:616:PRO:HD3	1.57	0.43
1:A:271:ALA:HB3	1:A:330:TRP:CZ3	2.54	0.43
1:A:449:TRP:HA	1:A:449:TRP:CE3	2.52	0.43
1:B:21:HIS:O	1:B:23:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLY:N	1:B:63:LYS:O	2.51	0.43
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.77	0.43
1:B:413:THR:HG21	1:B:595:GLN:NE2	2.34	0.43
1:B:447:PHE:CD1	1:B:447:PHE:C	2.94	0.43
1:C:102:LEU:HD11	1:C:155:TYR:CB	2.49	0.43
1:C:295:LEU:HG	1:C:330:TRP:CD1	2.53	0.43
1:C:298:ARG:HH12	1:C:615:ALA:HB3	1.83	0.43
1:C:394:MSE:HE2	1:C:394:MSE:HB3	1.90	0.43
1:D:513:PRO:HA	1:D:522:ILE:HG12	2.00	0.43
1:E:112:THR:HG23	1:E:125:THR:HG22	2.01	0.43
1:E:664:SER:OG	1:E:675:MSE:HB3	2.19	0.43
1:F:287:LEU:HD13	1:F:311:ILE:CD1	2.49	0.43
1:A:655:LEU:N	1:A:683:ASP:HB2	2.28	0.43
1:B:137:ARG:HH21	1:B:331:GLY:H	1.65	0.43
1:B:271:ALA:CB	1:B:330:TRP:CZ3	3.02	0.43
1:B:699:LEU:HD23	1:B:716:PHE:HB3	2.01	0.43
1:C:276:VAL:HG12	1:C:277:ILE:N	2.33	0.43
1:C:398:VAL:HB	1:C:628:ALA:HB3	2.00	0.43
1:C:489:MSE:HE3	1:C:489:MSE:HB2	1.90	0.43
1:E:17:SER:HB3	1:F:145:VAL:CG2	2.33	0.43
1:E:512:THR:HA	1:E:513:PRO:HD3	1.74	0.43
1:F:111:VAL:O	1:F:125:THR:HA	2.19	0.43
1:F:136:GLY:CA	1:F:268:VAL:HG21	2.31	0.43
1:F:690:VAL:HG22	1:F:729:LEU:HD23	2.01	0.43
1:A:10:SER:HA	1:A:50:GLN:NE2	2.33	0.43
1:A:18:TYR:C	1:A:18:TYR:CD2	2.97	0.43
1:A:69:LEU:HD22	1:A:69:LEU:HA	1.84	0.43
1:A:104:LYS:HD2	1:C:22:THR:CG2	2.34	0.43
1:B:547:TYR:OH	1:B:560:PHE:HB3	2.19	0.43
1:D:621:ILE:CD1	1:D:621:ILE:H	2.31	0.43
1:D:621:ILE:HD12	1:D:621:ILE:N	2.33	0.43
1:D:690:VAL:HG22	1:D:729:LEU:HD23	2.01	0.43
1:E:110:SER:HB2	1:E:126:LEU:O	2.18	0.43
1:E:657:SER:HA	1:E:732:LYS:HE3	2.01	0.43
1:F:699:LEU:HD23	1:F:716:PHE:HB3	2.00	0.43
1:A:136:GLY:CA	1:A:268:VAL:HG21	2.33	0.43
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.60	0.43
1:A:600:PHE:O	1:A:601:GLU:C	2.61	0.43
1:A:690:VAL:HG22	1:A:729:LEU:HD23	2.01	0.43
1:B:292:LEU:HD23	1:B:312:VAL:HG22	2.00	0.43
1:B:413:THR:HG23	1:B:468:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LEU:HD11	1:C:155:TYR:HB3	2.01	0.43
1:C:112:THR:HG23	1:C:125:THR:HG22	2.00	0.43
1:C:699:LEU:HD23	1:C:716:PHE:HB3	2.01	0.43
1:D:559:ALA:O	1:D:599:GLY:HA3	2.18	0.43
1:D:664:SER:OG	1:D:675:MSE:HB3	2.19	0.43
1:E:699:LEU:HD23	1:E:716:PHE:HB3	2.01	0.43
1:F:664:SER:OG	1:F:675:MSE:HB3	2.19	0.43
1:B:18:TYR:C	1:B:18:TYR:CD2	2.97	0.42
1:B:102:LEU:HD11	1:B:155:TYR:CB	2.48	0.42
1:B:137:ARG:H	1:B:332:ASN:HD22	1.67	0.42
1:B:287:LEU:HD22	1:B:330:TRP:CE2	2.54	0.42
1:B:328:TYR:O	1:B:328:TYR:CD1	2.72	0.42
1:B:491:VAL:O	1:B:505:ASP:HA	2.19	0.42
1:C:110:SER:HB2	1:C:126:LEU:O	2.19	0.42
1:C:400:PRO:HA	1:C:487:ALA:HB2	2.01	0.42
1:C:642:ILE:HB	1:C:647:PHE:HZ	1.83	0.42
1:D:655:LEU:HB2	1:D:683:ASP:CG	2.43	0.42
1:E:328:TYR:O	1:E:328:TYR:CD1	2.71	0.42
1:E:422:CYS:O	1:E:423:CYS:HB2	2.19	0.42
1:E:445:TYR:CG	1:E:451:GLY:HA3	2.53	0.42
1:F:71:GLN:C	1:F:73:HIS:H	2.25	0.42
1:F:445:TYR:O	1:F:460:ASN:ND2	2.52	0.42
2:K:2:NAG:HO3	2:K:3:BMA:C2	2.29	0.42
1:B:6:PHE:HA	1:B:57:GLY:O	2.19	0.42
1:C:108:GLY:CA	1:C:130:ILE:HB	2.47	0.42
1:D:137:ARG:H	1:D:332:ASN:HD22	1.66	0.42
1:D:303:ASN:HA	1:D:304:PRO:HD3	1.83	0.42
1:D:512:THR:HA	1:D:513:PRO:HD3	1.75	0.42
1:E:10:SER:HA	1:E:50:GLN:NE2	2.33	0.42
1:E:87:THR:OG1	1:E:106:PRO:HD2	2.19	0.42
1:F:292:LEU:HD23	1:F:312:VAL:HG22	2.01	0.42
1:F:642:ILE:HB	1:F:647:PHE:HZ	1.84	0.42
1:A:531:THR:HA	1:A:532:PRO:HD3	1.89	0.42
1:B:95:SER:OG	1:B:259:PHE:CZ	2.67	0.42
1:B:102:LEU:HD11	1:B:155:TYR:HB3	2.00	0.42
1:B:271:ALA:HB3	1:B:330:TRP:CZ3	2.55	0.42
1:B:299:ARG:NH1	1:B:305:GLU:CD	2.74	0.42
1:B:404:GLN:HA	1:B:482:ILE:HG12	2.00	0.42
1:B:655:LEU:N	1:B:683:ASP:HB2	2.27	0.42
1:C:18:TYR:C	1:C:18:TYR:CD2	2.97	0.42
1:D:300:LEU:CD1	1:D:337:ARG:HD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:531:THR:HA	1:D:532:PRO:HD3	1.89	0.42
1:E:72:ASP:O	1:E:73:HIS:HB2	2.19	0.42
1:E:489:MSE:HE3	1:E:489:MSE:HB2	1.92	0.42
1:F:398:VAL:O	1:F:400:PRO:HD3	2.19	0.42
1:A:413:THR:HG21	1:A:595:GLN:NE2	2.34	0.42
1:A:655:LEU:HB2	1:A:683:ASP:CG	2.43	0.42
1:B:385:ALA:HA	1:B:386:PRO:HD2	1.78	0.42
1:B:422:CYS:O	1:B:423:CYS:HB2	2.19	0.42
1:B:447:PHE:HA	1:B:454:CYS:O	2.20	0.42
1:B:449:TRP:C	1:B:451:GLY:N	2.77	0.42
1:C:407:ILE:HG22	1:C:408:THR:N	2.34	0.42
1:E:102:LEU:HD11	1:E:155:TYR:HB3	2.00	0.42
1:F:102:LEU:HD11	1:F:155:TYR:CB	2.49	0.42
1:A:664:SER:OG	1:A:675:MSE:HB3	2.19	0.42
1:C:385:ALA:HA	1:C:386:PRO:HD2	1.79	0.42
1:C:422:CYS:O	1:C:423:CYS:HB2	2.20	0.42
1:D:145:VAL:HG22	1:F:17:SER:CB	2.31	0.42
1:E:547:TYR:OH	1:E:560:PHE:HB3	2.20	0.42
1:E:649:ARG:H	1:E:649:ARG:HG3	1.52	0.42
1:F:389:LEU:HD12	1:F:389:LEU:HA	1.86	0.42
2:G:3:BMA:O3	2:G:4:MAN:C4	2.63	0.42
1:B:287:LEU:HD13	1:B:311:ILE:CD1	2.49	0.42
1:D:18:TYR:C	1:D:18:TYR:CD2	2.98	0.42
1:F:611:LEU:C	1:F:613:GLU:N	2.78	0.42
1:F:649:ARG:O	1:F:651:SER:HB2	2.20	0.42
3:H:3:BMA:H61	3:H:5:MAN:H2	1.32	0.42
1:B:72:ASP:O	1:B:73:HIS:HB2	2.19	0.42
1:B:555:MSE:HE3	1:B:555:MSE:HB2	1.65	0.42
1:B:625:PRO:HD2	1:B:627:ARG:HH12	1.84	0.42
1:C:72:ASP:O	1:C:73:HIS:HB2	2.18	0.42
1:C:111:VAL:O	1:C:125:THR:HA	2.20	0.42
1:C:287:LEU:HD13	1:C:311:ILE:CD1	2.50	0.42
1:C:304:PRO:O	1:C:305:GLU:C	2.62	0.42
1:C:404:GLN:HA	1:C:482:ILE:HG12	2.02	0.42
1:C:489:MSE:HG3	1:C:508:VAL:HB	2.00	0.42
1:C:690:VAL:HG22	1:C:729:LEU:HD23	2.01	0.42
1:D:591:VAL:HA	1:D:592:PRO:HD3	1.79	0.42
1:E:604:LYS:C	1:E:606:ASN:N	2.78	0.42
1:F:271:ALA:HB3	1:F:330:TRP:CZ3	2.54	0.42
1:F:657:SER:HA	1:F:732:LYS:HE3	2.01	0.42
1:A:413:THR:HG23	1:A:468:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:C	1:A:613:GLU:N	2.77	0.42
1:B:87:THR:OG1	1:B:106:PRO:HD2	2.20	0.42
1:B:378:LEU:HG	1:B:691:HIS:CB	2.50	0.42
1:C:87:THR:OG1	1:C:106:PRO:HD2	2.19	0.42
1:C:413:THR:HG23	1:C:468:VAL:HG12	2.02	0.42
1:D:37:GLU:OE1	1:D:473:ASP:OD2	2.37	0.42
1:D:688:CYS:HA	1:D:689:PRO:HD3	1.93	0.42
1:E:271:ALA:HB3	1:E:330:TRP:CZ3	2.54	0.42
1:E:378:LEU:HA	1:E:378:LEU:HD23	1.77	0.42
1:E:413:THR:HG21	1:E:595:GLN:NE2	2.35	0.42
1:F:18:TYR:C	1:F:18:TYR:CD2	2.97	0.42
1:F:102:LEU:HD11	1:F:155:TYR:HB3	2.01	0.42
1:F:299:ARG:NH1	1:F:305:GLU:CD	2.73	0.42
1:F:411:PHE:CD1	1:F:411:PHE:C	2.97	0.42
1:B:407:ILE:HG22	1:B:408:THR:N	2.34	0.42
1:B:436:TYR:O	1:B:437:THR:HG23	2.20	0.42
1:B:504:LEU:HD12	1:B:504:LEU:C	2.45	0.42
1:D:329:ILE:H	1:D:329:ILE:HG12	1.53	0.42
1:D:422:CYS:O	1:D:423:CYS:HB2	2.20	0.42
1:D:509:ASN:C	1:D:511:VAL:H	2.28	0.42
1:E:287:LEU:HD22	1:E:311:ILE:HD11	2.01	0.42
1:F:271:ALA:CB	1:F:330:TRP:CZ3	3.03	0.42
1:F:287:LEU:HD22	1:F:311:ILE:HD11	2.02	0.42
1:F:304:PRO:O	1:F:305:GLU:C	2.63	0.42
2:M:2:NAG:H83	2:M:2:NAG:O3	2.20	0.42
1:A:60:SER:CB	1:A:63:LYS:HB2	2.50	0.42
1:A:398:VAL:O	1:A:400:PRO:HD3	2.20	0.42
1:B:386:PRO:HG3	1:B:730:CYS:O	2.20	0.42
1:B:664:SER:OG	1:B:675:MSE:HB3	2.19	0.42
1:C:512:THR:HA	1:C:513:PRO:HD3	1.76	0.42
1:D:271:ALA:CB	1:D:330:TRP:CZ3	3.03	0.42
1:D:398:VAL:O	1:D:400:PRO:HD3	2.20	0.42
1:D:413:THR:HG23	1:D:468:VAL:HG12	2.02	0.42
1:E:33:GLN:O	1:E:34:VAL:HG23	2.19	0.42
1:F:69:LEU:HD22	1:F:69:LEU:HA	1.84	0.42
1:F:491:VAL:O	1:F:505:ASP:HA	2.20	0.42
1:A:52:GLY:N	1:A:63:LYS:O	2.51	0.41
1:B:591:VAL:HA	1:B:592:PRO:HD3	1.80	0.41
1:C:445:TYR:CB	1:C:452:ALA:H	2.32	0.41
1:C:625:PRO:HD2	1:C:627:ARG:HH12	1.84	0.41
1:D:436:TYR:O	1:D:437:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:513:PRO:HA	1:E:522:ILE:HG12	2.01	0.41
1:E:611:LEU:C	1:E:613:GLU:N	2.77	0.41
1:A:376:LYS:O	1:A:691:HIS:HE1	2.03	0.41
1:A:407:ILE:HG22	1:A:408:THR:N	2.34	0.41
1:B:489:MSE:HG3	1:B:508:VAL:HB	2.02	0.41
1:B:615:ALA:HA	1:B:616:PRO:HD3	1.56	0.41
1:B:657:SER:HA	1:B:732:LYS:HE3	2.01	0.41
1:C:426:LEU:HD23	1:C:426:LEU:HA	1.87	0.41
1:C:555:MSE:H	1:C:555:MSE:HE2	1.84	0.41
1:D:287:LEU:HD13	1:D:311:ILE:CD1	2.50	0.41
1:D:407:ILE:HG22	1:D:408:THR:N	2.34	0.41
1:D:491:VAL:O	1:D:505:ASP:HA	2.20	0.41
1:F:413:THR:HG23	1:F:468:VAL:HG12	2.02	0.41
1:A:6:PHE:HA	1:A:57:GLY:O	2.19	0.41
1:A:271:ALA:O	1:A:333:HIS:HE1	2.03	0.41
1:A:373:ILE:HA	1:A:374:PRO:HD2	1.91	0.41
1:A:657:SER:HA	1:A:732:LYS:HE3	2.01	0.41
1:C:271:ALA:O	1:C:333:HIS:HE1	2.02	0.41
1:D:328:TYR:CD1	1:D:328:TYR:O	2.73	0.41
1:E:111:VAL:O	1:E:125:THR:HA	2.20	0.41
1:E:426:LEU:HD23	1:E:426:LEU:HA	1.88	0.41
1:F:547:TYR:OH	1:F:560:PHE:HB3	2.19	0.41
1:A:287:LEU:HD13	1:A:311:ILE:CD1	2.49	0.41
1:A:300:LEU:CD1	1:A:337:ARG:HD3	2.50	0.41
1:C:51:PHE:CD2	1:C:80:MSE:SE	3.23	0.41
1:C:413:THR:HG21	1:C:595:GLN:HE22	1.83	0.41
1:D:102:LEU:HD11	1:D:155:TYR:CB	2.49	0.41
1:D:150:ILE:HG22	1:D:151:PRO:O	2.20	0.41
1:D:271:ALA:HB3	1:D:330:TRP:CZ3	2.55	0.41
1:D:321:VAL:CG1	1:D:340:ALA:HB2	2.50	0.41
1:D:334:GLU:HA	1:D:335:PRO:HD3	1.85	0.41
1:D:504:LEU:HB3	1:D:516:SER:HB2	2.03	0.41
1:D:691:HIS:HA	1:D:699:LEU:HD12	2.02	0.41
1:E:691:HIS:HA	1:E:699:LEU:HD12	2.02	0.41
1:A:552:TYR:HA	1:A:564:GLN:OE1	2.21	0.41
1:B:329:ILE:H	1:B:329:ILE:HG12	1.50	0.41
1:B:407:ILE:CG2	1:B:408:THR:N	2.84	0.41
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.61	0.41
1:C:649:ARG:O	1:C:650:THR:C	2.64	0.41
1:C:649:ARG:H	1:C:649:ARG:HG3	1.52	0.41
1:D:386:PRO:HG3	1:D:730:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:PHE:O	1:D:601:GLU:C	2.64	0.41
1:D:653:ALA:HB1	1:D:684:ARG:HD2	2.02	0.41
1:E:690:VAL:HG22	1:E:729:LEU:HD23	2.01	0.41
3:H:2:NAG:O3	3:H:3:BMA:H5	2.20	0.41
1:A:287:LEU:HD22	1:A:330:TRP:CE2	2.55	0.41
1:B:111:VAL:O	1:B:125:THR:HA	2.21	0.41
1:B:690:VAL:HG22	1:B:729:LEU:HD23	2.01	0.41
1:C:386:PRO:HB2	1:C:689:PRO:CG	2.50	0.41
1:C:509:ASN:C	1:C:511:VAL:H	2.29	0.41
1:D:271:ALA:O	1:D:333:HIS:HE1	2.02	0.41
1:D:292:LEU:CD2	1:D:312:VAL:HG22	2.51	0.41
1:D:489:MSE:HE3	1:D:489:MSE:HB2	1.89	0.41
1:E:287:LEU:HD22	1:E:330:TRP:CE2	2.56	0.41
1:E:491:VAL:O	1:E:505:ASP:HA	2.20	0.41
1:F:6:PHE:HA	1:F:57:GLY:O	2.21	0.41
1:A:407:ILE:CG2	1:A:408:THR:N	2.84	0.41
1:B:327:GLU:HA	1:B:337:ARG:HB3	2.03	0.41
1:B:649:ARG:O	1:B:650:THR:C	2.64	0.41
1:C:398:VAL:O	1:C:400:PRO:HD3	2.20	0.41
1:D:657:SER:HA	1:D:732:LYS:HE3	2.01	0.41
1:E:514:GLY:C	1:E:516:SER:H	2.26	0.41
1:F:287:LEU:CD2	1:F:330:TRP:NE1	2.80	0.41
1:F:404:GLN:HA	1:F:482:ILE:HG12	2.02	0.41
1:F:489:MSE:HG3	1:F:508:VAL:HB	2.03	0.41
4:N:1:NAG:O3	4:N:2:NAG:C7	2.69	0.41
1:B:373:ILE:HA	1:B:374:PRO:HD2	1.90	0.41
1:B:413:THR:HG21	1:B:595:GLN:HE22	1.86	0.41
1:B:604:LYS:C	1:B:606:ASN:N	2.77	0.41
1:B:612:GLN:HG2	1:B:612:GLN:H	1.50	0.41
1:C:42:THR:CG2	1:C:104:LYS:HG3	2.51	0.41
1:C:271:ALA:HB3	1:C:330:TRP:CZ3	2.56	0.41
1:C:602:MSE:HE3	1:C:602:MSE:HB3	1.60	0.41
1:D:426:LEU:HD23	1:D:426:LEU:HA	1.89	0.41
1:E:51:PHE:CD2	1:E:80:MSE:SE	3.23	0.41
1:B:44:ARG:NH1	1:B:258:PRO:HB2	2.36	0.41
1:B:544:VAL:N	1:B:612:GLN:HE22	2.18	0.41
1:B:691:HIS:HA	1:B:699:LEU:HD12	2.03	0.41
1:C:6:PHE:CD2	1:C:6:PHE:N	2.88	0.41
1:C:35:TRP:HB2	1:C:44:ARG:HB3	2.02	0.41
1:C:287:LEU:HD22	1:C:311:ILE:HD11	2.03	0.41
1:D:108:GLY:CA	1:D:130:ILE:HB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:O	1:D:125:THR:HA	2.21	0.41
1:D:287:LEU:CD2	1:D:330:TRP:NE1	2.83	0.41
1:D:433:HIS:O	1:D:434:ALA:C	2.64	0.41
1:D:547:TYR:OH	1:D:560:PHE:HB3	2.21	0.41
1:D:552:TYR:HA	1:D:564:GLN:OE1	2.21	0.41
1:D:556:LYS:HA	1:D:557:PRO:HD3	1.90	0.41
1:D:611:LEU:C	1:D:613:GLU:N	2.77	0.41
1:D:649:ARG:O	1:D:650:THR:C	2.64	0.41
1:D:655:LEU:N	1:D:683:ASP:HB2	2.27	0.41
1:E:44:ARG:NH1	1:E:258:PRO:HB2	2.35	0.41
1:E:150:ILE:HG22	1:E:151:PRO:O	2.21	0.41
1:E:568:LEU:H	1:E:568:LEU:HD22	1.85	0.41
1:F:271:ALA:O	1:F:333:HIS:HE1	2.04	0.41
1:F:373:ILE:HA	1:F:374:PRO:HD2	1.91	0.41
3:H:4:MAN:HO3	2:L:3:BMA:H5	1.81	0.41
3:P:2:NAG:H83	3:P:2:NAG:H2	1.94	0.41
1:A:33:GLN:O	1:A:34:VAL:HG23	2.21	0.41
1:B:287:LEU:CD2	1:B:330:TRP:CE2	3.04	0.41
1:C:287:LEU:CD2	1:C:330:TRP:NE1	2.82	0.41
1:C:547:TYR:OH	1:C:560:PHE:HB3	2.21	0.41
1:C:615:ALA:HA	1:C:616:PRO:HD3	1.55	0.41
1:C:657:SER:HA	1:C:732:LYS:HE3	2.02	0.41
1:D:44:ARG:NH1	1:D:258:PRO:HB2	2.36	0.41
1:D:148:LYS:HB3	1:D:150:ILE:CD1	2.51	0.41
1:E:287:LEU:HD13	1:E:311:ILE:CD1	2.50	0.41
1:E:287:LEU:CD2	1:E:330:TRP:CE2	3.03	0.41
1:F:80:MSE:HE2	1:F:80:MSE:HB3	1.93	0.41
1:F:422:CYS:O	1:F:423:CYS:HB2	2.20	0.41
1:F:504:LEU:HD12	1:F:504:LEU:C	2.46	0.41
1:A:107:PRO:CG	1:A:108:GLY:N	2.84	0.40
1:A:150:ILE:HG22	1:A:151:PRO:O	2.21	0.40
1:A:413:THR:HG21	1:A:595:GLN:HE22	1.86	0.40
1:A:422:CYS:O	1:A:423:CYS:HB2	2.20	0.40
1:C:481:ALA:HB1	1:C:549:PHE:CE1	2.57	0.40
1:D:407:ILE:CG2	1:D:408:THR:N	2.83	0.40
1:E:69:LEU:HD22	1:E:69:LEU:HA	1.85	0.40
1:E:433:HIS:O	1:E:434:ALA:C	2.64	0.40
1:F:107:PRO:CG	1:F:108:GLY:N	2.85	0.40
1:F:143:PRO:HA	1:F:144:PRO:HD3	1.96	0.40
1:F:292:LEU:CD2	1:F:312:VAL:HG22	2.52	0.40
1:F:509:ASN:C	1:F:511:VAL:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASN:C	1:A:511:VAL:H	2.29	0.40
1:A:557:PRO:C	1:A:559:ALA:H	2.29	0.40
1:A:604:LYS:C	1:A:606:ASN:N	2.79	0.40
1:A:649:ARG:O	1:A:650:THR:C	2.64	0.40
1:B:337:ARG:NH2	1:B:620:LYS:HE2	2.36	0.40
1:B:400:PRO:HB2	1:B:484:VAL:HG13	2.03	0.40
1:B:514:GLY:C	1:B:516:SER:H	2.25	0.40
1:C:407:ILE:CG2	1:C:408:THR:N	2.84	0.40
1:D:35:TRP:HB2	1:D:44:ARG:HB3	2.02	0.40
1:D:107:PRO:CG	1:D:108:GLY:N	2.84	0.40
1:D:361:TYR:HB2	1:D:381:ARG:HH21	1.86	0.40
1:E:300:LEU:CD1	1:E:337:ARG:HD3	2.50	0.40
1:F:137:ARG:HH21	1:F:331:GLY:H	1.69	0.40
1:F:287:LEU:HD22	1:F:330:TRP:CE2	2.56	0.40
1:F:591:VAL:HA	1:F:592:PRO:HD3	1.80	0.40
1:A:146:HIS:CD2	1:A:146:HIS:N	2.89	0.40
1:A:304:PRO:O	1:A:305:GLU:C	2.64	0.40
1:B:51:PHE:CD2	1:B:80:MSE:SE	3.25	0.40
1:B:60:SER:CB	1:B:63:LYS:HB2	2.51	0.40
1:B:143:PRO:HA	1:B:144:PRO:HD3	1.95	0.40
1:B:432:ALA:O	1:B:433:HIS:HB3	2.22	0.40
1:B:447:PHE:CE1	1:B:455:PHE:HA	2.54	0.40
1:B:552:TYR:HA	1:B:564:GLN:OE1	2.20	0.40
1:B:568:LEU:HD22	1:B:568:LEU:H	1.87	0.40
1:C:373:ILE:HA	1:C:374:PRO:HD2	1.91	0.40
1:C:604:LYS:C	1:C:606:ASN:N	2.79	0.40
1:C:654:PRO:HB3	1:C:684:ARG:H	1.87	0.40
1:D:544:VAL:N	1:D:612:GLN:HE22	2.19	0.40
1:F:287:LEU:CD2	1:F:330:TRP:CE2	3.04	0.40
1:F:407:ILE:CG2	1:F:408:THR:N	2.85	0.40
1:A:111:VAL:O	1:A:125:THR:HA	2.20	0.40
1:B:300:LEU:CD1	1:B:337:ARG:HD3	2.52	0.40
1:B:399:LEU:HD12	1:B:399:LEU:H	1.85	0.40
1:C:105:CYS:HA	1:C:106:PRO:HD3	1.89	0.40
1:C:292:LEU:CD2	1:C:312:VAL:HG22	2.51	0.40
1:C:300:LEU:CD1	1:C:337:ARG:HD3	2.51	0.40
1:C:504:LEU:HD12	1:C:504:LEU:C	2.47	0.40
1:D:331:GLY:O	1:D:332:ASN:C	2.64	0.40
1:E:504:LEU:HD12	1:E:504:LEU:C	2.46	0.40
1:F:92:ARG:HA	1:F:92:ARG:HD3	1.92	0.40
1:F:108:GLY:CA	1:F:130:ILE:HB	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:MSE:HE3	1:F:489:MSE:HB2	1.91	0.40
1:A:303:ASN:HA	1:A:304:PRO:HD3	1.84	0.40
1:A:547:TYR:OH	1:A:560:PHE:HB3	2.21	0.40
1:C:54:ASP:CG	1:C:55:GLN:N	2.80	0.40
1:C:491:VAL:O	1:C:505:ASP:HA	2.21	0.40
1:C:530:PHE:CE2	1:C:617:PHE:HD1	2.40	0.40
1:D:6:PHE:HA	1:D:57:GLY:O	2.22	0.40
1:D:398:VAL:HB	1:D:628:ALA:HB3	2.03	0.40
1:E:432:ALA:O	1:E:433:HIS:HB3	2.21	0.40
1:E:530:PHE:CE2	1:E:617:PHE:HD1	2.38	0.40
1:F:105:CYS:HA	1:F:106:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

