Full wwPDB X-ray Structure Validation Report (i)

May 7, 2024 – 10:11 AM EDT

PDB ID	:	8SUF
Title	:	The complex of TOL-1 ectodomain bound to LAT-1 Lectin domain
Authors	:	Carmona Rosas, G.; Li, J.; Arac, D.; Ozkan, E.
Deposited on	:	2023-05-12
Resolution	:	4.00 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:

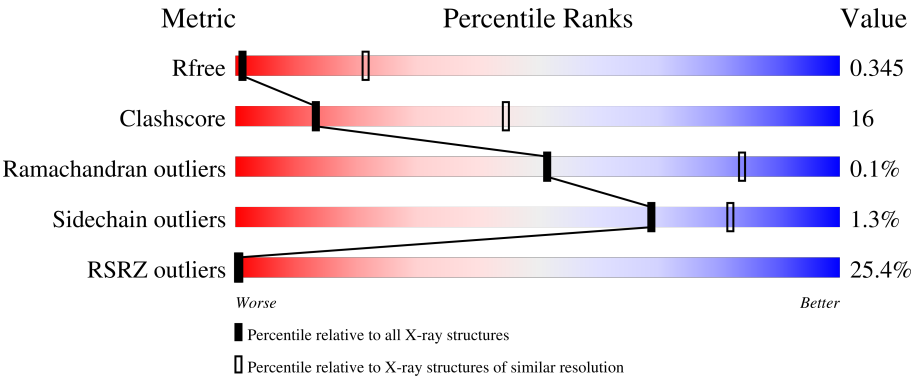
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	1007	19% 57% 36% 7%
1	B	1007	23% 58% 33% • 7%
1	C	1007	21% 62% 30% 7%
1	D	1007	23% 57% 36% 7%
2	E	114	39% 71% 23% • 5%

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Mol	Chain	Length	Quality of chain
2	F	114	46% 71% 24% 5%
2	G	114	40% 68% 24% 6%
2	H	114	44% 67% 25% 8%
3	I	4	25% 25% 50%
3	M	4	25% 50% 25%
4	J	2	50% 50%
4	K	2	100%
4	N	2	100%
4	O	2	50% 50%
4	R	2	100%
5	L	4	25% 75%
6	P	5	60% 40%
7	Q	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
3	MAN	I	4	-	-	-	X
4	NAG	K	1	-	-	-	X
4	NAG	N	2	-	-	-	X
4	NAG	O	2	-	-	-	X
8	NAG	A	1102	-	-	-	X
8	NAG	A	1103	-	-	-	X
8	NAG	B	1102	-	-	-	X
8	NAG	B	1103	-	-	-	X
8	NAG	C	1101	-	-	-	X
8	NAG	D	1101	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 32993 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 TIR domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	939	Total	C	N	O	S	0	0	0
			7315	4590	1278	1405	42			
1	B	935	Total	C	N	O	S	0	0	0
			7286	4570	1274	1401	41			
1	C	939	Total	C	N	O	S	0	0	0
			7315	4590	1278	1405	42			
1	D	939	Total	C	N	O	S	0	0	0
			7315	4590	1278	1405	42			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP Q9N5Z3
A	-5	ASP	-	expression tag	UNP Q9N5Z3
A	-4	PRO	-	expression tag	UNP Q9N5Z3
A	-3	HIS	-	expression tag	UNP Q9N5Z3
A	-2	HIS	-	expression tag	UNP Q9N5Z3
A	-1	HIS	-	expression tag	UNP Q9N5Z3
A	0	HIS	-	expression tag	UNP Q9N5Z3
A	1	HIS	-	expression tag	UNP Q9N5Z3
A	2	HIS	-	expression tag	UNP Q9N5Z3
A	3	GLY	-	expression tag	UNP Q9N5Z3
A	4	SER	-	expression tag	UNP Q9N5Z3
A	5	GLY	-	expression tag	UNP Q9N5Z3
A	6	LEU	-	expression tag	UNP Q9N5Z3
A	7	ASN	-	expression tag	UNP Q9N5Z3
A	8	ASP	-	expression tag	UNP Q9N5Z3
A	9	ILE	-	expression tag	UNP Q9N5Z3
A	10	PHE	-	expression tag	UNP Q9N5Z3
A	11	GLU	-	expression tag	UNP Q9N5Z3
A	12	ALA	-	expression tag	UNP Q9N5Z3
A	13	GLN	-	expression tag	UNP Q9N5Z3
A	14	LYS	-	expression tag	UNP Q9N5Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ILE	-	expression tag	UNP Q9N5Z3
A	16	GLU	-	expression tag	UNP Q9N5Z3
A	17	TRP	-	expression tag	UNP Q9N5Z3
A	18	HIS	-	expression tag	UNP Q9N5Z3
A	19	GLU	-	expression tag	UNP Q9N5Z3
A	20	ALA	-	expression tag	UNP Q9N5Z3
A	21	ASP	-	expression tag	UNP Q9N5Z3
A	22	PRO	-	expression tag	UNP Q9N5Z3
A	23	GLY	-	expression tag	UNP Q9N5Z3
A	24	TYR	-	expression tag	UNP Q9N5Z3
A	25	THR	-	expression tag	UNP Q9N5Z3
A	997	ASP	-	expression tag	UNP Q9N5Z3
A	998	ILE	-	expression tag	UNP Q9N5Z3
A	999	GLN	-	expression tag	UNP Q9N5Z3
A	1000	HIS	-	expression tag	UNP Q9N5Z3
B	-6	ALA	-	expression tag	UNP Q9N5Z3
B	-5	ASP	-	expression tag	UNP Q9N5Z3
B	-4	PRO	-	expression tag	UNP Q9N5Z3
B	-3	HIS	-	expression tag	UNP Q9N5Z3
B	-2	HIS	-	expression tag	UNP Q9N5Z3
B	-1	HIS	-	expression tag	UNP Q9N5Z3
B	0	HIS	-	expression tag	UNP Q9N5Z3
B	1	HIS	-	expression tag	UNP Q9N5Z3
B	2	HIS	-	expression tag	UNP Q9N5Z3
B	3	GLY	-	expression tag	UNP Q9N5Z3
B	4	SER	-	expression tag	UNP Q9N5Z3
B	5	GLY	-	expression tag	UNP Q9N5Z3
B	6	LEU	-	expression tag	UNP Q9N5Z3
B	7	ASN	-	expression tag	UNP Q9N5Z3
B	8	ASP	-	expression tag	UNP Q9N5Z3
B	9	ILE	-	expression tag	UNP Q9N5Z3
B	10	PHE	-	expression tag	UNP Q9N5Z3
B	11	GLU	-	expression tag	UNP Q9N5Z3
B	12	ALA	-	expression tag	UNP Q9N5Z3
B	13	GLN	-	expression tag	UNP Q9N5Z3
B	14	LYS	-	expression tag	UNP Q9N5Z3
B	15	ILE	-	expression tag	UNP Q9N5Z3
B	16	GLU	-	expression tag	UNP Q9N5Z3
B	17	TRP	-	expression tag	UNP Q9N5Z3
B	18	HIS	-	expression tag	UNP Q9N5Z3
B	19	GLU	-	expression tag	UNP Q9N5Z3
B	20	ALA	-	expression tag	UNP Q9N5Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	expression tag	UNP Q9N5Z3
B	22	PRO	-	expression tag	UNP Q9N5Z3
B	23	GLY	-	expression tag	UNP Q9N5Z3
B	24	TYR	-	expression tag	UNP Q9N5Z3
B	25	THR	-	expression tag	UNP Q9N5Z3
B	997	ASP	-	expression tag	UNP Q9N5Z3
B	998	ILE	-	expression tag	UNP Q9N5Z3
B	999	GLN	-	expression tag	UNP Q9N5Z3
B	1000	HIS	-	expression tag	UNP Q9N5Z3
C	-6	ALA	-	expression tag	UNP Q9N5Z3
C	-5	ASP	-	expression tag	UNP Q9N5Z3
C	-4	PRO	-	expression tag	UNP Q9N5Z3
C	-3	HIS	-	expression tag	UNP Q9N5Z3
C	-2	HIS	-	expression tag	UNP Q9N5Z3
C	-1	HIS	-	expression tag	UNP Q9N5Z3
C	0	HIS	-	expression tag	UNP Q9N5Z3
C	1	HIS	-	expression tag	UNP Q9N5Z3
C	2	HIS	-	expression tag	UNP Q9N5Z3
C	3	GLY	-	expression tag	UNP Q9N5Z3
C	4	SER	-	expression tag	UNP Q9N5Z3
C	5	GLY	-	expression tag	UNP Q9N5Z3
C	6	LEU	-	expression tag	UNP Q9N5Z3
C	7	ASN	-	expression tag	UNP Q9N5Z3
C	8	ASP	-	expression tag	UNP Q9N5Z3
C	9	ILE	-	expression tag	UNP Q9N5Z3
C	10	PHE	-	expression tag	UNP Q9N5Z3
C	11	GLU	-	expression tag	UNP Q9N5Z3
C	12	ALA	-	expression tag	UNP Q9N5Z3
C	13	GLN	-	expression tag	UNP Q9N5Z3
C	14	LYS	-	expression tag	UNP Q9N5Z3
C	15	ILE	-	expression tag	UNP Q9N5Z3
C	16	GLU	-	expression tag	UNP Q9N5Z3
C	17	TRP	-	expression tag	UNP Q9N5Z3
C	18	HIS	-	expression tag	UNP Q9N5Z3
C	19	GLU	-	expression tag	UNP Q9N5Z3
C	20	ALA	-	expression tag	UNP Q9N5Z3
C	21	ASP	-	expression tag	UNP Q9N5Z3
C	22	PRO	-	expression tag	UNP Q9N5Z3
C	23	GLY	-	expression tag	UNP Q9N5Z3
C	24	TYR	-	expression tag	UNP Q9N5Z3
C	25	THR	-	expression tag	UNP Q9N5Z3
C	997	ASP	-	expression tag	UNP Q9N5Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	998	ILE	-	expression tag	UNP Q9N5Z3
C	999	GLN	-	expression tag	UNP Q9N5Z3
C	1000	HIS	-	expression tag	UNP Q9N5Z3
D	-6	ALA	-	expression tag	UNP Q9N5Z3
D	-5	ASP	-	expression tag	UNP Q9N5Z3
D	-4	PRO	-	expression tag	UNP Q9N5Z3
D	-3	HIS	-	expression tag	UNP Q9N5Z3
D	-2	HIS	-	expression tag	UNP Q9N5Z3
D	-1	HIS	-	expression tag	UNP Q9N5Z3
D	0	HIS	-	expression tag	UNP Q9N5Z3
D	1	HIS	-	expression tag	UNP Q9N5Z3
D	2	HIS	-	expression tag	UNP Q9N5Z3
D	3	GLY	-	expression tag	UNP Q9N5Z3
D	4	SER	-	expression tag	UNP Q9N5Z3
D	5	GLY	-	expression tag	UNP Q9N5Z3
D	6	LEU	-	expression tag	UNP Q9N5Z3
D	7	ASN	-	expression tag	UNP Q9N5Z3
D	8	ASP	-	expression tag	UNP Q9N5Z3
D	9	ILE	-	expression tag	UNP Q9N5Z3
D	10	PHE	-	expression tag	UNP Q9N5Z3
D	11	GLU	-	expression tag	UNP Q9N5Z3
D	12	ALA	-	expression tag	UNP Q9N5Z3
D	13	GLN	-	expression tag	UNP Q9N5Z3
D	14	LYS	-	expression tag	UNP Q9N5Z3
D	15	ILE	-	expression tag	UNP Q9N5Z3
D	16	GLU	-	expression tag	UNP Q9N5Z3
D	17	TRP	-	expression tag	UNP Q9N5Z3
D	18	HIS	-	expression tag	UNP Q9N5Z3
D	19	GLU	-	expression tag	UNP Q9N5Z3
D	20	ALA	-	expression tag	UNP Q9N5Z3
D	21	ASP	-	expression tag	UNP Q9N5Z3
D	22	PRO	-	expression tag	UNP Q9N5Z3
D	23	GLY	-	expression tag	UNP Q9N5Z3
D	24	TYR	-	expression tag	UNP Q9N5Z3
D	25	THR	-	expression tag	UNP Q9N5Z3
D	997	ASP	-	expression tag	UNP Q9N5Z3
D	998	ILE	-	expression tag	UNP Q9N5Z3
D	999	GLN	-	expression tag	UNP Q9N5Z3
D	1000	HIS	-	expression tag	UNP Q9N5Z3

- Molecule 2 is a protein called Latrophilin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	108	Total	C	N	O	S	0	0	0
			815	507	133	166	9			
2	F	108	Total	C	N	O	S	0	0	0
			815	507	133	166	9			
2	G	107	Total	C	N	O	S	0	0	0
			808	502	132	165	9			
2	H	105	Total	C	N	O	S	0	0	0
			794	492	130	163	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	29	ALA	-	expression tag	UNP G5EDW2
E	30	ASP	-	expression tag	UNP G5EDW2
E	137	HIS	-	expression tag	UNP G5EDW2
E	138	HIS	-	expression tag	UNP G5EDW2
E	139	HIS	-	expression tag	UNP G5EDW2
E	140	HIS	-	expression tag	UNP G5EDW2
E	141	HIS	-	expression tag	UNP G5EDW2
E	142	HIS	-	expression tag	UNP G5EDW2
F	29	ALA	-	expression tag	UNP G5EDW2
F	30	ASP	-	expression tag	UNP G5EDW2
F	137	HIS	-	expression tag	UNP G5EDW2
F	138	HIS	-	expression tag	UNP G5EDW2
F	139	HIS	-	expression tag	UNP G5EDW2
F	140	HIS	-	expression tag	UNP G5EDW2
F	141	HIS	-	expression tag	UNP G5EDW2
F	142	HIS	-	expression tag	UNP G5EDW2
G	29	ALA	-	expression tag	UNP G5EDW2
G	30	ASP	-	expression tag	UNP G5EDW2
G	137	HIS	-	expression tag	UNP G5EDW2
G	138	HIS	-	expression tag	UNP G5EDW2
G	139	HIS	-	expression tag	UNP G5EDW2
G	140	HIS	-	expression tag	UNP G5EDW2
G	141	HIS	-	expression tag	UNP G5EDW2
G	142	HIS	-	expression tag	UNP G5EDW2
H	29	ALA	-	expression tag	UNP G5EDW2
H	30	ASP	-	expression tag	UNP G5EDW2
H	137	HIS	-	expression tag	UNP G5EDW2
H	138	HIS	-	expression tag	UNP G5EDW2
H	139	HIS	-	expression tag	UNP G5EDW2
H	140	HIS	-	expression tag	UNP G5EDW2
H	141	HIS	-	expression tag	UNP G5EDW2
H	142	HIS	-	expression tag	UNP G5EDW2

- Molecule 3 is an oligosaccharide called 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	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

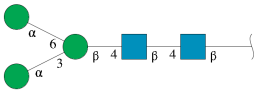
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.

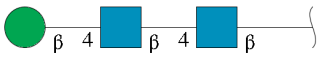
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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.



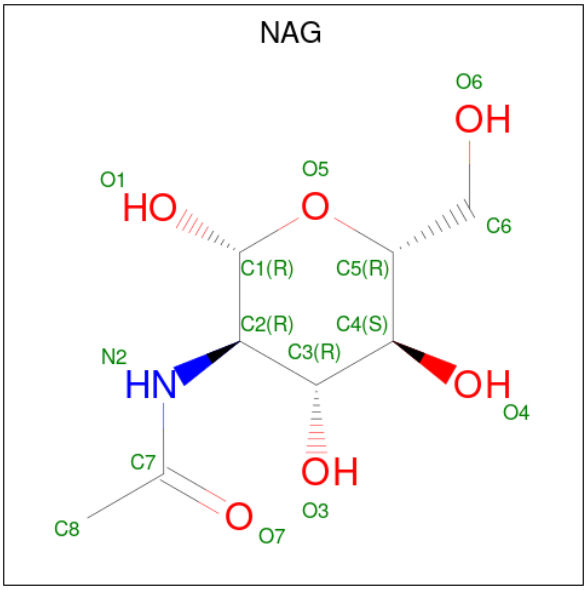
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	P	5	61	34	2	25	0	0	0

- Molecule 7 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			
7	Q	3	39	22	2	15	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



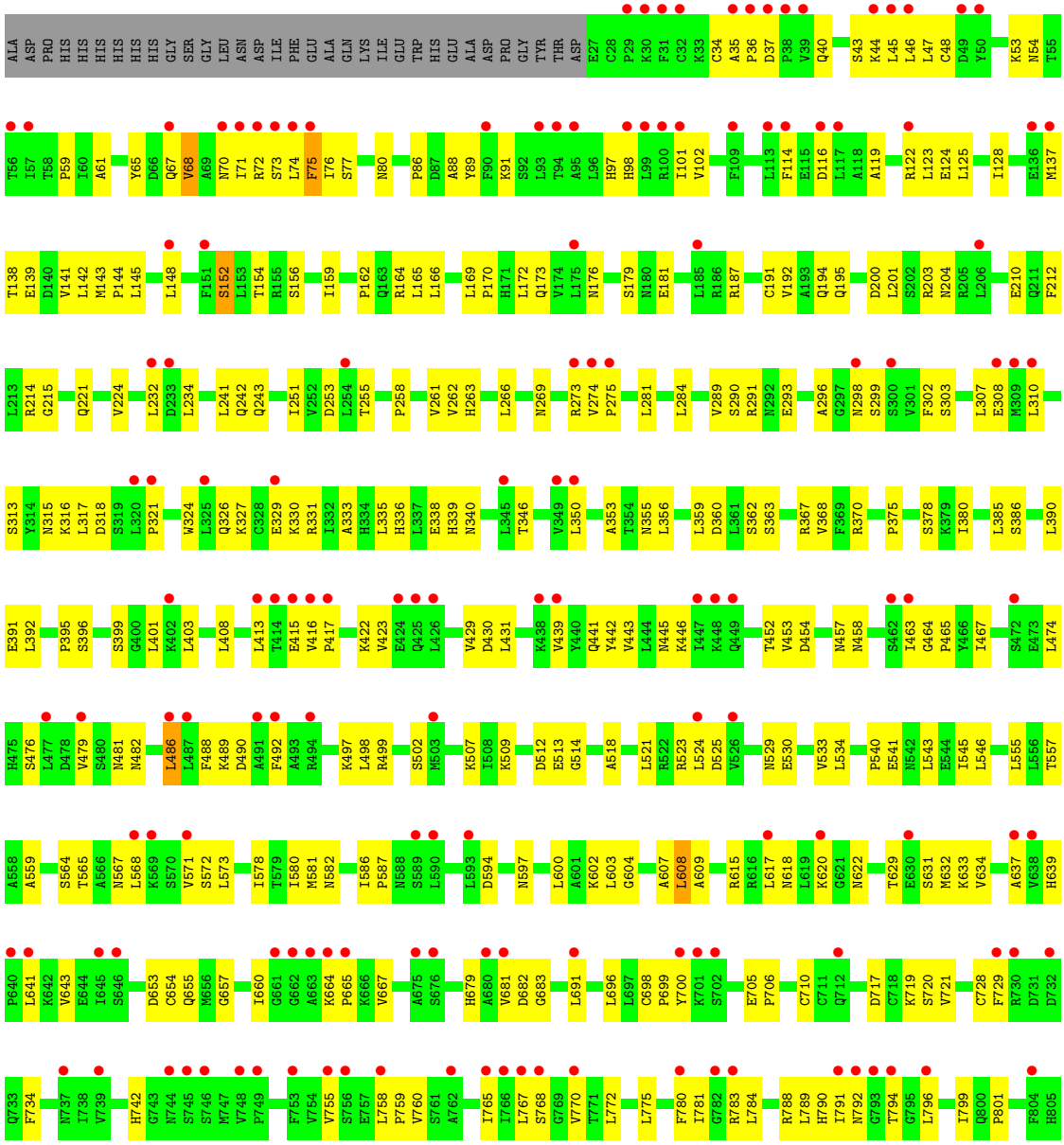
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

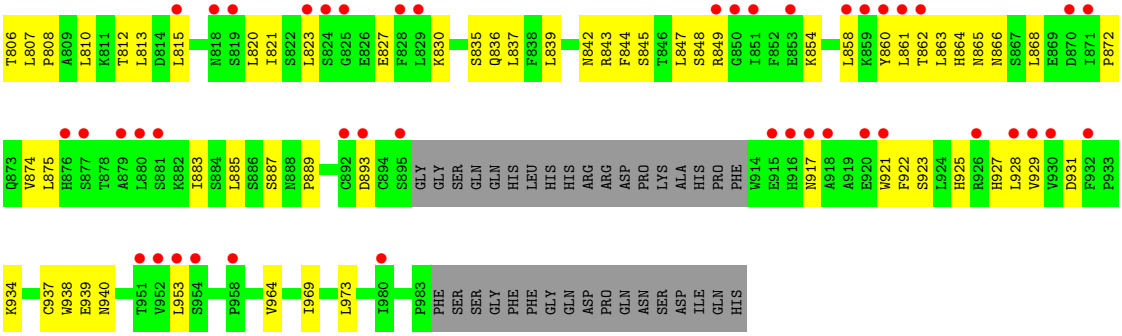
3 Residue-property plots (i)

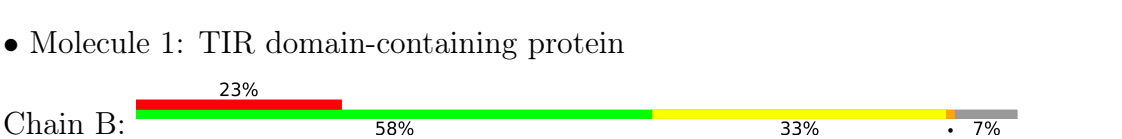
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

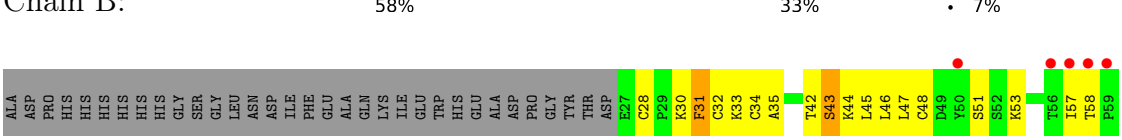
- Molecule 1: TIR domain-containing protein

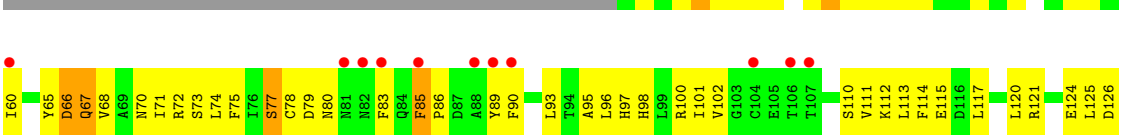
Chain A:

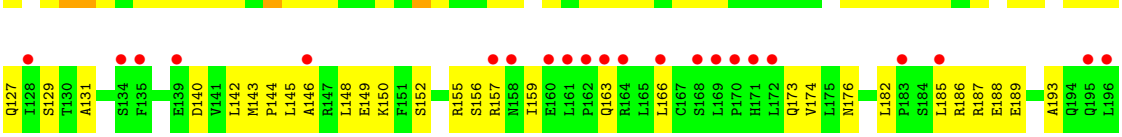


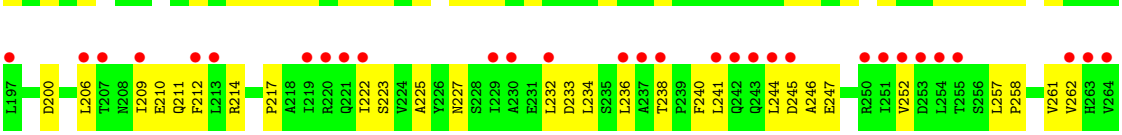


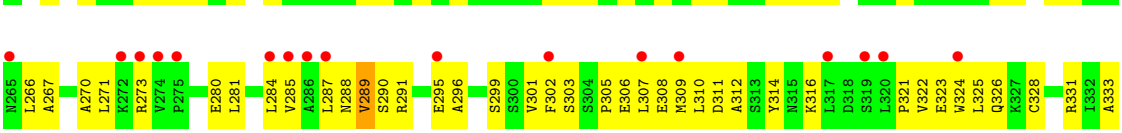


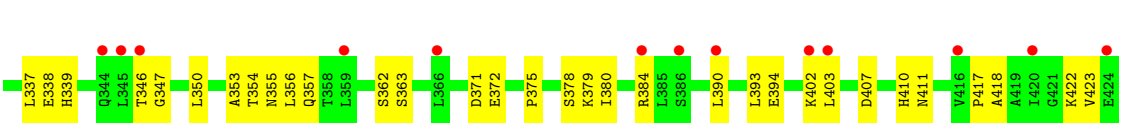


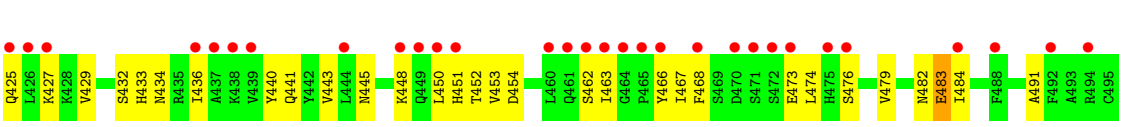


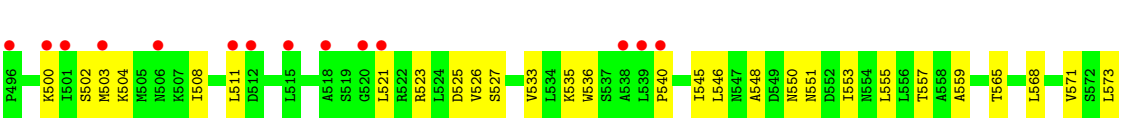


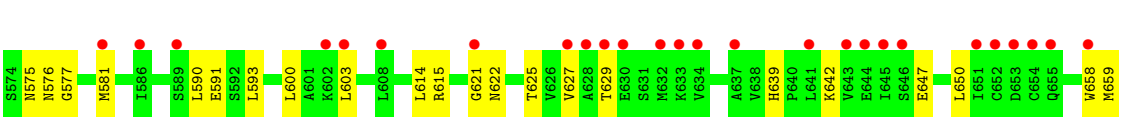


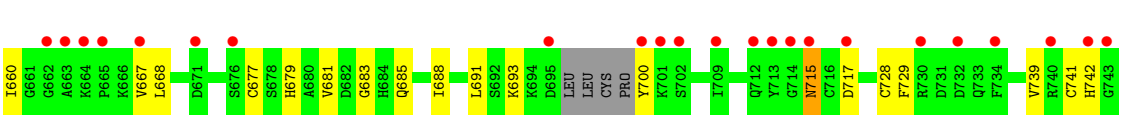






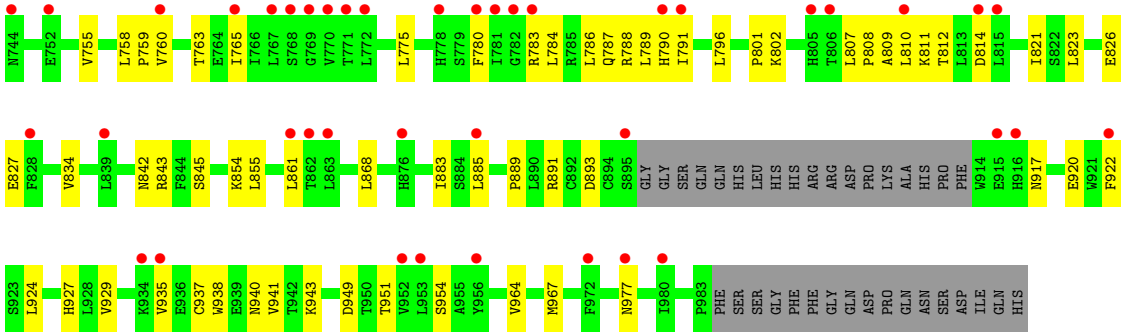






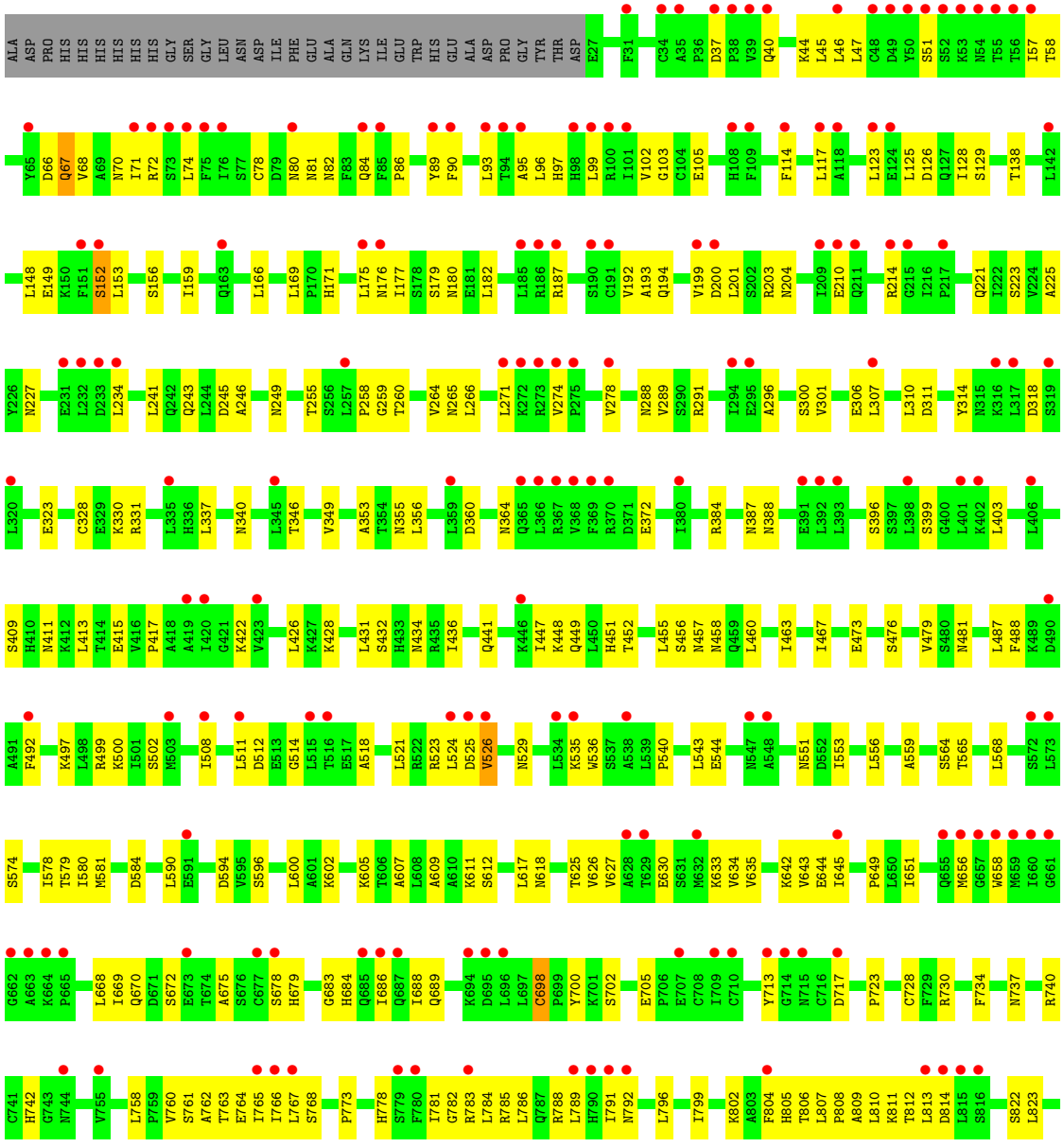
• Molecule 1: TIR domain-containing protein

