



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 8SUF / pdb_00008suf
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

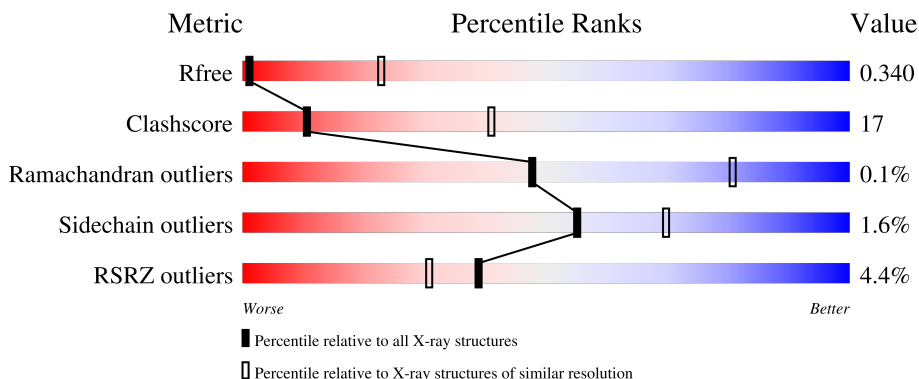
1 Overall quality at a glance

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1007	 2% 57% 36% 7%
1	B	1007	 5% 58% 34% 7%
1	C	1007	 3% 62% 31% 7%
1	D	1007	 3% 56% 37% 7%
2	E	114	 7% 71% 24% 5%

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Mol	Chain	Length	Quality of chain
2	F	114	
2	G	114	
2	H	114	
3	I	4	
3	M	4	
4	J	2	
4	K	2	
4	N	2	
4	O	2	
4	R	2	
5	L	4	
6	P	5	
7	Q	3	

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
			Total	C	N	O	S			
1	A	939	7315	4590	1278	1405	42	0	0	0
1	B	935	7286	4570	1274	1401	41	0	0	0
1	C	939	7315	4590	1278	1405	42	0	0	0
1	D	939	7315	4590	1278	1405	42	0	0	0

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
			Total	C	N	O	S			
2	E	108	815	507	133	166	9	0	0	0
2	F	108	815	507	133	166	9	0	0	0
2	G	107	808	502	132	165	9	0	0	0
2	H	105	794	492	130	163	9	0	0	0

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-mannopyranos e-(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			
3	I	4	50	28	2	20	0	0	0
3	M	4	50	28	2	20	0	0	0

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



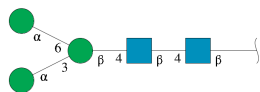
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	J	2	28	16	2	10	0	0	0
4	K	2	28	16	2	10	0	0	0
4	N	2	28	16	2	10	0	0	0
4	O	2	28	16	2	10	0	0	0
4	R	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



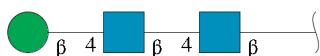
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	L	4	50	28	2	20	0	0	0

- 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.



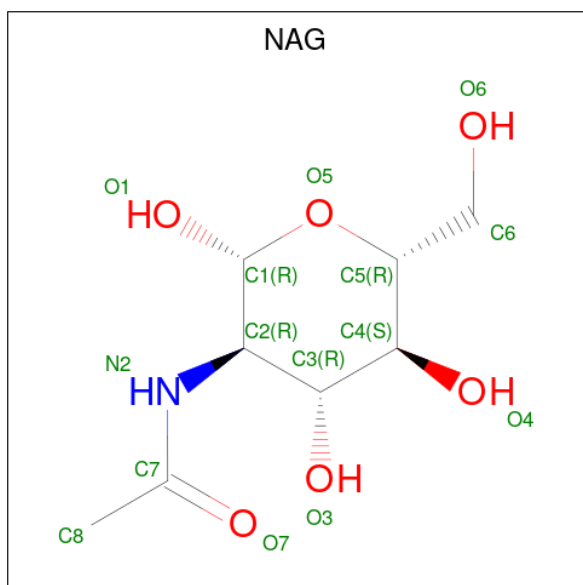
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	P	5	61	34	2	25	0	0	0

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).