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	617/750 (82%)	501 (81%)	92 (15%)	24 (4%)	2	16
1	B	616/750 (82%)	499 (81%)	96 (16%)	21 (3%)	3	18
1	C	616/750 (82%)	500 (81%)	92 (15%)	24 (4%)	2	16
1	D	616/750 (82%)	502 (82%)	92 (15%)	22 (4%)	2	17
1	E	617/750 (82%)	505 (82%)	90 (15%)	22 (4%)	2	17
1	F	612/750 (82%)	503 (82%)	87 (14%)	22 (4%)	2	17
All	All	3694/4500 (82%)	3010 (82%)	549 (15%)	135 (4%)	2	17

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO

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Mol	Chain	Res	Type
1	A	117	SER
1	A	434	ALA
1	A	650	THR
1	A	730	CYS
1	B	106	PRO
1	B	117	SER
1	B	434	ALA
1	B	650	THR
1	B	730	CYS
1	C	106	PRO
1	C	117	SER
1	C	434	ALA
1	C	447	PHE
1	C	650	THR
1	C	730	CYS
1	D	106	PRO
1	D	117	SER
1	D	434	ALA
1	D	650	THR
1	D	730	CYS
1	E	106	PRO
1	E	117	SER
1	E	434	ALA
1	E	650	THR
1	E	730	CYS
1	F	106	PRO
1	F	117	SER
1	F	434	ALA
1	F	447	PHE
1	F	650	THR
1	F	730	CYS
1	A	80	MSE
1	A	107	PRO
1	A	446	PRO
1	A	450	GLY
1	A	515	THR
1	B	80	MSE
1	B	107	PRO
1	B	515	THR
1	C	80	MSE
1	C	107	PRO
1	C	515	THR

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Mol	Chain	Res	Type
1	D	80	MSE
1	D	107	PRO
1	D	515	THR
1	E	80	MSE
1	E	107	PRO
1	E	515	THR
1	F	80	MSE
1	F	107	PRO
1	F	515	THR
1	A	257	LEU
1	A	624	ASN
1	B	255	LEU
1	B	257	LEU
1	B	624	ASN
1	C	257	LEU
1	C	624	ASN
1	D	257	LEU
1	D	624	ASN
1	E	257	LEU
1	E	423	CYS
1	E	624	ASN
1	F	624	ASN
1	A	70	LYS
1	A	322	ASP
1	A	386	PRO
1	A	423	CYS
1	A	721	PRO
1	B	322	ASP
1	B	332	ASN
1	B	423	CYS
1	B	721	PRO
1	C	22	THR
1	C	136	GLY
1	C	322	ASP
1	C	423	CYS
1	C	721	PRO
1	D	322	ASP
1	D	332	ASN
1	D	423	CYS
1	D	721	PRO
1	E	322	ASP
1	E	453	GLN

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Mol	Chain	Res	Type
1	E	721	PRO
1	F	22	THR
1	F	136	GLY
1	F	322	ASP
1	F	332	ASN
1	F	423	CYS
1	F	721	PRO
1	A	22	THR
1	A	332	ASN
1	A	430	PRO
1	B	70	LYS
1	B	136	GLY
1	B	386	PRO
1	B	430	PRO
1	C	70	LYS
1	C	386	PRO
1	C	430	PRO
1	D	70	LYS
1	D	386	PRO
1	D	430	PRO
1	E	70	LYS
1	E	136	GLY
1	E	332	ASN
1	E	386	PRO
1	E	430	PRO
1	F	70	LYS
1	F	386	PRO
1	F	430	PRO
1	A	119	ASN
1	A	136	GLY
1	B	444	VAL
1	C	332	ASN
1	C	449	TRP
1	C	653	ALA
1	D	22	THR
1	D	119	ASN
1	D	136	GLY
1	E	119	ASN
1	F	119	ASN
1	F	444	VAL
1	A	444	VAL
1	C	444	VAL

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Mol	Chain	Res	Type
1	D	444	VAL
1	E	444	VAL
1	F	610	PRO
1	E	610	PRO
1	A	610	PRO
1	C	610	PRO
1	D	610	PRO
1	B	610	PRO

5.3.2 Protein sidechains (i)

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	534/630 (85%)	459 (86%)	75 (14%)	3	15
1	B	533/630 (85%)	461 (86%)	72 (14%)	4	16
1	C	533/630 (85%)	455 (85%)	78 (15%)	3	14
1	D	533/630 (85%)	459 (86%)	74 (14%)	3	15
1	E	532/630 (84%)	457 (86%)	75 (14%)	3	14
1	F	529/630 (84%)	453 (86%)	76 (14%)	3	14
All	All	3194/3780 (84%)	2744 (86%)	450 (14%)	3	14

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	17	SER
1	A	20	HIS
1	A	34	VAL
1	A	68	SER
1	A	69	LEU
1	A	71	GLN
1	A	72	ASP
1	A	74	THR
1	A	77	GLU

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Mol	Chain	Res	Type
1	A	80	MSE
1	A	93	ARG
1	A	94	LEU
1	A	109	ASP
1	A	120	SER
1	A	122	THR
1	A	125	THR
1	A	146	HIS
1	A	261	LEU
1	A	262	ILE
1	A	267	MSE
1	A	268	VAL
1	A	282	HIS
1	A	288	ASP
1	A	289	THR
1	A	293	THR
1	A	294	LEU
1	A	295	LEU
1	A	296	THR
1	A	308	THR
1	A	312	VAL
1	A	317	ARG
1	A	326	LEU
1	A	329	ILE
1	A	333	HIS
1	A	336	VAL
1	A	341	GLN
1	A	343	SER
1	A	379	VAL
1	A	387	LEU
1	A	393	VAL
1	A	394	MSE
1	A	402	THR
1	A	405	GLU
1	A	407	ILE
1	A	409	CYS
1	A	413	THR
1	A	428	CYS
1	A	437	THR
1	A	439	LYS
1	A	474	CYS
1	A	490	LYS

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Mol	Chain	Res	Type
1	A	497	TYR
1	A	515	THR
1	A	516	SER
1	A	518	ASP
1	A	519	LEU
1	A	541	ARG
1	A	544	VAL
1	A	548	ASP
1	A	555	MSE
1	A	563	ILE
1	A	567	SER
1	A	573	LEU
1	A	578	ASP
1	A	581	LEU
1	A	591	VAL
1	A	597	SER
1	A	602	MSE
1	A	611	LEU
1	A	612	GLN
1	A	626	LEU
1	A	649	ARG
1	A	651	SER
1	A	655	LEU
1	B	8	LEU
1	B	17	SER
1	B	20	HIS
1	B	68	SER
1	B	69	LEU
1	B	71	GLN
1	B	72	ASP
1	B	74	THR
1	B	75	VAL
1	B	77	GLU
1	B	80	MSE
1	B	93	ARG
1	B	94	LEU
1	B	109	ASP
1	B	120	SER
1	B	122	THR
1	B	125	THR
1	B	146	HIS
1	B	261	LEU