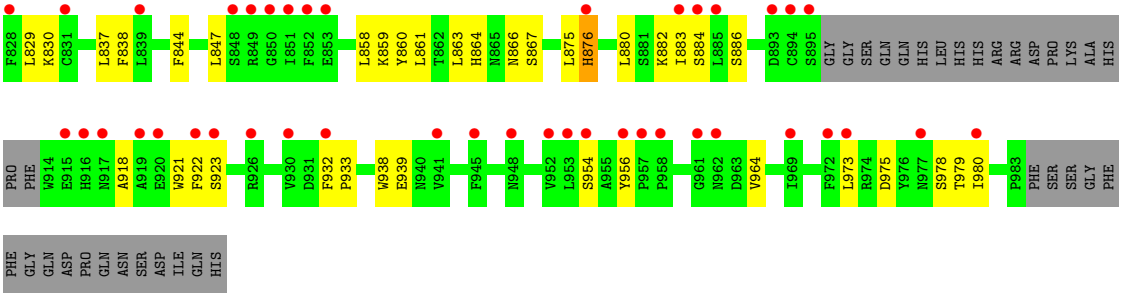
Chain B:



• Molecule 1: TIR domain-containing protein

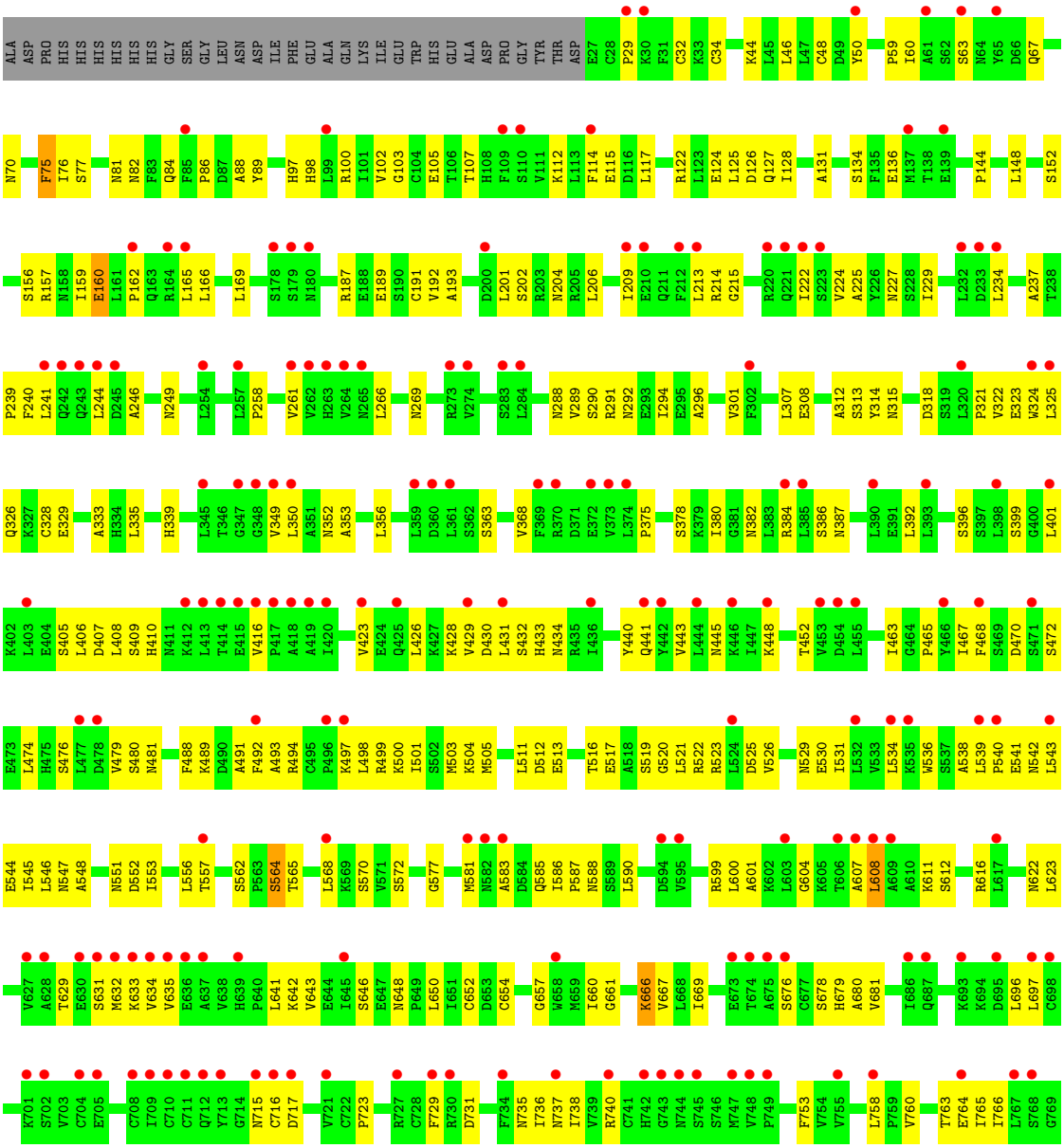
Chain C:

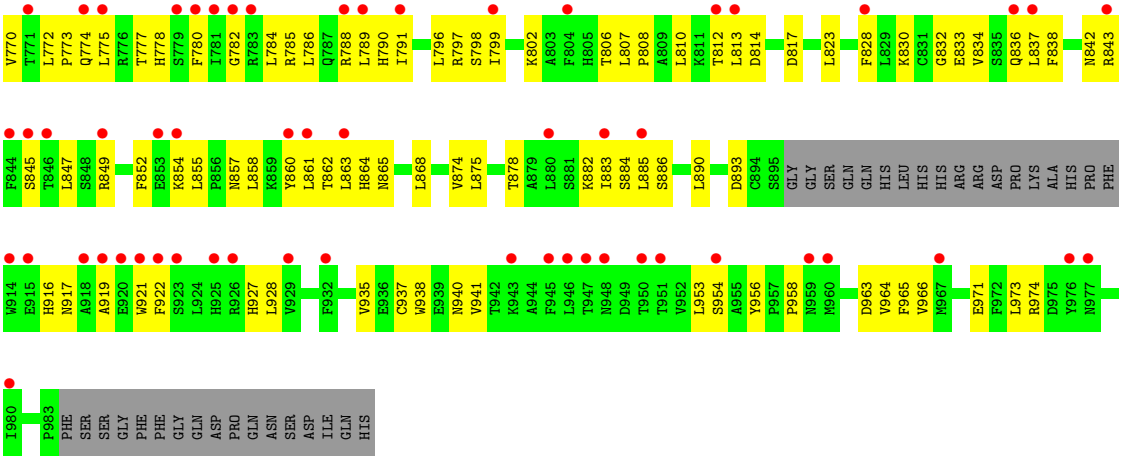




• Molecule 1: TIR domain-containing protein

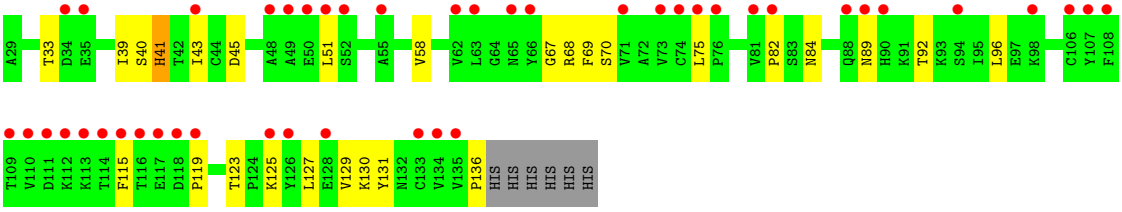
Chain D:





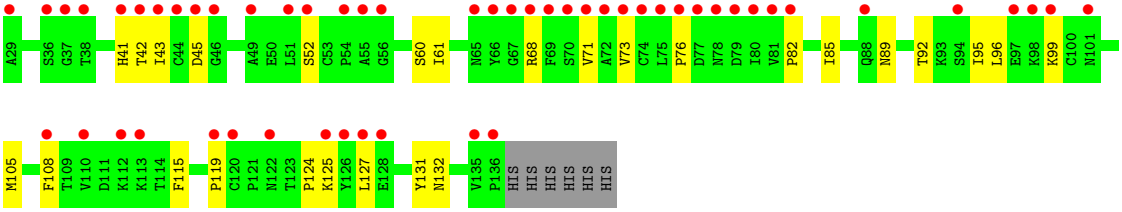
• Molecule 2: Latrophilin-like protein 1

Chain E:



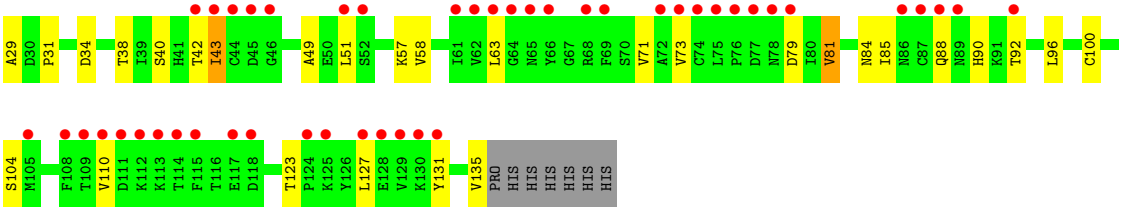
• Molecule 2: Latrophilin-like protein 1

Chain F:



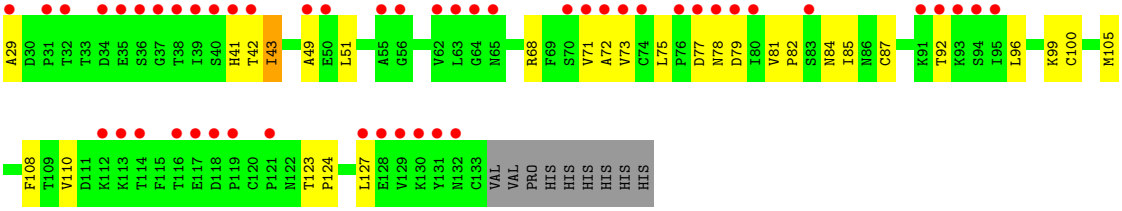
• Molecule 2: Latrophilin-like protein 1

Chain G:



• Molecule 2: Latrophilin-like protein 1

Chain H:

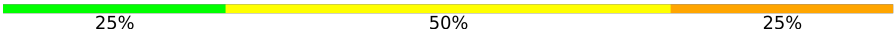


• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 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 M:

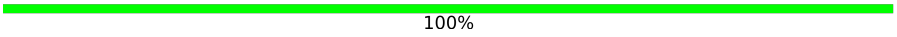


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

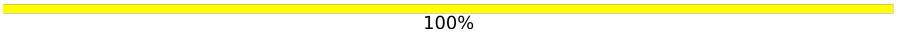
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain N:

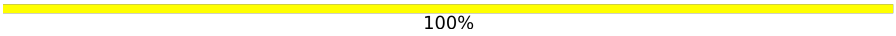


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain R:

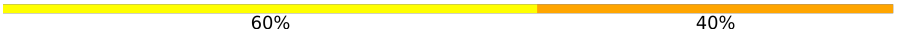


• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

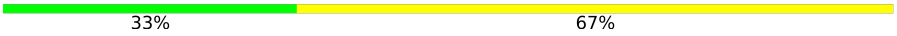
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.15Å 316.75Å 172.44Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	74.15 – 4.00 172.44 – 4.00	Depositor EDS
% Data completeness (in resolution range)	55.5 (74.15-4.00) 55.6 (172.44-4.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 4.02Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.288 , 0.338 0.293 , 0.345	Depositor DCC
R_{free} test set	1861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	139.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 381.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	32993	wwPDB-VP
Average B, all atoms (Å^2)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: BMA, MAN, 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	0.35	0/7436	0.66	0/10087
1	B	0.36	0/7405	0.67	0/10042
1	C	0.36	0/7436	0.68	0/10087
1	D	0.36	0/7436	0.66	1/10087 (0.0%)
2	E	0.29	0/831	0.54	0/1131
2	F	0.26	0/831	0.51	0/1131
2	G	0.29	0/823	0.58	0/1119
2	H	0.28	0/809	0.58	0/1099
All	All	0.35	0/33007	0.66	1/44783 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	160	GLU	C-N-CA	6.22	137.24	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7315	0	7381	262	0
1	B	7286	0	7348	253	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7315	0	7383	217	1
1	D	7315	0	7385	283	0
2	E	815	0	786	18	0
2	F	815	0	786	15	0
2	G	808	0	779	22	0
2	H	794	0	761	32	0
3	I	50	0	43	2	0
3	M	50	0	43	5	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	2	0
4	R	28	0	25	0	0
5	L	50	0	43	0	0
6	P	61	0	52	5	0
7	Q	39	0	34	0	0
8	A	42	0	39	3	0
8	B	42	0	39	2	0
8	C	28	0	26	1	0
8	D	28	0	26	2	0
All	All	32993	0	33079	1072	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1072) 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:407:ASP:HA	1:D:430:ASP:HB3	1.48	0.94
1:D:410:HIS:H	1:D:433:HIS:HB2	1.31	0.94
1:C:581:MET:HG3	1:C:600:LEU:HD21	1.50	0.91
1:A:86:PRO:HG2	1:A:89:TYR:HB2	1.53	0.90
1:A:799:ILE:HD12	1:A:823:LEU:HD21	1.51	0.89
1:B:758:LEU:HB2	1:B:783:ARG:HH21	1.38	0.87
1:D:632:MET:HE1	1:D:643:VAL:HG21	1.58	0.86
1:B:86:PRO:HG2	1:B:89:TYR:HB2	1.58	0.85
1:B:44:LYS:HG3	1:B:67:GLN:HG3	1.59	0.85
1:D:75:PHE:HE1	1:D:77:SER:HB2	1.42	0.85
1:B:267:ALA:HB1	3:M:1:NAG:H62	1.60	0.84
1:A:581:MET:HG3	1:A:600:LEU:HD21	1.59	0.83
1:A:187:ARG:NH2	1:A:214:ARG:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HB3	1:A:571:VAL:HG22	1.61	0.82
1:D:971:GLU:HG3	1:D:974:ARG:HH22	1.43	0.82
1:C:487:LEU:HB3	1:C:514:GLY:HA3	1.61	0.81
1:D:717:ASP:H	2:H:72:ALA:HB1	1.42	0.81
1:D:102:VAL:HA	1:D:126:ASP:HB3	1.59	0.81
1:C:536:TRP:O	1:C:564:SER:OG	1.99	0.80
1:C:51:SER:HA	1:C:78:CYS:HA	1.62	0.80
1:A:836:GLN:HG2	1:A:860:TYR:HB3	1.62	0.80
1:A:488:PHE:HZ	1:B:111:VAL:HG12	1.46	0.80
1:D:541:GLU:HA	1:D:564:SER:HB3	1.62	0.80
1:A:368:VAL:HG22	1:A:392:LEU:HB3	1.63	0.80
1:A:187:ARG:NH1	1:A:191:CYS:O	2.14	0.79
1:D:86:PRO:HG2	1:D:89:TYR:HB2	1.65	0.79
1:A:893:ASP:O	1:A:917:ASN:ND2	2.16	0.78
1:B:393:LEU:HB2	1:B:417:PRO:HG2	1.65	0.78
1:C:492:PHE:HB3	1:C:518:ALA:HB2	1.64	0.78
1:C:684:HIS:HB3	6:P:4:MAN:H4	1.66	0.78
1:D:522:ARG:O	1:D:545:ILE:N	2.18	0.77
1:B:679:HIS:HB3	1:B:683:GLY:H	1.48	0.77
1:A:35:ALA:O	1:A:45:LEU:N	2.17	0.77
1:D:498:LEU:O	1:D:521:LEU:HA	1.84	0.76
1:A:533:VAL:HG13	1:A:555:LEU:HB3	1.66	0.76
1:D:523:ARG:HG2	1:D:545:ILE:HB	1.66	0.76
1:B:535:LYS:HG2	1:B:557:THR:HG21	1.67	0.75
1:C:675:ALA:HB1	1:C:688:ILE:HD12	1.67	0.75
1:A:176:ASN:HA	1:A:200:ASP:HB3	1.68	0.75
1:C:187:ARG:NH2	1:C:214:ARG:O	2.19	0.75
1:C:201:LEU:O	1:C:204:ASN:ND2	2.19	0.75
1:A:330:LYS:O	1:A:355:ASN:ND2	2.19	0.75
1:B:788:ARG:HG2	1:B:812:THR:HB	1.69	0.74
1:B:57:ILE:HD13	1:B:86:PRO:HD3	1.68	0.74
1:B:940:ASN:HB3	1:B:943:LYS:HB3	1.68	0.74
1:D:488:PHE:HB2	1:D:491:ALA:HB2	1.67	0.74
1:C:609:ALA:HA	1:C:633:LYS:O	1.88	0.74
1:A:523:ARG:HG2	1:A:545:ILE:HB	1.69	0.74
1:B:353:ALA:HB1	1:B:356:LEU:HB2	1.68	0.74
1:D:633:LYS:HE2	1:D:635:VAL:HG22	1.68	0.74
1:D:213:LEU:HD13	1:D:234:LEU:HD21	1.69	0.73
1:D:565:THR:HA	1:D:568:LEU:HD12	1.70	0.73
1:D:428:LYS:HA	1:D:452:THR:O	1.87	0.73
1:D:29:PRO:HB3	1:D:63:SER:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:PRO:HG2	1:C:89:TYR:HB2	1.71	0.73
1:C:763:THR:HG22	1:C:785:ARG:HB3	1.71	0.73
1:D:201:LEU:O	1:D:204:ASN:ND2	2.22	0.72
2:H:96:LEU:O	2:H:100:CYS:N	2.23	0.72
1:B:452:THR:HG23	1:B:476:SER:HB3	1.72	0.72
1:B:893:ASP:H	1:B:917:ASN:HD21	1.35	0.72
1:D:775:LEU:HG	1:D:796:LEU:HD11	1.71	0.72
1:B:581:MET:HG3	1:B:600:LEU:HD21	1.72	0.72
1:B:273:ARG:HH12	8:B:1101:NAG:H82	1.54	0.72
1:B:384:ARG:HA	1:B:407:ASP:HB3	1.72	0.72
1:D:717:ASP:HA	1:D:760:VAL:HG21	1.71	0.72
1:B:891:ARG:NH1	1:B:949:ASP:OD2	2.21	0.71
1:D:479:VAL:HG23	1:D:503:MET:HG2	1.71	0.71
2:H:42:THR:HG21	2:H:73:VAL:HG11	1.73	0.71
1:C:723:PRO:HG2	1:C:758:LEU:HD23	1.73	0.71
1:D:225:ALA:O	1:D:227:ASN:ND2	2.23	0.71
1:B:333:ALA:HA	1:B:356:LEU:HA	1.72	0.71
1:A:166:LEU:HD11	1:A:212:PHE:HE1	1.56	0.70
1:B:176:ASN:HA	1:B:200:ASP:HB2	1.72	0.70
2:H:43:ILE:HB	2:H:110:VAL:HG21	1.73	0.70
1:B:758:LEU:HD13	1:B:765:ILE:HD13	1.73	0.70
1:A:700:TYR:CE2	1:A:728:CYS:HB3	2.27	0.69
1:B:222:ILE:HD12	1:B:241:LEU:HD13	1.72	0.69
1:B:688:ILE:HA	1:B:691:LEU:HB2	1.73	0.69
1:C:301:VAL:HA	1:C:323:GLU:HB3	1.73	0.69
1:A:326:GLN:OE1	1:C:449:GLN:NE2	2.25	0.68
1:A:586:ILE:HD12	1:A:607:ALA:HB1	1.75	0.68
1:B:32:CYS:HA	1:B:48:CYS:HA	1.75	0.68
1:A:565:THR:HA	1:A:568:LEU:HD12	1.75	0.68
1:B:33:LYS:HB2	1:B:47:LEU:HB2	1.76	0.68
1:A:845:SER:HA	1:A:868:LEU:HA	1.75	0.67
1:A:784:LEU:HA	1:A:808:PRO:HD2	1.76	0.67
1:C:830:LYS:NZ	2:G:79:ASP:O	2.22	0.67
1:A:67:GLN:HB3	1:A:70:ASN:HB2	1.77	0.67
1:A:465:PRO:HD2	1:B:143:MET:HB3	1.75	0.67
1:D:511:LEU:HD11	1:D:526:VAL:HG11	1.77	0.67
1:D:919:ALA:HB1	1:D:973:LEU:HD21	1.75	0.67
1:C:426:LEU:HB3	1:C:447:ILE:HG21	1.76	0.67
1:C:456:SER:O	1:C:458:ASN:ND2	2.29	0.66
2:F:61:ILE:HD13	2:F:131:TYR:HB3	1.76	0.66
1:D:717:ASP:N	2:H:72:ALA:HB1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:O	1:A:255:THR:OG1	2.12	0.66
1:A:266:LEU:HB2	1:A:289:VAL:HG12	1.77	0.66
2:E:92:THR:HG23	2:E:115:PHE:CE1	2.31	0.66
1:B:124:GLU:HG2	1:B:152:SER:HB3	1.77	0.66
1:B:331:ARG:HA	1:B:355:ASN:HD22	1.61	0.66
1:C:617:LEU:HB3	1:C:643:VAL:HG22	1.76	0.66
1:A:416:VAL:HB	1:A:443:VAL:HG11	1.78	0.66
1:C:502:SER:HA	1:C:525:ASP:HB3	1.78	0.66
1:D:512:ASP:HA	1:D:538:ALA:HB1	1.78	0.66
1:D:772:LEU:HD21	1:D:775:LEU:HD21	1.78	0.66
1:D:122:ARG:NH2	1:D:124:GLU:OE2	2.29	0.65
1:B:775:LEU:HG	1:B:796:LEU:HD11	1.79	0.65
1:D:832:GLY:O	1:D:857:ASN:ND2	2.29	0.65
1:A:770:VAL:O	1:A:794:THR:HA	1.97	0.65
1:A:243:GLN:HG3	1:A:263:HIS:HB2	1.80	0.64
2:F:60:SER:HB3	2:F:132:ASN:HB2	1.78	0.64
1:D:237:ALA:O	1:D:239:PRO:HD3	1.98	0.64
1:D:836:GLN:HG2	1:D:860:TYR:HB3	1.79	0.64
1:A:452:THR:HG23	1:A:476:SER:HB3	1.80	0.64
1:A:308:GLU:HG3	1:A:331:ARG:O	1.96	0.64
1:D:322:VAL:HG13	1:D:349:VAL:HG13	1.79	0.64
1:D:581:MET:HG3	1:D:600:LEU:HD21	1.80	0.64
1:D:806:THR:HG21	2:H:78:ASN:HA	1.78	0.64
1:C:452:THR:HG23	1:C:476:SER:HB3	1.79	0.64
1:D:290:SER:O	1:D:292:ASN:ND2	2.30	0.63
1:D:307:LEU:HB3	1:D:328:CYS:SG	2.38	0.63
1:D:353:ALA:HB1	1:D:356:LEU:HB2	1.80	0.63
1:A:486:LEU:HB2	1:B:112:LYS:HE3	1.80	0.63
1:C:96:LEU:HD21	1:C:99:LEU:HD13	1.80	0.63
1:C:274:VAL:HB	1:C:300:SER:HB2	1.81	0.63
1:A:839:LEU:HB2	1:A:863:LEU:HD23	1.80	0.63
1:D:814:ASP:HA	1:D:838:PHE:HB2	1.78	0.63
1:D:409:SER:HA	1:D:432:SER:O	1.99	0.63
1:D:520:GLY:HA2	1:D:542:ASN:HD22	1.63	0.63
1:D:788:ARG:HG2	1:D:812:THR:HB	1.80	0.63
1:A:299:SER:HB3	1:A:321:PRO:HB3	1.81	0.63
1:C:360:ASP:OD2	1:C:384:ARG:NH1	2.32	0.63
1:C:837:LEU:HB2	1:C:858:LEU:HD11	1.81	0.63
1:D:864:HIS:HB3	1:D:886:SER:H	1.63	0.63
1:A:430:ASP:HA	1:A:454:ASP:HB3	1.81	0.63
1:B:247:GLU:OE2	3:M:1:NAG:O6	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD21	1:A:310:LEU:HD13	1.80	0.62
1:C:46:LEU:HD23	1:C:74:LEU:HD13	1.81	0.62
1:A:679:HIS:HB3	1:A:683:GLY:H	1.64	0.62
1:D:187:ARG:NH2	1:D:214:ARG:O	2.32	0.62
1:A:632:MET:HE3	1:A:643:VAL:HG21	1.80	0.62
1:B:440:TYR:HB2	1:B:443:VAL:HG23	1.81	0.62
1:D:806:THR:HG22	1:D:830:LYS:HD2	1.79	0.62
1:C:307:LEU:HB3	1:C:328:CYS:SG	2.38	0.62
1:D:465:PRO:HA	1:D:491:ALA:HA	1.81	0.62
1:D:493:ALA:HB2	1:D:517:GLU:OE1	2.00	0.62
1:B:811:LYS:HA	1:B:834:VAL:HA	1.80	0.62
1:D:60:ILE:HA	1:D:63:SER:HB3	1.82	0.62
1:D:187:ARG:NH1	1:D:191:CYS:O	2.33	0.62
1:A:401:LEU:HB2	1:A:423:VAL:HG22	1.81	0.61
1:A:931:ASP:HB2	1:A:934:LYS:HB2	1.82	0.61
1:C:524:LEU:HB2	1:C:543:LEU:HD11	1.81	0.61
1:D:753:PHE:HB2	1:D:770:VAL:HB	1.82	0.61
1:A:600:LEU:HB2	1:A:622:ASN:OD1	2.00	0.61
1:B:45:LEU:HA	1:B:73:SER:O	2.00	0.61
1:B:502:SER:HA	1:B:525:ASP:HB3	1.82	0.61
1:C:210:GLU:O	1:C:214:ARG:HB2	2.00	0.61
1:C:266:LEU:HB2	1:C:289:VAL:HG12	1.82	0.61
1:A:336:HIS:HA	1:A:360:ASP:HB3	1.82	0.61
1:A:657:GLY:O	1:A:660:ILE:HG12	2.00	0.61
1:C:605:LYS:O	1:C:630:GLU:HB3	1.99	0.61
1:D:408:LEU:O	1:D:434:ASN:ND2	2.31	0.61
1:D:543:LEU:HD21	1:D:546:LEU:HD13	1.82	0.61
1:D:536:TRP:HD1	1:D:557:THR:H	1.48	0.61
1:D:717:ASP:H	2:H:72:ALA:CB	2.12	0.61
1:D:777:THR:HG23	1:D:802:LYS:HB2	1.83	0.61
1:D:883:ILE:HG22	1:D:928:LEU:HB3	1.82	0.61
1:B:403:LEU:HD12	1:B:423:VAL:HG21	1.82	0.61
1:D:562:SER:OG	1:D:564:SER:OG	2.18	0.61
1:B:523:ARG:HG2	1:B:545:ILE:HB	1.82	0.61
1:C:258:PRO:C	1:C:260:THR:H	2.04	0.61
1:A:540:PRO:O	1:A:564:SER:HB2	2.00	0.61
1:A:923:SER:HB3	1:A:973:LEU:HD22	1.83	0.61
1:C:799:ILE:HD12	1:C:823:LEU:HD21	1.83	0.61
1:D:201:LEU:HD12	1:D:224:VAL:HG12	1.83	0.61
1:D:737:ASN:HB3	1:D:763:THR:HG23	1.81	0.61
1:C:176:ASN:HA	1:C:200:ASP:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:HB2	1:A:317:LEU:HD22	1.83	0.60
1:D:125:LEU:N	1:D:152:SER:O	2.33	0.60
1:A:142:LEU:HB3	1:A:169:LEU:HD21	1.84	0.60
1:D:410:HIS:N	1:D:433:HIS:HB2	2.08	0.60
1:A:581:MET:O	1:A:604:GLY:N	2.29	0.60
1:B:479:VAL:HG23	1:B:503:MET:HG2	1.84	0.60
1:D:519:SER:O	1:D:542:ASN:ND2	2.34	0.60
1:D:519:SER:HB2	1:D:541:GLU:HB2	1.83	0.60
1:B:43:SER:OG	1:B:44:LYS:N	2.34	0.60
1:B:784:LEU:HA	1:B:808:PRO:HD2	1.83	0.60
1:D:780:PHE:HB3	1:D:807:LEU:HD21	1.84	0.60
1:B:780:PHE:HA	1:B:783:ARG:NH1	2.17	0.59
1:B:451:HIS:CE1	1:B:473:GLU:HB3	2.37	0.59
1:B:546:LEU:HB3	1:B:571:VAL:HG22	1.84	0.59
1:C:792:ASN:HB3	6:P:1:NAG:O5	2.02	0.59
2:G:96:LEU:O	2:G:100:CYS:N	2.33	0.59
1:C:809:ALA:O	1:C:811:LYS:HG3	2.03	0.59
2:H:68:ARG:NE	2:H:124:PRO:O	2.23	0.59
1:D:301:VAL:HG22	1:D:323:GLU:HB3	1.84	0.59
1:A:654:CYS:HA	1:A:696:LEU:HB3	1.83	0.59
1:B:429:VAL:HG11	1:B:450:LEU:HD21	1.85	0.59
1:C:679:HIS:HB3	1:C:683:GLY:H	1.68	0.59
1:A:36:PRO:HG3	1:A:44:LYS:NZ	2.18	0.59
1:B:715:ASN:N	1:B:715:ASN:OD1	2.36	0.59
1:A:863:LEU:HB2	1:A:885:LEU:HD23	1.85	0.59
1:D:740:ARG:HG3	1:D:766:ILE:HG13	1.85	0.59
1:C:245:ASP:OD1	1:C:265:ASN:ND2	2.36	0.58
1:B:681:VAL:HG22	1:B:729:PHE:HE2	1.67	0.58
1:A:780:PHE:HA	1:A:783:ARG:NH1	2.18	0.58
1:D:834:VAL:HB	1:D:855:LEU:HD22	1.85	0.58
1:B:681:VAL:HG22	1:B:729:PHE:CE2	2.39	0.58
2:G:29:ALA:N	2:G:42:THR:O	2.36	0.58
2:G:42:THR:HG21	2:G:73:VAL:HG11	1.86	0.58
1:A:44:LYS:O	1:A:71:ILE:HA	2.04	0.57
1:A:48:CYS:HB2	1:A:76:ILE:HG12	1.84	0.57
1:A:274:VAL:HG11	1:A:302:PHE:HE1	1.67	0.57
1:C:432:SER:HA	1:C:458:ASN:HD21	1.68	0.57
1:A:862:THR:HB	1:A:864:HIS:CE1	2.39	0.57
1:B:700:TYR:CZ	1:B:728:CYS:HB3	2.38	0.57
1:C:156:SER:HB2	1:C:159:ILE:HD11	1.85	0.57
1:B:131:ALA:HB2	1:B:157:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:SER:HA	1:D:500:LYS:HB3	1.85	0.57
1:D:763:THR:HA	1:D:786:LEU:HA	1.85	0.57
1:C:802:LYS:NZ	2:G:79:ASP:OD2	2.23	0.57
1:A:45:LEU:HD21	1:A:47:LEU:HD21	1.86	0.57
1:B:267:ALA:CB	3:M:1:NAG:H62	2.33	0.57
1:A:331:ARG:HA	1:A:355:ASN:HD22	1.70	0.57
1:D:499:ARG:O	1:D:523:ARG:N	2.38	0.57
1:D:657:GLY:O	1:D:660:ILE:HG12	2.05	0.57
1:D:860:TYR:HD1	1:D:882:LYS:HB2	1.68	0.57
1:B:355:ASN:HA	1:B:379:LYS:HD2	1.85	0.57
1:D:246:ALA:O	1:D:249:ASN:ND2	2.37	0.57
1:D:854:LYS:O	1:D:855:LEU:HD23	2.04	0.57
1:A:375:PRO:HG2	1:A:378:SER:HB2	1.86	0.57
1:A:302:PHE:HB2	1:A:324:TRP:O	2.05	0.57
1:A:634:VAL:H	1:A:665:PRO:HG3	1.69	0.57
1:A:788:ARG:HG2	1:A:812:THR:HB	1.87	0.57
1:C:876:HIS:ND1	1:C:921:TRP:HD1	2.03	0.57
1:D:288:ASN:OD1	1:D:290:SER:OG	2.11	0.56
1:A:489:LYS:HB2	1:A:513:GLU:HB3	1.86	0.56
1:C:740:ARG:HG2	1:C:742:HIS:CE1	2.39	0.56
1:B:34:CYS:HA	1:B:46:LEU:HD12	1.86	0.56
1:C:786:LEU:HD23	1:C:810:LEU:HD13	1.87	0.56
1:D:650:LEU:HD12	1:D:676:SER:O	2.05	0.56
1:D:953:LEU:HD22	1:D:965:PHE:HE2	1.71	0.56
1:B:71:ILE:HG22	1:B:96:LEU:HD13	1.88	0.56
1:C:544:GLU:HA	1:C:568:LEU:HA	1.87	0.56
1:D:440:TYR:HB2	1:D:443:VAL:HG23	1.87	0.56
1:D:543:LEU:O	1:D:568:LEU:HD23	2.06	0.56
1:A:210:GLU:O	1:A:214:ARG:HB2	2.06	0.56
1:B:110:SER:HB3	1:B:113:LEU:HB2	1.88	0.56
1:B:448:LYS:O	1:B:473:GLU:HB2	2.05	0.56
1:C:102:VAL:HA	1:C:126:ASP:HB3	1.86	0.56
1:D:401:LEU:O	1:D:423:VAL:HG13	2.05	0.56
1:D:556:LEU:O	1:D:585:GLN:NE2	2.39	0.56
1:C:353:ALA:HB1	1:C:356:LEU:HB2	1.88	0.56
1:D:773:PRO:O	1:D:797:ARG:N	2.38	0.56
1:C:864:HIS:HB3	1:C:886:SER:H	1.71	0.56
1:A:37:ASP:OD2	1:A:72:ARG:HB2	2.07	0.55
1:D:166:LEU:HD22	1:D:193:ALA:HB2	1.87	0.55
1:A:46:LEU:HD22	1:A:71:ILE:HD13	1.88	0.55
1:B:241:LEU:HD21	1:B:244:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:LEU:HD23	1:C:540:PRO:HG3	1.88	0.55
1:A:474:LEU:HD23	1:A:498:LEU:HD22	1.87	0.55
1:C:330:LYS:O	1:C:355:ASN:ND2	2.40	0.55
1:C:802:LYS:HD3	2:G:79:ASP:OD2	2.06	0.55
1:D:239:PRO:HG2	1:D:240:PHE:CE2	2.41	0.55
1:A:700:TYR:CZ	1:A:728:CYS:HB3	2.41	0.55
1:B:46:LEU:HB3	1:B:74:LEU:HD13	1.88	0.55
1:D:266:LEU:HB3	1:D:269:ASN:HD22	1.70	0.55
1:A:75:PHE:HE1	1:A:77:SER:HB2	1.71	0.55
1:D:784:LEU:HD21	2:H:79:ASP:HB3	1.88	0.55
1:B:66:ASP:HB2	1:B:67:GLN:OE1	2.07	0.55
1:B:536:TRP:CG	1:B:559:ALA:HB2	2.42	0.55
1:C:307:LEU:HD21	1:C:310:LEU:HD13	1.89	0.55
1:D:643:VAL:O	1:D:669:ILE:HA	2.07	0.55
1:A:154:THR:HG21	8:A:1101:NAG:O5	2.07	0.55
1:A:609:ALA:HA	1:A:633:LYS:O	2.07	0.55
1:B:451:HIS:ND1	1:B:473:GLU:O	2.39	0.55
1:D:463:ILE:HD13	1:D:492:PHE:HZ	1.71	0.55
1:D:784:LEU:HA	1:D:808:PRO:HD2	1.88	0.55
1:D:156:SER:HB2	1:D:159:ILE:HD11	1.88	0.54
1:D:516:THR:HG22	1:D:538:ALA:HA	1.88	0.54
1:B:97:HIS:O	1:B:121:ARG:N	2.33	0.54
1:B:755:VAL:HG13	1:B:758:LEU:HD12	1.87	0.54
1:C:149:GLU:HA	1:C:171:HIS:O	2.08	0.54
1:A:429:VAL:HG13	1:A:453:VAL:HA	1.89	0.54
1:D:375:PRO:HG2	1:D:378:SER:HB2	1.89	0.54
1:D:544:GLU:O	1:D:570:SER:HB3	2.07	0.54
1:D:600:LEU:HB2	1:D:622:ASN:OD1	2.06	0.54
1:C:102:VAL:HG22	1:C:126:ASP:HB3	1.88	0.54
1:D:34:CYS:HA	1:D:46:LEU:HD12	1.88	0.54
1:D:97:HIS:HB3	1:D:98:HIS:CE1	2.43	0.54
1:D:531:ILE:HB	1:D:551:ASN:OD1	2.06	0.54
1:D:953:LEU:HA	1:D:956:TYR:HD2	1.73	0.54
1:A:755:VAL:HG13	1:A:758:LEU:HD12	1.88	0.54
1:B:333:ALA:O	1:B:357:GLN:N	2.38	0.54
2:F:68:ARG:NH1	2:F:82:PRO:HG2	2.23	0.54
1:B:295:GLU:HG2	1:B:316:LYS:HB2	1.89	0.54
1:B:536:TRP:CD1	1:B:559:ALA:HB2	2.43	0.54
1:C:760:VAL:O	1:C:783:ARG:HG2	2.07	0.54
1:D:521:LEU:HD23	1:D:540:PRO:HG3	1.89	0.54
1:A:125:LEU:HD13	1:A:128:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:LEU:HB2	1:A:631:SER:O	2.08	0.54
1:A:615:ARG:HH12	1:A:639:HIS:CE1	2.26	0.54
1:B:521:LEU:HD23	1:B:540:PRO:HG3	1.90	0.54
1:D:82:ASN:O	1:D:84:GLN:HG3	2.07	0.54
1:D:885:LEU:O	1:D:935:VAL:HG22	2.08	0.54
1:A:114:PHE:CD2	1:A:141:VAL:HG13	2.42	0.54
1:A:807:LEU:HB3	1:A:810:LEU:HB2	1.89	0.54
1:B:290:SER:HB2	1:B:314:TYR:HD2	1.72	0.54
1:C:939:GLU:HG3	1:C:954:SER:HB3	1.89	0.54
1:A:634:VAL:HB	1:A:637:ALA:HB2	1.89	0.53
1:A:114:PHE:HD2	1:A:141:VAL:HG13	1.74	0.53
1:B:86:PRO:HG2	1:B:89:TYR:CB	2.35	0.53
1:B:758:LEU:HB2	1:B:783:ARG:NH2	2.18	0.53
1:C:441:GLN:HA	1:C:467:ILE:HG22	1.89	0.53
1:C:684:HIS:CB	6:P:4:MAN:H4	2.37	0.53
1:A:137:MET:O	1:A:162:PRO:HD3	2.09	0.53
1:A:806:THR:HG22	1:A:830:LYS:HD2	1.90	0.53
1:D:426:LEU:HD21	1:D:429:VAL:HB	1.90	0.53
1:B:187:ARG:HD3	1:B:212:PHE:CD1	2.43	0.53
1:C:810:LEU:HD21	1:C:813:LEU:HD22	1.91	0.53
1:D:386:SER:HB3	1:D:409:SER:H	1.74	0.53
1:D:715:ASN:O	2:H:73:VAL:HG22	2.08	0.53
1:B:629:THR:HA	1:B:658:TRP:CD1	2.43	0.53
2:H:84:ASN:HB3	2:H:123:THR:HG21	1.90	0.53
1:D:296:ALA:HB1	1:D:321:PRO:HG3	1.91	0.53
1:D:312:ALA:C	1:D:315:ASN:HD22	2.11	0.53
1:D:922:PHE:CZ	1:D:935:VAL:HG11	2.44	0.53
1:A:541:GLU:O	1:A:567:ASN:ND2	2.40	0.53
1:A:849:ARG:HA	1:A:874:VAL:HG21	1.91	0.53
1:B:67:GLN:HB2	1:B:70:ASN:HB2	1.91	0.53
1:A:97:HIS:ND1	1:A:119:ALA:O	2.42	0.53
1:B:660:ILE:HD12	1:B:693:LYS:HG2	1.90	0.53
1:C:67:GLN:HB2	1:C:70:ASN:HB2	1.91	0.53
1:C:409:SER:O	1:C:411:ASN:ND2	2.42	0.53
1:D:849:ARG:HA	1:D:874:VAL:HG21	1.91	0.53
1:A:717:ASP:HA	1:A:760:VAL:HG21	1.90	0.52
1:C:806:THR:HG21	2:G:81:VAL:HG21	1.91	0.52
1:D:480:SER:HB2	1:D:504:LYS:HG2	1.91	0.52
1:A:580:ILE:HD11	1:A:602:LYS:HD3	1.92	0.52
1:C:125:LEU:HB2	1:C:153:LEU:HD13	1.92	0.52
1:D:291:ARG:HA	1:D:314:TYR:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:ASN:HA	1:D:505:MET:O	2.09	0.52
2:G:43:ILE:HB	2:G:110:VAL:HG21	1.90	0.52
1:B:187:ARG:HD3	1:B:212:PHE:HD1	1.74	0.52
1:A:395:PRO:O	1:A:422:LYS:HE3	2.09	0.52
1:B:920:GLU:O	1:B:924:LEU:HG	2.09	0.52
1:C:399:SER:OG	1:C:422:LYS:HG3	2.10	0.52
1:D:852:PHE:CD2	1:D:878:THR:HG21	2.44	0.52
1:A:597:ASN:N	1:A:620:LYS:O	2.30	0.52
1:B:225:ALA:HA	1:B:247:GLU:O	2.09	0.52
1:C:451:HIS:CE1	1:C:473:GLU:HB3	2.45	0.52
1:A:274:VAL:HG11	1:A:302:PHE:CE1	2.45	0.52
1:B:787:GLN:HG2	1:B:809:ALA:HB1	1.92	0.52
1:C:698:CYS:N	1:C:730:ARG:O	2.40	0.52
1:D:416:VAL:HG13	1:D:431:LEU:HD11	1.92	0.52
1:B:977:ASN:HD22	8:B:1103:NAG:H83	1.73	0.52
1:C:301:VAL:HG22	1:C:323:GLU:HG2	1.92	0.52
1:C:346:THR:O	1:C:349:VAL:HG23	2.10	0.52
2:E:40:SER:HA	2:E:130:LYS:HA	1.92	0.52
1:A:497:LYS:O	1:A:499:ARG:HG3	2.10	0.52
1:A:938:TRP:CD2	1:A:964:VAL:HG11	2.45	0.52
1:D:32:CYS:HA	1:D:48:CYS:HA	1.90	0.52
1:D:333:ALA:HA	1:D:356:LEU:HA	1.91	0.52
1:D:731:ASP:CG	1:D:736:ILE:H	2.12	0.52
2:F:52:SER:HB3	2:F:105:MET:HE3	1.91	0.52
1:A:457:ASN:OD1	1:A:481:ASN:ND2	2.31	0.52
1:C:814:ASP:HA	1:C:838:PHE:HB2	1.91	0.52
1:D:448:LYS:HG2	1:D:470:ASP:O	2.10	0.52
1:D:604:GLY:O	1:D:631:SER:OG	2.17	0.52
1:A:36:PRO:HG3	1:A:44:LYS:HZ3	1.75	0.51
1:A:192:VAL:HG12	1:A:194:GLN:HG3	1.91	0.51
1:B:679:HIS:HB3	1:B:683:GLY:N	2.22	0.51
1:A:775:LEU:HG	1:A:796:LEU:HD11	1.92	0.51
1:B:741:CYS:O	1:B:742:HIS:ND1	2.43	0.51
1:D:335:LEU:HD23	1:D:350:LEU:HD11	1.91	0.51
1:A:67:GLN:O	1:A:71:ILE:HG13	2.11	0.51
1:A:164:ARG:HA	1:A:191:CYS:SG	2.51	0.51
1:A:488:PHE:HD1	1:B:115:GLU:HG3	1.75	0.51
1:D:75:PHE:CD2	1:D:100:ARG:HD3	2.45	0.51
1:B:46:LEU:HB3	1:B:74:LEU:CD1	2.41	0.51
1:B:339:HIS:H	1:B:363:SER:HB2	1.74	0.51
1:B:356:LEU:HD23	1:B:380:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:THR:HG21	2:G:81:VAL:CG2	2.41	0.51
1:A:488:PHE:CZ	1:B:111:VAL:HG12	2.37	0.51
1:B:257:LEU:HD22	1:B:261:VAL:HG21	1.92	0.51
1:C:258:PRO:O	1:C:260:THR:N	2.41	0.51
1:D:59:PRO:HB3	1:D:88:ALA:O	2.10	0.51
1:A:258:PRO:O	1:A:261:VAL:HG23	2.11	0.51
1:A:486:LEU:HD11	1:A:488:PHE:CE2	2.46	0.51
1:B:96:LEU:HD23	1:B:117:LEU:HD22	1.93	0.51
1:D:289:VAL:HB	1:D:294:ILE:HD11	1.92	0.51
2:G:88:GLN:OE1	2:G:90:HIS:NE2	2.44	0.51
1:A:573:LEU:N	1:A:594:ASP:O	2.39	0.51
1:A:768:SER:HB2	8:A:1103:NAG:HN2	1.76	0.51
1:C:46:LEU:HD22	1:C:71:ILE:HD13	1.93	0.51
1:C:802:LYS:HE2	1:C:829:LEU:HD22	1.91	0.51
1:A:35:ALA:N	1:A:45:LEU:O	2.43	0.51
1:A:664:LYS:HA	1:A:665:PRO:C	2.29	0.51
1:D:661:GLY:HA2	1:D:666:LYS:HE3	1.92	0.51
1:A:176:ASN:HD22	8:A:1101:NAG:H83	1.76	0.51
1:B:185:LEU:HD23	1:B:209:ILE:HG22	1.92	0.51
1:B:445:ASN:ND2	1:B:466:TYR:O	2.43	0.51
1:B:511:LEU:HD11	1:B:526:VAL:HG11	1.93	0.51
1:C:717:ASP:HA	1:C:760:VAL:HG21	1.91	0.51
1:D:112:LYS:HG2	1:D:115:GLU:OE1	2.10	0.51
1:D:131:ALA:HB2	1:D:157:ARG:HH11	1.76	0.51
1:D:817:ASP:OD1	8:D:1102:NAG:H5	2.11	0.51
4:O:1:NAG:H61	4:O:2:NAG:HN2	1.75	0.51
1:B:307:LEU:HB3	1:B:328:CYS:SG	2.51	0.50
1:B:357:GLN:HA	1:B:379:LYS:O	2.11	0.50
1:C:761:SER:O	1:C:785:ARG:HD2	2.11	0.50
1:D:148:LEU:HD23	1:D:169:LEU:HD13	1.92	0.50
1:D:474:LEU:HB3	1:D:498:LEU:HD13	1.94	0.50
1:A:98:HIS:ND1	1:A:122:ARG:HB3	2.25	0.50
1:A:641:LEU:HB3	1:A:667:VAL:HG22	1.93	0.50
1:B:296:ALA:HB1	1:B:321:PRO:HG3	1.92	0.50
1:A:617:LEU:HB3	1:A:643:VAL:HG22	1.92	0.50
1:A:883:ILE:O	1:A:929:VAL:HA	2.11	0.50
1:B:101:ILE:O	1:B:126:ASP:N	2.45	0.50
1:C:245:ASP:HA	1:C:265:ASN:HB3	1.93	0.50
1:D:862:THR:HA	1:D:884:SER:HB3	1.94	0.50
1:A:65:TYR:HB3	1:A:68:VAL:HG13	1.93	0.50
1:A:303:SER:O	1:C:448:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:O	1:A:423:VAL:HG13	2.12	0.50
1:B:600:LEU:HB2	1:B:622:ASN:OD1	2.11	0.50
1:B:807:LEU:HB3	1:B:810:LEU:HB2	1.93	0.50
1:C:57:ILE:HG22	1:C:89:TYR:CE1	2.47	0.50
1:C:511:LEU:HD21	1:C:526:VAL:HG11	1.92	0.50
1:C:594:ASP:HA	1:C:618:ASN:HB3	1.93	0.50
1:D:806:THR:HG21	2:H:78:ASN:C	2.31	0.50
1:A:378:SER:HB3	1:A:380:ILE:HG13	1.93	0.50
1:B:31:PHE:CE1	1:B:53:LYS:HG2	2.46	0.50
1:B:210:GLU:O	1:B:214:ARG:HB2	2.12	0.50
1:B:309:MET:CE	3:M:1:NAG:H83	2.42	0.50
2:E:41:HIS:N	2:E:129:VAL:O	2.42	0.50
1:A:937:CYS:HB3	1:A:953:LEU:HD11	1.93	0.50
1:B:861:LEU:O	1:B:883:ILE:HA	2.12	0.50
1:C:152:SER:OG	1:C:176:ASN:HB3	2.12	0.50
1:D:808:PRO:O	1:D:833:GLU:HG3	2.12	0.50
1:A:742:HIS:ND1	1:A:768:SER:O	2.44	0.50
1:B:427:LYS:O	1:B:451:HIS:HB2	2.12	0.50
1:D:222:ILE:HD12	1:D:241:LEU:HD13	1.93	0.50
1:C:387:ASN:ND2	4:O:1:NAG:O7	2.45	0.50
1:C:428:LYS:HG3	1:C:452:THR:HB	1.94	0.50
1:C:508:ILE:HB	1:C:529:ASN:OD1	2.12	0.50
1:C:565:THR:HA	1:C:568:LEU:HD12	1.92	0.50
2:E:68:ARG:NH1	2:E:82:PRO:HG2	2.27	0.50
1:B:350:LEU:O	1:B:375:PRO:HD3	2.12	0.50
1:C:114:PHE:HD1	1:C:117:LEU:HD12	1.77	0.50
1:C:413:LEU:HD12	1:C:431:LEU:HD22	1.93	0.50
1:C:822:SER:HA	1:C:844:PHE:CE1	2.47	0.50
1:D:103:GLY:HA2	1:D:127:GLN:HB2	1.92	0.50
1:A:46:LEU:HB3	1:A:74:LEU:HD13	1.94	0.49
1:B:305:PRO:HA	1:B:328:CYS:HB3	1.94	0.49
1:A:329:GLU:O	1:A:353:ALA:HA	2.12	0.49
1:A:362:SER:HB3	1:A:386:SER:H	1.77	0.49
1:A:641:LEU:HD23	1:A:667:VAL:HG22	1.94	0.49
1:B:629:THR:HA	1:B:658:TRP:HD1	1.77	0.49
1:D:500:LYS:HA	1:D:523:ARG:HB2	1.94	0.49
1:A:114:PHE:O	1:A:144:PRO:HB2	2.11	0.49
1:A:691:LEU:HD21	1:A:696:LEU:HD21	1.94	0.49
1:C:291:ARG:H	1:C:314:TYR:HB2	1.77	0.49
1:C:864:HIS:CG	1:C:884:SER:HG	2.28	0.49
1:D:114:PHE:HD1	1:D:117:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ILE:HG13	1:D:468:PHE:CD1	2.47	0.49
1:D:654:CYS:HA	1:D:696:LEU:HB3	1.94	0.49
1:A:463:ILE:HG23	1:A:467:ILE:HD11	1.94	0.49
1:B:885:LEU:O	1:B:935:VAL:HG22	2.12	0.49
1:C:221:GLN:HG3	1:C:243:GLN:HB3	1.95	0.49
1:C:698:CYS:O	1:C:730:ARG:N	2.42	0.49
1:D:479:VAL:CG2	1:D:503:MET:HG2	2.42	0.49
1:D:806:THR:HG21	2:H:78:ASN:CA	2.40	0.49
1:B:591:GLU:HA	1:B:614:LEU:HA	1.94	0.49
1:B:780:PHE:CZ	1:B:791:ILE:HD11	2.46	0.49
1:A:61:ALA:HB2	1:A:91:LYS:HB3	1.93	0.49
2:F:95:ILE:HD13	2:F:115:PHE:HA	1.93	0.49
2:G:31:PRO:HA	2:G:40:SER:O	2.13	0.49
1:A:489:LYS:CB	1:A:513:GLU:HB3	2.42	0.49
1:B:462:SER:HA	1:B:484:ILE:HG23	1.94	0.49
1:B:551:ASN:HB3	1:B:553:ILE:HG13	1.95	0.49
1:C:192:VAL:HG12	1:C:194:GLN:HG3	1.94	0.49
1:D:406:LEU:O	1:D:430:ASP:N	2.42	0.49
1:B:131:ALA:HB2	1:B:157:ARG:NH1	2.27	0.49
1:B:402:LYS:HB3	1:B:425:GLN:HG3	1.95	0.49
1:B:463:ILE:HG22	1:B:491:ALA:HB1	1.94	0.49
1:C:175:LEU:HD23	1:C:199:VAL:HG13	1.95	0.49
2:H:71:VAL:HB	2:H:82:PRO:HD2	1.94	0.49
1:A:241:LEU:HB3	1:A:258:PRO:HG3	1.94	0.49
1:A:442:TYR:HB2	1:A:446:LYS:HE3	1.94	0.49
1:B:51:SER:HA	1:B:78:CYS:HA	1.94	0.49
1:C:396:SER:HA	1:C:399:SER:OG	2.13	0.49
1:C:672:SER:HB2	1:C:689:GLN:HA	1.95	0.49
1:A:77:SER:HA	1:A:102:VAL:O	2.12	0.49
1:C:399:SER:HA	1:C:422:LYS:HB2	1.95	0.49
1:C:813:LEU:HB3	1:C:837:LEU:HD12	1.94	0.49
1:D:526:VAL:O	1:D:529:ASN:ND2	2.46	0.49
2:E:84:ASN:HB3	2:E:123:THR:HG21	1.95	0.49
2:G:58:VAL:HA	2:G:104:SER:HA	1.95	0.49
6:P:3:BMA:H3	6:P:4:MAN:H2	1.60	0.49
1:A:327:LYS:HG3	1:C:448:LYS:NZ	2.28	0.48
1:A:502:SER:HA	1:A:525:ASP:HB3	1.95	0.48
1:B:246:ALA:HB3	1:B:266:LEU:HD23	1.95	0.48
1:D:206:LEU:HD13	1:D:209:ILE:HG21	1.95	0.48
1:D:258:PRO:O	1:D:261:VAL:HG23	2.13	0.48
1:B:922:PHE:CE1	1:B:929:VAL:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ASN:HA	1:C:481:ASN:HB3	1.95	0.48
1:D:784:LEU:HG	2:H:79:ASP:OD2	2.13	0.48
1:D:941:VAL:N	1:D:963:ASP:O	2.45	0.48
2:F:76:PRO:HG3	2:F:124:PRO:HG2	1.95	0.48
1:A:681:VAL:HG22	1:A:729:PHE:CE2	2.47	0.48
1:B:85:PHE:HD1	1:B:86:PRO:HD2	1.78	0.48
1:C:129:SER:OG	1:C:156:SER:HB3	2.14	0.48
1:D:679:HIS:CE1	1:D:697:LEU:HD12	2.48	0.48
1:B:280:GLU:HA	1:B:303:SER:OG	2.13	0.48
1:D:441:GLN:HA	1:D:467:ILE:HG22	1.95	0.48