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Mol	Chain	Res	Type
1	B	262	ILE
1	B	267	MSE
1	B	268	VAL
1	B	282	HIS
1	B	288	ASP
1	B	289	THR
1	B	293	THR
1	B	294	LEU
1	B	295	LEU
1	B	296	THR
1	B	308	THR
1	B	312	VAL
1	B	317	ARG
1	B	326	LEU
1	B	329	ILE
1	B	333	HIS
1	B	336	VAL
1	B	379	VAL
1	B	387	LEU
1	B	393	VAL
1	B	394	MSE
1	B	402	THR
1	B	405	GLU
1	B	407	ILE
1	B	409	CYS
1	B	413	THR
1	B	428	CYS
1	B	437	THR
1	B	474	CYS
1	B	490	LYS
1	B	497	TYR
1	B	515	THR
1	B	516	SER
1	B	518	ASP
1	B	519	LEU
1	B	541	ARG
1	B	544	VAL
1	B	548	ASP
1	B	555	MSE
1	B	563	ILE
1	B	567	SER
1	B	573	LEU

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Mol	Chain	Res	Type
1	B	578	ASP
1	B	581	LEU
1	B	591	VAL
1	B	597	SER
1	B	602	MSE
1	B	611	LEU
1	B	612	GLN
1	B	626	LEU
1	B	649	ARG
1	B	651	SER
1	B	655	LEU
1	C	8	LEU
1	C	17	SER
1	C	20	HIS
1	C	34	VAL
1	C	68	SER
1	C	69	LEU
1	C	71	GLN
1	C	72	ASP
1	C	74	THR
1	C	75	VAL
1	C	77	GLU
1	C	80	MSE
1	C	93	ARG
1	C	94	LEU
1	C	109	ASP
1	C	120	SER
1	C	122	THR
1	C	125	THR
1	C	146	HIS
1	C	255	LEU
1	C	261	LEU
1	C	262	ILE
1	C	267	MSE
1	C	268	VAL
1	C	282	HIS
1	C	288	ASP
1	C	289	THR
1	C	293	THR
1	C	294	LEU
1	C	295	LEU
1	C	296	THR

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Mol	Chain	Res	Type
1	C	308	THR
1	C	312	VAL
1	C	317	ARG
1	C	326	LEU
1	C	329	ILE
1	C	333	HIS
1	C	336	VAL
1	C	341	GLN
1	C	379	VAL
1	C	387	LEU
1	C	393	VAL
1	C	394	MSE
1	C	402	THR
1	C	405	GLU
1	C	407	ILE
1	C	409	CYS
1	C	413	THR
1	C	428	CYS
1	C	437	THR
1	C	439	LYS
1	C	447	PHE
1	C	448	MSE
1	C	474	CYS
1	C	490	LYS
1	C	497	TYR
1	C	515	THR
1	C	516	SER
1	C	518	ASP
1	C	519	LEU
1	C	541	ARG
1	C	544	VAL
1	C	548	ASP
1	C	555	MSE
1	C	563	ILE
1	C	567	SER
1	C	573	LEU
1	C	578	ASP
1	C	581	LEU
1	C	591	VAL
1	C	597	SER
1	C	602	MSE
1	C	611	LEU

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Mol	Chain	Res	Type
1	C	612	GLN
1	C	626	LEU
1	C	649	ARG
1	C	651	SER
1	C	655	LEU
1	D	8	LEU
1	D	17	SER
1	D	20	HIS
1	D	34	VAL
1	D	68	SER
1	D	69	LEU
1	D	71	GLN
1	D	72	ASP
1	D	74	THR
1	D	75	VAL
1	D	77	GLU
1	D	80	MSE
1	D	93	ARG
1	D	94	LEU
1	D	109	ASP
1	D	120	SER
1	D	122	THR
1	D	125	THR
1	D	146	HIS
1	D	261	LEU
1	D	262	ILE
1	D	267	MSE
1	D	268	VAL
1	D	282	HIS
1	D	288	ASP
1	D	289	THR
1	D	293	THR
1	D	294	LEU
1	D	295	LEU
1	D	296	THR
1	D	308	THR
1	D	312	VAL
1	D	317	ARG
1	D	326	LEU
1	D	329	ILE
1	D	333	HIS
1	D	336	VAL

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Mol	Chain	Res	Type
1	D	379	VAL
1	D	387	LEU
1	D	393	VAL
1	D	394	MSE
1	D	402	THR
1	D	405	GLU
1	D	407	ILE
1	D	409	CYS
1	D	413	THR
1	D	428	CYS
1	D	437	THR
1	D	439	LYS
1	D	474	CYS
1	D	490	LYS
1	D	497	TYR
1	D	515	THR
1	D	516	SER
1	D	518	ASP
1	D	519	LEU
1	D	541	ARG
1	D	544	VAL
1	D	548	ASP
1	D	555	MSE
1	D	563	ILE
1	D	567	SER
1	D	573	LEU
1	D	578	ASP
1	D	581	LEU
1	D	591	VAL
1	D	597	SER
1	D	602	MSE
1	D	611	LEU
1	D	612	GLN
1	D	626	LEU
1	D	649	ARG
1	D	651	SER
1	D	655	LEU
1	E	8	LEU
1	E	17	SER
1	E	20	HIS
1	E	34	VAL
1	E	68	SER

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Mol	Chain	Res	Type
1	E	69	LEU
1	E	71	GLN
1	E	72	ASP
1	E	74	THR
1	E	75	VAL
1	E	77	GLU
1	E	80	MSE
1	E	93	ARG
1	E	94	LEU
1	E	109	ASP
1	E	120	SER
1	E	122	THR
1	E	125	THR
1	E	146	HIS
1	E	261	LEU
1	E	262	ILE
1	E	267	MSE
1	E	268	VAL
1	E	282	HIS
1	E	288	ASP
1	E	289	THR
1	E	293	THR
1	E	294	LEU
1	E	295	LEU
1	E	296	THR
1	E	308	THR
1	E	312	VAL
1	E	317	ARG
1	E	326	LEU
1	E	329	ILE
1	E	333	HIS
1	E	336	VAL
1	E	341	GLN
1	E	379	VAL
1	E	387	LEU
1	E	393	VAL
1	E	394	MSE
1	E	402	THR
1	E	405	GLU
1	E	407	ILE
1	E	409	CYS
1	E	413	THR

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Mol	Chain	Res	Type
1	E	428	CYS
1	E	437	THR
1	E	439	LYS
1	E	474	CYS
1	E	490	LYS
1	E	497	TYR
1	E	515	THR
1	E	516	SER
1	E	518	ASP
1	E	519	LEU
1	E	541	ARG
1	E	544	VAL
1	E	548	ASP
1	E	555	MSE
1	E	563	ILE
1	E	567	SER
1	E	573	LEU
1	E	578	ASP
1	E	581	LEU
1	E	591	VAL
1	E	597	SER
1	E	602	MSE
1	E	611	LEU
1	E	612	GLN
1	E	626	LEU
1	E	649	ARG
1	E	651	SER
1	E	655	LEU
1	F	8	LEU
1	F	17	SER
1	F	20	HIS
1	F	34	VAL
1	F	68	SER
1	F	69	LEU
1	F	71	GLN
1	F	72	ASP
1	F	74	THR
1	F	75	VAL
1	F	77	GLU
1	F	80	MSE
1	F	93	ARG
1	F	94	LEU

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Mol	Chain	Res	Type
1	F	109	ASP
1	F	120	SER
1	F	122	THR
1	F	125	THR
1	F	146	HIS
1	F	261	LEU
1	F	262	ILE
1	F	267	MSE
1	F	268	VAL
1	F	282	HIS
1	F	288	ASP
1	F	289	THR
1	F	293	THR
1	F	294	LEU
1	F	295	LEU
1	F	296	THR
1	F	308	THR
1	F	312	VAL
1	F	317	ARG
1	F	326	LEU
1	F	329	ILE
1	F	333	HIS
1	F	336	VAL
1	F	341	GLN
1	F	379	VAL
1	F	387	LEU
1	F	393	VAL
1	F	394	MSE
1	F	402	THR
1	F	405	GLU
1	F	407	ILE
1	F	409	CYS
1	F	413	THR
1	F	428	CYS
1	F	437	THR
1	F	439	LYS
1	F	448	MSE
1	F	474	CYS
1	F	490	LYS
1	F	497	TYR
1	F	515	THR
1	F	516	SER

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Mol	Chain	Res	Type
1	F	518	ASP
1	F	519	LEU
1	F	541	ARG
1	F	544	VAL
1	F	548	ASP
1	F	555	MSE
1	F	563	ILE
1	F	567	SER
1	F	573	LEU
1	F	578	ASP
1	F	581	LEU
1	F	591	VAL
1	F	597	SER
1	F	602	MSE
1	F	611	LEU
1	F	612	GLN
1	F	626	LEU
1	F	649	ARG
1	F	651	SER
1	F	655	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	62	ASN
1	A	146	HIS
1	A	275	ASN
1	A	291	HIS
1	A	332	ASN
1	A	333	HIS
1	A	341	GLN
1	A	540	HIS
1	A	546	ASN
1	A	595	GLN
1	A	612	GLN
1	A	691	HIS
1	A	715	HIS
1	B	46	GLN
1	B	50	GLN
1	B	62	ASN
1	B	146	HIS

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Mol	Chain	Res	Type
1	B	272	HIS
1	B	291	HIS
1	B	332	ASN
1	B	333	HIS
1	B	540	HIS
1	B	546	ASN
1	B	595	GLN
1	B	612	GLN
1	B	691	HIS
1	B	715	HIS
1	C	46	GLN
1	C	50	GLN
1	C	62	ASN
1	C	146	HIS
1	C	256	HIS
1	C	291	HIS
1	C	332	ASN
1	C	333	HIS
1	C	540	HIS
1	C	546	ASN
1	C	595	GLN
1	C	612	GLN
1	C	691	HIS
1	C	715	HIS
1	D	46	GLN
1	D	50	GLN
1	D	62	ASN
1	D	146	HIS
1	D	291	HIS
1	D	332	ASN
1	D	333	HIS
1	D	453	GLN
1	D	540	HIS
1	D	546	ASN
1	D	595	GLN
1	D	612	GLN
1	D	691	HIS
1	D	715	HIS
1	E	46	GLN
1	E	50	GLN
1	E	62	ASN
1	E	146	HIS

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Mol	Chain	Res	Type
1	E	272	HIS
1	E	291	HIS
1	E	332	ASN
1	E	333	HIS
1	E	540	HIS
1	E	546	ASN
1	E	595	GLN
1	E	612	GLN
1	E	691	HIS
1	E	705	HIS
1	E	715	HIS
1	F	46	GLN
1	F	50	GLN
1	F	62	ASN
1	F	146	HIS
1	F	291	HIS
1	F	332	ASN
1	F	333	HIS
1	F	540	HIS
1	F	546	ASN
1	F	595	GLN
1	F	612	GLN
1	F	691	HIS
1	F	715	HIS

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

50 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	NAG	G	1	2,1	14,14,15	0.41	0	17,19,21	2.09	2 (11%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	2.05	5 (29%)
2	BMA	G	3	2	11,11,12	1.71	2 (18%)	15,15,17	4.14	10 (66%)
2	MAN	G	4	2	11,11,12	0.89	1 (9%)	15,15,17	2.00	4 (26%)
3	NAG	H	1	1,3	14,14,15	0.71	0	17,19,21	1.35	2 (11%)
3	NAG	H	2	3	14,14,15	0.48	0	17,19,21	1.15	1 (5%)
3	BMA	H	3	3	11,11,12	2.11	4 (36%)	15,15,17	3.03	9 (60%)
3	MAN	H	4	3	11,11,12	0.41	0	15,15,17	1.54	2 (13%)
3	MAN	H	5	3	11,11,12	0.50	0	15,15,17	1.40	1 (6%)
2	NAG	I	1	2,1	14,14,15	0.76	0	17,19,21	1.01	0
2	NAG	I	2	2	14,14,15	0.83	0	17,19,21	1.96	3 (17%)
2	BMA	I	3	2	11,11,12	2.20	5 (45%)	15,15,17	2.89	7 (46%)
2	MAN	I	4	2	11,11,12	0.52	0	15,15,17	1.05	1 (6%)
2	NAG	J	1	2,1	14,14,15	0.55	0	17,19,21	1.45	2 (11%)
2	NAG	J	2	2	14,14,15	0.59	0	17,19,21	1.53	3 (17%)
2	BMA	J	3	2	11,11,12	1.82	3 (27%)	15,15,17	3.54	9 (60%)
2	MAN	J	4	2	11,11,12	0.61	0	15,15,17	0.69	0
2	NAG	K	1	2,1	14,14,15	0.69	0	17,19,21	1.18	1 (5%)
2	NAG	K	2	2	14,14,15	0.63	0	17,19,21	1.00	2 (11%)
2	BMA	K	3	2	11,11,12	2.04	4 (36%)	15,15,17	3.66	10 (66%)
2	MAN	K	4	2	11,11,12	0.77	1 (9%)	15,15,17	1.79	5 (33%)
2	NAG	L	1	2,1	14,14,15	0.46	0	17,19,21	1.97	4 (23%)
2	NAG	L	2	2	14,14,15	0.49	0	17,19,21	2.90	5 (29%)
2	BMA	L	3	2	11,11,12	1.82	3 (27%)	15,15,17	3.30	8 (53%)
2	MAN	L	4	2	11,11,12	0.44	0	15,15,17	1.71	1 (6%)
2	NAG	M	1	2,1	14,14,15	0.78	1 (7%)	17,19,21	2.21	6 (35%)
2	NAG	M	2	2	14,14,15	0.58	0	17,19,21	1.67	4 (23%)
2	BMA	M	3	2	11,11,12	1.89	4 (36%)	15,15,17	3.29	12 (80%)
2	MAN	M	4	2	11,11,12	0.55	0	15,15,17	0.91	0
4	NAG	N	1	1,4	14,14,15	0.39	0	17,19,21	2.14	2 (11%)
4	NAG	N	2	4	14,14,15	0.52	0	17,19,21	1.25	2 (11%)
4	BMA	N	3	4	11,11,12	2.00	4 (36%)	15,15,17	3.29	9 (60%)
2	NAG	O	1	2,1	14,14,15	0.62	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	O	2	2	14,14,15	0.67	0	17,19,21	1.88	4 (23%)
2	BMA	O	3	2	11,11,12	1.95	4 (36%)	15,15,17	3.65	10 (66%)
2	MAN	O	4	2	11,11,12	0.65	0	15,15,17	0.63	0
3	NAG	P	1	1,3	14,14,15	0.52	0	17,19,21	2.22	4 (23%)
3	NAG	P	2	3	14,14,15	0.66	1 (7%)	17,19,21	2.53	5 (29%)
3	BMA	P	3	3	11,11,12	1.81	3 (27%)	15,15,17	3.74	8 (53%)
3	MAN	P	4	3	11,11,12	0.57	0	15,15,17	1.07	1 (6%)
3	MAN	P	5	3	11,11,12	0.61	0	15,15,17	0.50	0
2	NAG	Q	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	1.83	2 (11%)
2	NAG	Q	2	2	14,14,15	0.48	0	17,19,21	3.23	5 (29%)
2	BMA	Q	3	2	11,11,12	2.05	4 (36%)	15,15,17	4.14	10 (66%)
2	MAN	Q	4	2	11,11,12	0.51	0	15,15,17	1.33	2 (13%)
3	NAG	R	1	1,3	14,14,15	0.43	0	17,19,21	1.94	3 (17%)
3	NAG	R	2	3	14,14,15	0.45	0	17,19,21	2.23	3 (17%)
3	BMA	R	3	3	11,11,12	2.09	4 (36%)	15,15,17	1.99	6 (40%)
3	MAN	R	4	3	11,11,12	0.60	0	15,15,17	0.60	0
3	MAN	R	5	3	11,11,12	0.46	0	15,15,17	1.51	4 (26%)