1:D:489:LYS:HB2	1:D:513:GLU:HB3	1.95	0.48
1:D:616:ARG:HH21	1:D:642:LYS:HZ1	1.61	0.48
1:D:681:VAL:HG13	1:D:729:PHE:CE2	2.49	0.48
1:D:60:ILE:HD11	1:D:89:TYR:CZ	2.48	0.48
1:D:296:ALA:HB3	1:D:318:ASP:OD1	2.13	0.48
2:E:51:LEU:HD22	2:E:131:TYR:CE1	2.48	0.48
1:A:717:ASP:O	1:A:760:VAL:HB	2.13	0.48
1:B:252:VAL:HG22	1:B:270:ALA:HB3	1.95	0.48
1:B:299:SER:CB	1:B:321:PRO:HB3	2.44	0.48
1:D:863:LEU:HB2	1:D:885:LEU:HD23	1.95	0.48
2:E:58:VAL:HG13	2:E:136:PRO:HG3	1.95	0.48
2:H:92:THR:HG21	2:H:127:LEU:HD13	1.95	0.48
1:C:580:ILE:HG13	1:C:602:LYS:HB3	1.94	0.48
1:D:441:GLN:HA	1:D:467:ILE:HA	1.96	0.48
1:A:123:LEU:HB3	1:A:148:LEU:HD21	1.94	0.48
1:B:287:LEU:HD11	1:B:289:VAL:HG13	1.94	0.48
2:F:92:THR:HG23	2:F:115:PHE:CE1	2.47	0.48
1:B:425:GLN:O	1:B:427:LYS:HG3	2.14	0.48
1:C:626:VAL:HA	1:C:656:MET:HE3	1.95	0.48
1:D:234:LEU:HD13	1:D:241:LEU:HD22	1.95	0.48
1:D:241:LEU:HD21	1:D:244:LEU:HB2	1.96	0.48
1:D:463:ILE:HG21	1:D:492:PHE:CZ	2.48	0.48
1:D:806:THR:HG22	1:D:830:LYS:CD	2.42	0.48
1:A:291:ARG:HH21	3:I:2:NAG:H2	1.78	0.48
1:A:543:LEU:HD21	1:A:546:LEU:HD13	1.96	0.48
1:D:136:GLU:HG3	1:D:160:GLU:O	2.14	0.48
2:E:33:THR:OG1	2:E:39:ILE:HG12	2.14	0.48
2:E:45:ASP:HB2	2:E:125:LYS:O	2.14	0.48
1:B:390:LEU:HB2	1:B:411:ASN:OD1	2.14	0.47
1:C:975:ASP:HB3	1:C:979:THR:OG1	2.14	0.47
1:D:44:LYS:N	1:D:70:ASN:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:HIS:CD2	2:E:43:ILE:HD11	2.49	0.47
1:A:415:GLU:O	1:A:417:PRO:HD3	2.15	0.47
1:A:705:GLU:HA	1:A:734:PHE:CE2	2.49	0.47
1:B:187:ARG:NH2	1:B:189:GLU:HA	2.28	0.47
1:D:790:HIS:HA	1:D:814:ASP:HB3	1.95	0.47
1:B:187:ARG:NH1	1:B:188:GLU:O	2.47	0.47
1:B:615:ARG:HH12	1:B:639:HIS:CE1	2.33	0.47
1:B:763:THR:HA	1:B:786:LEU:HA	1.95	0.47
1:A:582:ASN:HA	1:A:604:GLY:HA3	1.95	0.47
1:B:47:LEU:HD23	1:B:75:PHE:HB3	1.96	0.47
1:C:448:LYS:O	1:C:473:GLU:HB2	2.14	0.47
1:C:932:PHE:HB3	1:C:933:PRO:HD3	1.97	0.47
1:D:50:TYR:HD2	1:D:76:ILE:HG23	1.79	0.47
1:D:239:PRO:HG2	1:D:240:PHE:CD2	2.49	0.47
1:D:717:ASP:O	1:D:760:VAL:HB	2.14	0.47
1:A:293:GLU:HG2	1:A:316:LYS:HE3	1.96	0.47
1:C:574:SER:HA	1:C:596:SER:O	2.14	0.47
1:C:786:LEU:HD21	1:C:789:LEU:HB2	1.96	0.47
1:C:860:TYR:HD1	1:C:882:LYS:HB2	1.79	0.47
1:D:350:LEU:C	1:D:352:ASN:H	2.18	0.47
2:G:43:ILE:HD13	2:G:49:ALA:CB	2.45	0.47
1:A:781:ILE:HD13	2:E:75:LEU:HD21	1.96	0.47
1:C:540:PRO:O	1:C:564:SER:HB2	2.14	0.47
1:D:100:ARG:HE	1:D:102:VAL:CG2	2.28	0.47
1:D:499:ARG:HG2	1:D:522:ARG:HG3	1.97	0.47
1:D:612:SER:HA	1:D:634:VAL:HG12	1.96	0.47
2:G:84:ASN:HB3	2:G:123:THR:HG21	1.96	0.47
1:A:706:PRO:HD3	1:A:734:PHE:CD1	2.50	0.47
1:A:835:SER:HA	1:A:858:LEU:HA	1.97	0.47
1:A:883:ILE:HG22	1:A:928:LEU:HB3	1.97	0.47
1:A:939:GLU:H	1:A:964:VAL:HG13	1.80	0.47
1:D:641:LEU:O	1:D:667:VAL:HA	2.15	0.47
1:D:782:GLY:HA3	2:H:75:LEU:HD13	1.97	0.47
2:E:96:LEU:HD11	2:E:127:LEU:HD11	1.95	0.47
2:H:99:LYS:HE2	2:H:108:PHE:HB3	1.96	0.47
1:A:162:PRO:HD2	1:A:165:LEU:HD13	1.97	0.47
1:A:439:VAL:HB	1:A:467:ILE:HD12	1.97	0.47
1:B:223:SER:HA	1:B:245:ASP:HB3	1.96	0.47
1:B:262:VAL:HB	1:B:285:VAL:HG23	1.96	0.47
1:B:301:VAL:HA	1:B:323:GLU:HB3	1.97	0.47
1:C:415:GLU:O	1:C:417:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:GLY:HA3	2:G:71:VAL:HG21	1.97	0.47
1:C:860:TYR:CD1	1:C:882:LYS:HB2	2.49	0.47
1:A:59:PRO:HB3	1:A:88:ALA:O	2.15	0.47
1:B:102:VAL:HG22	1:B:126:ASP:HB3	1.96	0.47
1:B:225:ALA:O	1:B:227:ASN:ND2	2.48	0.47
1:B:642:LYS:HA	1:B:668:LEU:O	2.15	0.47
1:B:780:PHE:HA	1:B:783:ARG:HH11	1.79	0.47
1:C:644:GLU:HG2	1:C:670:GLN:HB2	1.96	0.47
1:C:799:ILE:HG21	1:C:804:PHE:HE2	1.79	0.47
1:A:221:GLN:HG3	1:A:243:GLN:HB3	1.97	0.46
1:A:464:GLY:HA3	1:B:143:MET:SD	2.55	0.46
1:A:573:LEU:HD13	1:A:578:ILE:HD11	1.95	0.46
1:A:767:LEU:HD12	1:A:791:ILE:HG22	1.97	0.46
1:B:146:ALA:C	1:B:148:LEU:H	2.18	0.46
1:D:753:PHE:HB2	1:D:770:VAL:CB	2.46	0.46
1:D:938:TRP:NE1	1:D:966:VAL:HG13	2.31	0.46
1:A:156:SER:CB	1:A:159:ILE:HD11	2.45	0.46
1:A:847:LEU:HB2	1:A:872:PRO:HG2	1.95	0.46
1:B:75:PHE:HE1	1:B:77:SER:HB3	1.80	0.46
1:C:72:ARG:HD2	1:C:97:HIS:ND1	2.31	0.46
1:C:166:LEU:HD22	1:C:193:ALA:HB2	1.97	0.46
1:C:847:LEU:HD13	1:C:863:LEU:HD11	1.96	0.46
1:D:763:THR:HG22	1:D:785:ARG:HB3	1.98	0.46
1:B:807:LEU:HD12	1:B:810:LEU:HD22	1.97	0.46
1:D:202:SER:HA	1:D:225:ALA:O	2.15	0.46
1:D:601:ALA:HA	1:D:623:LEU:O	2.14	0.46
1:D:927:HIS:CE1	1:D:928:LEU:HG	2.51	0.46
2:F:89:ASN:HB2	2:F:119:PRO:HG3	1.96	0.46
2:H:43:ILE:HD12	2:H:127:LEU:HD23	1.97	0.46
2:H:68:ARG:H	2:H:87:CYS:HB3	1.80	0.46
1:A:453:VAL:HG23	1:A:474:LEU:HD11	1.97	0.46
1:B:211:GLN:HA	1:B:214:ARG:HD2	1.96	0.46
1:B:479:VAL:CG2	1:B:503:MET:HG2	2.46	0.46
1:C:559:ALA:N	1:C:584:ASP:O	2.41	0.46
1:C:807:LEU:HD13	1:C:810:LEU:HD22	1.96	0.46
1:D:971:GLU:HG3	1:D:974:ARG:NH2	2.20	0.46
1:A:173:GLN:HA	1:A:195:GLN:O	2.14	0.46
1:A:201:LEU:HB2	1:A:224:VAL:HG12	1.97	0.46
1:A:799:ILE:HG22	1:A:827:GLU:HG2	1.97	0.46
1:B:302:PHE:HB2	1:B:324:TRP:O	2.16	0.46
1:B:309:MET:HE1	3:M:1:NAG:H83	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LEU:HB3	1:D:590:LEU:HD21	1.97	0.46
1:D:586:ILE:O	1:D:611:LYS:HE3	2.15	0.46
1:A:608:LEU:HD12	1:A:641:LEU:HD21	1.97	0.46
1:B:33:LYS:N	1:B:47:LEU:O	2.47	0.46
1:B:114:PHE:O	1:B:144:PRO:HB2	2.15	0.46
1:B:790:HIS:HA	1:B:814:ASP:HB3	1.98	0.46
1:C:823:LEU:HG	1:C:844:PHE:HZ	1.81	0.46
1:D:539:LEU:HB3	1:D:540:PRO:HD2	1.98	0.46
1:B:266:LEU:HB3	1:B:271:LEU:HD11	1.96	0.46
1:B:603:LEU:HD22	1:B:627:VAL:HG13	1.97	0.46
1:C:153:LEU:O	1:C:180:ASN:ND2	2.35	0.46
1:C:241:LEU:HB3	1:C:258:PRO:HG3	1.97	0.46
1:D:813:LEU:HB3	1:D:837:LEU:HD12	1.98	0.46
2:E:67:GLY:HA2	2:E:125:LYS:HG2	1.97	0.46
2:F:71:VAL:HG13	2:F:85:ILE:HG21	1.98	0.46
2:F:99:LYS:HE2	2:F:108:PHE:HB3	1.97	0.46
1:A:73:SER:HA	1:A:98:HIS:O	2.16	0.46
1:A:889:PRO:HB3	1:A:938:TRP:CE3	2.50	0.46
1:B:48:CYS:O	1:B:77:SER:OG	2.32	0.46
1:B:72:ARG:HD3	1:B:95:ALA:O	2.15	0.46
1:B:187:ARG:HH22	1:B:189:GLU:HA	1.80	0.46
1:C:340:ASN:HB2	1:C:364:ASN:OD1	2.16	0.46
1:C:497:LYS:O	1:C:499:ARG:HG3	2.16	0.46
1:D:329:GLU:O	1:D:353:ALA:HA	2.16	0.46
2:H:43:ILE:HD13	2:H:49:ALA:CB	2.46	0.46
1:A:253:ASP:OD1	1:A:275:PRO:HB3	2.16	0.46
1:A:281:LEU:HD13	1:A:284:LEU:HD13	1.97	0.46
1:D:941:VAL:HG11	1:D:958:PRO:HD3	1.97	0.46
1:A:790:HIS:HB3	1:A:792:ASN:OD1	2.15	0.46
1:C:291:ARG:HA	1:C:314:TYR:HB2	1.98	0.46
1:C:764:GLU:OE2	1:C:766:ILE:HD11	2.16	0.46
1:B:142:LEU:HA	1:B:145:LEU:HD12	1.97	0.45
1:C:737:ASN:HB3	1:C:762:ALA:HA	1.98	0.45
1:A:321:PRO:HG2	1:A:324:TRP:CE2	2.51	0.45
1:B:234:LEU:HD13	1:B:241:LEU:HD22	1.98	0.45
1:B:854:LYS:O	1:B:855:LEU:HD23	2.16	0.45
1:C:773:PRO:C	1:C:796:LEU:HD12	2.36	0.45
1:D:308:GLU:HG2	1:D:333:ALA:HB3	1.97	0.45
1:D:837:LEU:HB3	1:D:861:LEU:CD1	2.45	0.45
1:D:837:LEU:HB3	1:D:861:LEU:HD12	1.99	0.45
1:D:847:LEU:HD12	1:D:847:LEU:HA	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:HG2	1:B:333:ALA:HB3	1.98	0.45
1:D:499:ARG:HB3	1:D:522:ARG:HB2	1.98	0.45
1:D:765:ILE:HG13	1:D:786:LEU:HD11	1.97	0.45
1:D:893:ASP:O	1:D:917:ASN:ND2	2.50	0.45
2:F:60:SER:N	2:F:132:ASN:O	2.48	0.45
1:C:159:ILE:HB	1:C:182:LEU:HD21	1.99	0.45
1:C:200:ASP:OD2	8:C:1101:NAG:N2	2.49	0.45
1:D:204:ASN:HB2	1:D:227:ASN:OD1	2.17	0.45
1:D:324:TRP:C	1:D:326:GLN:H	2.20	0.45
1:D:382:ASN:OD1	1:D:405:SER:HB3	2.16	0.45
1:D:384:ARG:HA	1:D:407:ASP:HB3	1.98	0.45
1:A:40:GLN:OE1	1:A:72:ARG:NH1	2.50	0.45
1:B:378:SER:HB3	1:B:380:ILE:HG13	1.98	0.45
1:B:658:TRP:CE3	1:B:667:VAL:HG11	2.52	0.45
1:D:588:ASN:HA	1:D:611:LYS:HD2	1.99	0.45
1:D:780:PHE:CZ	1:D:789:LEU:HD21	2.52	0.45
1:A:261:VAL:HB	1:A:281:LEU:HD21	1.99	0.45
1:A:821:ILE:HG12	1:A:843:ARG:HB2	1.99	0.45
1:C:805:HIS:CD2	1:C:806:THR:HG23	2.51	0.45
1:D:105:GLU:HA	1:D:128:ILE:HA	1.99	0.45
1:D:890:LEU:O	1:D:937:CYS:HA	2.16	0.45
1:A:413:LEU:HD12	1:A:431:LEU:HD22	1.98	0.45
1:B:434:ASN:HB3	1:B:436:ILE:HG13	1.98	0.45
1:B:467:ILE:HG13	1:B:468:PHE:CD1	2.51	0.45
1:C:705:GLU:HG2	1:C:734:PHE:CD2	2.52	0.45
1:C:778:HIS:HB3	1:C:781:ILE:HG21	1.98	0.45
1:D:536:TRP:HD1	1:D:557:THR:N	2.12	0.45
1:D:953:LEU:HB3	1:D:965:PHE:CD2	2.52	0.45
1:B:159:ILE:HB	1:B:182:LEU:HD21	1.99	0.45
1:B:393:LEU:HB2	1:B:417:PRO:CG	2.40	0.45
1:C:105:GLU:HA	1:C:128:ILE:HA	1.99	0.45
1:C:223:SER:HA	1:C:245:ASP:HB3	1.98	0.45
1:C:568:LEU:HB3	1:C:590:LEU:HD21	1.97	0.45
2:F:96:LEU:HD11	2:F:127:LEU:HD11	1.98	0.45
2:G:51:LEU:HD22	2:G:131:TYR:CE1	2.52	0.45
1:A:512:ASP:O	1:A:514:GLY:N	2.48	0.45
1:A:719:LYS:HG2	1:A:721:VAL:HG23	1.98	0.45
1:B:238:THR:O	1:B:258:PRO:HG3	2.16	0.45
1:B:291:ARG:H	1:B:314:TYR:HB2	1.81	0.45
1:C:148:LEU:HD23	1:C:169:LEU:HD13	1.98	0.45
1:C:859:LYS:HA	1:C:880:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PHE:CE1	1:D:77:SER:HB2	2.35	0.45
1:D:652:CYS:HB2	1:D:678:SER:O	2.16	0.45
2:G:57:LYS:HE2	2:G:135:VAL:HG23	1.97	0.45
1:A:315:ASN:O	1:A:340:ASN:HA	2.17	0.45
1:A:367:ARG:HD3	1:A:391:GLU:OE2	2.16	0.45
1:A:572:SER:HA	1:A:594:ASP:HB3	1.98	0.45
1:B:100:ARG:HD2	1:B:124:GLU:OE1	2.17	0.45
1:B:786:LEU:HD23	1:B:810:LEU:HD13	1.99	0.45
1:B:845:SER:O	1:B:868:LEU:HD23	2.16	0.45
1:D:774:GLN:HA	1:D:798:SER:O	2.16	0.45
6:P:1:NAG:O7	6:P:1:NAG:O3	2.28	0.45
1:A:313:SER:O	1:A:315:ASN:ND2	2.50	0.44
1:A:399:SER:HA	1:A:422:LYS:CB	2.48	0.44
1:A:580:ILE:HG13	1:A:602:LYS:HB3	1.98	0.44
1:A:791:ILE:HG13	1:A:815:LEU:HD23	1.99	0.44
1:B:150:LYS:HG3	1:B:174:VAL:HB	1.97	0.44
1:B:166:LEU:HD22	1:B:193:ALA:HB2	1.99	0.44
1:B:568:LEU:HB3	1:B:590:LEU:HD21	1.99	0.44
2:H:71:VAL:HG13	2:H:85:ILE:HG21	1.98	0.44
1:A:474:LEU:HD12	1:A:474:LEU:HA	1.83	0.44
1:A:801:PRO:HA	1:A:827:GLU:HA	1.97	0.44
1:A:922:PHE:CG	1:A:969:ILE:HD11	2.52	0.44
1:C:82:ASN:O	1:C:84:GLN:HG3	2.18	0.44
1:D:67:GLN:HB3	1:D:70:ASN:ND2	2.32	0.44
1:D:353:ALA:O	1:D:375:PRO:HG3	2.18	0.44
1:D:697:LEU:HD21	1:D:736:ILE:HG21	1.98	0.44
1:D:775:LEU:HB2	1:D:799:ILE:HG23	1.99	0.44
2:F:42:THR:HG21	2:F:73:VAL:HG11	1.99	0.44
1:A:179:SER:H	1:A:203:ARG:HB2	1.82	0.44
1:B:60:ILE:HD13	1:B:93:LEU:HD11	2.00	0.44
1:B:140:ASP:HA	1:B:143:MET:HG3	1.99	0.44
1:B:232:LEU:HG	1:B:234:LEU:HG	1.99	0.44
1:B:559:ALA:HB1	1:B:565:THR:HG21	2.00	0.44
1:C:225:ALA:O	1:C:227:ASN:ND2	2.51	0.44
1:C:463:ILE:HD11	1:C:479:VAL:HG21	1.99	0.44
1:C:556:LEU:HD11	1:C:578:ILE:HD13	1.99	0.44
1:C:627:VAL:HG21	1:C:645:ILE:HD11	2.00	0.44
1:C:861:LEU:O	1:C:883:ILE:HA	2.18	0.44
1:C:923:SER:HB3	1:C:973:LEU:HD13	1.99	0.44
1:D:738:ILE:HG23	1:D:764:GLU:OE1	2.17	0.44
1:D:828:PHE:O	1:D:854:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:LEU:HB3	1:A:794:THR:HB	1.99	0.44
1:B:85:PHE:CD1	1:B:86:PRO:HD2	2.53	0.44
1:B:807:LEU:HD13	1:B:810:LEU:HD13	1.99	0.44
1:D:940:ASN:HA	1:D:964:VAL:HA	2.00	0.44
1:A:335:LEU:HD23	1:A:359:LEU:HD13	1.99	0.44
1:A:492:PHE:HB3	1:A:518:ALA:HB2	1.99	0.44
1:B:802:LYS:H	1:B:827:GLU:HA	1.81	0.44
1:D:115:GLU:HA	1:D:144:PRO:HG2	2.00	0.44
1:D:246:ALA:HB3	1:D:266:LEU:HD23	1.98	0.44
1:D:586:ILE:HD12	1:D:607:ALA:HB1	1.98	0.44
1:A:75:PHE:HD1	1:A:76:ILE:N	2.15	0.44
1:A:396:SER:HA	1:A:399:SER:OG	2.18	0.44
1:B:677:CYS:O	1:B:685:GLN:HA	2.18	0.44
1:B:823:LEU:HD23	1:B:823:LEU:HA	1.87	0.44
1:D:501:ILE:N	1:D:523:ARG:O	2.41	0.44
2:E:115:PHE:HZ	2:E:127:LEU:HD22	1.82	0.44
1:A:293:GLU:HB3	1:A:316:LYS:HD2	2.00	0.44
1:A:458:ASN:H	1:A:482:ASN:HD21	1.66	0.44
1:A:617:LEU:O	1:A:643:VAL:HA	2.17	0.44
1:B:307:LEU:HD23	1:B:325:LEU:HD23	1.99	0.44
1:B:576:ASN:HB3	1:B:577:GLY:H	1.59	0.44
1:B:889:PRO:HA	1:B:938:TRP:HB2	1.98	0.44
1:D:356:LEU:HD23	1:D:380:ILE:HD11	2.00	0.44
1:D:731:ASP:OD2	1:D:735:ASN:HB2	2.18	0.44
1:A:403:LEU:HD12	1:A:423:VAL:HG21	1.99	0.44
1:B:44:LYS:HD3	1:B:44:LYS:HA	1.70	0.44
1:B:149:GLU:O	1:B:173:GLN:HB2	2.18	0.44
1:D:189:GLU:OE2	1:D:214:ARG:HD3	2.17	0.44
2:H:43:ILE:HD13	2:H:49:ALA:HB1	2.00	0.44
1:A:720:SER:HA	1:A:759:PRO:HB3	2.00	0.44
1:B:71:ILE:O	1:B:96:LEU:HA	2.18	0.44
1:B:440:TYR:HB2	1:B:443:VAL:CG2	2.47	0.44
1:B:504:LYS:HA	1:B:527:SER:O	2.18	0.44
1:B:801:PRO:HB3	1:B:826:GLU:HB2	1.98	0.44
1:C:93:LEU:HD13	1:C:96:LEU:HD22	2.00	0.44
1:C:266:LEU:HD13	1:C:271:LEU:HD11	2.00	0.44
1:C:512:ASP:OD1	1:C:535:LYS:HD2	2.18	0.44
1:C:526:VAL:O	1:C:529:ASN:ND2	2.51	0.44
1:D:100:ARG:HE	1:D:102:VAL:HG21	1.83	0.44
1:D:481:ASN:N	1:D:504:LYS:O	2.28	0.44
1:D:525:ASP:HA	1:D:547:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:ASP:HB2	2:F:125:LYS:O	2.17	0.44
2:H:51:LEU:O	2:H:105:MET:HA	2.18	0.44
1:A:116:ASP:OD1	1:A:116:ASP:N	2.50	0.43
1:A:170:PRO:C	1:A:172:LEU:H	2.22	0.43
1:A:385:LEU:HD22	1:A:390:LEU:HD11	2.00	0.43
1:A:679:HIS:ND1	1:A:682:ASP:OD1	2.51	0.43
1:A:842:ASN:HB3	1:A:843:ARG:H	1.54	0.43
1:C:37:ASP:HB3	1:C:40:GLN:O	2.17	0.43
1:D:81:ASN:HA	1:D:105:GLU:HB2	2.00	0.43
1:D:588:ASN:HA	1:D:611:LYS:CD	2.48	0.43
1:D:971:GLU:HA	1:D:974:ARG:NH1	2.33	0.43
2:H:96:LEU:HD11	2:H:127:LEU:HD21	2.00	0.43
1:A:251:ILE:HD12	1:A:269:ASN:ND2	2.32	0.43
1:A:338:GLU:HA	1:A:362:SER:O	2.18	0.43
1:A:350:LEU:O	1:A:375:PRO:HD3	2.18	0.43
1:B:821:ILE:HG12	1:B:843:ARG:HB2	2.00	0.43
1:A:156:SER:HB2	1:A:159:ILE:HD11	1.99	0.43
1:A:844:PHE:HB2	1:A:866:ASN:OD1	2.18	0.43
1:A:938:TRP:CG	1:A:964:VAL:HG11	2.53	0.43
1:B:120:LEU:HD23	1:B:145:LEU:HD22	2.00	0.43
1:B:163:GLN:NE2	1:B:186:ARG:HD3	2.33	0.43
1:C:156:SER:CB	1:C:159:ILE:HD11	2.49	0.43
1:C:939:GLU:CG	1:C:954:SER:HB3	2.48	0.43
1:C:956:TYR:OH	1:C:980:ILE:HG12	2.18	0.43
1:D:534:LEU:HB3	1:D:553:ILE:HG23	2.01	0.43
1:B:476:SER:HA	1:B:500:LYS:HB3	2.00	0.43
1:C:90:PHE:HB3	1:C:117:LEU:HD21	2.01	0.43
1:C:125:LEU:O	1:C:153:LEU:HA	2.17	0.43
1:C:455:LEU:HB3	1:C:460:LEU:HD11	1.99	0.43
1:A:273:ARG:HD2	1:A:298:ASN:HB3	2.01	0.43
1:A:594:ASP:HA	1:A:618:ASN:HB3	2.00	0.43
1:A:784:LEU:HD22	1:A:808:PRO:HG3	2.00	0.43
1:B:418:ALA:O	1:B:422:LYS:HE2	2.19	0.43
1:C:331:ARG:HA	1:C:355:ASN:HD22	1.82	0.43
1:C:612:SER:HB3	1:C:635:VAL:O	2.18	0.43
1:C:651:ILE:HG12	1:C:678:SER:OG	2.18	0.43
1:C:713:TYR:CE2	2:G:63:LEU:HD21	2.54	0.43
1:D:409:SER:HB2	1:D:433:HIS:CD2	2.54	0.43
1:D:807:LEU:HB3	1:D:810:LEU:HB2	1.99	0.43
1:A:463:ILE:HD11	1:A:479:VAL:HG21	2.00	0.43
1:A:813:LEU:HB3	1:A:837:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CD2	1:B:113:LEU:HG	2.53	0.43
1:B:842:ASN:HB3	1:B:843:ARG:H	1.66	0.43
1:C:78:CYS:HB2	1:C:103:GLY:O	2.19	0.43
1:D:790:HIS:CE1	8:D:1101:NAG:H61	2.54	0.43
1:D:834:VAL:CB	1:D:855:LEU:HD22	2.47	0.43
1:D:845:SER:O	1:D:868:LEU:HD23	2.18	0.43
1:A:299:SER:HA	1:A:324:TRP:HE1	1.84	0.43
1:A:368:VAL:HG12	1:A:370:ARG:HG3	2.00	0.43
1:A:758:LEU:HD13	1:A:765:ILE:HD13	2.00	0.43
1:B:65:TYR:CE2	1:B:71:ILE:HD11	2.54	0.43
1:B:590:LEU:HD13	1:B:593:LEU:HD13	2.01	0.43
1:B:700:TYR:CE2	1:B:728:CYS:HB3	2.54	0.43
1:C:875:LEU:HD13	1:C:883:ILE:CD1	2.49	0.43
1:D:789:LEU:HD11	1:D:791:ILE:HD11	2.01	0.43
1:B:331:ARG:HA	1:B:355:ASN:ND2	2.32	0.43
1:B:940:ASN:HA	1:B:964:VAL:HG22	2.01	0.43
1:C:411:ASN:HB2	1:C:434:ASN:OD1	2.19	0.43
1:D:522:ARG:HD3	1:D:544:GLU:OE1	2.19	0.43
1:D:529:ASN:HB3	1:D:530:GLU:H	1.68	0.43
1:D:778:HIS:CD2	2:H:77:ASP:OD2	2.72	0.43
1:D:858:LEU:HD12	1:D:858:LEU:HA	1.79	0.43
2:E:68:ARG:NH1	2:E:70:SER:O	2.51	0.43
2:H:29:ALA:O	2:H:41:HIS:NE2	2.52	0.43
1:A:125:LEU:N	1:A:152:SER:O	2.34	0.43
1:A:242:GLN:O	1:A:262:VAL:HG22	2.18	0.43
1:B:568:LEU:HB3	1:B:590:LEU:CD2	2.49	0.43
1:D:75:PHE:CD1	1:D:75:PHE:C	2.91	0.43
1:D:534:LEU:HD21	1:D:539:LEU:HD11	2.01	0.43
1:A:699:PRO:HA	1:A:729:PHE:HA	2.01	0.43
1:B:533:VAL:HG13	1:B:555:LEU:HB3	2.00	0.43
1:B:550:ASN:HA	1:B:575:ASN:O	2.18	0.43
1:B:739:VAL:HG21	1:B:759:PRO:HD2	2.00	0.43
1:C:72:ARG:HD3	1:C:95:ALA:O	2.19	0.43
1:A:441:GLN:O	1:A:445:ASN:HB2	2.19	0.42
1:A:559:ALA:HB1	1:A:587:PRO:HG3	2.01	0.42
1:B:125:LEU:N	1:B:152:SER:O	2.33	0.42
1:B:371:ASP:OD1	1:B:394:GLU:HB2	2.19	0.42
1:B:937:CYS:N	1:B:967:MET:O	2.42	0.42
1:C:44:LYS:HA	1:C:44:LYS:HD3	1.74	0.42
1:C:705:GLU:HA	1:C:734:PHE:CE2	2.53	0.42
1:C:788:ARG:HG2	1:C:812:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:VAL:HA	1:D:215:GLY:O	2.19	0.42
2:G:71:VAL:HG13	2:G:85:ILE:HG21	2.01	0.42
1:A:34:CYS:HA	1:A:46:LEU:HD12	2.01	0.42
1:A:124:GLU:HG2	1:A:152:SER:HB2	2.01	0.42
1:A:820:LEU:HB2	1:A:844:PHE:HE1	1.84	0.42
1:C:234:LEU:HD13	1:C:241:LEU:CD2	2.48	0.42
1:C:938:TRP:CE3	1:C:964:VAL:HG11	2.54	0.42
1:D:162:PRO:HD2	1:D:165:LEU:HD13	2.01	0.42
1:D:339:HIS:HA	1:D:363:SER:HB2	2.01	0.42
1:D:543:LEU:O	1:D:568:LEU:HA	2.18	0.42
1:D:616:ARG:HG2	1:D:642:LYS:HD2	2.01	0.42
1:A:234:LEU:HD13	1:A:241:LEU:HD22	2.00	0.42
1:B:30:LYS:HG2	1:B:31:PHE:CE1	2.54	0.42
1:C:78:CYS:HB2	1:C:103:GLY:C	2.40	0.42
1:C:700:TYR:CZ	1:C:728:CYS:HB3	2.54	0.42
1:C:705:GLU:HG2	1:C:734:PHE:HD2	1.84	0.42
1:D:396:SER:HA	1:D:399:SER:OG	2.19	0.42
1:D:681:VAL:HG22	1:D:729:PHE:CD2	2.54	0.42
3:I:2:NAG:O6	3:I:3:BMA:O5	2.29	0.42
1:A:385:LEU:O	1:A:408:LEU:HA	2.19	0.42
1:A:632:MET:CE	1:A:643:VAL:HG21	2.48	0.42
1:B:322:VAL:O	1:B:326:GLN:HB2	2.20	0.42
1:B:482:ASN:HB3	1:B:483:GLU:H	1.63	0.42
1:B:650:LEU:HD13	1:B:659:MET:HE1	2.00	0.42
1:C:551:ASN:HB3	1:C:553:ILE:HG13	2.00	0.42
1:C:763:THR:HG22	1:C:785:ARG:CB	2.46	0.42
1:D:156:SER:CB	1:D:159:ILE:HD11	2.50	0.42
2:F:41:HIS:ND1	2:F:43:ILE:HD11	2.35	0.42
1:A:54:ASN:OD1	1:A:80:ASN:ND2	2.53	0.42
1:A:75:PHE:CE1	1:A:77:SER:HB2	2.51	0.42
1:A:139:GLU:O	1:A:143:MET:HG3	2.20	0.42
1:A:333:ALA:HA	1:A:356:LEU:HA	2.01	0.42
1:A:629:THR:OG1	1:A:655:GLN:O	2.32	0.42
1:B:347:GLY:HA3	1:B:372:GLU:CG	2.49	0.42
1:C:179:SER:H	1:C:203:ARG:HB2	1.84	0.42
1:D:224:VAL:HB	1:D:229:ILE:CD1	2.50	0.42
1:D:472:SER:HB3	1:D:494:ARG:O	2.19	0.42
1:D:568:LEU:HD13	1:D:587:PRO:HG2	2.01	0.42
1:A:43:SER:H	1:A:43:SER:HG	1.63	0.42
1:A:53:LYS:HE3	1:A:53:LYS:HB2	1.75	0.42
1:A:290:SER:HA	1:A:315:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:HIS:HA	1:A:927:HIS:CE1	2.54	0.42
1:B:281:LEU:HD13	1:B:284:LEU:HD13	2.01	0.42
1:B:453:VAL:HG23	1:B:474:LEU:HD11	2.02	0.42
1:C:301:VAL:HG22	1:C:323:GLU:CG	2.49	0.42
1:C:918:ALA:O	1:C:922:PHE:HD2	2.03	0.42
1:D:474:LEU:O	1:D:498:LEU:HA	2.20	0.42
1:D:531:ILE:O	1:D:552:ASP:HB2	2.19	0.42
1:D:646:SER:O	1:D:648:ASN:ND2	2.52	0.42
1:D:652:CYS:O	1:D:680:ALA:HB2	2.19	0.42
1:A:581:MET:HE2	1:A:603:LEU:HD11	2.01	0.42
1:A:653:ASP:HB2	1:A:698:CYS:HB3	2.01	0.42
1:B:90:PHE:CE2	1:B:113:LEU:HG	2.55	0.42
1:B:941:VAL:HG22	1:B:954:SER:HA	2.01	0.42
1:D:842:ASN:HB3	1:D:843:ARG:H	1.64	0.42
2:G:92:THR:HG21	2:G:127:LEU:HD13	2.02	0.42
2:H:42:THR:CG2	2:H:73:VAL:HG11	2.47	0.42
1:A:865:ASN:HA	1:A:887:SER:HB2	2.02	0.42
1:B:717:ASP:O	1:B:760:VAL:HB	2.19	0.42
1:C:45:LEU:HD21	1:C:47:LEU:HD21	2.02	0.42
1:C:81:ASN:HA	1:C:105:GLU:HB2	2.02	0.42
1:C:264:VAL:HG12	1:C:266:LEU:HG	2.01	0.42
1:C:765:ILE:HG22	1:C:767:LEU:HG	2.01	0.42
1:C:844:PHE:HB2	1:C:866:ASN:OD1	2.20	0.42
1:C:866:ASN:HB3	1:C:867:SER:H	1.56	0.42
1:D:313:SER:O	1:D:315:ASN:ND2	2.53	0.42
1:D:387:ASN:N	1:D:409:SER:O	2.36	0.42
1:D:875:LEU:O	1:D:921:TRP:NE1	2.53	0.42
2:E:89:ASN:HB2	2:E:119:PRO:HG3	2.01	0.42
2:G:34:ASP:OD1	2:G:38:THR:N	2.49	0.42
1:A:486:LEU:HD13	1:B:112:LYS:HG3	2.02	0.42
1:B:347:GLY:HA3	1:B:372:GLU:HG3	2.02	0.42
1:B:441:GLN:HA	1:B:467:ILE:HA	2.02	0.42
1:B:508:ILE:HG21	1:B:511:LEU:HD23	2.01	0.42
1:C:658:TRP:CZ3	1:C:669:ILE:HD11	2.53	0.42
1:C:679:HIS:HD2	1:C:686:ILE:HD11	1.83	0.42
1:D:823:LEU:HD23	1:D:823:LEU:HA	1.83	0.42
1:B:252:VAL:HA	1:B:270:ALA:O	2.19	0.42
1:B:893:ASP:OD2	1:B:951:THR:HG22	2.19	0.42
1:C:713:TYR:CD2	2:G:63:LEU:HD11	2.55	0.42
1:A:789:LEU:O	1:A:813:LEU:HD12	2.20	0.41
1:B:129:SER:OG	1:B:156:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASP:OD2	1:B:236:LEU:HD12	2.19	0.41
1:B:854:LYS:HD3	1:B:854:LYS:HA	1.87	0.41
1:C:123:LEU:HB3	1:C:148:LEU:HD21	2.02	0.41
1:D:409:SER:HB3	1:D:432:SER:OG	2.19	0.41
1:D:723:PRO:HG2	1:D:758:LEU:HD23	2.02	0.41
1:D:773:PRO:HA	1:D:796:LEU:HA	2.01	0.41
1:A:101:ILE:HB	1:A:125:LEU:HD23	2.03	0.41
1:A:339:HIS:H	1:A:363:SER:HB2	1.86	0.41
1:A:710:CYS:HB3	2:E:69:PHE:CD2	2.56	0.41
1:B:548:ALA:HB3	1:B:573:LEU:HD23	2.02	0.41
1:C:288:ASN:HA	1:C:311:ASP:HB3	2.01	0.41
1:C:607:ALA:O	1:C:611:LYS:HE2	2.19	0.41
1:D:546:LEU:O	1:D:572:SER:HB3	2.20	0.41
1:B:35:ALA:N	1:B:45:LEU:O	2.53	0.41
1:B:775:LEU:HD23	1:B:775:LEU:HA	1.85	0.41
1:C:364:ASN:HB2	1:C:388:ASN:HD21	1.85	0.41
1:C:457:ASN:OD1	1:C:481:ASN:ND2	2.48	0.41
1:C:488:PHE:O	1:C:514:GLY:HA2	2.20	0.41
1:C:642:LYS:HA	1:C:668:LEU:O	2.20	0.41
1:D:548:ALA:HB1	1:D:553:ILE:HD11	2.02	0.41
1:A:91:LYS:HG3	1:A:116:ASP:OD2	2.20	0.41
1:A:296:ALA:HB3	1:A:318:ASP:OD1	2.21	0.41
1:B:72:ARG:O	1:B:98:HIS:N	2.49	0.41
1:B:100:ARG:HA	1:B:124:GLU:O	2.19	0.41
1:B:288:ASN:HA	1:B:311:ASP:HB3	2.03	0.41
1:B:338:GLU:HA	1:B:362:SER:O	2.20	0.41
1:C:72:ARG:CZ	1:C:95:ALA:HB1	2.51	0.41
1:C:125:LEU:HB3	1:C:128:ILE:HD13	2.02	0.41
1:C:148:LEU:HD12	1:C:148:LEU:HA	1.89	0.41
1:C:768:SER:HA	1:C:792:ASN:O	2.21	0.41
1:C:975:ASP:HA	1:C:978:SER:OG	2.21	0.41
1:D:568:LEU:C	1:D:590:LEU:HD23	2.41	0.41
1:D:583:ALA:HA	1:D:607:ALA:HA	2.01	0.41
1:A:353:ALA:HB1	1:A:356:LEU:HB2	2.02	0.41
1:A:854:LYS:HD3	1:A:854:LYS:HA	1.55	0.41
1:B:312:ALA:HB3	1:B:337:LEU:CD2	2.50	0.41
1:B:780:PHE:CE2	1:B:791:ILE:HD11	2.55	0.41
1:C:246:ALA:O	1:C:249:ASN:ND2	2.54	0.41
1:C:403:LEU:O	1:C:426:LEU:HA	2.21	0.41
1:C:784:LEU:HA	1:C:808:PRO:HD2	2.01	0.41
1:D:124:GLU:HA	1:D:152:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:941:VAL:HG13	1:D:954:SER:O	2.21	0.41
2:H:84:ASN:HB3	2:H:123:THR:CG2	2.51	0.41
1:A:507:LYS:O	1:A:509:LYS:HG3	2.21	0.41
1:B:258:PRO:O	1:B:261:VAL:HG23	2.20	0.41
1:B:621:GLY:H	1:B:647:GLU:HB2	1.85	0.41
1:D:187:ARG:NH2	1:D:189:GLU:HA	2.35	0.41
1:D:616:ARG:HH21	1:D:642:LYS:NZ	2.18	0.41
1:D:953:LEU:HB3	1:D:965:PHE:HD2	1.85	0.41
2:H:71:VAL:HA	2:H:82:PRO:HG2	2.02	0.41
1:A:192:VAL:HG13	1:A:215:GLY:O	2.20	0.41
1:B:28:CYS:SG	1:B:34:CYS:N	2.92	0.41
1:C:441:GLN:HA	1:C:467:ILE:HA	2.03	0.41
1:C:579:THR:HA	1:C:600:LEU:HA	2.03	0.41
1:D:778:HIS:HB3	2:H:77:ASP:CG	2.41	0.41
1:A:600:LEU:HB2	1:A:622:ASN:CG	2.40	0.41
1:A:705:GLU:HA	1:A:734:PHE:CD2	2.55	0.41
1:B:57:ILE:HG12	1:B:83:PHE:CZ	2.55	0.41
1:B:232:LEU:HD21	1:B:234:LEU:HD11	2.03	0.41
1:B:432:SER:HB3	1:B:454:ASP:OD1	2.21	0.41
1:C:415:GLU:HA	1:C:436:ILE:HG23	2.02	0.41
1:D:368:VAL:HG22	1:D:392:LEU:HB3	2.02	0.41
1:D:568:LEU:HB3	1:D:590:LEU:CD2	2.51	0.41
1:A:142:LEU:HA	1:A:145:LEU:HD12	2.03	0.41
1:A:262:VAL:HA	1:A:284:LEU:HA	2.03	0.41
1:A:534:LEU:O	1:A:557:THR:HG23	2.21	0.41
1:A:875:LEU:O	1:A:921:TRP:NE1	2.49	0.41
1:B:354:THR:O	1:B:379:LYS:HG3	2.21	0.41
1:B:410:HIS:HA	1:B:433:HIS:HB2	2.02	0.41
1:C:102:VAL:HG22	1:C:126:ASP:CB	2.51	0.41
1:C:296:ALA:HB3	1:C:318:ASP:OD1	2.20	0.41
1:C:612:SER:HA	1:C:634:VAL:HG12	2.03	0.41
1:C:625:THR:HG22	1:C:649:PRO:O	2.20	0.41
1:D:440:TYR:O	1:D:467:ILE:HB	2.21	0.41
1:D:489:LYS:CB	1:D:513:GLU:HB3	2.50	0.41
1:D:557:THR:O	1:D:585:GLN:HG2	2.21	0.41
1:D:577:GLY:HA2	1:D:599:ARG:HD2	2.02	0.41
1:A:315:ASN:HB2	1:A:340:ASN:OD1	2.20	0.41
1:A:940:ASN:HA	1:A:964:VAL:HG22	2.03	0.41
1:B:126:ASP:OD1	1:B:127:GLN:HG3	2.21	0.41
1:B:187:ARG:HG2	1:B:188:GLU:N	2.35	0.41
1:B:291:ARG:HA	1:B:314:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LEU:O	1:C:340:ASN:ND2	2.54	0.41
1:C:399:SER:HA	1:C:422:LYS:CB	2.51	0.41
1:C:500:LYS:HG3	1:C:523:ARG:HB2	2.02	0.41
1:C:536:TRP:NE1	1:C:559:ALA:HB2	2.36	0.41
1:D:301:VAL:HG13	1:D:323:GLU:O	2.21	0.41
1:A:474:LEU:HG	1:A:498:LEU:HD13	2.03	0.40
1:B:306:GLU:HA	1:B:331:ARG:HD3	2.01	0.40
1:B:625:THR:HA	1:B:650:LEU:HA	2.03	0.40
1:C:153:LEU:HB3	1:C:177:ILE:HG22	2.02	0.40
1:C:306:GLU:HA	1:C:331:ARG:HD3	2.03	0.40
1:D:497:LYS:O	1:D:499:ARG:HG3	2.21	0.40
1:D:608:LEU:HB2	1:D:631:SER:O	2.21	0.40
1:A:717:ASP:CG	2:E:70:SER:HA	2.42	0.40
1:D:474:LEU:HD12	1:D:474:LEU:HA	1.85	0.40
1:A:401:LEU:HB3	1:A:403:LEU:HG	2.02	0.40
1:A:529:ASN:HB3	1:A:530:GLU:H	1.54	0.40
1:A:641:LEU:HD23	1:A:667:VAL:CG2	2.52	0.40
1:B:126:ASP:OD1	1:B:155:ARG:HB2	2.22	0.40
1:B:217:PRO:O	1:B:240:PHE:HD2	2.04	0.40
1:D:107:THR:HA	1:D:134:SER:O	2.21	0.40
1:D:335:LEU:CD2	1:D:350:LEU:HD11	2.51	0.40
1:D:407:ASP:OD1	1:D:408:LEU:N	2.55	0.40
1:A:187:ARG:NE	1:A:212:PHE:O	2.53	0.40
1:A:861:LEU:O	1:A:883:ILE:HA	2.21	0.40
1:B:187:ARG:NH1	1:B:189:GLU:HA	2.37	0.40
1:B:660:ILE:CD1	1:B:693:LYS:HG2	2.52	0.40
1:C:264:VAL:HG21	1:C:278:VAL:HG13	2.02	0.40
1:A:181:GLU:HA	1:A:204:ASN:HA	2.02	0.40
1:A:521:LEU:HD21	1:A:524:LEU:HB2	2.03	0.40
1:B:206:LEU:HB2	1:B:227:ASN:OD1	2.21	0.40
1:B:287:LEU:HB3	1:B:310:LEU:CD1	2.51	0.40
1:B:780:PHE:CE2	1:B:789:LEU:HD21	2.56	0.40
1:C:46:LEU:HB3	1:C:74:LEU:HD13	2.04	0.40
1:D:716:CYS:HA	2:H:72:ALA:HB1	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:HIS:NE2	1:C:702:SER:OG[2_654]	2.09	0.11