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	NAG	G	1	2,1	1/1/5/7	6/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	1/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	2/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	1/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	BMA	M	3	2	-	2/2/19/22	0/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
2	NAG	O	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	2/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	MAN	P	4	3	-	0/2/19/22	1/1/1/1
3	MAN	P	5	3	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	2,1	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	2/2/19/22	1/1/1/1
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	BMA	R	3	3	-	1/2/19/22	0/1/1/1
3	MAN	R	4	3	-	1/2/19/22	0/1/1/1
3	MAN	R	5	3	-	2/2/19/22	1/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	3	BMA	C4-C5	4.32	1.62	1.53
2	I	3	BMA	C4-C5	4.25	1.62	1.53
3	H	3	BMA	C4-C5	4.08	1.61	1.53
4	N	3	BMA	C4-C5	3.99	1.61	1.53
3	R	3	BMA	C4-C5	3.88	1.61	1.53
2	K	3	BMA	C2-C3	-3.72	1.46	1.52
2	L	3	BMA	O4-C4	3.64	1.52	1.43
2	Q	3	BMA	O4-C4	3.62	1.51	1.43
2	G	3	BMA	O4-C4	3.57	1.51	1.43
2	J	3	BMA	O4-C4	3.55	1.51	1.43
4	N	3	BMA	O4-C4	3.53	1.51	1.43
2	O	3	BMA	C4-C5	3.52	1.60	1.53
3	P	3	BMA	O4-C4	3.47	1.51	1.43
2	J	3	BMA	C4-C5	3.45	1.60	1.53
2	K	3	BMA	O4-C4	3.43	1.51	1.43
2	M	3	BMA	O4-C4	3.42	1.51	1.43
3	R	3	BMA	O4-C4	3.40	1.51	1.43
2	M	3	BMA	C4-C5	3.39	1.60	1.53
2	K	3	BMA	C4-C5	3.39	1.60	1.53
2	L	3	BMA	C4-C5	3.37	1.60	1.53
2	O	3	BMA	O4-C4	3.35	1.51	1.43
3	H	3	BMA	O4-C4	3.35	1.51	1.43
2	I	3	BMA	O4-C4	3.27	1.51	1.43
3	P	3	BMA	C4-C5	3.22	1.59	1.53
2	G	3	BMA	C4-C5	3.11	1.59	1.53
2	I	3	BMA	C2-C3	-3.02	1.47	1.52
3	R	3	BMA	C2-C3	-3.02	1.47	1.52
2	I	3	BMA	C4-C3	2.91	1.59	1.52
2	M	3	BMA	C2-C3	-2.78	1.48	1.52
3	H	3	BMA	C4-C3	2.77	1.59	1.52
2	O	3	BMA	C2-C3	-2.75	1.48	1.52
2	Q	3	BMA	C4-C3	2.73	1.59	1.52
3	P	3	BMA	C2-C3	-2.69	1.48	1.52
3	H	3	BMA	C2-C3	-2.67	1.48	1.52
4	N	3	BMA	C2-C3	-2.66	1.48	1.52
2	L	3	BMA	C4-C3	2.49	1.58	1.52
3	R	3	BMA	C4-C3	2.38	1.58	1.52
2	O	3	BMA	C4-C3	2.37	1.58	1.52
2	J	3	BMA	C4-C3	2.34	1.58	1.52
3	P	2	NAG	C1-C2	2.29	1.55	1.52
4	N	3	BMA	C4-C3	2.27	1.58	1.52
2	G	4	MAN	O5-C1	-2.26	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	3	BMA	C4-C3	2.24	1.58	1.52
2	K	3	BMA	C4-C3	2.20	1.58	1.52
2	I	3	BMA	C1-C2	-2.12	1.47	1.52
2	Q	1	NAG	C1-C2	2.11	1.55	1.52
2	K	4	MAN	O5-C1	-2.09	1.40	1.43
2	Q	3	BMA	C2-C3	-2.07	1.49	1.52
2	M	1	NAG	C1-C2	2.06	1.55	1.52

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	2	NAG	C4-C3-C2	-10.25	96.00	111.02
2	Q	3	BMA	C1-O5-C5	-9.65	99.26	112.19
2	L	2	NAG	C1-O5-C5	8.34	123.36	112.19
3	H	3	BMA	C1-O5-C5	-8.11	101.31	112.19
2	O	3	BMA	C1-O5-C5	-7.76	101.78	112.19
4	N	1	NAG	C1-O5-C5	7.63	122.42	112.19
3	R	2	NAG	C1-O5-C5	7.56	122.31	112.19
2	G	1	NAG	C1-O5-C5	7.26	121.92	112.19
3	P	3	BMA	O5-C5-C6	7.24	121.75	107.66
2	G	3	BMA	O3-C3-C2	7.05	124.44	110.05
2	J	3	BMA	O3-C3-C2	7.03	124.40	110.05
3	P	3	BMA	O3-C3-C2	6.97	124.27	110.05
3	P	2	NAG	C1-O5-C5	6.91	121.45	112.19
2	G	3	BMA	O5-C5-C6	6.86	121.01	107.66
2	G	3	BMA	O4-C4-C5	6.72	125.87	109.32
2	I	3	BMA	C1-O5-C5	-6.68	103.23	112.19
3	P	1	NAG	C1-O5-C5	6.62	121.06	112.19
2	M	3	BMA	O5-C5-C6	6.35	120.02	107.66
2	L	1	NAG	C1-O5-C5	6.30	120.64	112.19
2	Q	3	BMA	O5-C5-C6	6.25	119.83	107.66
2	L	2	NAG	C4-C3-C2	-6.09	102.09	111.02
2	K	3	BMA	O5-C5-C6	6.02	119.39	107.66
2	O	3	BMA	O5-C5-C6	6.00	119.34	107.66
2	L	3	BMA	O5-C5-C6	5.92	119.18	107.66
4	N	3	BMA	C1-O5-C5	-5.83	104.37	112.19
2	K	3	BMA	O4-C4-C5	5.83	123.68	109.32
3	P	3	BMA	O4-C4-C5	5.77	123.52	109.32
2	L	4	MAN	C1-O5-C5	5.75	119.90	112.19
2	G	3	BMA	O4-C4-C3	5.75	123.93	110.38
2	K	3	BMA	O4-C4-C3	5.66	123.73	110.38
2	Q	3	BMA	O3-C3-C2	5.66	121.61	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	1	NAG	C1-O5-C5	5.64	119.75	112.19
2	M	1	NAG	O4-C4-C3	5.59	123.55	110.38
4	N	3	BMA	O4-C4-C5	5.57	123.03	109.32
2	K	3	BMA	C2-C3-C4	-5.50	101.19	110.86
2	G	2	NAG	C1-O5-C5	5.46	119.51	112.19
2	M	3	BMA	O4-C4-C5	5.42	122.69	109.32
2	J	3	BMA	O4-C4-C5	5.39	122.60	109.32
2	J	3	BMA	O4-C4-C3	5.36	123.01	110.38
2	J	3	BMA	O5-C5-C6	5.26	117.91	107.66
2	L	3	BMA	O4-C4-C5	5.25	122.25	109.32
2	G	3	BMA	C3-C4-C5	-5.20	100.80	110.23
2	Q	3	BMA	C1-C2-C3	-5.20	102.07	109.64
2	Q	2	NAG	O4-C4-C3	5.16	122.54	110.38
2	Q	1	NAG	C1-O5-C5	5.16	119.10	112.19
4	N	3	BMA	O5-C5-C6	5.15	117.69	107.66
2	L	3	BMA	O3-C3-C2	5.14	120.55	110.05
2	L	3	BMA	C1-O5-C5	-5.07	105.39	112.19
2	I	2	NAG	O5-C1-C2	-5.05	103.48	111.29
3	P	2	NAG	C4-C3-C2	-5.03	103.65	111.02
2	O	3	BMA	O4-C4-C5	5.01	121.66	109.32
2	K	3	BMA	O3-C3-C4	4.94	122.02	110.38
2	M	3	BMA	O4-C4-C3	4.85	121.82	110.38
2	Q	2	NAG	C2-N2-C7	-4.81	116.46	122.90
2	Q	3	BMA	O4-C4-C5	4.74	121.00	109.32
3	H	5	MAN	C1-O5-C5	4.74	118.54	112.19
2	I	3	BMA	O5-C5-C6	4.73	116.88	107.66
3	P	3	BMA	O4-C4-C3	4.68	121.40	110.38
2	L	3	BMA	O4-C4-C3	4.46	120.89	110.38
3	H	3	BMA	O5-C5-C6	4.45	116.32	107.66
2	G	4	MAN	C3-C4-C5	4.37	118.16	110.23
4	N	3	BMA	O3-C3-C2	4.37	118.97	110.05
3	H	4	MAN	C1-O5-C5	4.37	118.04	112.19
2	O	2	NAG	O5-C1-C2	-4.20	104.80	111.29
2	Q	4	MAN	C1-O5-C5	4.15	117.74	112.19
2	O	3	BMA	O4-C4-C3	4.11	120.06	110.38
3	P	3	BMA	C2-C3-C4	-4.02	103.79	110.86
2	O	2	NAG	C2-N2-C7	-3.95	117.61	122.90
4	N	3	BMA	O4-C4-C3	3.88	119.52	110.38
3	R	5	MAN	C1-O5-C5	3.87	117.37	112.19
2	M	2	NAG	C1-O5-C5	-3.86	107.01	112.19
2	G	3	BMA	C2-C3-C4	-3.86	104.08	110.86
2	M	3	BMA	O3-C3-C2	3.76	117.73	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	2	NAG	C4-C3-C2	-3.74	105.54	111.02
2	O	3	BMA	O3-C3-C2	3.72	117.64	110.05
2	I	3	BMA	C3-C4-C5	3.69	116.93	110.23
2	J	3	BMA	O3-C3-C4	3.67	119.03	110.38
2	K	1	NAG	O5-C1-C2	-3.66	105.62	111.29
3	P	1	NAG	C4-C3-C2	-3.66	105.65	111.02
2	K	4	MAN	C3-C4-C5	3.66	116.87	110.23
2	I	2	NAG	C3-C4-C5	3.63	116.82	110.23
2	G	4	MAN	O5-C1-C2	-3.60	102.21	110.79
2	J	3	BMA	C2-C3-C4	-3.59	104.55	110.86
3	R	3	BMA	O4-C4-C5	3.58	118.15	109.32
3	H	1	NAG	C4-C3-C2	3.56	116.23	111.02
2	M	3	BMA	O3-C3-C4	3.55	118.74	110.38
2	J	1	NAG	O5-C1-C2	-3.48	105.90	111.29
3	P	3	BMA	C1-O5-C5	-3.46	107.55	112.19
3	R	3	BMA	O5-C5-C6	3.45	114.38	107.66
2	G	2	NAG	C3-C4-C5	3.43	116.46	110.23
3	R	2	NAG	O5-C5-C4	3.37	119.02	110.83
2	G	2	NAG	O5-C5-C4	3.33	118.92	110.83
2	O	3	BMA	O3-C3-C4	3.33	118.22	110.38
2	Q	3	BMA	O2-C2-C1	3.30	116.78	109.22
3	R	1	NAG	C4-C3-C2	-3.27	106.23	111.02
3	H	3	BMA	O4-C4-C5	3.25	117.33	109.32
2	K	3	BMA	O3-C3-C2	3.22	116.62	110.05
4	N	3	BMA	O3-C3-C4	3.21	117.94	110.38
2	I	2	NAG	C2-N2-C7	-3.21	118.60	122.90
2	Q	3	BMA	O2-C2-C3	3.20	116.79	110.15
2	M	1	NAG	C3-C4-C5	-3.18	104.47	110.23
2	K	3	BMA	C3-C4-C5	-3.17	104.48	110.23
2	L	2	NAG	O4-C4-C3	3.17	117.84	110.38
2	G	4	MAN	C1-O5-C5	-3.14	107.98	112.19
2	O	3	BMA	C6-C5-C4	3.12	120.68	113.02
2	M	1	NAG	C1-O5-C5	3.10	116.33	112.19
2	G	3	BMA	O3-C3-C4	3.08	117.64	110.38
2	M	3	BMA	C1-O5-C5	-3.03	108.12	112.19
2	J	2	NAG	C1-O5-C5	-3.03	108.13	112.19
3	R	3	BMA	C3-C4-C5	3.03	115.72	110.23
2	Q	1	NAG	O4-C4-C3	3.03	117.51	110.38
2	L	1	NAG	O5-C5-C4	3.00	118.13	110.83
3	P	4	MAN	C1-O5-C5	2.98	116.18	112.19
2	Q	3	BMA	O4-C4-C3	2.96	117.36	110.38
2	K	3	BMA	C6-C5-C4	2.95	120.27	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3	BMA	O2-C2-C1	2.94	115.97	109.22
2	I	3	BMA	O2-C2-C3	2.94	116.24	110.15
4	N	3	BMA	C6-C5-C4	2.93	120.22	113.02
2	M	1	NAG	C4-C3-C2	-2.93	106.72	111.02
2	J	3	BMA	C3-C4-C5	-2.93	104.93	110.23
3	P	1	NAG	O4-C4-C3	2.92	117.26	110.38
2	I	3	BMA	O4-C4-C5	2.88	116.41	109.32
3	H	2	NAG	C1-O5-C5	2.84	116.00	112.19
2	M	1	NAG	C2-N2-C7	-2.83	119.11	122.90
3	P	2	NAG	O5-C1-C2	2.82	115.66	111.29
3	H	4	MAN	C2-C3-C4	-2.81	105.91	110.86
2	M	2	NAG	O5-C1-C2	-2.81	106.94	111.29
2	G	3	BMA	C6-C5-C4	2.81	119.92	113.02
2	L	2	NAG	C2-N2-C7	-2.81	119.14	122.90
2	G	4	MAN	C1-C2-C3	-2.81	105.56	109.64
2	M	2	NAG	C3-C4-C5	2.78	115.28	110.23
3	H	3	BMA	O3-C3-C4	2.77	116.91	110.38
2	O	3	BMA	C1-C2-C3	-2.75	105.64	109.64
2	O	3	BMA	O2-C2-C3	2.74	115.82	110.15
3	H	3	BMA	O2-C2-C3	2.73	115.80	110.15
2	K	4	MAN	O5-C5-C4	2.73	117.46	110.83
3	P	2	NAG	O4-C4-C3	2.71	116.78	110.38
3	P	3	BMA	C3-C4-C5	-2.71	105.32	110.23
2	K	2	NAG	C1-C2-N2	2.70	114.68	110.43
4	N	1	NAG	O5-C5-C4	2.69	117.38	110.83
2	J	1	NAG	C1-O5-C5	2.67	115.77	112.19
2	M	3	BMA	C2-C3-C4	-2.66	106.18	110.86
2	K	4	MAN	C6-C5-C4	-2.64	106.53	113.02
2	J	2	NAG	C4-C3-C2	2.63	114.88	111.02
2	I	3	BMA	O3-C3-C4	2.63	116.58	110.38
2	M	3	BMA	C6-C5-C4	2.62	119.45	113.02
2	G	3	BMA	O5-C5-C4	-2.60	104.50	110.83
3	P	3	BMA	C1-C2-C3	2.58	113.40	109.64
2	J	3	BMA	C6-C5-C4	2.57	119.34	113.02
2	J	3	BMA	O2-C2-C3	2.55	115.44	110.15
4	N	2	NAG	O5-C1-C2	-2.55	107.35	111.29
2	J	2	NAG	C3-C4-C5	2.54	114.84	110.23
3	H	1	NAG	C3-C4-C5	2.52	114.81	110.23
4	N	3	BMA	C2-C3-C4	-2.52	106.42	110.86
2	L	2	NAG	O5-C5-C4	2.48	116.85	110.83
3	R	1	NAG	O5-C5-C4	2.47	116.83	110.83
2	L	3	BMA	C6-C5-C4	2.45	119.05	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	5	MAN	C3-C4-C5	-2.43	105.82	110.23
2	L	3	BMA	O2-C2-C3	2.43	115.19	110.15
2	K	4	MAN	C1-O5-C5	2.42	115.44	112.19
3	H	3	BMA	O3-C3-C2	2.40	114.95	110.05
2	M	2	NAG	C2-N2-C7	-2.39	119.70	122.90
2	O	3	BMA	O2-C2-C1	2.38	114.66	109.22
2	L	3	BMA	O2-C2-C1	2.34	114.58	109.22
2	Q	2	NAG	O5-C1-C2	-2.34	107.67	111.29
3	R	3	BMA	O5-C1-C2	-2.31	105.28	110.79
3	H	3	BMA	O4-C4-C3	2.31	115.82	110.38
2	O	2	NAG	C3-C4-C5	2.30	114.41	110.23
2	G	3	BMA	O2-C2-C3	2.30	114.92	110.15
3	R	3	BMA	O4-C4-C3	2.29	115.78	110.38
2	I	4	MAN	C1-O5-C5	2.29	115.25	112.19
2	Q	2	NAG	O3-C3-C4	2.27	115.72	110.38
2	G	1	NAG	O5-C5-C4	2.26	116.33	110.83
3	R	3	BMA	O3-C3-C2	2.25	114.64	110.05
2	G	2	NAG	C4-C3-C2	2.24	114.31	111.02
2	K	4	MAN	O5-C5-C6	-2.24	103.30	107.66
2	L	1	NAG	O5-C5-C6	-2.22	103.35	107.66
3	P	2	NAG	O4-C4-C5	2.21	114.78	109.32
2	L	1	NAG	C2-N2-C7	-2.21	119.94	122.90
3	H	3	BMA	C3-C4-C5	2.19	114.21	110.23
3	R	5	MAN	C2-C3-C4	-2.19	107.00	110.86
3	H	3	BMA	C6-C5-C4	2.19	118.40	113.02
3	R	2	NAG	C3-C4-C5	2.19	114.20	110.23
4	N	3	BMA	O2-C2-C3	2.18	114.67	110.15
3	R	5	MAN	O5-C5-C6	2.18	111.90	107.66
2	M	3	BMA	C3-C4-C5	-2.16	106.31	110.23
2	Q	3	BMA	C6-C5-C4	2.15	118.30	113.02
2	I	3	BMA	O3-C3-C2	2.15	114.44	110.05
4	N	2	NAG	C3-C4-C5	2.15	114.12	110.23
2	G	2	NAG	C1-C2-N2	-2.12	107.09	110.43
2	Q	4	MAN	O5-C5-C6	2.11	111.76	107.66
3	P	1	NAG	C2-N2-C7	-2.10	120.08	122.90
2	K	3	BMA	O5-C5-C4	-2.10	105.73	110.83
2	M	3	BMA	O2-C2-C3	2.07	114.43	110.15
2	M	3	BMA	O2-C2-C1	2.06	113.94	109.22
2	K	2	NAG	O5-C1-C2	-2.06	108.11	111.29
2	M	1	NAG	O5-C1-C2	2.06	114.47	111.29
2	M	3	BMA	O5-C5-C4	-2.05	105.83	110.83
2	Q	3	BMA	O3-C3-C4	2.03	115.17	110.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	Q	1	NAG	C1