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	935/1007 (93%)	813 (87%)	122 (13%)	0	100 100
1	B	929/1007 (92%)	805 (87%)	123 (13%)	1 (0%)	51 84
1	C	935/1007 (93%)	802 (86%)	132 (14%)	1 (0%)	51 84
1	D	935/1007 (93%)	812 (87%)	122 (13%)	1 (0%)	51 84
2	E	106/114 (93%)	101 (95%)	5 (5%)	0	100 100
2	F	106/114 (93%)	101 (95%)	5 (5%)	0	100 100
2	G	105/114 (92%)	101 (96%)	4 (4%)	0	100 100
2	H	103/114 (90%)	98 (95%)	5 (5%)	0	100 100
All	All	4154/4484 (93%)	3633 (88%)	518 (12%)	3 (0%)	51 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	LEU
1	B	346	THR
1	C	259	GLY

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	851/908 (94%)	842 (99%)	9 (1%)	73 85
1	B	847/908 (93%)	833 (98%)	14 (2%)	60 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	851/908 (94%)	838 (98%)	13 (2%)	65 80
1	D	851/908 (94%)	843 (99%)	8 (1%)	78 88
2	E	97/103 (94%)	96 (99%)	1 (1%)	76 86
2	F	97/103 (94%)	97 (100%)	0	100 100
2	G	96/103 (93%)	94 (98%)	2 (2%)	53 72
2	H	94/103 (91%)	92 (98%)	2 (2%)	53 72
All	All	3784/4044 (94%)	3735 (99%)	49 (1%)	69 82

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	75	PHE
1	A	138	THR
1	A	152	SER
1	A	346	THR
1	A	486	LEU
1	A	490	ASP
1	A	608	LEU
1	A	848	SER
1	B	31	PHE
1	B	42	THR
1	B	43	SER
1	B	58	THR
1	B	66	ASP
1	B	67	GLN
1	B	68	VAL
1	B	77	SER
1	B	79	ASP
1	B	80	ASN
1	B	85	PHE
1	B	289	VAL
1	B	483	GLU
1	B	715	ASN
1	C	58	THR
1	C	66	ASP
1	C	67	GLN
1	C	68	VAL
1	C	80	ASN
1	C	138	THR

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Mol	Chain	Res	Type
1	C	152	SER
1	C	255	THR
1	C	372	GLU
1	C	526	VAL
1	C	698	CYS
1	C	791	ILE
1	C	876	HIS
1	D	75	PHE
1	D	445	ASN
1	D	564	SER
1	D	608	LEU
1	D	629	THR
1	D	666	LYS
1	D	865	ASN
1	D	916	HIS
2	E	41	HIS
2	G	43	ILE
2	G	81	VAL
2	H	43	ILE
2	H	81	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
1	A	774	GLN
1	B	355	ASN
1	B	917	ASN
1	C	249	ASN
1	C	355	ASN
1	C	388	ASN
1	C	458	ASN
1	D	108	HIS
1	D	292	ASN
1	D	340	ASN
1	D	410	HIS
1	D	433	HIS
1	D	542	ASN
1	D	778	HIS
1	D	916	HIS
2	E	41	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

30 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	$\#\|Z\| > 2$
3	NAG	I	1	3,1	14,14,15	0.47	0	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
3	BMA	I	3	3	11,11,12	0.98	1 (9%)	15,15,17	1.17	1 (6%)
3	MAN	I	4	3	11,11,12	1.02	0	15,15,17	1.04	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
4	NAG	J	2	4	14,14,15	0.57	0	17,19,21	0.40	0
4	NAG	K	1	4,1	14,14,15	0.33	0	17,19,21	0.54	0
4	NAG	K	2	4	14,14,15	0.41	0	17,19,21	0.38	0
5	NAG	L	1	1,5	14,14,15	0.64	1 (7%)	17,19,21	0.89	1 (5%)
5	NAG	L	2	5	14,14,15	0.18	0	17,19,21	0.64	0
5	BMA	L	3	5	11,11,12	1.61	2 (18%)	15,15,17	1.31	2 (13%)
5	MAN	L	4	5	11,11,12	1.55	3 (27%)	15,15,17	1.23	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.31	0	17,19,21	1.06	1 (5%)
3	NAG	M	2	3	14,14,15	0.58	1 (7%)	17,19,21	0.42	0
3	BMA	M	3	3	11,11,12	0.89	0	15,15,17	0.91	0
3	MAN	M	4	3	11,11,12	1.00	0	15,15,17	1.32	1 (6%)
4	NAG	N	1	4,1	14,14,15	0.22	0	17,19,21	0.96	1 (5%)
4	NAG	N	2	4	14,14,15	0.85	1 (7%)	17,19,21	0.47	0
4	NAG	O	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.72	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	O	2	4	14,14,15	0.68	0	17,19,21	0.40	0
6	NAG	P	1	1,6	14,14,15	0.30	0	17,19,21	0.63	0
6	NAG	P	2	6	14,14,15	0.49	0	17,19,21	0.82	1 (5%)
6	BMA	P	3	6	11,11,12	1.72	3 (27%)	15,15,17	2.10	6 (40%)
6	MAN	P	4	6	11,11,12	1.57	2 (18%)	15,15,17	1.27	2 (13%)
6	MAN	P	5	6	11,11,12	2.05	3 (27%)	15,15,17	1.65	1 (6%)
7	NAG	Q	1	1,7	14,14,15	0.76	1 (7%)	17,19,21	0.51	0
7	NAG	Q	2	7	14,14,15	0.30	0	17,19,21	0.63	0
7	BMA	Q	3	7	11,11,12	1.33	2 (18%)	15,15,17	1.14	0
4	NAG	R	1	4,1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)
4	NAG	R	2	4	14,14,15	0.90	1 (7%)	17,19,21	0.73	0

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

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

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	3	BMA	C1-C2	3.86	1.61	1.52
6	P	5	MAN	O5-C5	3.72	1.51	1.43
6	P	5	MAN	C2-C3	3.69	1.58	1.52
6	P	4	MAN	C1-C2	3.40	1.60	1.52
4	R	2	NAG	C1-C2	3.18	1.57	1.52
5	L	3	BMA	O3-C3	3.08	1.50	1.43
7	Q	3	BMA	O5-C1	-3.06	1.38	1.43
6	P	5	MAN	C1-C2	2.93	1.58	1.52
5	L	4	MAN	C2-C3	2.82	1.56	1.52
5	L	4	MAN	O5-C5	2.75	1.49	1.43
6	P	4	MAN	C2-C3	2.74	1.56	1.52
5	L	3	BMA	C2-C3	2.62	1.56	1.52
4	N	2	NAG	C1-C2	2.61	1.56	1.52
3	I	3	BMA	C1-C2	2.53	1.58	1.52
6	P	3	BMA	O5-C1	2.45	1.47	1.43
5	L	4	MAN	C1-C2	2.38	1.57	1.52
6	P	3	BMA	C2-C3	2.35	1.56	1.52
7	Q	3	BMA	C4-C5	2.32	1.57	1.53
7	Q	1	NAG	C1-C2	2.09	1.55	1.52
5	L	1	NAG	C1-C2	2.08	1.55	1.52
4	O	1	NAG	O5-C1	-2.04	1.40	1.43
3	M	2	NAG	O5-C1	-2.02	1.40	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	5	MAN	C1-O5-C5	4.91	118.85	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	3	BMA	C1-O5-C5	4.45	118.23	112.19
3	M	4	MAN	C1-O5-C5	4.03	117.66	112.19
5	L	4	MAN	C1-O5-C5	3.64	117.12	112.19
6	P	3	BMA	O5-C1-C2	3.08	115.53	110.77
6	P	3	BMA	C3-C4-C5	-3.02	104.85	110.24
6	P	3	BMA	O3-C3-C2	3.00	115.74	109.99
5	L	3	BMA	O3-C3-C2	2.92	115.58	109.99
3	I	4	MAN	C1-O5-C5	2.87	116.08	112.19
3	I	3	BMA	C1-O5-C5	2.84	116.04	112.19
3	M	1	NAG	C2-N2-C7	2.75	126.81	122.90
6	P	4	MAN	C1-O5-C5	2.60	115.71	112.19
4	N	1	NAG	C1-O5-C5	2.56	115.66	112.19
6	P	3	BMA	O2-C2-C1	2.54	114.35	109.15
5	L	1	NAG	C1-O5-C5	2.51	115.59	112.19
4	J	1	NAG	C1-O5-C5	2.49	115.56	112.19
3	I	2	NAG	C1-O5-C5	2.40	115.44	112.19
6	P	4	MAN	C1-C2-C3	2.29	112.49	109.67
4	R	1	NAG	C1-O5-C5	2.27	115.26	112.19
6	P	2	NAG	C2-N2-C7	2.26	126.11	122.90
5	L	3	BMA	C1-O5-C5	2.12	115.06	112.19
4	O	1	NAG	O4-C4-C5	2.08	114.46	109.30
6	P	3	BMA	O5-C5-C4	-2.04	105.87	110.83

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	1	NAG	C3-C2-N2-C7
6	P	1	NAG	C1-C2-N2-C7
6	P	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	L	4	MAN	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	M	4	MAN	O5-C5-C6-O6
5	L	4	MAN	O5-C5-C6-O6
6	P	4	MAN	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
3	M	4	MAN	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
6	P	2	NAG	C1-C2-N2-C7
4	N	1	NAG	C4-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
6	P	5	MAN	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
3	I	2	NAG	C3-C2-N2-C7
3	M	3	BMA	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C3-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7
6	P	1	NAG	C3-C2-N2-C7
4	K	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C3-C2-N2-C7

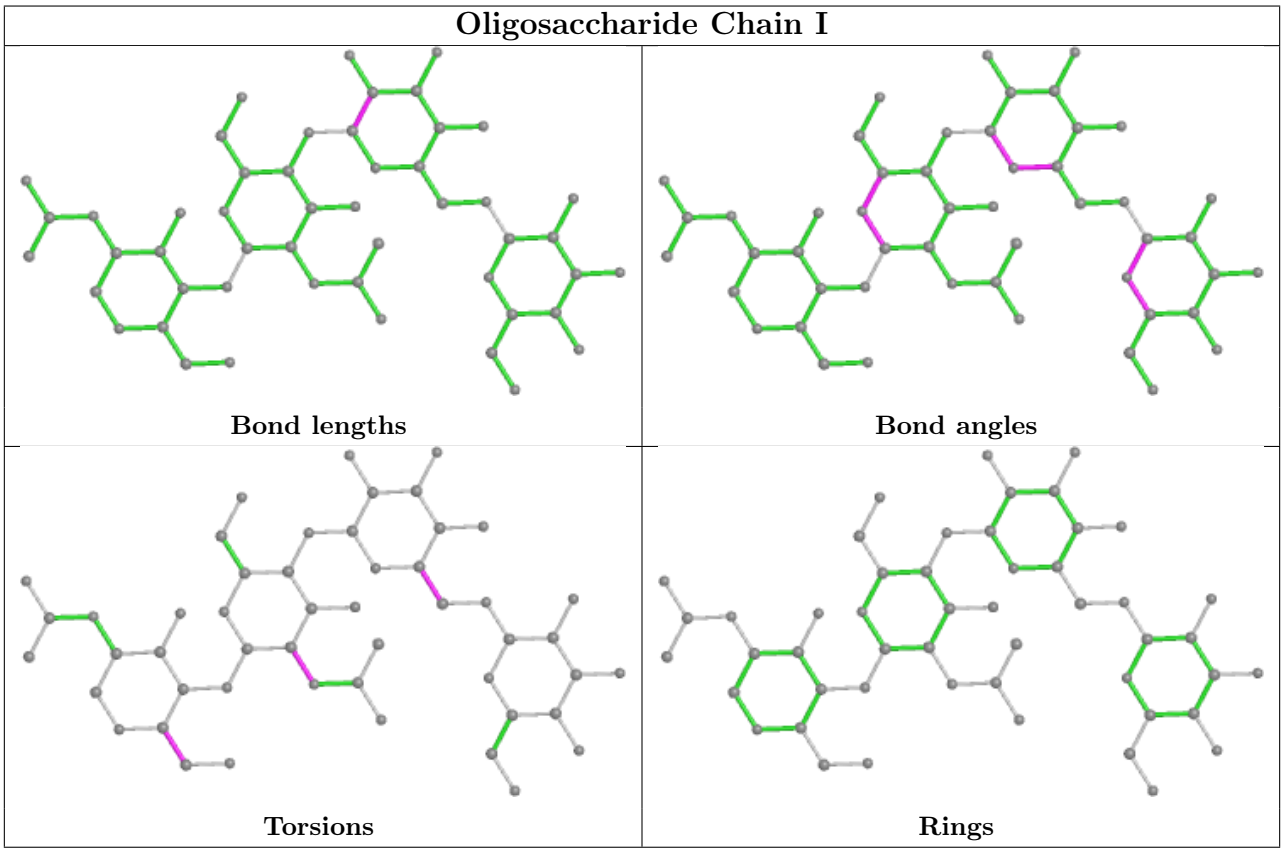
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	4	MAN	C1-C2-C3-C4-C5-O5

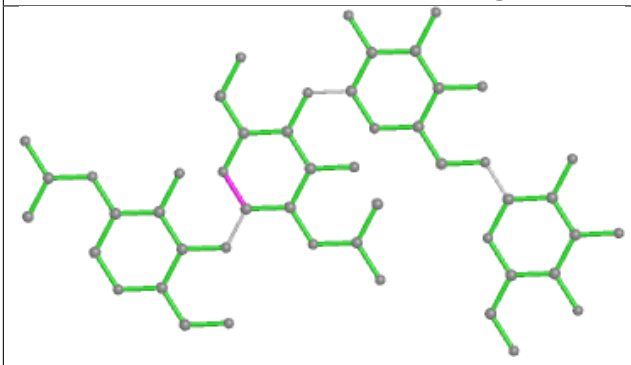
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	5	0
6	P	4	MAN	3	0
4	O	1	NAG	2	0
6	P	3	BMA	1	0
3	I	3	BMA	1	0
3	I	2	NAG	2	0
6	P	1	NAG	2	0
4	O	2	NAG	1	0

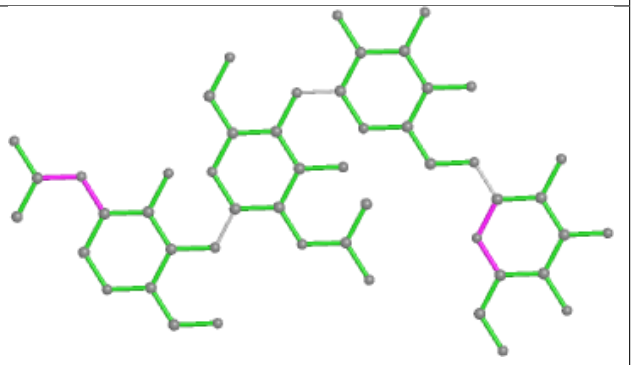
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