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	Q	1	NAG	C1-C2-N2-C7
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2
3	R	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Q	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
2	J	4	MAN	O5-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	J	4	MAN	C4-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	M	3	BMA	C4-C5-C6-O6
3	R	5	MAN	C4-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
2	G	4	MAN	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
2	O	4	MAN	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
2	O	4	MAN	C4-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
2	G	4	MAN	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
2	Q	4	MAN	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	J	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	R	5	MAN	O5-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
3	R	3	BMA	C4-C5-C6-O6
2	Q	4	MAN	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	Q	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
3	R	1	NAG	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
4	N	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C1-C2-N2-C7
2	O	1	NAG	C1-C2-N2-C7
3	R	4	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	4	MAN	C1-C2-C3-C4-C5-O5
3	P	4	MAN	C1-C2-C3-C4-C5-O5
3	R	5	MAN	C1-C2-C3-C4-C5-O5
3	H	5	MAN	C1-C2-C3-C4-C5-O5
2	Q	4	MAN	C1-C2-C3-C4-C5-O5

23 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	4	MAN	1	0
2	G	3	BMA	1	0
2	K	3	BMA	1	0
2	L	3	BMA	2	0
3	P	3	BMA	2	0

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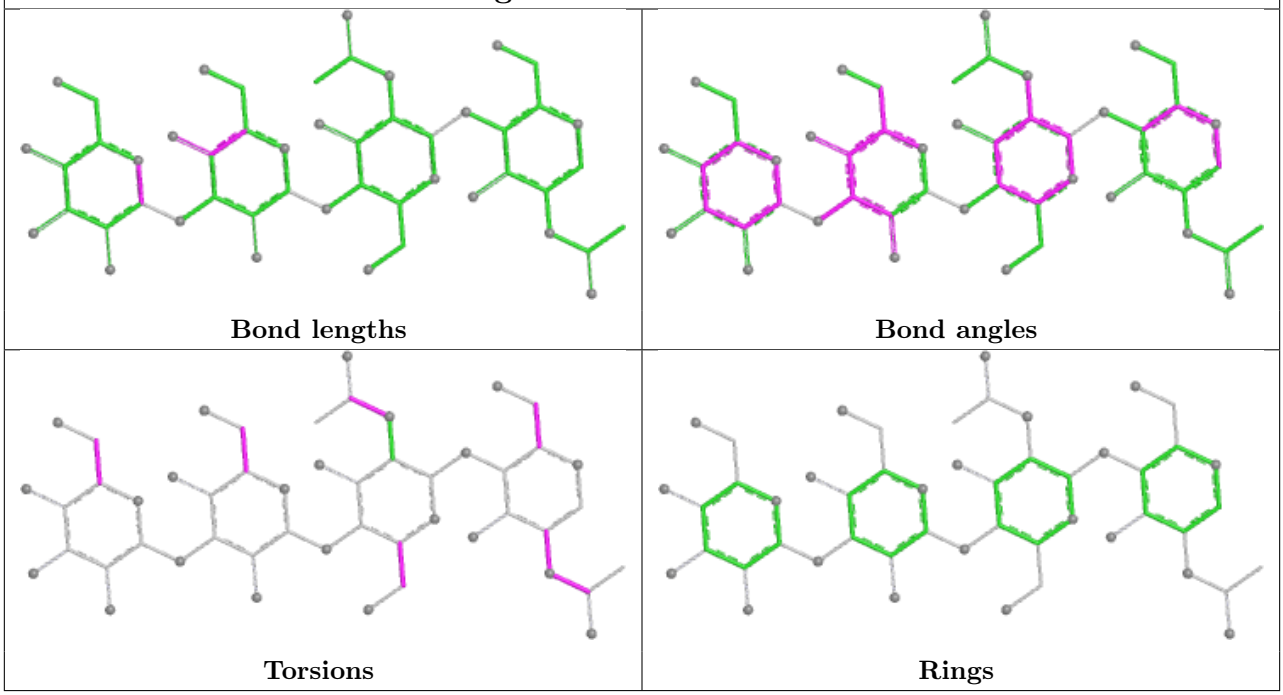
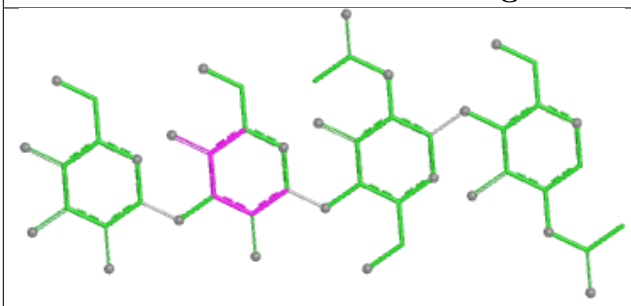
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	NAG	1	0
3	H	3	BMA	2	0
2	M	2	NAG	1	0
2	L	2	NAG	1	0
2	J	4	MAN	2	0
3	H	2	NAG	1	0
2	K	1	NAG	2	0
3	R	5	MAN	3	0
2	J	3	BMA	2	0
2	K	2	NAG	3	0
3	H	4	MAN	2	0
4	N	2	NAG	1	0
2	G	1	NAG	1	0
3	H	5	MAN	1	0
3	R	1	NAG	4	0
2	L	1	NAG	1	0
4	N	1	NAG	2	0
3	R	2	NAG	4	0

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

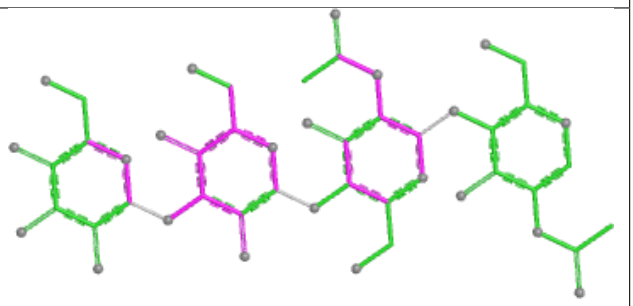
Oligosaccharide Chain G



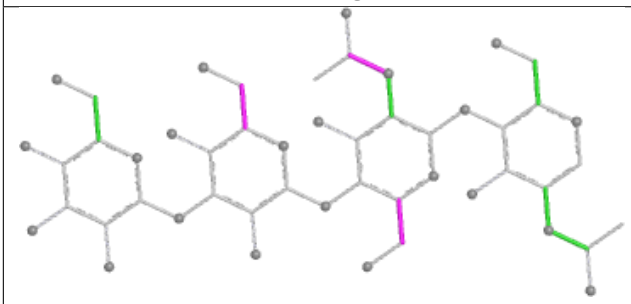
Oligosaccharide Chain I



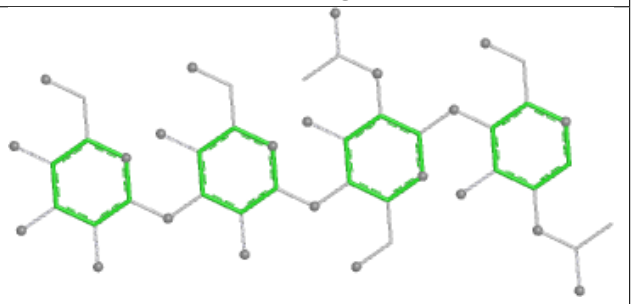
Bond lengths



Bond angles

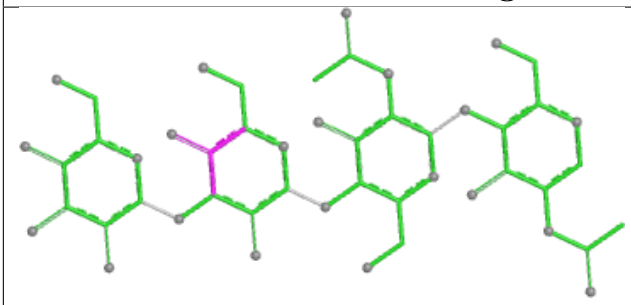


Torsions

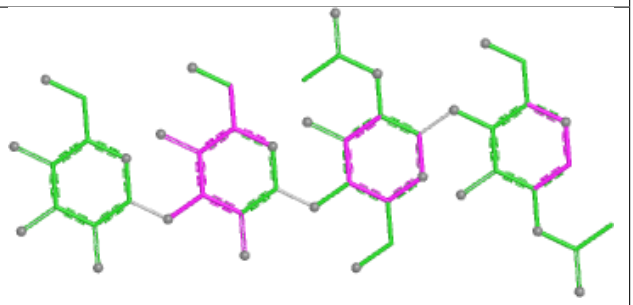


Rings

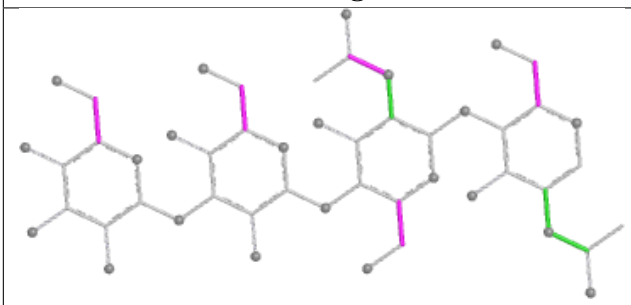
Oligosaccharide Chain J



Bond lengths



Bond angles



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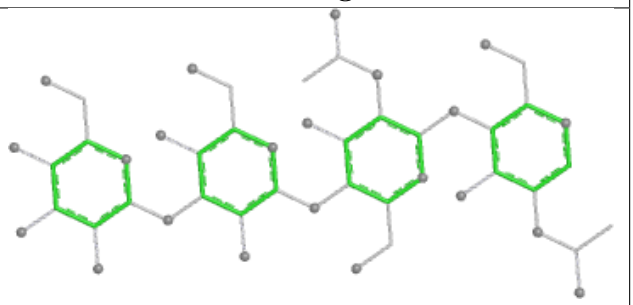
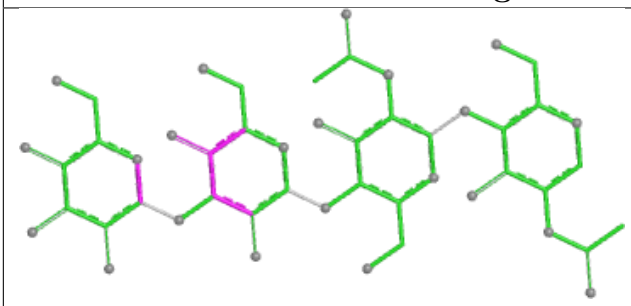
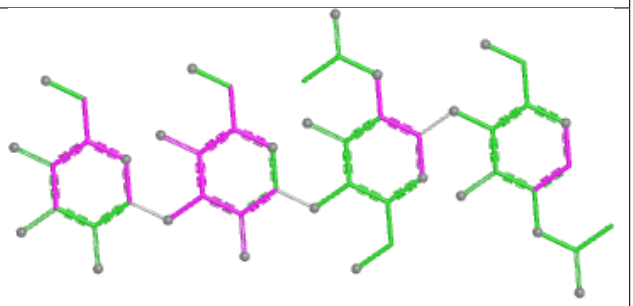


Rings

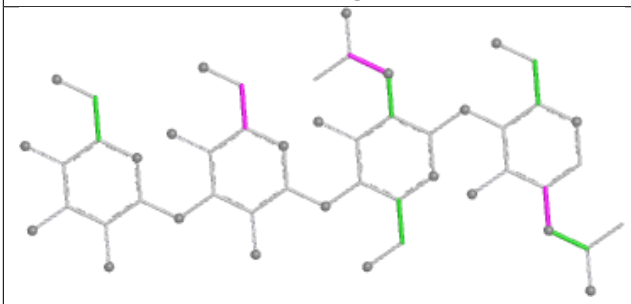
Oligosaccharide Chain K



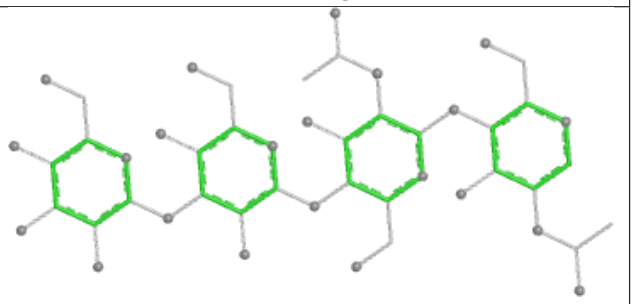
Bond lengths



Bond angles

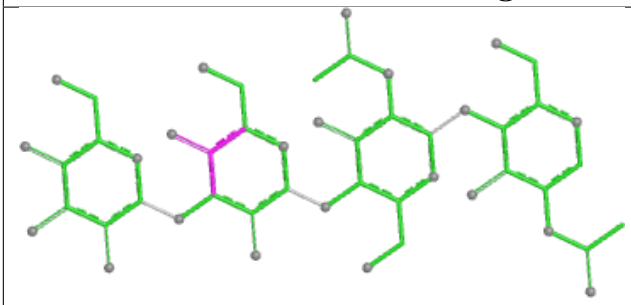


Torsions

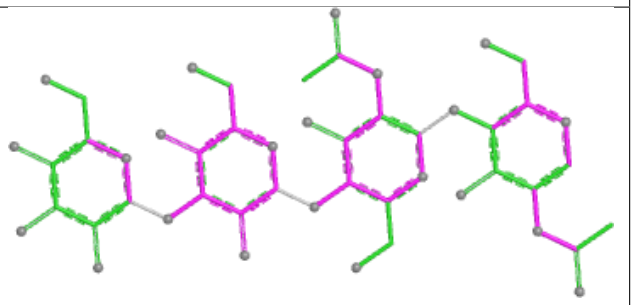


Rings

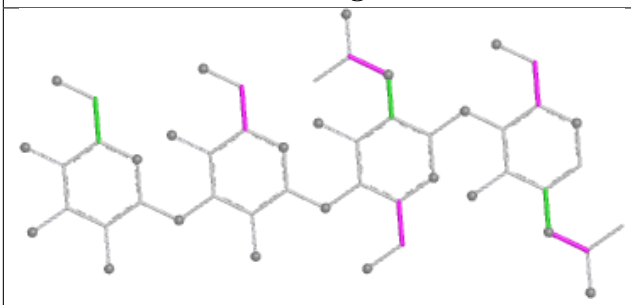
Oligosaccharide Chain L



Bond lengths



Bond angles



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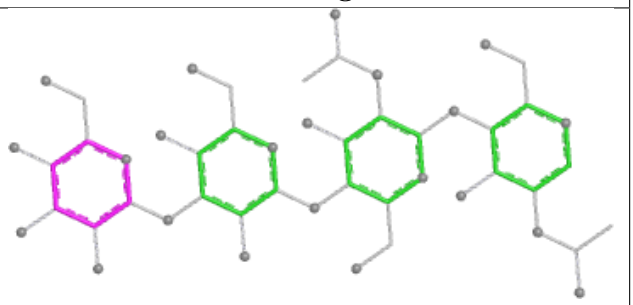
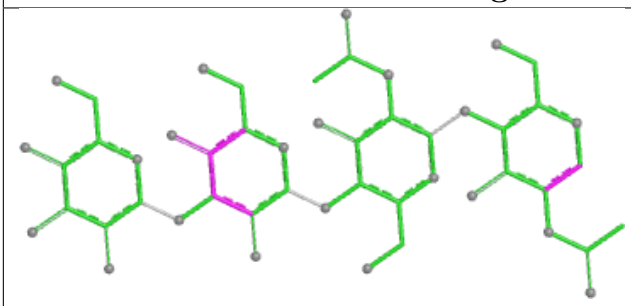
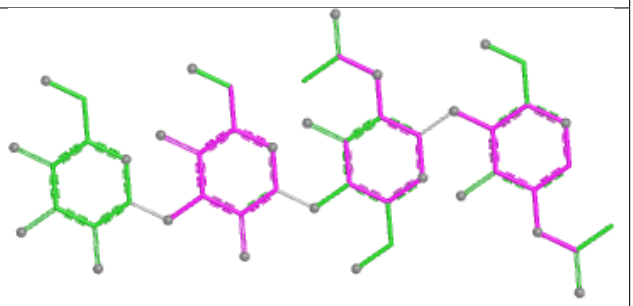


Rings

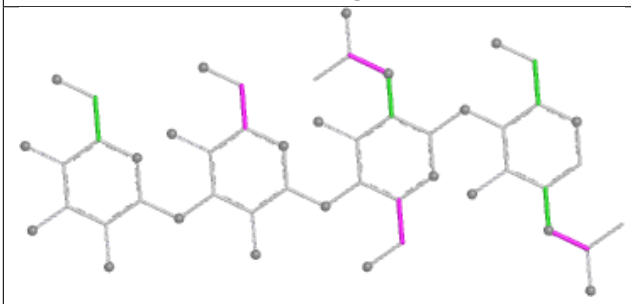
Oligosaccharide Chain M



Bond lengths



Bond angles



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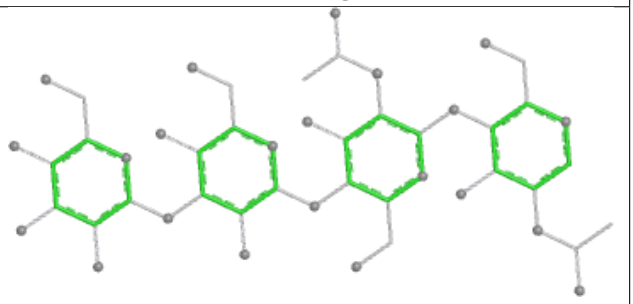
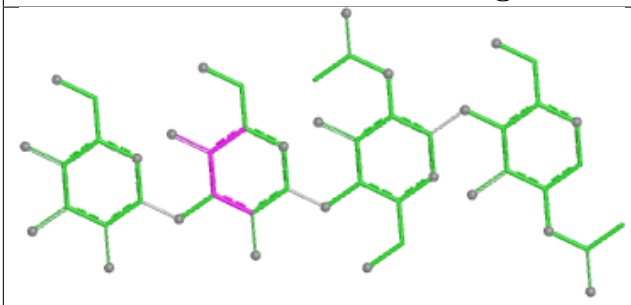
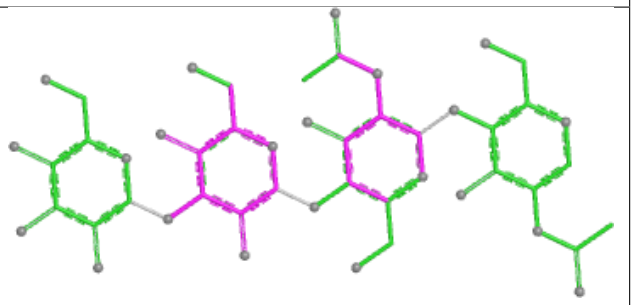