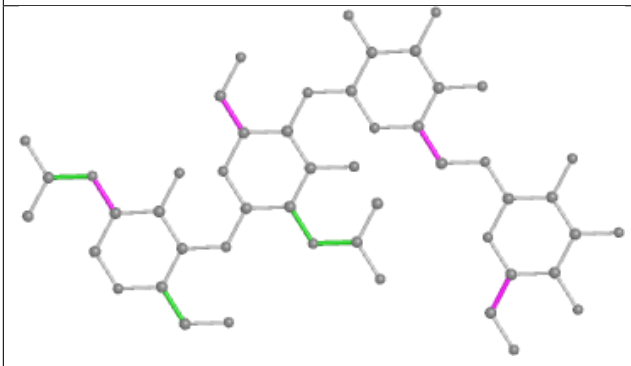
Oligosaccharide Chain M



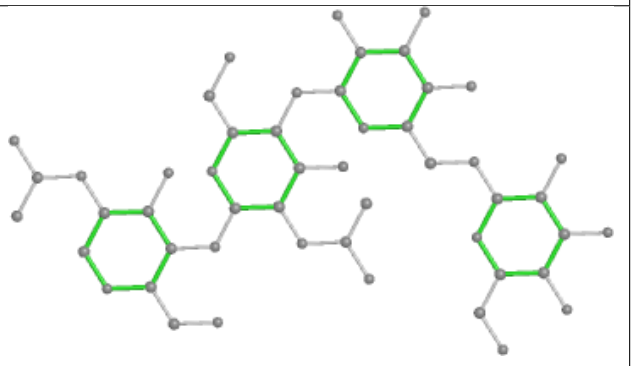
Bond lengths



Bond angles

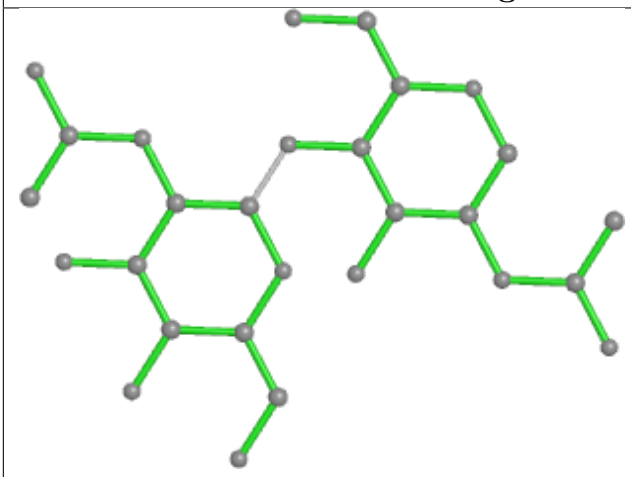


Torsions

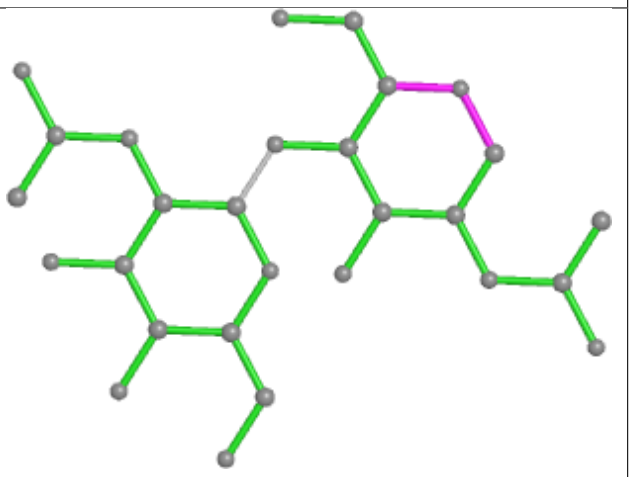


Rings

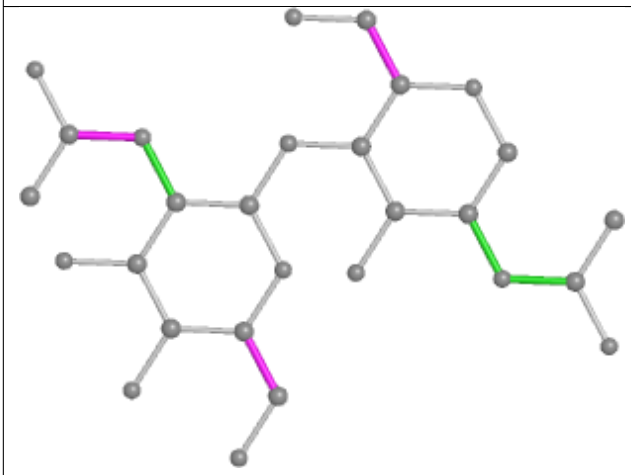
Oligosaccharide Chain J



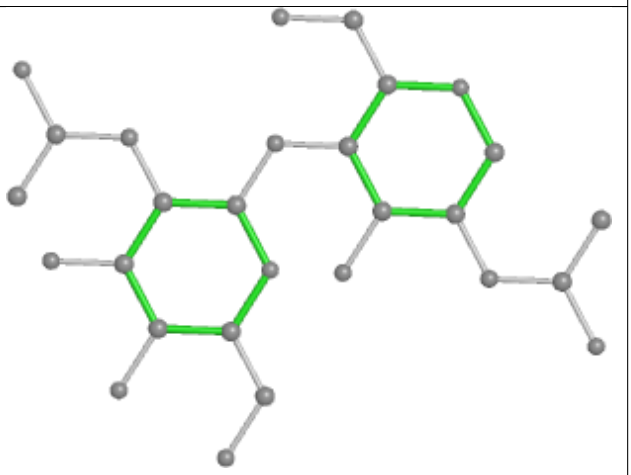
Bond lengths



Bond angles

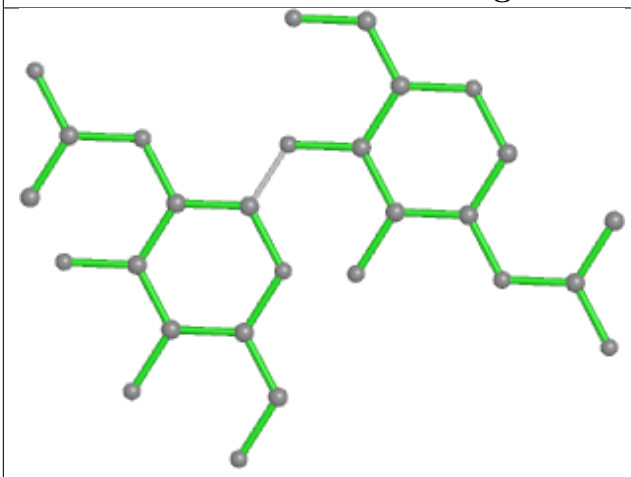


Torsions

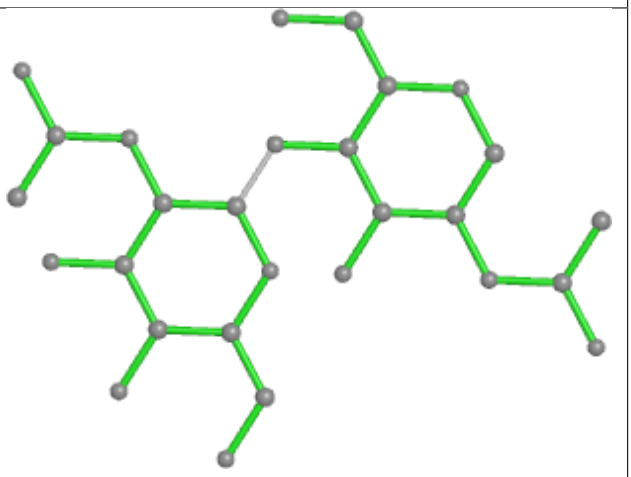


Rings

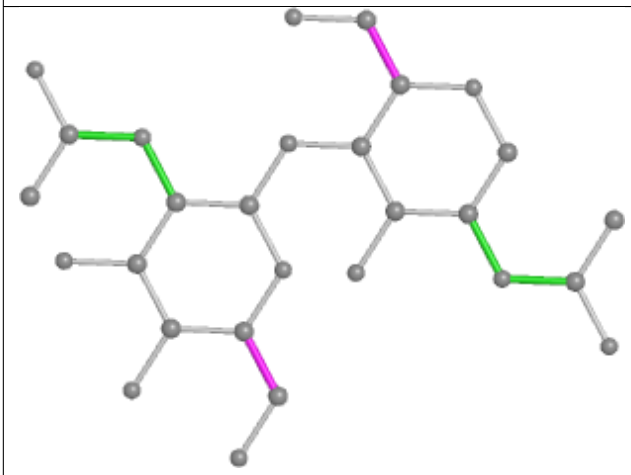
Oligosaccharide Chain K



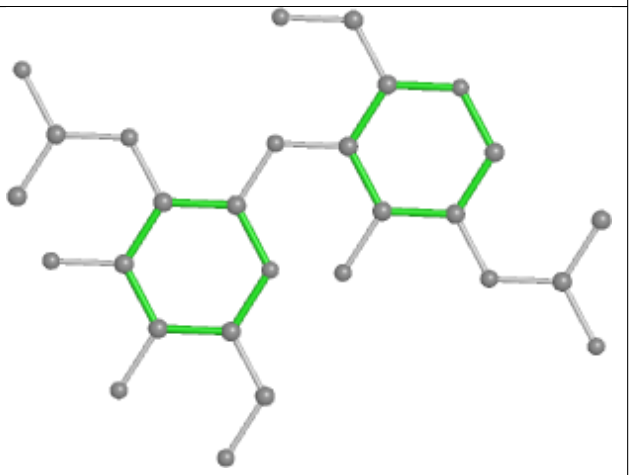
Bond lengths



Bond angles

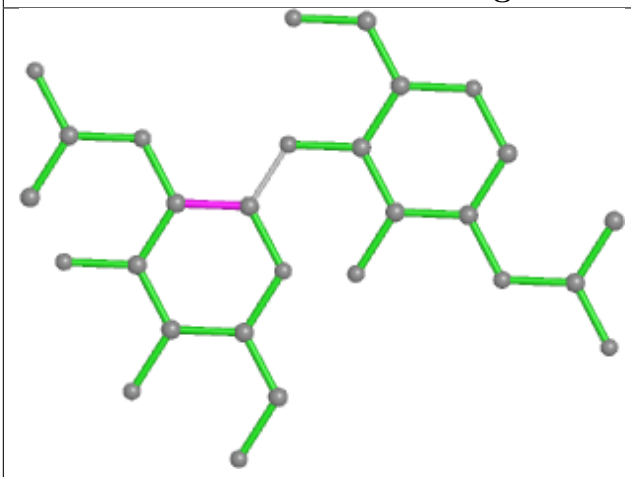


Torsions

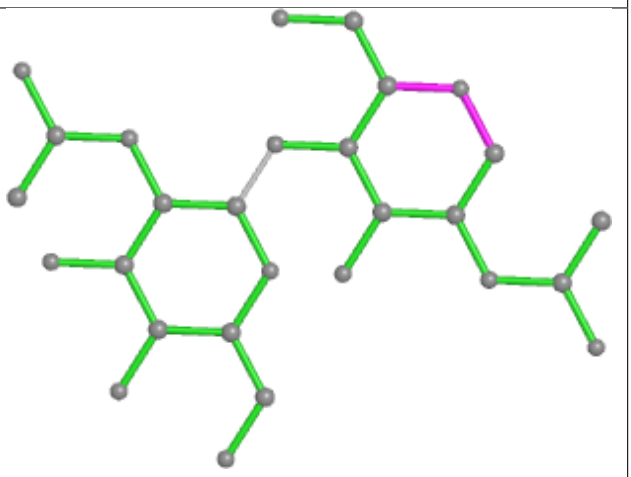


Rings

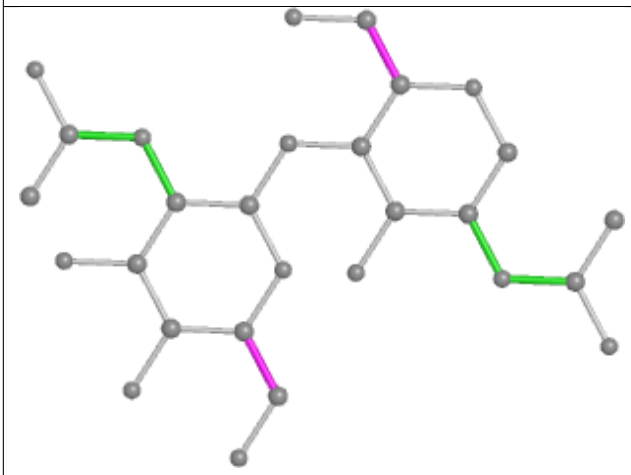
Oligosaccharide Chain N



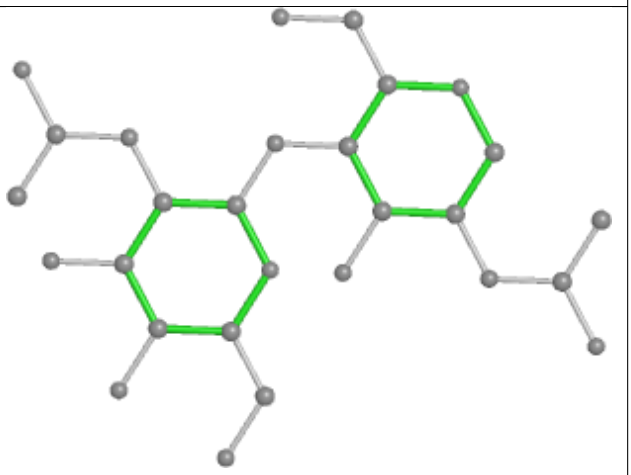
Bond lengths



Bond angles

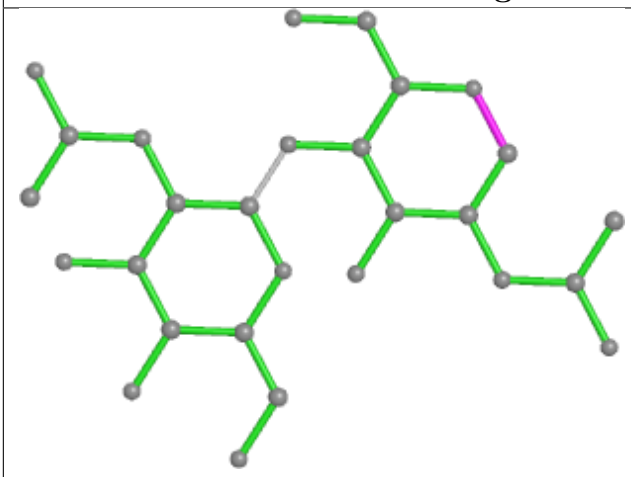


Torsions

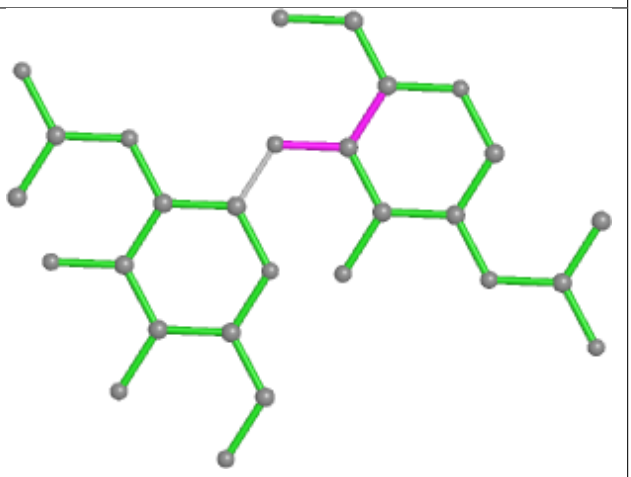


Rings

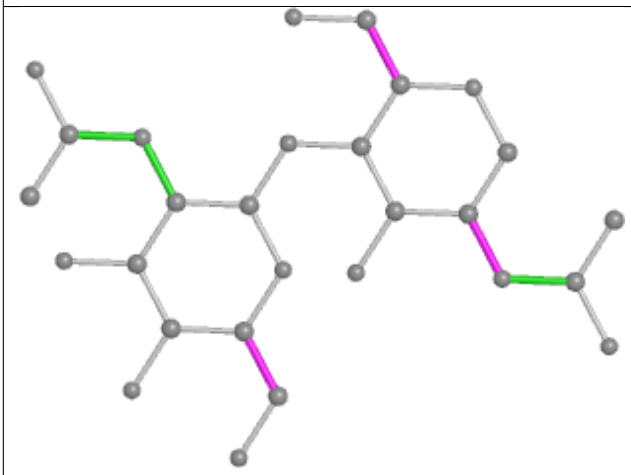
Oligosaccharide Chain O



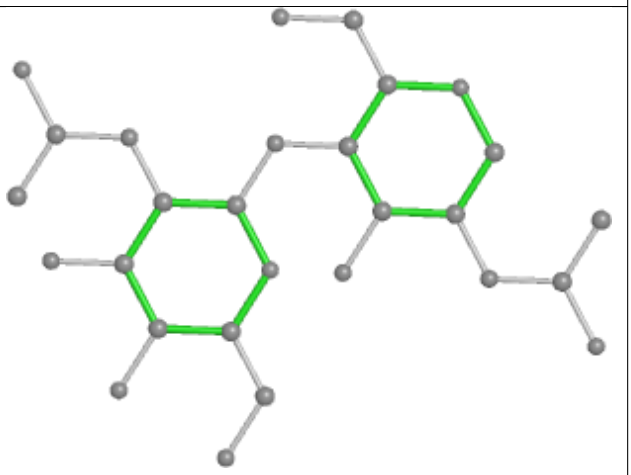
Bond lengths



Bond angles

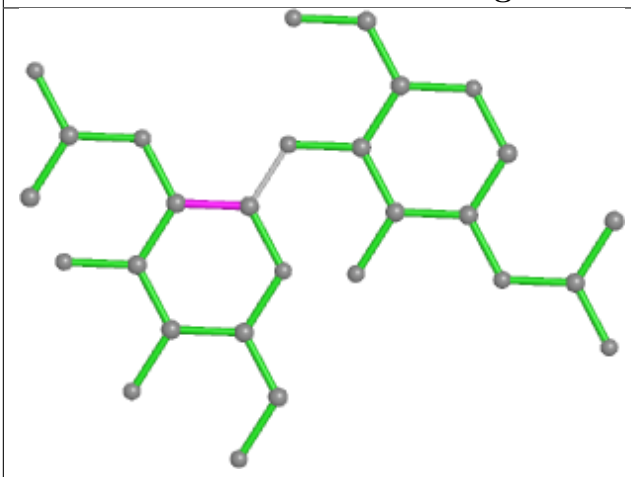


Torsions

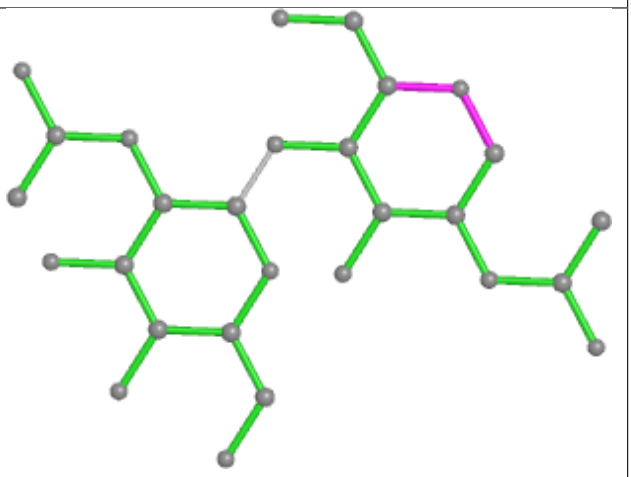


Rings

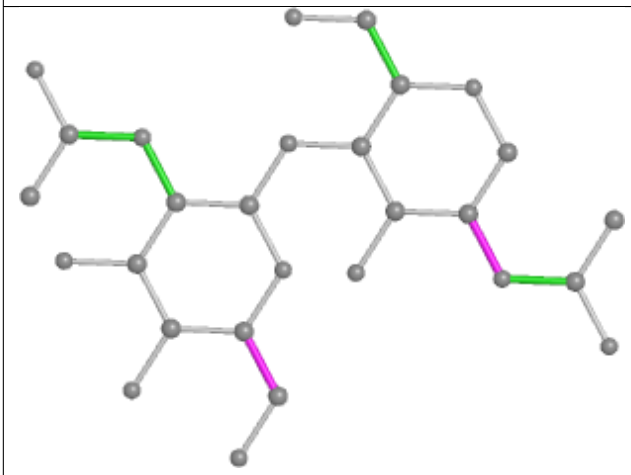
Oligosaccharide Chain R



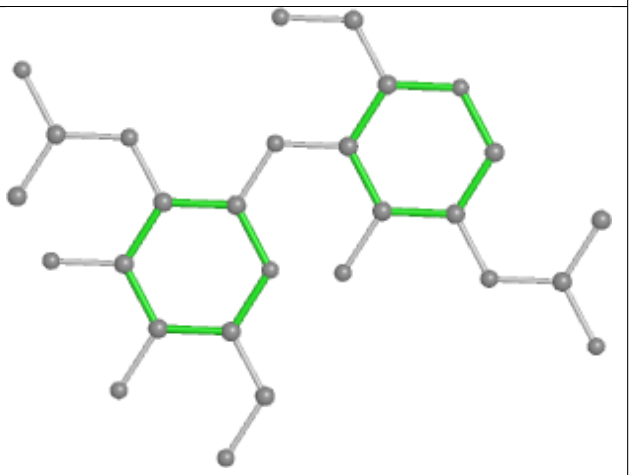
Bond lengths



Bond angles

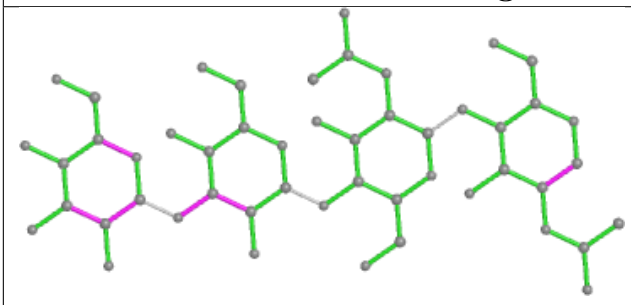


Torsions

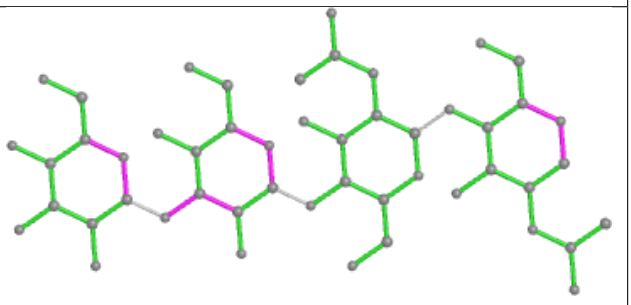


Rings

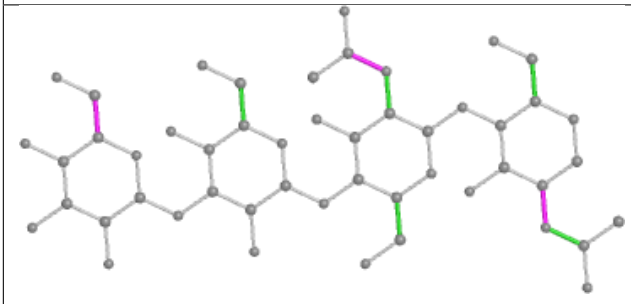
Oligosaccharide Chain L



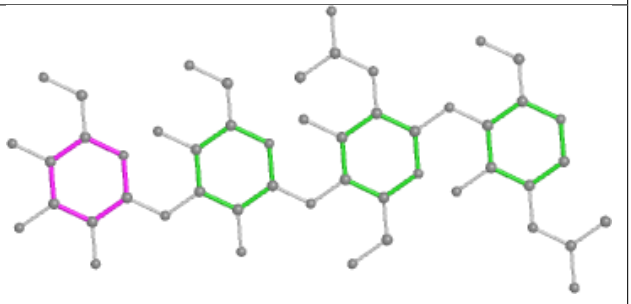
Bond lengths



Bond angles

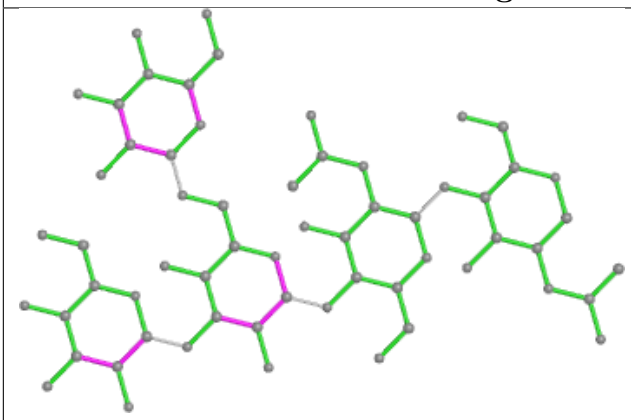


Torsions

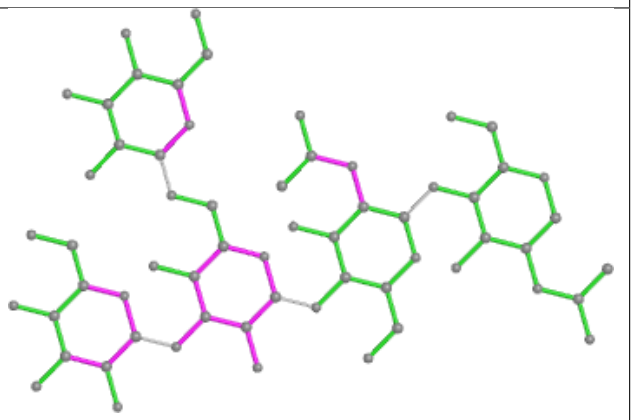


Rings

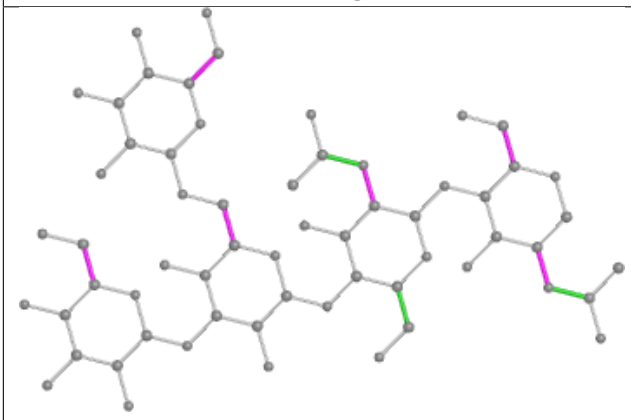
Oligosaccharide Chain P



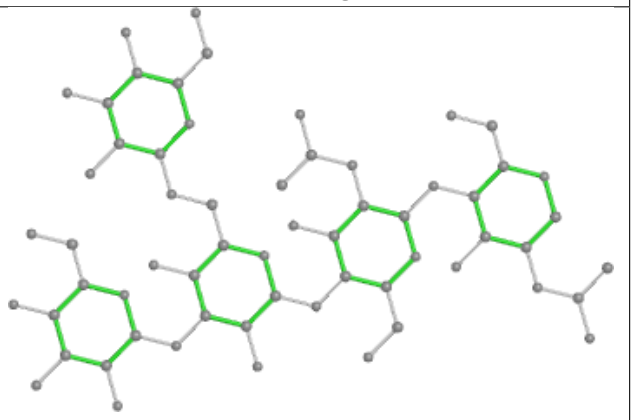
Bond lengths



Bond angles

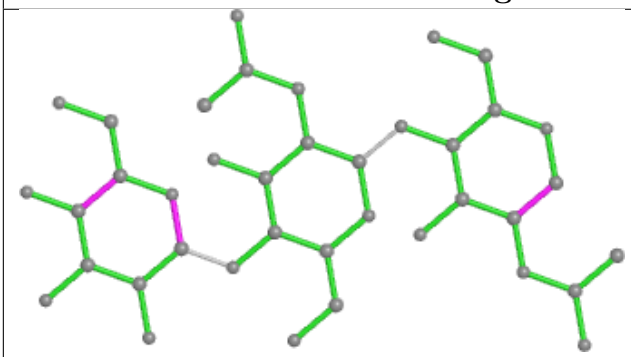


Torsions

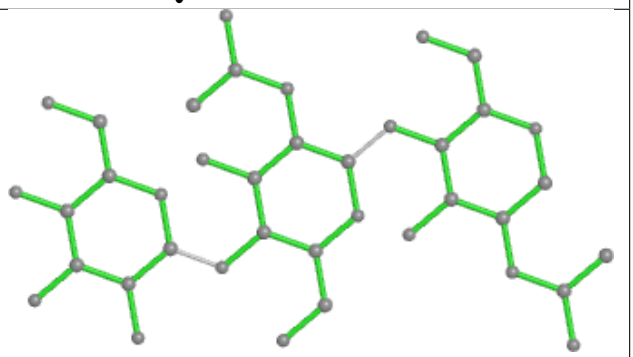


Rings

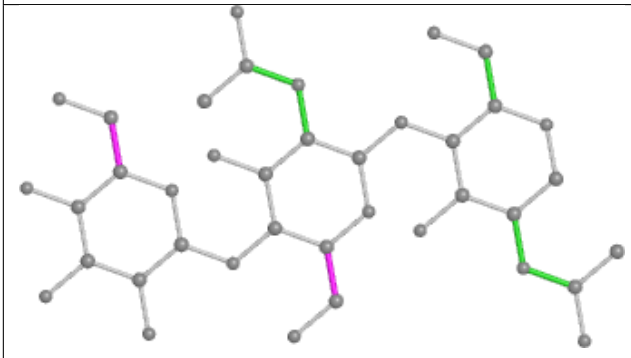
Oligosaccharide Chain Q



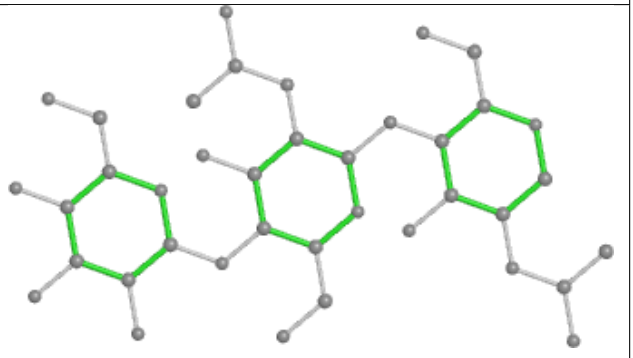
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