Rings

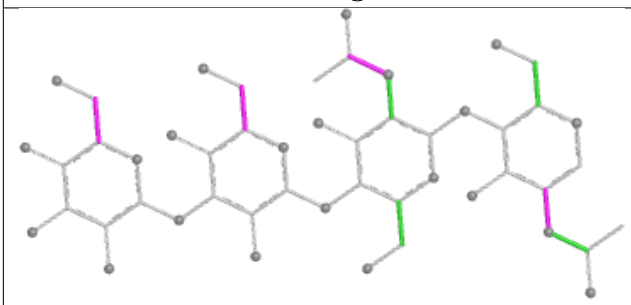
Oligosaccharide Chain O



Bond lengths



Bond angles



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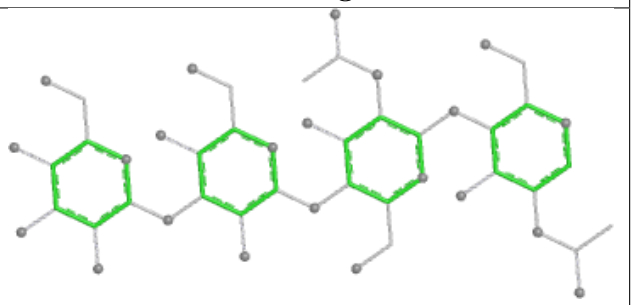
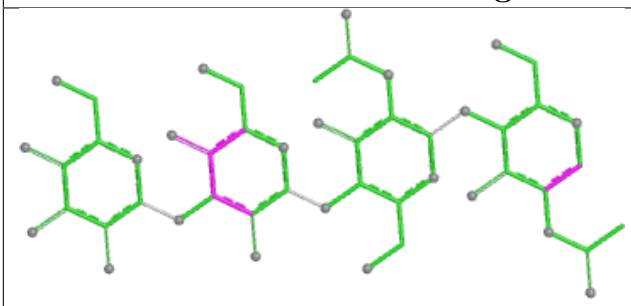


Rings

Oligosaccharide Chain Q



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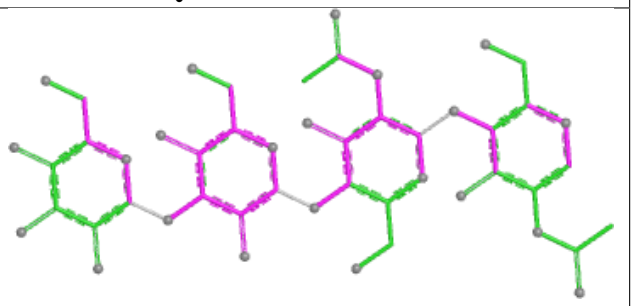
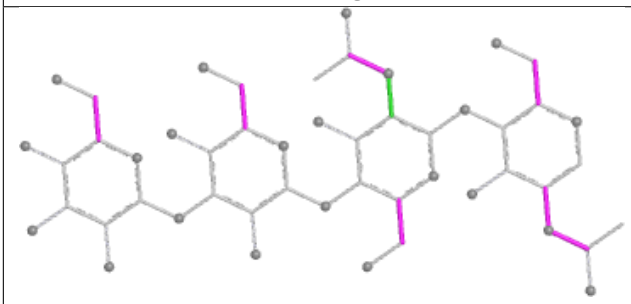


Bond angles



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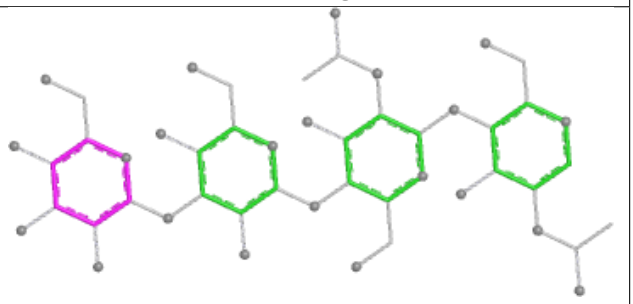
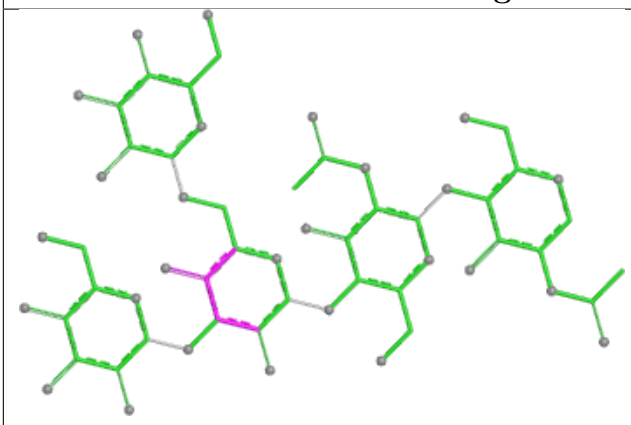


Rings

Oligosaccharide Chain H



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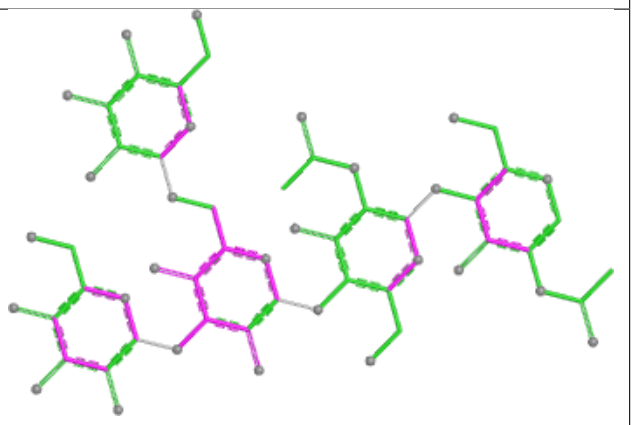
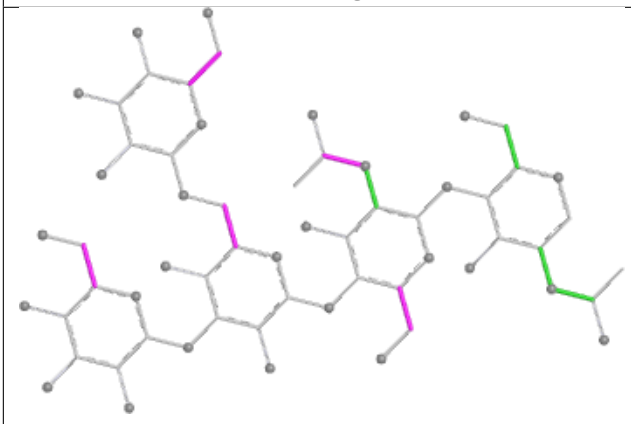


Bond angles



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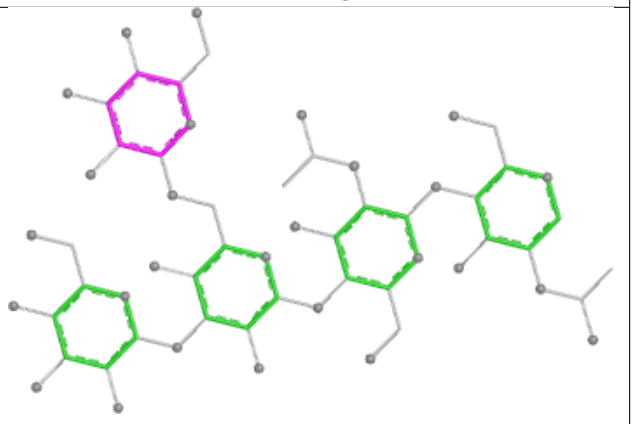
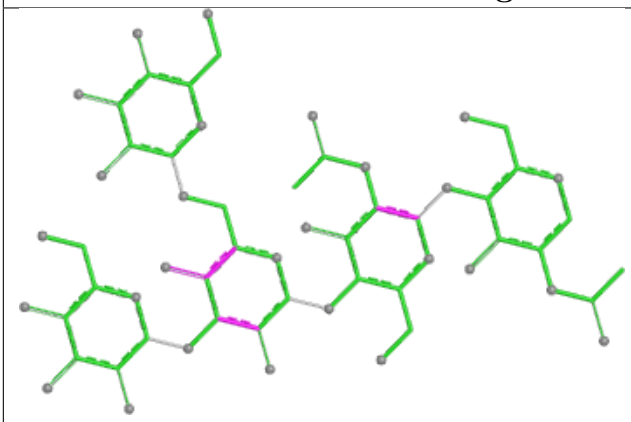


Rings

Oligosaccharide Chain P



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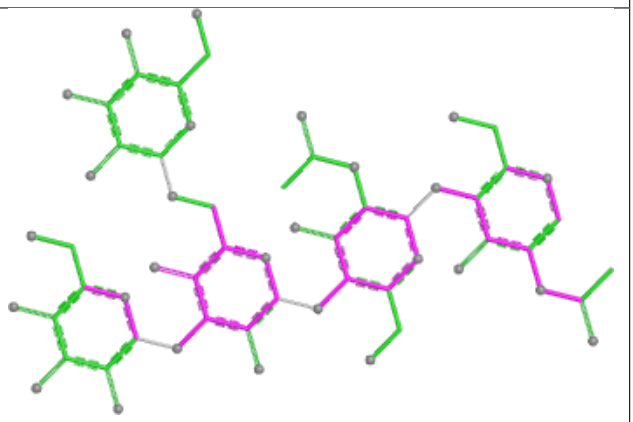
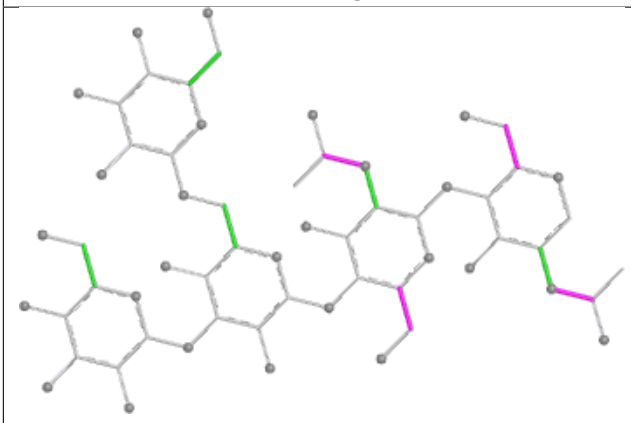


Bond angles



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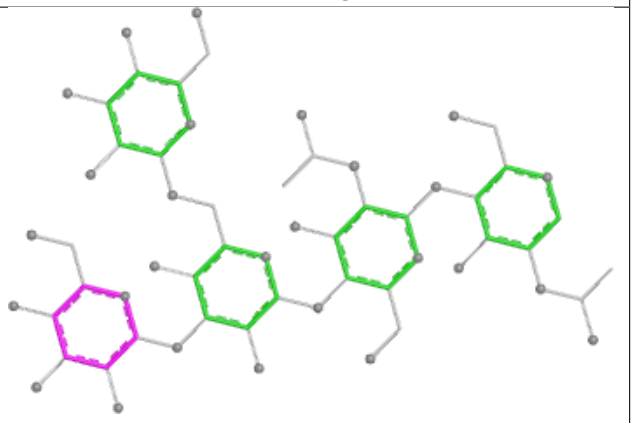
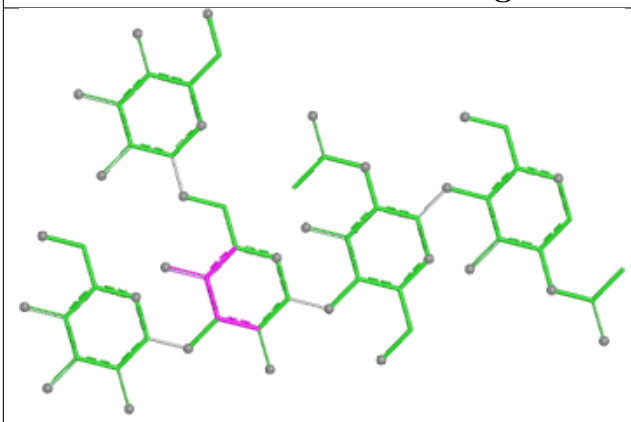
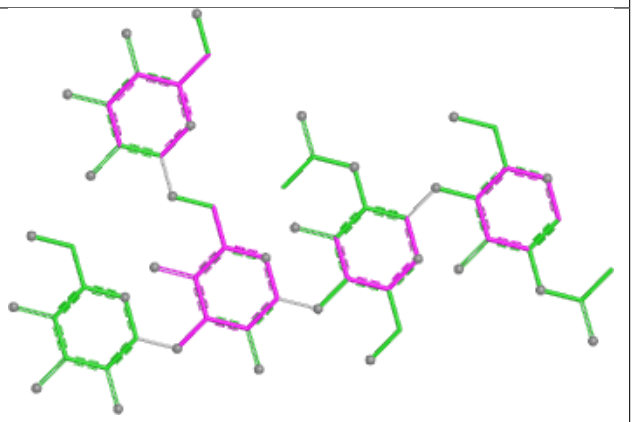


Rings

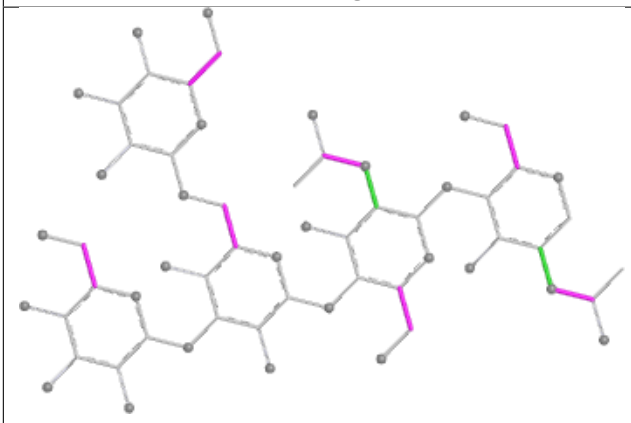
Oligosaccharide Chain R



Bond lengths



Bond angles



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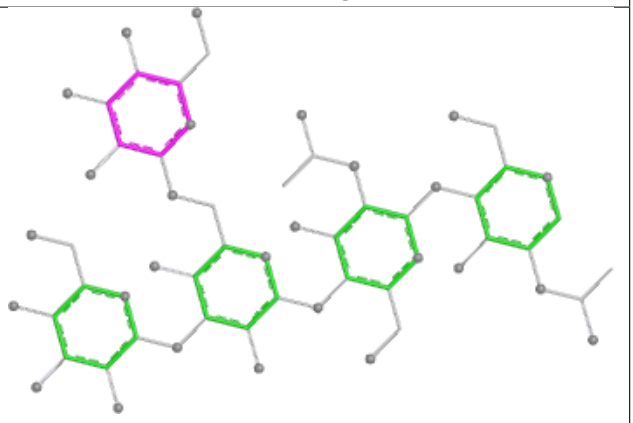
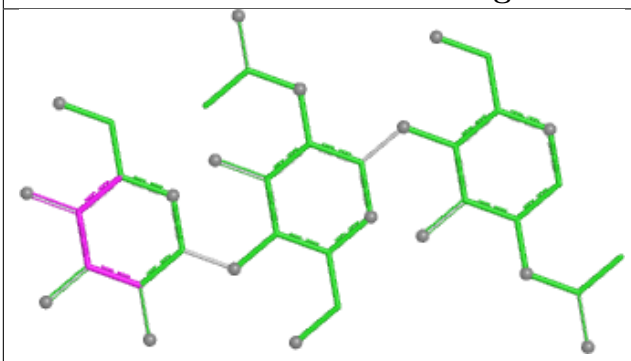
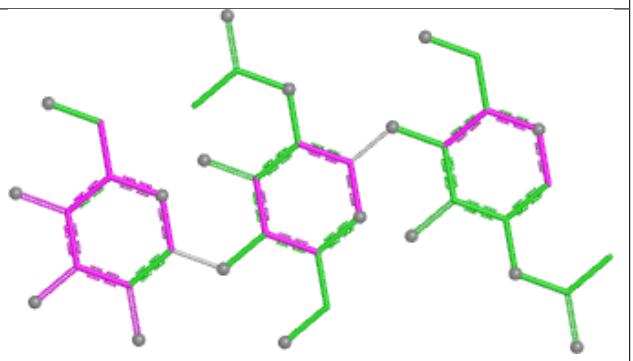