10 ligands 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	$\#\|Z\| > 2$
8	NAG	B	1103	1	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	D	1101	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
8	NAG	A	1103	1	14,14,15	0.60	1 (7%)	17,19,21	0.50	0
8	NAG	B	1101	1	14,14,15	0.82	1 (7%)	17,19,21	0.62	0
8	NAG	A	1101	1	14,14,15	0.57	0	17,19,21	0.52	0
8	NAG	C	1102	1	14,14,15	0.47	0	17,19,21	0.47	0
8	NAG	C	1101	1	14,14,15	0.65	0	17,19,21	0.76	0
8	NAG	D	1102	1	14,14,15	0.60	1 (7%)	17,19,21	0.62	0
8	NAG	A	1102	1	14,14,15	0.64	0	17,19,21	0.60	0
8	NAG	B	1102	1	14,14,15	0.48	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	1103	1	-	2/6/23/26	0/1/1/1
8	NAG	D	1101	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1103	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1101	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1101	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1102	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1101	1	-	2/6/23/26	0/1/1/1
8	NAG	D	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1102	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1101	NAG	O5-C1	2.35	1.47	1.43
8	A	1103	NAG	C1-C2	2.04	1.55	1.52
8	D	1102	NAG	C1-C2	2.03	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	1101	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1102	NAG	C4-C5-C6-O6
8	A	1101	NAG	O5-C5-C6-O6
8	B	1102	NAG	O5-C5-C6-O6
8	A	1101	NAG	C4-C5-C6-O6
8	A	1101	NAG	C8-C7-N2-C2
8	A	1101	NAG	O7-C7-N2-C2
8	B	1103	NAG	C8-C7-N2-C2
8	B	1103	NAG	O7-C7-N2-C2
8	C	1101	NAG	C8-C7-N2-C2
8	C	1101	NAG	O7-C7-N2-C2
8	C	1102	NAG	O5-C5-C6-O6
8	A	1102	NAG	O5-C5-C6-O6
8	B	1101	NAG	O5-C5-C6-O6
8	D	1101	NAG	O5-C5-C6-O6
8	D	1101	NAG	C1-C2-N2-C7
8	A	1102	NAG	C3-C2-N2-C7
8	A	1103	NAG	C4-C5-C6-O6
8	D	1102	NAG	O5-C5-C6-O6
8	D	1102	NAG	C4-C5-C6-O6
8	D	1101	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1103	NAG	1	0
8	D	1101	NAG	1	0
8	A	1103	NAG	1	0
8	B	1101	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1101	NAG	2	0
8	C	1101	NAG	1	0
8	D	1102	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	939/1007 (93%)	0.93	191 (20%)	1	1	136, 195, 266, 306	0
1	B	935/1007 (92%)	1.17	232 (24%)	0	0	156, 213, 258, 322	0
1	C	939/1007 (93%)	1.05	210 (22%)	0	1	109, 198, 254, 299	0
1	D	939/1007 (93%)	1.11	233 (24%)	0	0	123, 224, 290, 319	0
2	E	108/114 (94%)	2.23	45 (41%)	0	0	227, 296, 318, 335	0
2	F	108/114 (94%)	2.44	53 (49%)	0	0	277, 350, 369, 379	0
2	G	107/114 (93%)	1.72	46 (42%)	0	0	221, 264, 284, 289	0
2	H	105/114 (92%)	2.67	50 (47%)	0	0	295, 346, 370, 382	0
All	All	4180/4484 (93%)	1.19	1060 (25%)	0	0	109, 213, 315, 382	0

All (1060) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	76	PRO	14.0
1	B	243	GLN	13.0
2	E	115	PHE	13.0
2	H	70	SER	12.2
1	C	52	SER	11.7
2	E	114	THR	11.5
1	B	237	ALA	11.4
2	F	42	THR	11.4
2	E	109	THR	11.3
1	B	449	GLN	11.2
2	H	128	GLU	10.8
1	C	50	TYR	10.6
2	E	108	PHE	10.5
2	H	129	VAL	10.4
1	C	915	GLU	10.3
1	B	715	ASN	9.7

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Mol	Chain	Res	Type	RSRZ
1	D	744	ASN	9.6
1	B	263	HIS	9.5
1	D	417	PRO	9.4
2	H	118	ASP	9.4
2	E	119	PRO	9.3
2	F	43	ILE	9.3
1	B	220	ARG	9.3
1	D	915	GLU	9.2
2	H	94	SER	9.1
2	E	135	VAL	9.1
1	D	951	THR	9.1
1	B	915	GLU	8.8
1	C	916	HIS	8.7
1	B	730	ARG	8.6
2	H	73	VAL	8.6
1	C	662	GLY	8.3
2	H	92	THR	8.3
2	F	73	VAL	8.3
2	H	72	ALA	8.3
1	C	744	ASN	8.3
1	B	743	GLY	8.2
2	G	63	LEU	8.1
2	H	130	LYS	8.1
1	A	783	ARG	8.1
1	C	663	ALA	8.0
1	B	244	LEU	8.0
1	A	662	GLY	8.0
2	H	35	GLU	7.9
1	B	221	GLN	7.9
2	F	71	VAL	7.8
1	C	814	ASP	7.7
1	C	273	ARG	7.7
2	H	55	ALA	7.6
1	A	29	PRO	7.5
2	G	128	GLU	7.4
1	D	711	CYS	7.4
2	H	63	LEU	7.4
1	B	470	ASP	7.4
1	B	662	GLY	7.4
1	B	465	PRO	7.3
2	F	70	SER	7.2
1	B	242	GLN	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	186	ARG	7.1
1	D	715	ASN	7.1
2	H	39	ILE	7.1
1	A	915	GLU	7.0
2	H	113	LYS	7.0
2	H	114	THR	7.0
1	B	782	GLY	6.8
1	C	53	LYS	6.8
2	E	51	LEU	6.8
2	E	117	GLU	6.8
2	F	79	ASP	6.7
2	H	91	LYS	6.7
2	H	95	ILE	6.7
1	D	676	SER	6.6
1	A	73	SER	6.6
1	A	916	HIS	6.5
1	A	589	SER	6.5
1	D	632	MET	6.5
1	C	953	LEU	6.5
1	C	100	ARG	6.5
2	G	76	PRO	6.5
2	G	111	ASP	6.4
2	F	51	LEU	6.4
1	B	781	ILE	6.4
2	F	119	PRO	6.4
1	B	783	ARG	6.3
1	C	99	LEU	6.3
2	G	77	ASP	6.3
2	G	110	VAL	6.3
2	H	79	ASP	6.3
1	D	742	HIS	6.3
2	H	78	ASN	6.3
2	F	41	HIS	6.3
1	A	893	ASP	6.3
2	F	128	GLU	6.2
1	D	413	LEU	6.2
1	D	727	ARG	6.2
2	F	56	GLY	6.2
2	H	36	SER	6.1
1	B	768	SER	6.1
1	B	448	LYS	6.1
1	D	743	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	438	LYS	6.1
1	D	914	TRP	6.1
1	C	713	TYR	6.1
1	B	262	VAL	6.0
2	G	115	PHE	6.0
2	E	49	ALA	6.0
1	A	895	SER	6.0
2	F	108	PHE	6.0
1	B	645	ILE	6.0
1	B	264	VAL	5.9
1	A	447	ILE	5.9
2	E	133	CYS	5.9
1	A	920	GLU	5.9
2	G	45	ASP	5.9
1	B	805	HIS	5.9
1	B	644	GLU	5.8
1	B	712	GLN	5.8
2	H	127	LEU	5.8
1	C	715	ASN	5.8
1	D	416	VAL	5.8
2	E	66	TYR	5.8
1	C	664	LYS	5.7
1	A	30	LYS	5.7
1	D	262	VAL	5.7
1	D	372	GLU	5.7
1	C	977	ASN	5.7
1	B	60	ILE	5.7
2	G	124	PRO	5.7
1	B	58	THR	5.6
1	C	56	THR	5.6
1	D	209	ILE	5.5
2	H	40	SER	5.5
1	B	934	LYS	5.5
1	A	680	ALA	5.5
1	B	633	LYS	5.5
1	D	945	PHE	5.5
2	E	52	SER	5.5
1	B	540	PRO	5.5
2	H	34	ASP	5.5
1	B	663	ALA	5.4
2	H	37	GLY	5.4
2	F	110	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
2	E	73	VAL	5.4
1	C	84	GLN	5.4
1	B	791	ILE	5.4
2	H	131	TYR	5.4
2	F	127	LEU	5.4
1	D	349	VAL	5.4
2	E	76	PRO	5.4
2	G	129	VAL	5.3
1	B	512	ASP	5.3
1	D	607	ALA	5.3
1	B	815	LEU	5.3
2	F	97	GLU	5.3
1	B	653	ASP	5.3
1	D	414	THR	5.3
1	C	109	PHE	5.3
1	D	448	LYS	5.3
1	A	274	VAL	5.3
1	C	884	SER	5.3
2	F	72	ALA	5.3
2	H	116	THR	5.3
1	B	714	GLY	5.3
1	A	36	PRO	5.3
1	A	448	LYS	5.3
1	A	486	LEU	5.3
1	D	781	ILE	5.3
1	C	883	ILE	5.2
1	A	744	ASN	5.2
1	D	348	GLY	5.2
1	A	50	TYR	5.2
2	E	110	VAL	5.2
1	A	94	THR	5.2
2	F	126	TYR	5.2
2	F	55	ALA	5.2
1	B	238	THR	5.2
1	C	392	LEU	5.1
2	H	74	CYS	5.1
1	C	209	ILE	5.1
1	B	59	PRO	5.1
1	D	347	GLY	5.1
2	E	35	GLU	5.1
1	C	35	ALA	5.0
1	B	632	MET	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	420	ILE	5.0
1	C	849	ARG	5.0
1	C	274	VAL	5.0
2	H	77	ASP	5.0
1	D	415	GLU	5.0
1	C	210	GLU	5.0
1	A	828	PHE	5.0
1	B	57	ILE	5.0
1	B	770	VAL	5.0
1	D	812	THR	5.0
1	C	659	MET	4.9
1	D	233	ASP	4.9
1	A	93	LEU	4.9
1	A	953	LEU	4.9
1	C	791	ILE	4.9
1	D	425	GLN	4.9
2	H	42	THR	4.9
1	C	658	TRP	4.9
2	H	38	THR	4.9
2	F	135	VAL	4.9
1	D	373	VAL	4.8
1	D	967	MET	4.8
1	D	628	ALA	4.8
1	C	790	HIS	4.8
1	D	234	LEU	4.8
1	A	46	LEU	4.8
1	C	393	LEU	4.8
1	B	466	TYR	4.8
1	B	344	GLN	4.8
1	C	57	ILE	4.8
1	C	709	ILE	4.8
2	H	121	PRO	4.8
1	D	947	THR	4.7
2	E	50	GLU	4.7
1	B	767	LEU	4.7
2	H	64	GLY	4.7
1	C	34	CYS	4.7
1	A	952	VAL	4.7
2	E	134	VAL	4.7
1	A	425	GLN	4.7
1	D	709	ILE	4.7
1	B	916	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
2	G	86	ASN	4.7
1	B	511	LEU	4.7
1	A	449	GLN	4.6
1	A	109	PHE	4.6
1	B	254	LEU	4.6
1	C	54	ASN	4.6
1	B	732	ASP	4.6
1	D	710	CYS	4.6
1	A	850	GLY	4.6
1	B	701	LYS	4.6
1	C	51	SER	4.6
2	G	51	LEU	4.6
2	F	75	LEU	4.6
1	B	274	VAL	4.6
2	G	64	GLY	4.6
1	B	654	CYS	4.6
2	E	106	CYS	4.5
1	C	954	SER	4.5
1	B	89	TYR	4.5
1	B	172	LEU	4.5
1	B	646	SER	4.5
2	E	118	ASP	4.5
1	B	629	THR	4.5
2	E	74	CYS	4.5
1	D	730	ARG	4.5
2	F	52	SER	4.4
1	C	74	LEU	4.4
1	D	179	SER	4.4
1	B	139	GLU	4.4
1	B	769	GLY	4.4
1	A	100	ARG	4.4
1	B	345	LEU	4.4
1	D	768	SER	4.4
1	A	753	PHE	4.3
1	B	253	ASP	4.3
1	B	416	VAL	4.3
1	D	712	GLN	4.3
1	C	661	GLY	4.3
1	D	164	ARG	4.3
1	D	686	ILE	4.3
1	C	767	LEU	4.3
1	A	273	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	66	TYR	4.3
1	B	655	GLN	4.3
1	B	222	ILE	4.3
1	B	778	HIS	4.3
1	D	441	GLN	4.3
1	A	663	ALA	4.3
2	G	112	LYS	4.3
1	D	633	LYS	4.3
1	D	429	VAL	4.3
1	A	780	PHE	4.3
1	C	85	PHE	4.3
1	D	783	ARG	4.3
1	C	815	LEU	4.3
1	C	211	GLN	4.2
1	D	261	VAL	4.2
1	D	109	PHE	4.2
1	C	695	ASP	4.2
1	C	714	GLY	4.2
1	D	369	PHE	4.2
1	D	263	HIS	4.2
1	A	876	HIS	4.2
1	B	229	ILE	4.2
1	A	782	GLY	4.2
2	F	94	SER	4.2
1	D	740	ARG	4.2
1	B	634	VAL	4.2
1	B	643	VAL	4.2
1	A	31	PHE	4.2
1	B	765	ILE	4.2
2	G	88	GLN	4.2
1	B	252	VAL	4.1
1	C	525	ASP	4.1
1	D	627	VAL	4.1
1	C	655	GLN	4.1
1	C	895	SER	4.1
2	E	116	THR	4.1
1	C	686	ILE	4.1
2	E	82	PRO	4.1
1	A	463	ILE	4.1
1	A	829	LEU	4.1
1	D	454	ASP	4.1
1	A	45	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	823	LEU	4.1
1	C	316	LYS	4.1
1	C	547	ASN	4.1
1	A	151	PHE	4.1
1	A	300	SER	4.0
1	D	212	PHE	4.0
1	D	631	SER	4.0
1	D	788	ARG	4.0
1	C	804	PHE	4.0
2	E	88	GLN	4.0
1	C	766	ILE	4.0
1	A	99	LEU	4.0
1	D	540	PRO	4.0
1	B	520	GLY	4.0
1	C	391	GLU	4.0
2	E	90	HIS	4.0
1	B	603	LEU	4.0
2	G	130	LYS	4.0
2	H	119	PRO	3.9
1	D	582	ASN	3.9
1	A	56	THR	3.9
2	H	50	GLU	3.9
1	C	124	GLU	3.9
2	F	29	ALA	3.9
1	B	195	GLN	3.9
1	C	885	LEU	3.9
1	A	954	SER	3.9
1	B	273	ARG	3.9
1	D	929	VAL	3.9
1	D	324	TRP	3.9
1	D	849	ARG	3.9
1	D	468	PHE	3.9
1	B	168	SER	3.9
1	D	747	MET	3.9
1	C	789	LEU	3.9
1	A	38	PRO	3.9
1	A	879	ALA	3.9
1	D	637	ALA	3.9
1	B	295	GLU	3.9
1	A	462	SER	3.9
1	A	185	LEU	3.8
1	D	926	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	767	LEU	3.8
1	D	243	GLN	3.8
1	D	764	GLU	3.8
1	B	515	LEU	3.8
1	C	49	ASP	3.8
1	C	851	ILE	3.8
1	D	948	ASN	3.8
1	A	862	THR	3.8
1	A	951	THR	3.8
1	C	665	PRO	3.8
1	D	635	VAL	3.8
1	D	780	PHE	3.8
1	B	134	SER	3.8
1	C	93	LEU	3.7
1	D	139	GLU	3.7
1	A	791	ILE	3.7
1	B	265	ASN	3.7
1	D	63	SER	3.7
1	D	634	VAL	3.7
2	F	136	PRO	3.7
1	B	106	THR	3.7
1	C	55	THR	3.7
1	C	369	PHE	3.7
1	A	892	CYS	3.7
1	C	123	LEU	3.7
2	E	65	ASN	3.7
2	H	112	LYS	3.7
1	D	880	LEU	3.7
1	D	919	ALA	3.7
1	B	284	LEU	3.7
1	D	65	TYR	3.7
1	A	57	ILE	3.7
1	B	302	PHE	3.7
1	B	320	LEU	3.7
2	E	98	LYS	3.7
1	A	824	SER	3.7
1	B	196	LEU	3.7
1	A	871	ILE	3.7
1	D	232	LEU	3.7
1	C	65	TYR	3.7
1	B	82	ASN	3.6
1	B	170	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	40	GLN	3.6
2	G	74	CYS	3.6
1	B	212	PHE	3.6
1	C	232	LEU	3.6
1	A	487	LEU	3.6
1	C	932	PHE	3.6
1	C	90	PHE	3.6
1	D	636	GLU	3.6
1	B	162	PRO	3.6
1	D	713	TYR	3.6
1	D	813	LEU	3.6
1	C	657	GLY	3.6
1	B	171	HIS	3.6
2	G	108	PHE	3.6
2	F	65	ASN	3.6
1	A	730	ARG	3.6
1	B	444	LEU	3.6
1	A	74	LEU	3.5
1	A	568	LEU	3.5
1	A	32	CYS	3.5
1	D	210	GLU	3.5
1	D	922	PHE	3.5
1	B	608	LEU	3.5
2	H	56	GLY	3.5
1	C	972	PHE	3.5
2	G	92	THR	3.5
1	C	114	PHE	3.5
1	D	885	LEU	3.5
2	H	76	PRO	3.5
1	D	946	LEU	3.5
1	C	231	GLU	3.5
1	D	774	GLN	3.5
1	B	839	LEU	3.5
1	C	685	GLN	3.5
1	C	278	VAL	3.5
1	C	956	TYR	3.5
1	D	701	LYS	3.5
1	D	789	LEU	3.5
1	C	917	ASN	3.5
1	D	455	LEU	3.5
1	D	717	ASP	3.5
1	C	94	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	335	LEU	3.4
1	A	590	LEU	3.4
1	C	317	LEU	3.4
1	C	677	CYS	3.4
1	B	206	LEU	3.4
1	B	245	ASP	3.4
1	D	697	LEU	3.4
2	F	80	ILE	3.4
1	B	286	ALA	3.4
1	B	232	LEU	3.4
1	C	359	LEU	3.4
1	D	932	PHE	3.4
1	C	272	LYS	3.4
1	B	307	LEU	3.4
1	B	464	GLY	3.4
1	D	673	GLU	3.4
1	C	39	VAL	3.4
1	C	765	ILE	3.4
1	D	492	PHE	3.4
2	F	67	GLY	3.4
1	A	849	ARG	3.4
1	C	117	LEU	3.4
1	D	716	CYS	3.4
1	D	846	THR	3.4
1	D	921	TRP	3.4
1	B	667	VAL	3.3
2	H	41	HIS	3.3
1	D	162	PRO	3.3
1	C	101	ILE	3.3
1	C	294	ILE	3.3
1	A	804	PHE	3.3
1	B	538	ALA	3.3
1	A	98	HIS	3.3
1	C	423	VAL	3.3
1	D	749	PRO	3.3
1	B	752	GLU	3.3
1	B	627	VAL	3.3
1	B	471	SER	3.3
1	C	850	GLY	3.3
2	F	69	PHE	3.3
1	B	473	GLU	3.3
1	A	739	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	3.3
1	B	56	THR	3.3
1	D	283	SER	3.3
1	A	851	ILE	3.3
1	B	83	PHE	3.3
1	D	446	LYS	3.3
1	D	977	ASN	3.3
1	A	880	LEU	3.3
1	B	236	LEU	3.3
1	B	602	LYS	3.3
1	C	142	LEU	3.3
1	C	973	LEU	3.3
1	B	420	ILE	3.3
1	C	152	SER	3.3
1	C	295	GLU	3.3
1	B	439	VAL	3.3
1	D	30	LYS	3.3
1	C	200	ASP	3.3
2	G	131	TYR	3.3
1	B	169	LEU	3.3
1	B	451	HIS	3.3
1	D	708	CYS	3.3
1	B	319	SER	3.3
1	D	960	MET	3.3
1	D	920	GLU	3.3
2	F	99	LYS	3.3
1	B	324	TRP	3.2
1	C	320	LEU	3.2
1	D	350	LEU	3.2
1	A	494	ARG	3.2
1	A	113	LEU	3.2
1	B	806	THR	3.2
1	D	606	THR	3.2
1	A	765	ILE	3.2
1	D	178	SER	3.2
1	B	309	MET	3.2
2	G	117	GLU	3.2
1	B	250	ARG	3.2
1	C	187	ARG	3.2
1	C	919	ALA	3.2
1	D	782	GLY	3.2
2	F	49	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	497	LYS	3.2
1	D	442	TYR	3.2
1	C	185	LEU	3.2
1	D	698	CYS	3.2
1	B	665	PRO	3.2
1	A	439	VAL	3.2
1	B	539	LEU	3.2
2	F	37	GLY	3.2
1	A	980	ILE	3.2
1	A	298	ASN	3.2
1	D	853	GLU	3.2
1	B	450	LEU	3.2
2	F	36	SER	3.2
1	B	209	ILE	3.2
1	C	962	ASN	3.2
1	A	39	VAL	3.2
2	F	45	ASP	3.2
1	A	792	ASN	3.1
1	D	675	ALA	3.1
1	A	117	LEU	3.1
1	B	652	CYS	3.1
1	C	199	VAL	3.1
2	G	109	THR	3.1
1	A	309	MET	3.1
1	B	641	LEU	3.1
1	B	463	ILE	3.1
1	C	367	ARG	3.1
1	D	943	LYS	3.1
1	B	386	SER	3.1
1	B	461	GLN	3.1
1	B	50	TYR	3.1
1	B	207	THR	3.1
1	C	780	PHE	3.1
1	A	413	LEU	3.1
1	A	700	TYR	3.1
1	A	825	GLY	3.1
1	A	49	ASP	3.1
2	E	111	ASP	3.1
1	C	632	MET	3.1
1	A	664	LYS	3.1
1	C	76	ILE	3.1
1	D	61	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	492	PHE	3.1
1	B	437	ALA	3.1
1	D	320	LEU	3.1
1	D	244	LEU	3.1
1	C	952	VAL	3.1
1	A	870	ASP	3.1
1	C	783	ARG	3.1
1	D	734	PHE	3.1
1	D	29	PRO	3.1
1	B	272	LYS	3.1
1	B	436	ILE	3.1
1	C	401	LEU	3.1
1	D	431	LEU	3.1
1	C	957	PRO	3.1
1	C	696	LEU	3.1
2	H	80	ILE	3.1
1	B	863	LEU	3.0
2	G	125	LYS	3.0
1	B	135	PHE	3.0
2	F	98	LYS	3.0
1	B	956	TYR	3.0
1	B	255	THR	3.0
1	C	402	LYS	3.0
1	D	50	TYR	3.0
1	A	794	THR	3.0
1	D	702	SER	3.0
2	G	114	THR	3.0
2	E	34	ASP	3.0
1	A	930	VAL	3.0
1	B	935	VAL	3.0
2	E	113	LYS	3.0
1	D	245	ASP	3.0
1	D	836	GLN	3.0
1	B	161	LEU	3.0
2	H	93	LYS	3.0
1	A	416	VAL	3.0
1	B	695	ASP	3.0
2	E	107	TYR	3.0
1	B	790	HIS	3.0
1	A	114	PHE	3.0
1	A	116	ASP	3.0
1	D	639	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	43	ILE	3.0
2	G	62	VAL	3.0
1	A	72	ARG	3.0
1	A	737	ASN	3.0
1	A	861	LEU	3.0
2	F	125	LYS	3.0
2	G	61	ILE	3.0
2	H	49	ALA	3.0
1	A	853	GLU	3.0
1	B	771	THR	3.0
2	F	44	CYS	3.0
1	C	948	ASN	3.0
1	A	90	PHE	2.9
1	D	345	LEU	2.9
1	D	385	LEU	2.9
1	A	645	ILE	2.9
1	B	185	LEU	2.9
1	B	521	LEU	2.9
2	F	113	LYS	2.9
1	B	213	LEU	2.9
1	C	38	PRO	2.9
1	D	674	THR	2.9
1	C	572	SER	2.9
1	D	524	LEU	2.9
1	A	417	PRO	2.9
1	B	810	LEU	2.9
1	B	742	HIS	2.9
1	D	419	ALA	2.9
1	A	691	LEU	2.9
1	A	758	LEU	2.9
1	A	70	ASN	2.9
2	G	89	ASN	2.9
1	B	628	ALA	2.9
1	B	828	PHE	2.9
1	D	594	ASP	2.9
2	F	54	PRO	2.9
1	A	859	LYS	2.9
1	C	852	PHE	2.9
2	G	66	TYR	2.9
1	A	479	VAL	2.9
1	D	359	LEU	2.9
1	B	676	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	628	ALA	2.9
1	D	693	LYS	2.9
1	D	539	LEU	2.9
1	D	861	LEU	2.9
1	B	980	ILE	2.9
1	D	687	GLN	2.8
2	G	105	MET	2.8
1	D	581	MET	2.8
1	D	302	PHE	2.8
1	A	349	VAL	2.8
1	C	503	MET	2.8
1	D	828	PHE	2.8
2	F	101	ASN	2.8
1	A	350	LEU	2.8
1	A	641	LEU	2.8
2	E	75	LEU	2.8
1	D	110	SER	2.8
2	E	55	ALA	2.8
1	C	687	GLN	2.8
1	D	242	GLN	2.8
1	C	958	PRO	2.8
1	B	581	MET	2.8
1	B	496	PRO	2.8
1	A	95	ALA	2.8
1	A	415	GLU	2.8
1	D	954	SER	2.8
1	B	972	PHE	2.8
1	D	221	GLN	2.8
1	C	275	PRO	2.8
1	D	213	LEU	2.8
1	D	361	LEU	2.8
1	D	478	ASP	2.8
1	A	424	GLU	2.8
1	A	310	LEU	2.8
1	C	853	GLU	2.8
1	C	548	ALA	2.8
1	C	214	ARG	2.8
1	C	792	ASN	2.8
1	B	518	ALA	2.7
1	B	501	ILE	2.7
1	B	90	PHE	2.7
1	D	837	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	779	SER	2.7
1	A	746	SER	2.7
1	B	241	LEU	2.7
1	C	257	LEU	2.7
1	B	651	ILE	2.7
1	B	157	ARG	2.7
1	B	780	PHE	2.7
1	B	359	LEU	2.7
1	D	860	TYR	2.7
1	C	73	SER	2.7
1	B	163	GLN	2.7
1	C	526	VAL	2.7
1	C	694	LYS	2.7
1	C	271	LEU	2.7
2	F	81	VAL	2.7
1	C	707	GLU	2.7
1	B	183	PRO	2.7
1	D	423	VAL	2.7
1	A	320	LEU	2.7
1	B	403	LEU	2.7
1	D	617	LEU	2.7
1	D	950	THR	2.7
1	B	460	LEU	2.7
1	D	137	MET	2.7
1	D	883	ILE	2.7
1	A	254	LEU	2.7
1	B	384	ARG	2.7
1	B	500	LYS	2.7
1	C	72	ARG	2.7
1	C	420	ILE	2.7
1	C	319	SER	2.7
1	D	844	PHE	2.6
1	A	640	PRO	2.6
1	C	48	CYS	2.6
1	C	980	ILE	2.6
1	D	532	LEU	2.6
1	A	917	ASN	2.6
1	A	136	GLU	2.6
2	G	118	ASP	2.6
1	B	85	PHE	2.6
2	G	42	THR	2.6
1	D	200	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	62	VAL	2.6
1	B	128	ILE	2.6
1	C	945	PHE	2.6
1	B	862	THR	2.6
1	A	877	SER	2.6
1	D	630	GLU	2.6
1	B	658	TRP	2.6
1	C	961	GLY	2.6
1	D	393	LEU	2.6
2	G	127	LEU	2.6
1	A	928	LEU	2.6
1	D	257	LEU	2.6
2	G	87	CYS	2.6
1	C	813	LEU	2.6
1	C	930	VAL	2.6
1	B	484	ILE	2.6
1	A	681	VAL	2.6
1	D	608	LEU	2.6
1	D	695	ASP	2.6
1	C	876	HIS	2.6
1	A	732	ASP	2.6
1	C	31	PHE	2.6
1	C	75	PHE	2.6
1	B	285	VAL	2.6
1	C	368	VAL	2.6
1	A	321	PRO	2.6
1	A	472	SER	2.6
1	D	360	ASP	2.6
2	E	62	VAL	2.5
1	C	71	ILE	2.5
1	C	673	GLU	2.5
1	B	197	LEU	2.5
1	D	466	TYR	2.5
1	A	929	VAL	2.5
2	H	31	PRO	2.5
1	D	374	LEU	2.5
1	D	477	LEU	2.5
1	A	819	SER	2.5
1	C	848	SER	2.5
2	G	46	GLY	2.5
1	B	275	PRO	2.5
2	F	38	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	89	TYR	2.5
1	D	85	PHE	2.5
1	C	831	CYS	2.5
1	C	969	ILE	2.5
1	A	926	ARG	2.5
1	C	118	ALA	2.5
1	B	438	LYS	2.5
1	B	488	PHE	2.5
2	F	112	LYS	2.5
1	C	535	LYS	2.5
2	E	89	ASN	2.5
1	D	758	LEU	2.5
1	B	424	GLU	2.5
1	B	700	TYR	2.5
2	G	44	CYS	2.5
1	B	952	VAL	2.5
2	F	88	GLN	2.5
1	C	217	PRO	2.5
1	A	646	SER	2.5
1	B	462	SER	2.5
1	D	241	LEU	2.5
1	B	160	GLU	2.5
2	G	68	ARG	2.5
1	D	959	ASN	2.5
1	A	232	LEU	2.5
1	A	818	ASN	2.5
1	D	401	LEU	2.5
1	D	412	LYS	2.5
1	D	471	SER	2.5
1	A	308	GLU	2.5
1	A	745	SER	2.5
1	C	660	ILE	2.5
1	D	804	PHE	2.5
1	C	629	THR	2.4
2	E	128	GLU	2.4
1	A	414	THR	2.4
1	B	709	ILE	2.4
1	B	230	ALA	2.4
1	B	468	PHE	2.4
1	D	114	PHE	2.4
2	F	74	CYS	2.4
1	D	609	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	755	VAL	2.4
1	D	398	LEU	2.4
1	D	767	LEU	2.4
1	C	108	HIS	2.4
2	G	69	PHE	2.4
1	B	717	ASP	2.4
2	G	75	LEU	2.4
1	C	163	GLN	2.4
1	A	402	LYS	2.4
1	D	418	ALA	2.4
1	A	860	TYR	2.4
1	D	925	HIS	2.4
2	F	82	PRO	2.4
1	A	729	PHE	2.4
1	A	756	SER	2.4
1	B	317	LEU	2.4
1	B	402	LYS	2.4
1	B	251	ILE	2.4
1	A	796	LEU	2.4
1	A	768	SER	2.4
1	D	923	SER	2.4
2	E	112	LYS	2.4
1	B	146	ALA	2.4
1	B	702	SER	2.4
1	D	658	TRP	2.4
1	D	863	LEU	2.4
1	A	638	VAL	2.4
2	H	71	VAL	2.4
1	A	37	ASP	2.4
1	A	71	ILE	2.4
1	C	151	PHE	2.4
1	C	380	ILE	2.4
1	D	729	PHE	2.4
1	C	215	GLY	2.4
1	D	721	VAL	2.4
1	D	748	VAL	2.4
1	A	815	LEU	2.4
1	B	637	ALA	2.4
1	D	845	SER	2.3
1	B	107	THR	2.3
1	B	475	HIS	2.3
2	E	71	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	165	LEU	2.3
1	D	775	LEU	2.3
1	D	854	LYS	2.3
1	B	287	LEU	2.3
2	E	63	LEU	2.3
1	B	734	PHE	2.3
1	D	799	ILE	2.3
1	B	713	TYR	2.3
1	D	453	VAL	2.3
1	D	645	ILE	2.3
1	A	233	ASP	2.3
1	A	637	ALA	2.3
1	D	220	ARG	2.3
1	D	254	LEU	2.3
1	C	80	ASN	2.3
1	D	265	ASN	2.3
1	B	164	ARG	2.3
1	B	492	PHE	2.3
1	D	705	GLU	2.3
1	C	534	LEU	2.3
1	A	175	LEU	2.3
1	C	515	LEU	2.3
1	C	524	LEU	2.3
1	D	745	SER	2.3
2	F	120	CYS	2.3
1	B	166	LEU	2.3
1	C	233	ASP	2.3
1	C	345	LEU	2.3
1	C	656	MET	2.3
1	C	816	SER	2.3
1	B	104	CYS	2.3
1	B	390	LEU	2.3
1	D	444	LEU	2.3
1	A	571	VAL	2.3
1	A	345	LEU	2.3
1	B	81	ASN	2.3
1	C	893	ASP	2.3
1	B	589	SER	2.3
1	D	843	ARG	2.3
1	C	307	LEU	2.3
1	C	398	LEU	2.3
1	C	717	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	770	VAL	2.3
1	A	524	LEU	2.3
1	C	516	THR	2.3
2	H	83	SER	2.3
1	D	918	ALA	2.3
1	C	511	LEU	2.3
1	C	645	ILE	2.3
1	C	573	LEU	2.2
1	C	710	CYS	2.2
1	B	630	GLU	2.2
1	B	744	ASN	2.2
1	B	977	ASN	2.2
1	C	926	ARG	2.2
1	A	569	LYS	2.2
1	D	791	ILE	2.2
1	A	35	ALA	2.2
2	G	113	LYS	2.2
1	D	543	LEU	2.2
2	F	46	GLY	2.2
1	A	701	LYS	2.2
1	A	137	MET	2.2
1	C	490	ASP	2.2
1	C	839	LEU	2.2
2	E	48	ALA	2.2
1	A	526	VAL	2.2
1	B	426	LEU	2.2
1	B	772	LEU	2.2
1	D	370	ARG	2.2
1	A	675	ALA	2.2
1	A	702	SER	2.2
2	E	126	TYR	2.2
1	A	593	LEU	2.2
1	A	75	PHE	2.2
1	A	148	LEU	2.2
1	A	275	PRO	2.2
1	B	503	MET	2.2
1	D	273	ARG	2.2
1	D	384	ARG	2.2
1	C	190	SER	2.2
1	D	403	LEU	2.2
2	F	77	ASP	2.2
1	B	895	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	941	VAL	2.2
2	H	32	THR	2.2
1	A	676	SER	2.2
1	B	472	SER	2.2
1	D	223	SER	2.2
1	A	665	PRO	2.2
1	A	122	ARG	2.2
1	A	918	ALA	2.2
2	G	43	ILE	2.2
1	C	191	CYS	2.2
1	A	329	GLU	2.2
1	B	494	ARG	2.2
1	B	586	ILE	2.2
1	B	427	LYS	2.2
1	C	366	LEU	2.2
1	D	704	CYS	2.2
1	A	858	LEU	2.1
1	B	158	ASN	2.1
1	D	595	VAL	2.1
1	A	44	LYS	2.1
1	C	365	GLN	2.1
1	B	953	LEU	2.1
1	D	274	VAL	2.1
2	F	122	ASN	2.1
1	A	426	LEU	2.1
1	A	921	TRP	2.1
1	B	506	ASN	2.1
1	B	861	LEU	2.1
1	C	37	ASP	2.1
2	G	79	ASP	2.1
1	D	180	ASN	2.1
1	D	976	TYR	2.1
1	A	762	ALA	2.1
2	G	65	ASN	2.1
2	G	72	ALA	2.1
2	G	78	ASN	2.1
1	B	346	THR	2.1
1	D	557	THR	2.1
1	A	503	MET	2.1
1	A	881	SER	2.1
1	C	923	SER	2.1
1	D	568	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	885	LEU	2.1
1	D	325	LEU	2.1
2	F	68	ARG	2.1
1	A	325	LEU	2.1
2	H	29	ALA	2.1
1	A	932	PHE	2.1
1	C	755	VAL	2.1
1	D	436	ILE	2.1
1	A	491	ALA	2.1
1	C	538	ALA	2.1
1	A	206	LEU	2.1
1	A	617	LEU	2.1
1	B	621	GLY	2.1
1	D	222	ILE	2.1
1	A	748	VAL	2.1
1	B	876	HIS	2.1
2	E	94	SER	2.1
1	A	630	GLU	2.1
1	D	980	ILE	2.1
1	B	425	GLN	2.1
1	B	476	SER	2.1
1	B	922	PHE	2.1
1	C	95	ALA	2.1
1	C	176	ASN	2.1
1	C	922	PHE	2.1
1	C	175	LEU	2.1
1	A	67	GLN	2.1
1	B	671	ASP	2.1
1	A	958	PRO	2.1
1	D	496	PRO	2.1
1	A	766	ILE	2.1
1	A	749	PRO	2.1
1	C	779	SER	2.1
2	E	125	LYS	2.1
1	B	740	ARG	2.1
1	A	712	GLN	2.1
1	C	446	LYS	2.1
1	D	534	LEU	2.1
1	B	219	ILE	2.1
1	A	477	LEU	2.0
1	C	370	ARG	2.0
1	D	603	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	101	ILE	2.0
1	C	492	PHE	2.0
1	C	591	GLU	2.0
1	D	737	ASN	2.0
2	H	132	ASN	2.0
1	D	583	ALA	2.0
1	C	46	LEU	2.0
2	H	117	GLU	2.0
2	F	78	ASN	2.0
2	H	65	ASN	2.0
1	D	99	LEU	2.0
1	C	98	HIS	2.0
2	G	52	SER	2.0
1	B	664	LYS	2.0
1	C	406	LEU	2.0
1	C	419	ALA	2.0
1	D	535	LYS	2.0
1	B	814	ASP	2.0
1	D	264	VAL	2.0
2	G	73	VAL	2.0
1	C	828	PHE	2.0
1	A	620	LYS	2.0
1	A	661	GLY	2.0
2	E	81	VAL	2.0
1	A	793	GLY	2.0
1	B	88	ALA	2.0
1	D	284	LEU	2.0
1	B	760	VAL	2.0
1	C	894	CYS	2.0
1	D	771	THR	2.0
1	C	678	SER	2.0
1	B	366	LEU	2.0
1	C	234	LEU	2.0
1	D	755	VAL	2.0
1	C	508	ILE	2.0
1	C	920	GLU	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)