Rings

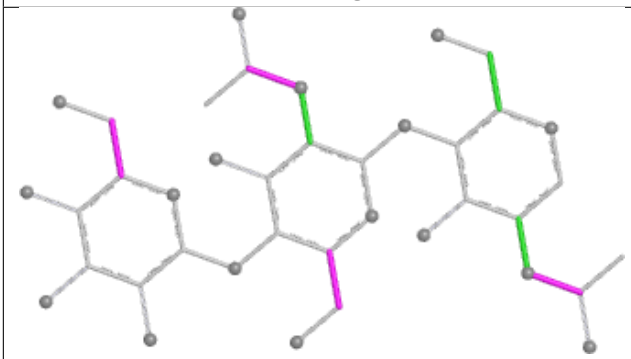
Oligosaccharide Chain N



Bond lengths



Bond angles



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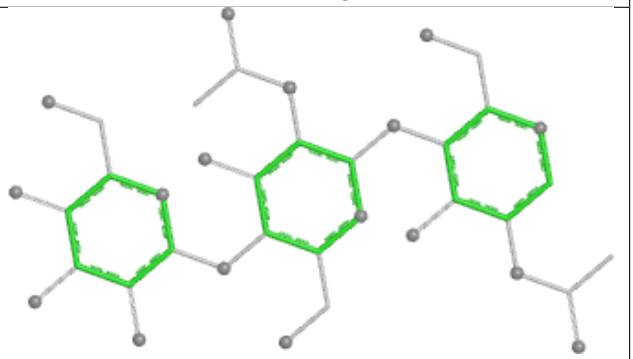

Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	613/750 (81%)	0.32	20 (3%)	49	33	52, 123, 277, 384	0
1	B	612/750 (81%)	0.34	25 (4%)	41	27	53, 123, 278, 384	0
1	C	612/750 (81%)	0.34	26 (4%)	40	26	53, 123, 276, 384	0
1	D	612/750 (81%)	0.33	23 (3%)	44	30	52, 123, 275, 384	0
1	E	613/750 (81%)	0.31	24 (3%)	43	29	52, 123, 278, 384	0
1	F	608/750 (81%)	0.33	25 (4%)	41	27	52, 122, 277, 376	0
All	All	3670/4500 (81%)	0.33	143 (3%)	43	29	52, 123, 278, 384	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	95	SER	5.1
1	B	95	SER	5.0
1	E	95	SER	5.0
1	D	95	SER	4.8
1	C	95	SER	4.6
1	A	95	SER	4.5
1	F	452	ALA	3.7
1	B	714	VAL	3.7
1	D	714	VAL	3.5
1	B	472	ALA	3.5
1	D	623	VAL	3.4
1	C	704	VAL	3.4
1	A	714	VAL	3.3
1	F	472	ALA	3.3
1	F	704	VAL	3.3
1	D	127	ALA	3.3
1	E	10	SER	3.2
1	F	276	VAL	3.2
1	B	432	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	94	LEU	3.2
1	E	472	ALA	3.0
1	F	420	ILE	3.0
1	A	623	VAL	3.0
1	D	704	VAL	3.0
1	F	714	VAL	3.0
1	F	451	GLY	2.9
1	C	377	ALA	2.9
1	E	714	VAL	2.9
1	A	472	ALA	2.9
1	F	656	VAL	2.9
1	F	623	VAL	2.9
1	B	94	LEU	2.9
1	B	623	VAL	2.8
1	B	716	PHE	2.8
1	C	10	SER	2.8
1	D	472	ALA	2.8
1	B	729	LEU	2.8
1	D	723	ALA	2.8
1	F	258	PRO	2.8
1	B	10	SER	2.7
1	C	276	VAL	2.7
1	C	698	THR	2.7
1	F	388	ASN	2.7
1	C	729	LEU	2.7
1	E	698	THR	2.7
1	C	689	PRO	2.7
1	D	377	ALA	2.7
1	B	656	VAL	2.7
1	C	714	VAL	2.7
1	D	94	LEU	2.7
1	A	656	VAL	2.6
1	B	516	SER	2.6
1	C	472	ALA	2.6
1	F	127	ALA	2.6
1	F	10	SER	2.6
1	F	71	GLN	2.6
1	B	377	ALA	2.6
1	C	590	HIS	2.5
1	C	94	LEU	2.5
1	C	717	SER	2.5
1	A	127	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	127	ALA	2.5
1	B	132	PRO	2.5
1	D	590	HIS	2.5
1	C	623	VAL	2.5
1	D	656	VAL	2.5
1	B	713	THR	2.5
1	A	94	LEU	2.5
1	A	590	HIS	2.5
1	D	712	VAL	2.5
1	D	518	ASP	2.4
1	D	713	THR	2.4
1	B	590	HIS	2.4
1	C	656	VAL	2.4
1	F	96	TYR	2.4
1	A	518	ASP	2.4
1	A	704	VAL	2.4
1	B	676	ALA	2.4
1	E	516	SER	2.4
1	A	713	THR	2.4
1	D	515	THR	2.4
1	F	689	PRO	2.4
1	C	716	PHE	2.3
1	D	716	PHE	2.3
1	D	132	PRO	2.3
1	E	657	SER	2.3
1	E	127	ALA	2.3
1	F	590	HIS	2.3
1	A	562	ASP	2.3
1	B	712	VAL	2.3
1	B	706	VAL	2.3
1	E	656	VAL	2.3
1	E	432	ALA	2.3
1	A	657	SER	2.3
1	F	713	THR	2.3
1	E	71	GLN	2.3
1	D	698	THR	2.3
1	D	725	PHE	2.3
1	E	623	VAL	2.3
1	D	88	SER	2.2
1	E	88	SER	2.2
1	A	698	THR	2.2
1	C	713	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	657	SER	2.2
1	C	591	VAL	2.2
1	D	457	ASP	2.2
1	A	414	VAL	2.2
1	A	377	ALA	2.2
1	C	388	ASN	2.2
1	E	676	ALA	2.2
1	B	725	PHE	2.2
1	A	276	VAL	2.1
1	A	343	SER	2.1
1	C	88	SER	2.1
1	C	702	SER	2.1
1	F	27	SER	2.1
1	E	515	THR	2.1
1	E	699	LEU	2.1
1	B	71	GLN	2.1
1	B	723	ALA	2.1
1	E	717	SER	2.1
1	E	666	CYS	2.1
1	C	71	GLN	2.1
1	F	432	ALA	2.1
1	B	689	PRO	2.1
1	B	88	SER	2.1
1	D	676	ALA	2.1
1	E	716	PHE	2.1
1	F	716	PHE	2.1
1	C	699	LEU	2.1
1	D	432	ALA	2.1
1	F	377	ALA	2.1
1	E	414	VAL	2.0
1	B	157	ARG	2.0
1	A	457	ASP	2.0
1	C	676	ALA	2.0
1	E	518	ASP	2.0
1	E	510	GLY	2.0
1	F	94	LEU	2.0
1	C	705	HIS	2.0
1	E	713	THR	2.0
1	B	57	GLY	2.0
1	A	157	ARG	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	H	2	14/15	0.35	0.14	218,228,238,243	0
3	MAN	P	5	11/12	0.39	0.12	193,208,213,216	0
2	BMA	I	3	11/12	0.40	0.10	185,193,201,201	0
3	MAN	R	5	11/12	0.40	0.12	209,236,246,247	0
2	BMA	J	3	11/12	0.44	0.10	234,243,255,256	0
3	BMA	H	3	11/12	0.46	0.11	194,229,252,253	0
2	BMA	K	3	11/12	0.47	0.11	159,180,190,193	0
3	NAG	R	2	14/15	0.48	0.10	199,205,211,212	0
2	NAG	J	2	14/15	0.52	0.13	165,190,204,219	0
3	MAN	H	4	11/12	0.54	0.13	176,202,226,228	0
2	NAG	L	2	14/15	0.55	0.12	218,236,246,251	0
3	NAG	P	2	14/15	0.56	0.11	189,205,217,222	0
3	BMA	R	3	11/12	0.59	0.08	195,209,234,236	0
2	BMA	M	3	11/12	0.60	0.09	176,190,223,224	0
2	MAN	K	4	11/12	0.60	0.13	177,187,197,202	0
2	MAN	L	4	11/12	0.60	0.15	248,250,254,260	0
2	BMA	G	3	11/12	0.62	0.10	165,169,197,213	0
2	BMA	O	3	11/12	0.66	0.09	173,180,196,200	0
3	NAG	P	1	14/15	0.68	0.14	144,163,174,188	0
2	NAG	J	1	14/15	0.69	0.12	144,161,170,183	0
4	NAG	N	1	14/15	0.69	0.13	154,177,186,194	0
4	BMA	N	3	11/12	0.72	0.10	176,193,202,203	0
2	BMA	Q	3	11/12	0.73	0.10	137,172,188,193	0
2	BMA	L	3	11/12	0.73	0.13	138,178,231,243	0
2	MAN	J	4	11/12	0.73	0.13	244,259,266,268	0
2	NAG	K	2	14/15	0.75	0.13	124,164,186,188	0
3	NAG	R	1	14/15	0.76	0.11	129,152,172,190	0
3	BMA	P	3	11/12	0.76	0.07	195,214,225,225	0
3	NAG	H	1	14/15	0.77	0.13	138,164,178,204	0
3	MAN	H	5	11/12	0.77	0.13	174,195,201,207	0
2	MAN	I	4	11/12	0.77	0.13	164,189,195,195	0
2	NAG	I	2	14/15	0.77	0.10	113,130,175,175	0

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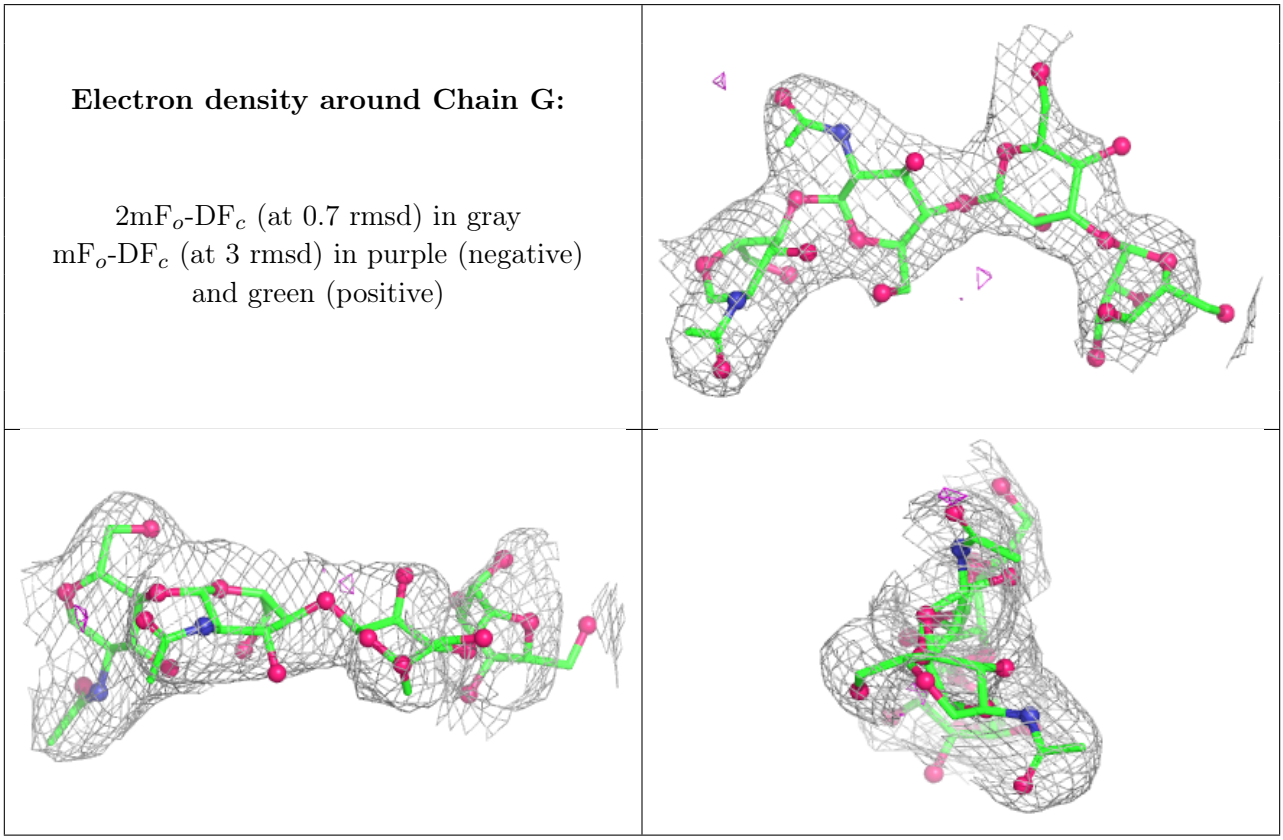
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	L	1	14/15	0.79	0.10	127,150,176,205	0
2	NAG	G	2	14/15	0.79	0.10	113,136,144,151	0
3	MAN	R	4	11/12	0.80	0.12	241,253,263,265	0
4	NAG	N	2	14/15	0.80	0.12	184,194,201,202	0
2	NAG	O	2	14/15	0.80	0.09	113,124,164,165	0
2	MAN	Q	4	11/12	0.82	0.11	185,192,197,199	0
2	NAG	Q	2	14/15	0.82	0.10	98,134,160,166	0
2	NAG	M	2	14/15	0.83	0.09	110,131,162,178	0
2	MAN	M	4	11/12	0.86	0.10	176,185,193,194	0
2	MAN	O	4	11/12	0.88	0.10	191,196,204,207	0
3	MAN	P	4	11/12	0.89	0.10	114,174,187,188	0
2	NAG	G	1	14/15	0.89	0.08	77,100,126,131	0
2	NAG	M	1	14/15	0.91	0.08	92,103,130,136	0
2	NAG	K	1	14/15	0.91	0.08	92,108,127,134	0
2	NAG	Q	1	14/15	0.92	0.08	78,105,124,134	0
2	NAG	O	1	14/15	0.92	0.08	93,108,125,132	0
2	NAG	I	1	14/15	0.93	0.07	91,98,122,133	0
2	MAN	G	4	11/12	0.93	0.09	225,228,240,247	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.

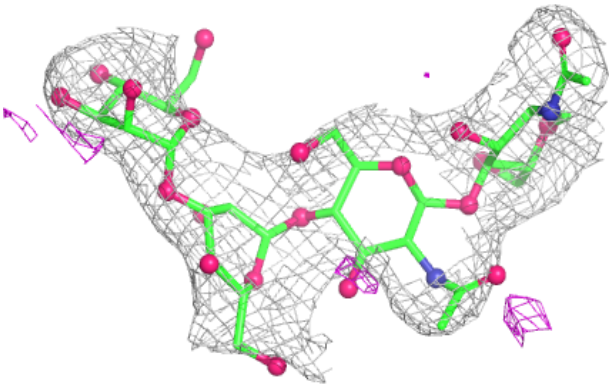
Electron density around Chain G:

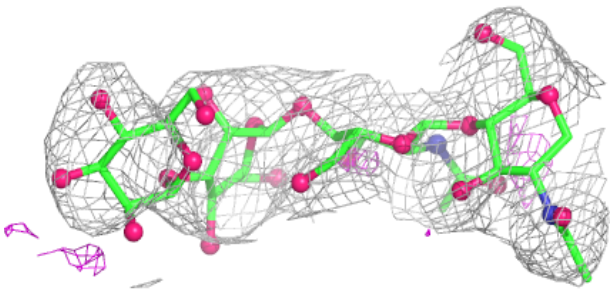
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

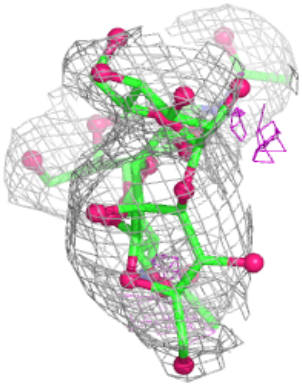


Electron density around Chain I:

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

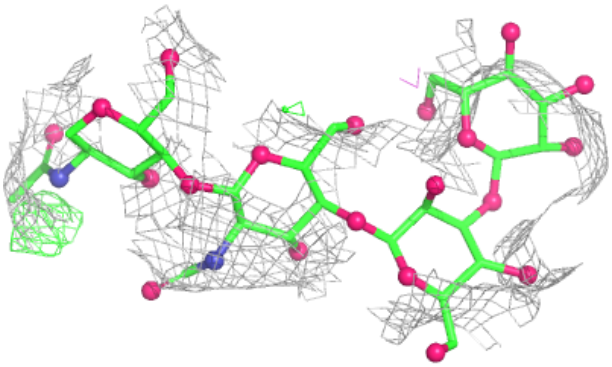


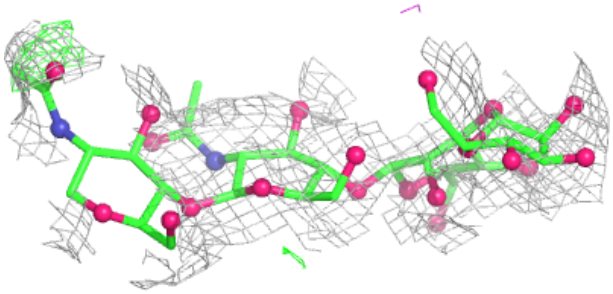


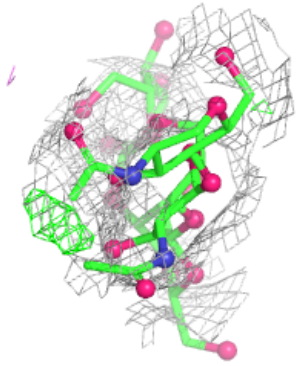


Electron density around Chain J:

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

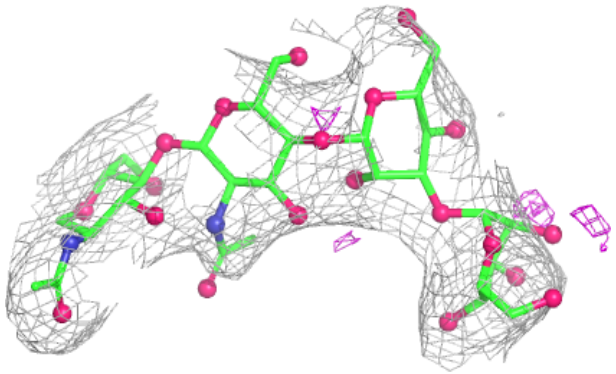


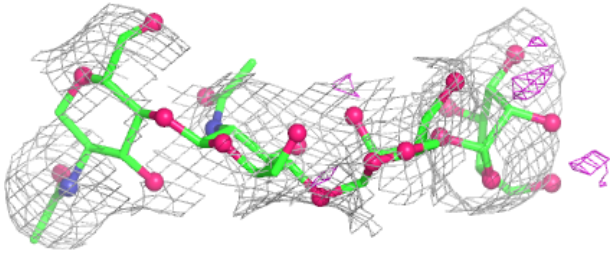


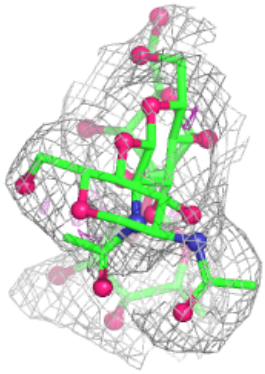


Electron density around Chain K:

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

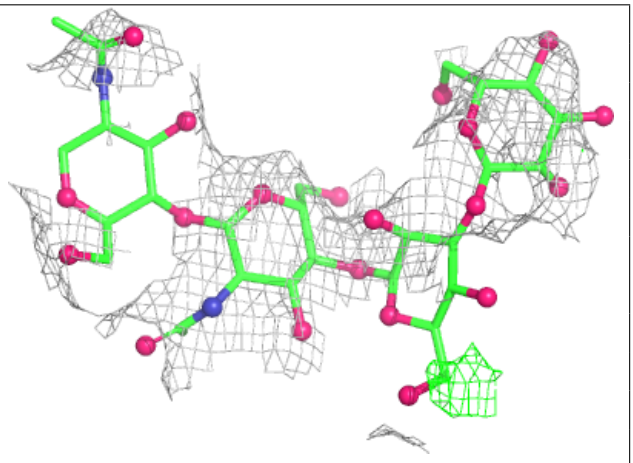


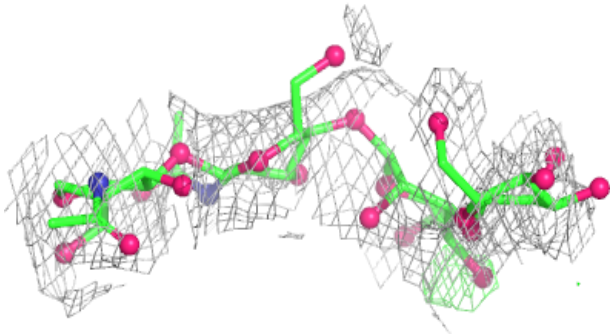


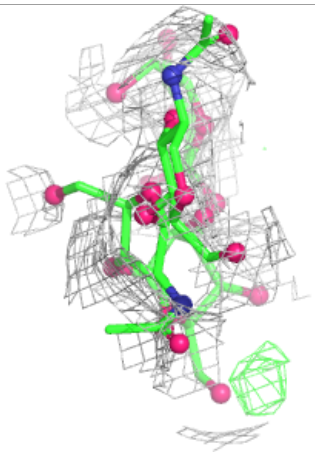


Electron density around Chain L:

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

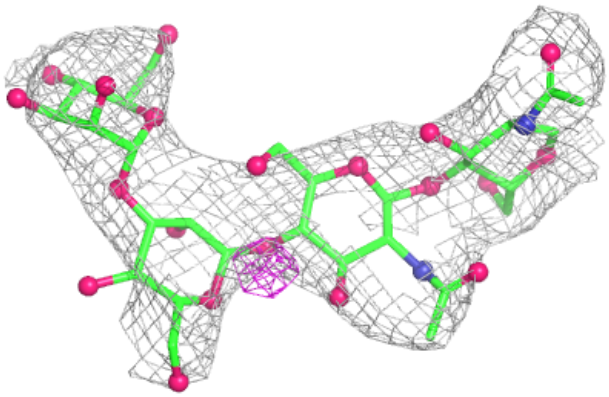


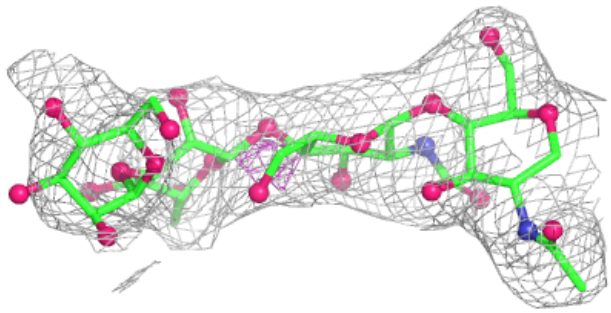


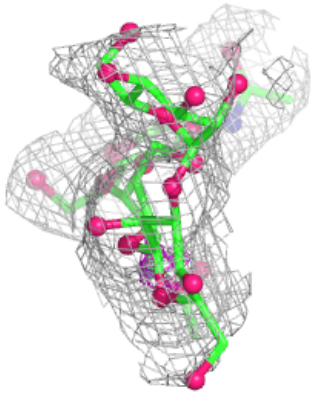


Electron density around Chain M:

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

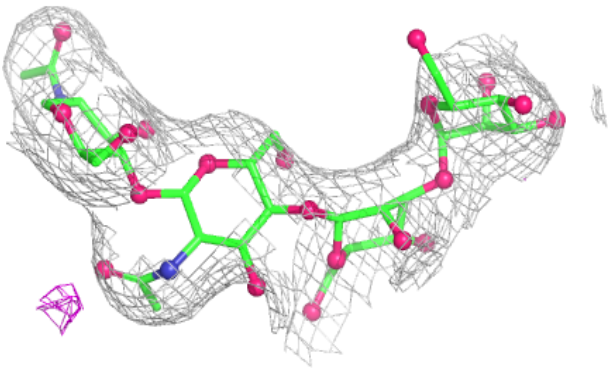


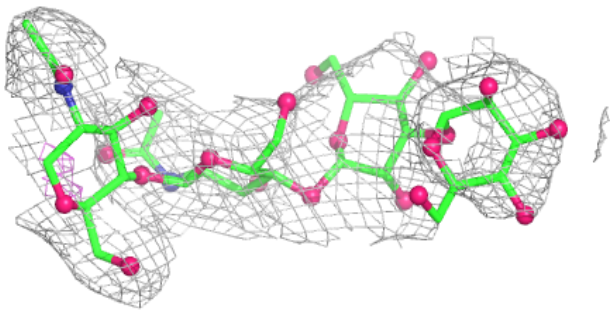


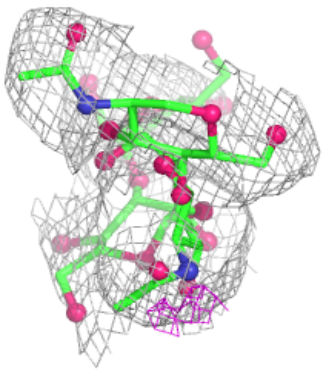


Electron density around Chain O:

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

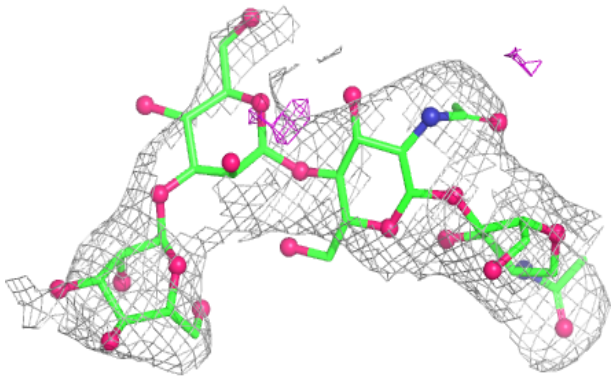


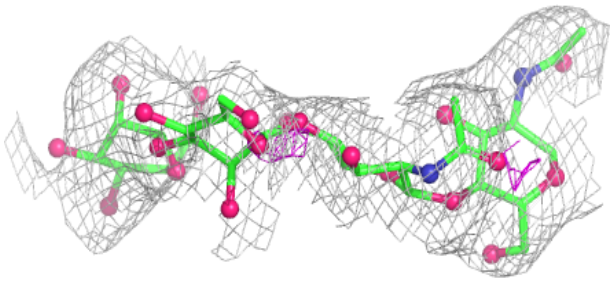


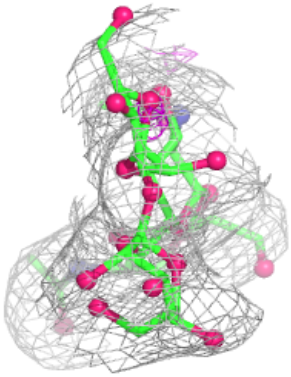


Electron density around Chain Q:

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

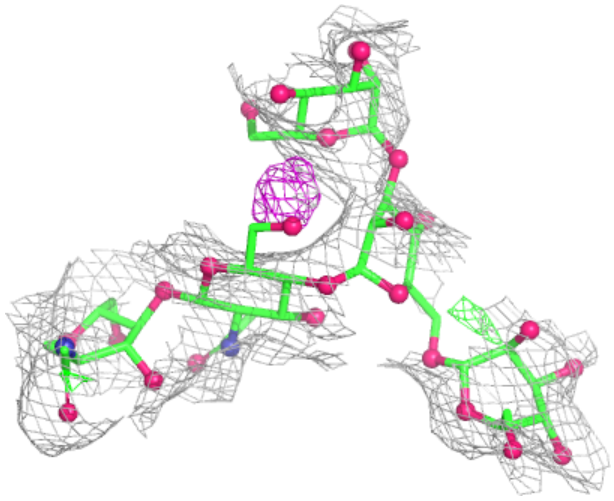


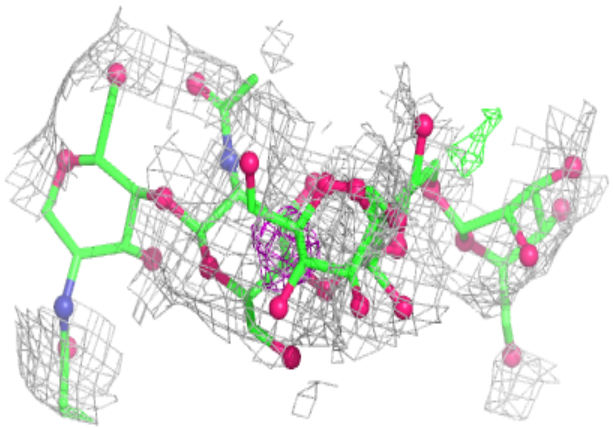


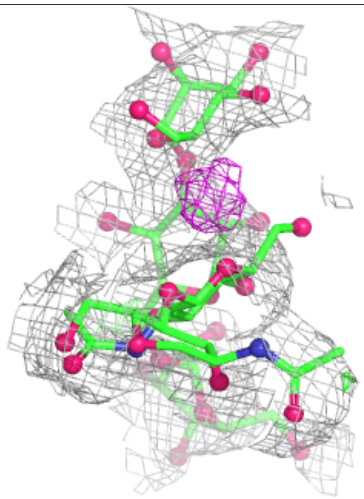


Electron density around Chain H:

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

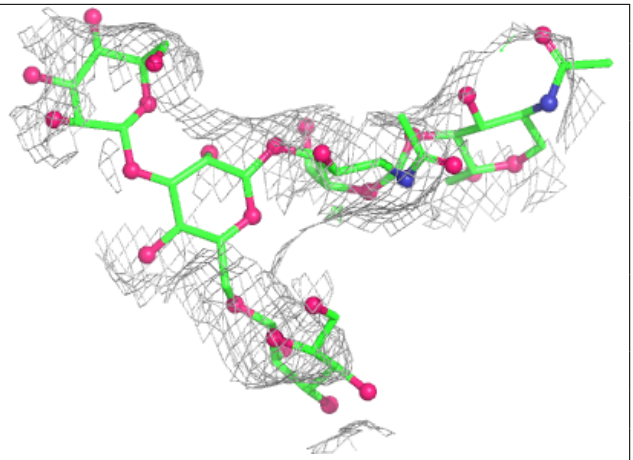


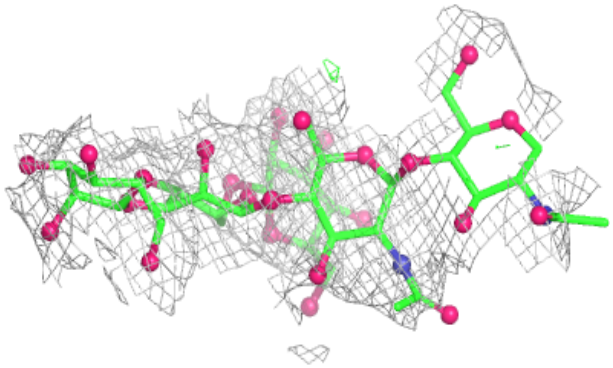


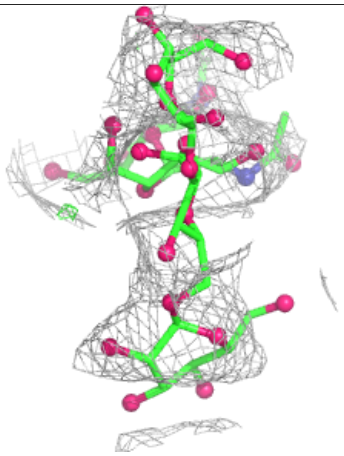


Electron density around Chain P:

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

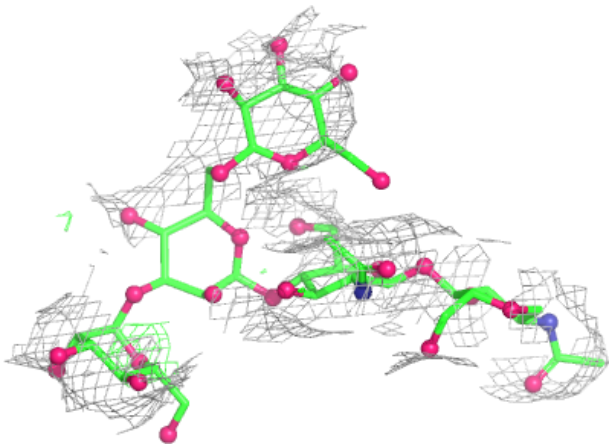


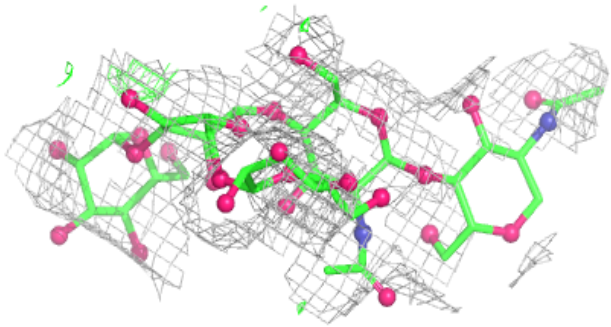


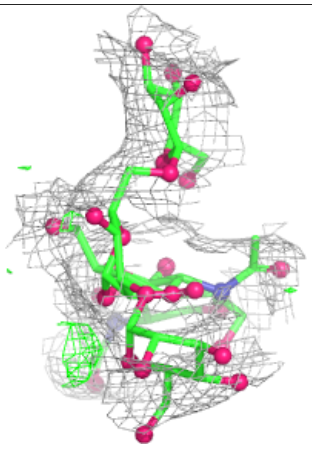


Electron density around Chain R:

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

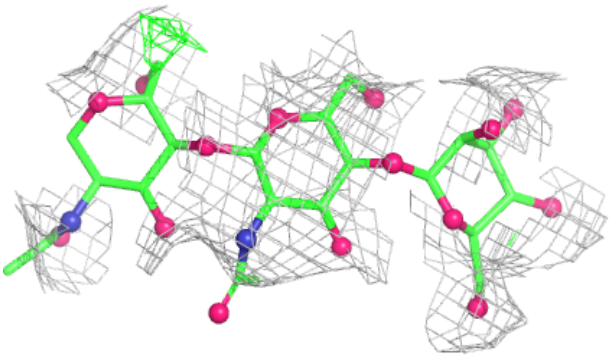


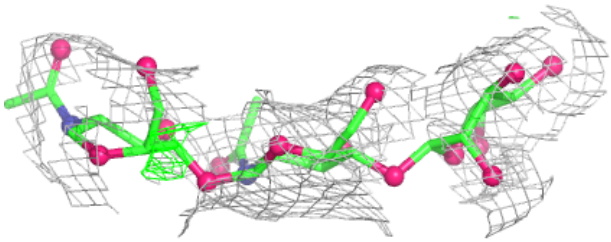


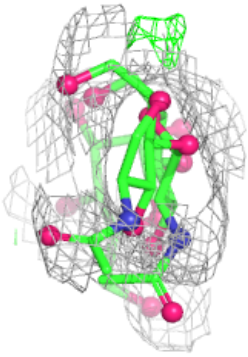


Electron density around Chain N:

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







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.