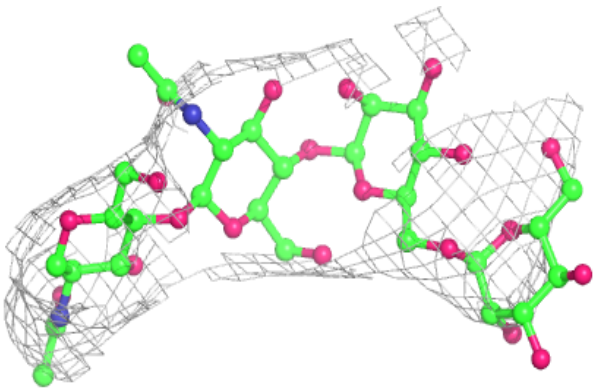
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

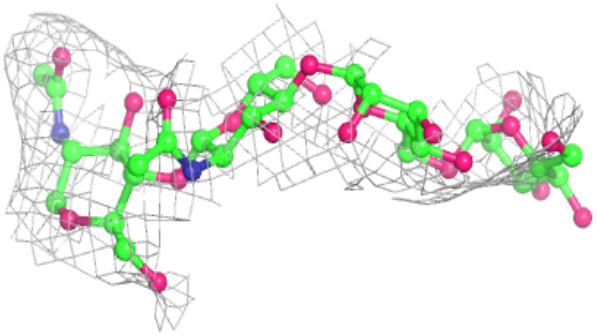
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	N	2	14/15	0.50	0.42	226,226,226,226	0
4	NAG	K	1	14/15	0.59	0.45	225,225,225,225	0
5	MAN	L	4	11/12	0.62	0.36	257,257,257,257	0
6	MAN	P	4	11/12	0.67	0.23	222,222,222,222	0
7	NAG	Q	1	14/15	0.72	0.29	199,199,199,199	0
3	NAG	I	1	14/15	0.73	0.28	199,199,199,199	0
3	MAN	I	4	11/12	0.74	0.57	246,246,246,246	0
4	NAG	R	2	14/15	0.75	0.28	253,253,253,253	0
4	NAG	N	1	14/15	0.77	0.25	233,233,233,233	0
6	MAN	P	5	11/12	0.77	0.33	229,229,229,229	0
3	BMA	I	3	11/12	0.77	0.27	230,230,230,230	0
3	MAN	M	4	11/12	0.78	0.32	251,251,251,251	0
5	NAG	L	2	14/15	0.78	0.31	191,191,191,191	0
6	NAG	P	1	14/15	0.79	0.37	224,224,224,224	0
4	NAG	O	2	14/15	0.79	0.51	228,228,228,228	0
4	NAG	J	1	14/15	0.81	0.49	211,211,211,211	0
7	BMA	Q	3	11/12	0.81	0.32	234,234,234,234	0
3	NAG	M	1	14/15	0.82	0.20	210,210,210,210	0
3	BMA	M	3	11/12	0.82	0.31	230,230,230,230	0
4	NAG	J	2	14/15	0.82	0.65	239,239,239,239	0
3	NAG	I	2	14/15	0.84	0.33	224,224,224,224	0
6	NAG	P	2	14/15	0.85	0.40	234,234,234,234	0
4	NAG	R	1	14/15	0.86	0.51	255,255,255,255	0
6	BMA	P	3	11/12	0.88	0.22	233,233,233,233	0
5	NAG	L	1	14/15	0.89	0.25	199,199,199,199	0
4	NAG	O	1	14/15	0.89	0.27	202,202,202,202	0
7	NAG	Q	2	14/15	0.90	0.49	221,221,221,221	0
4	NAG	K	2	14/15	0.90	0.32	246,246,246,246	0
5	BMA	L	3	11/12	0.91	0.17	234,234,234,234	0
3	NAG	M	2	14/15	0.93	0.22	212,212,212,212	0

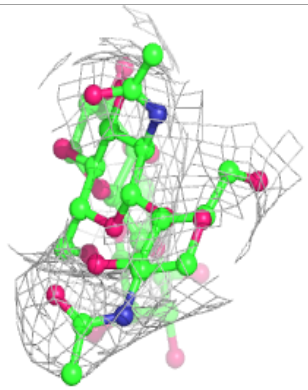
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

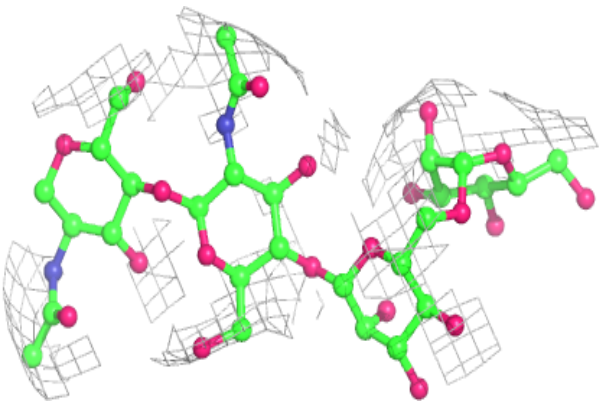


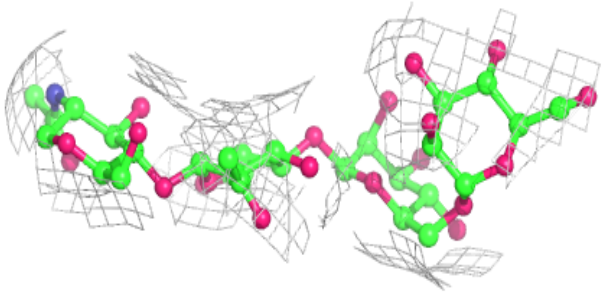


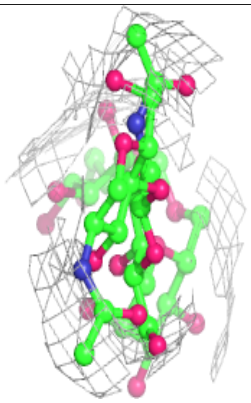


Electron density around Chain M:

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

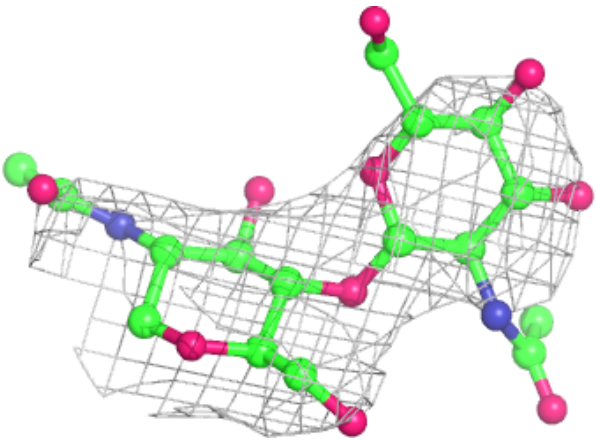


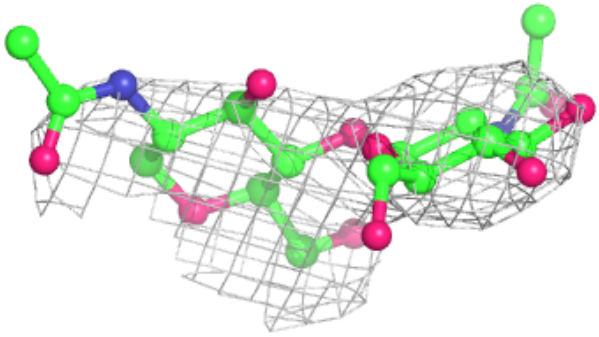


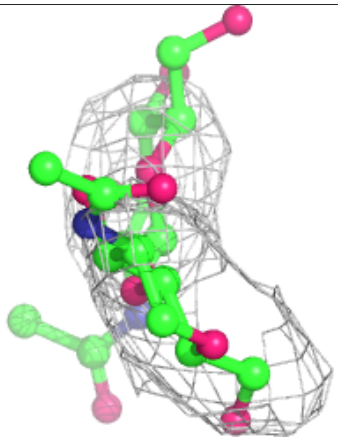


Electron density around Chain J:

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

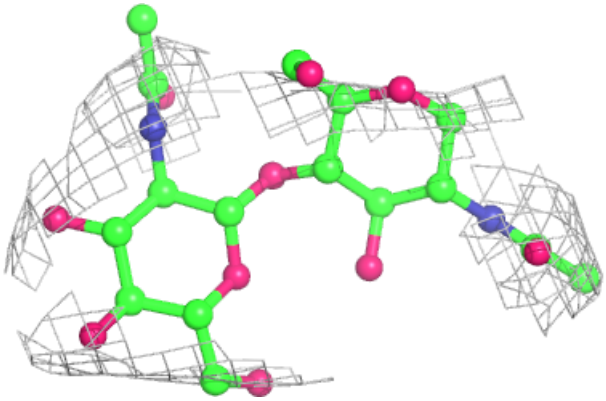


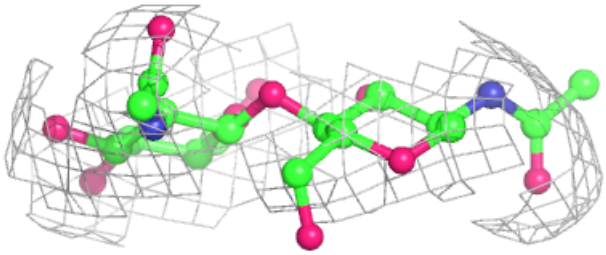


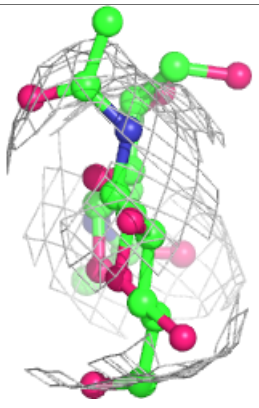


Electron density around Chain K:

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

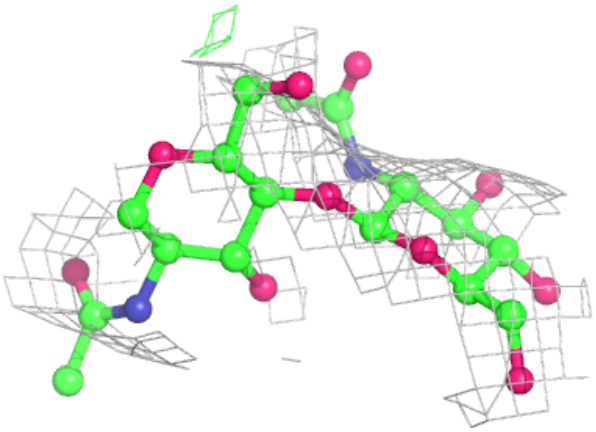


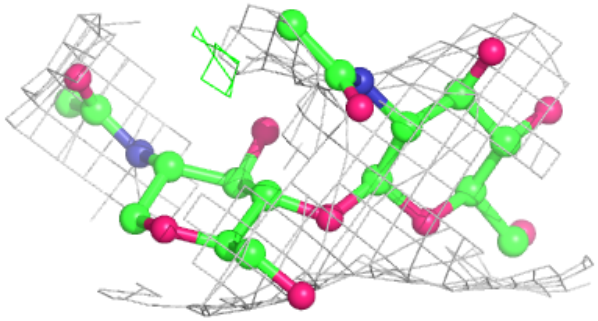


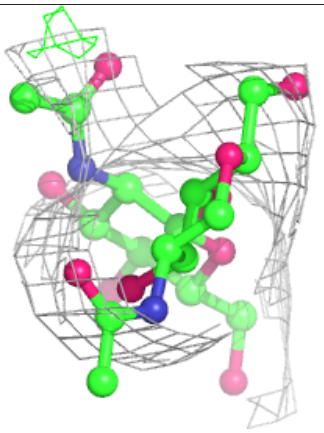


Electron density around Chain N:

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

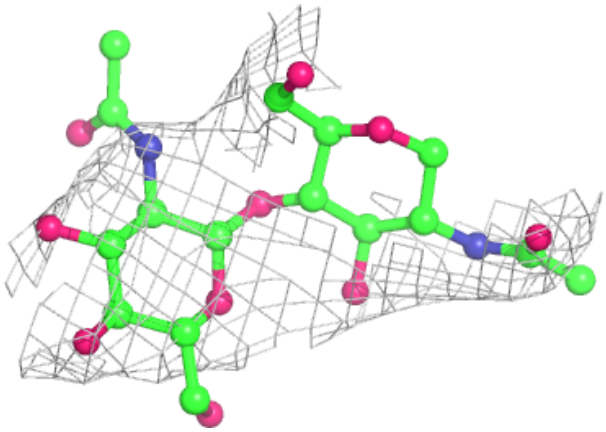


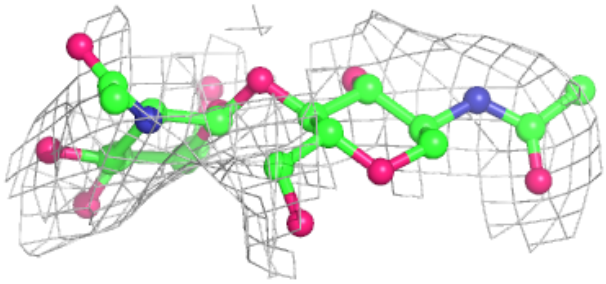


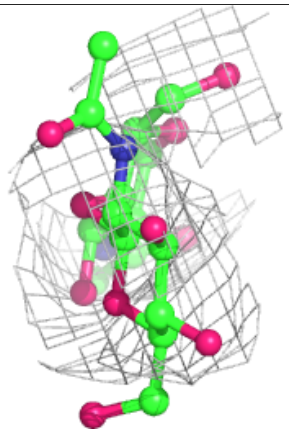


Electron density around Chain O:

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

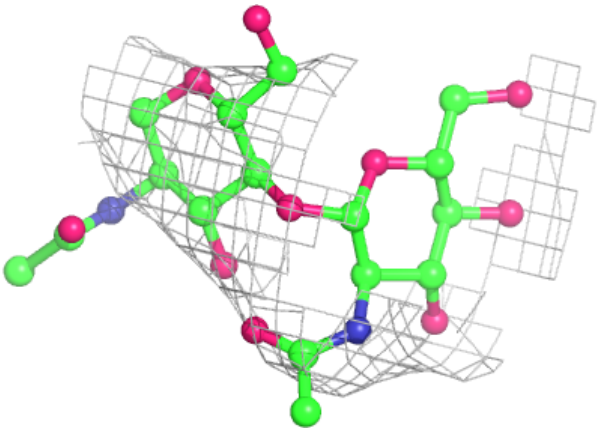


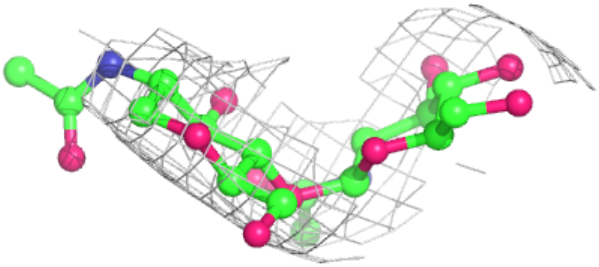


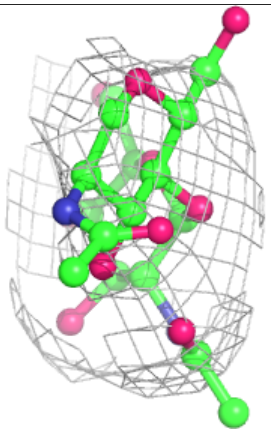


Electron density around Chain R:

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

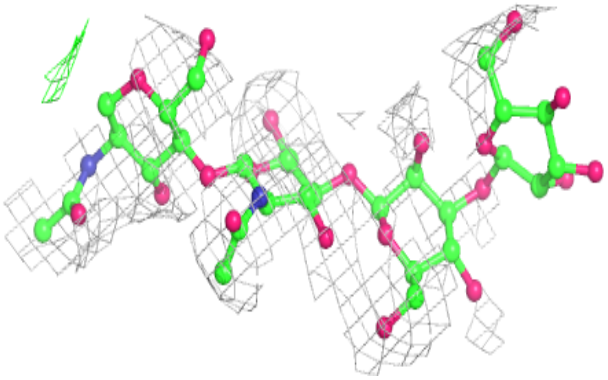


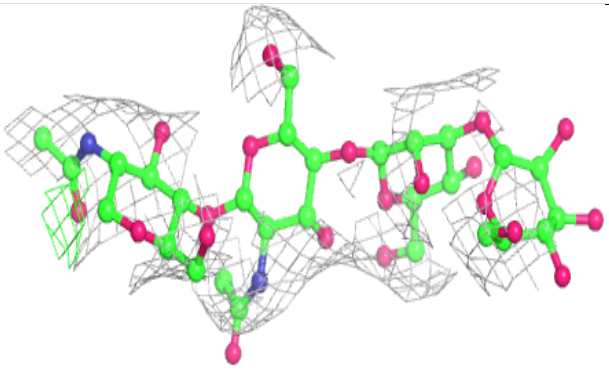


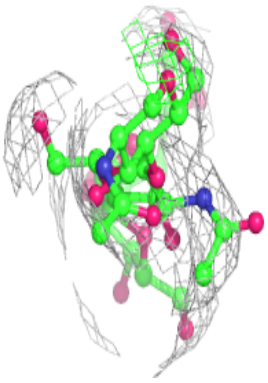


Electron density around Chain L:

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

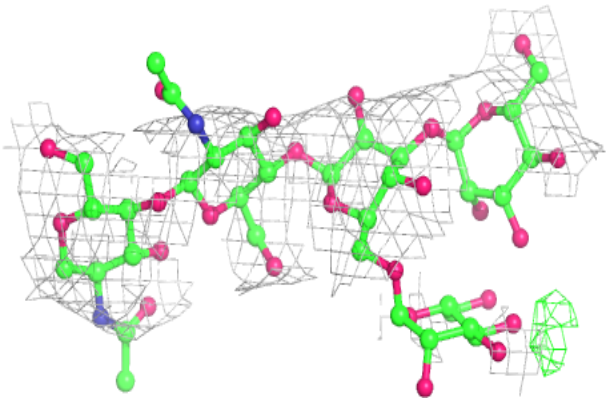


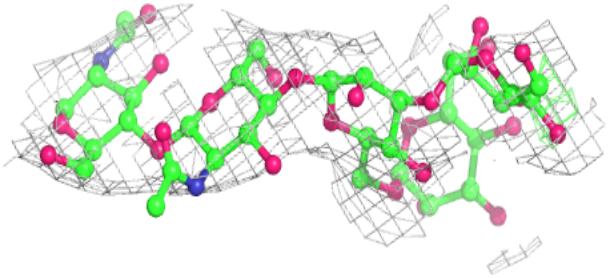


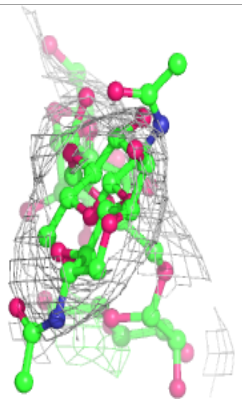


Electron density around Chain P:

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

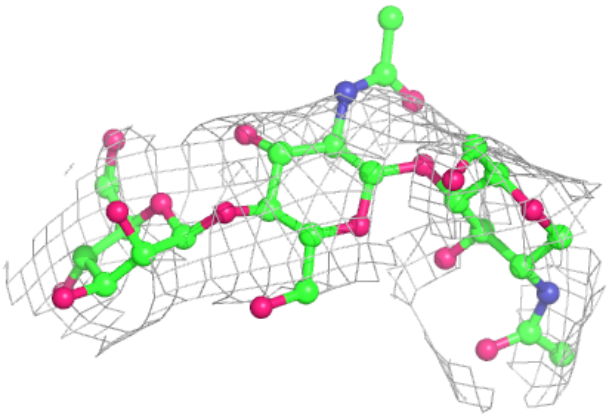


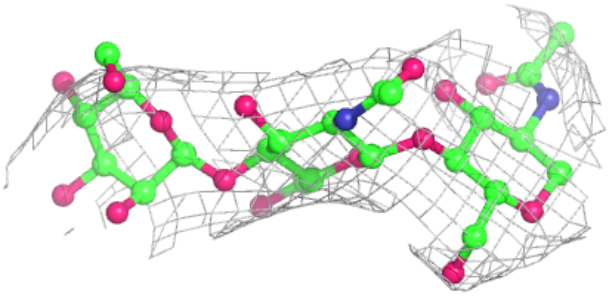


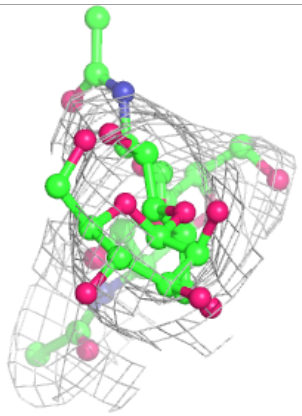


Electron density around Chain Q:

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







6.4 Ligands

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, 95^{th} 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
8	NAG	C	1101	14/15	0.47	0.54	175,175,175,175	0
8	NAG	A	1102	14/15	0.54	0.87	254,254,254,254	0
8	NAG	B	1102	14/15	0.61	0.43	235,235,235,235	0
8	NAG	A	1103	14/15	0.63	0.70	204,204,204,204	0
8	NAG	D	1101	14/15	0.70	0.76	246,246,246,246	0
8	NAG	B	1103	14/15	0.73	0.68	234,234,234,234	0
8	NAG	B	1101	14/15	0.78	0.29	264,264,264,264	0
8	NAG	C	1102	14/15	0.84	0.26	220,220,220,220	0
8	NAG	A	1101	14/15	0.91	0.28	209,209,209,209	0
8	NAG	D	1102	14/15	0.92	0.27	234,234,234,234	0

6.5 Other polymers

There are no such residues in this entry.