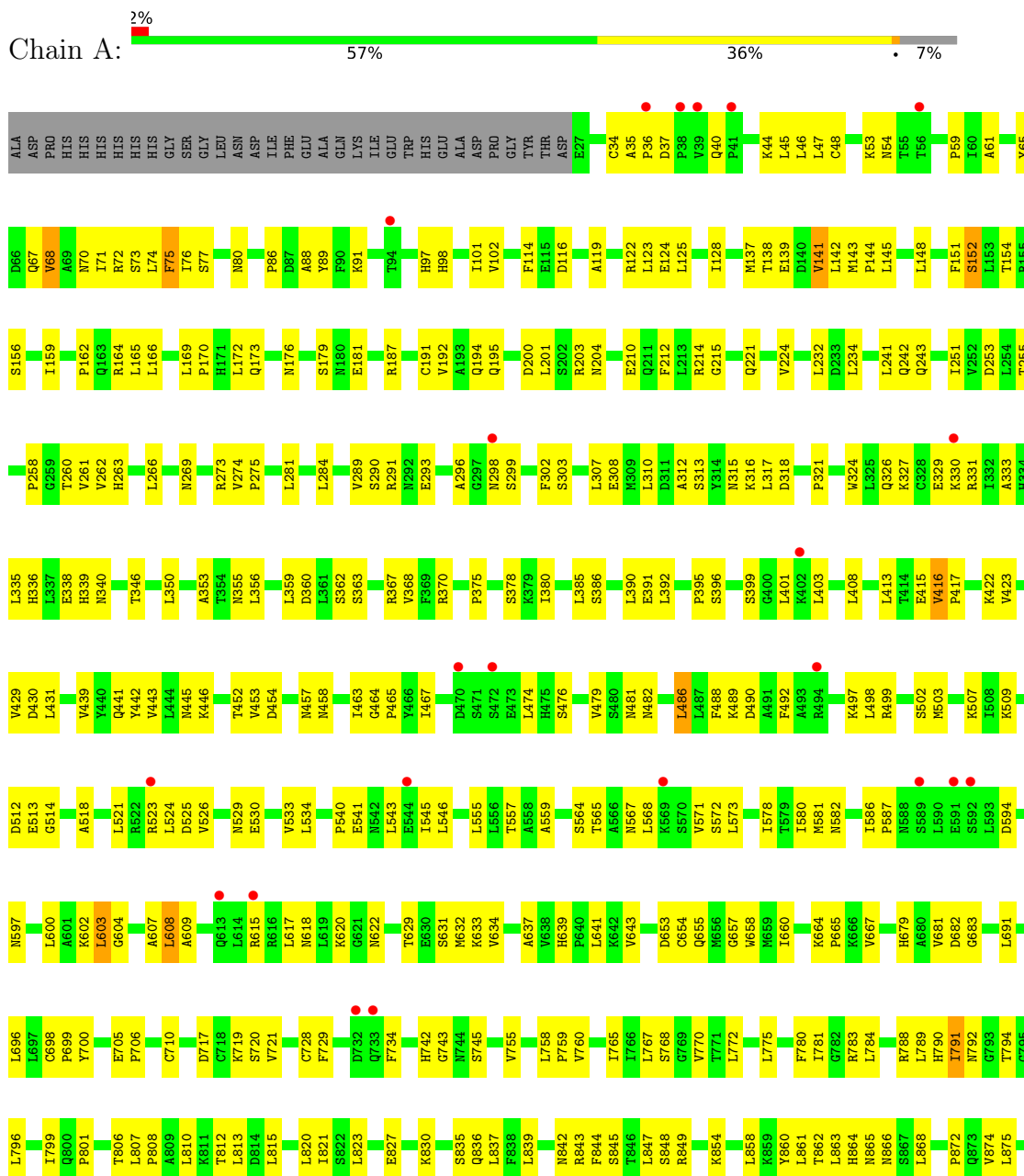


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1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

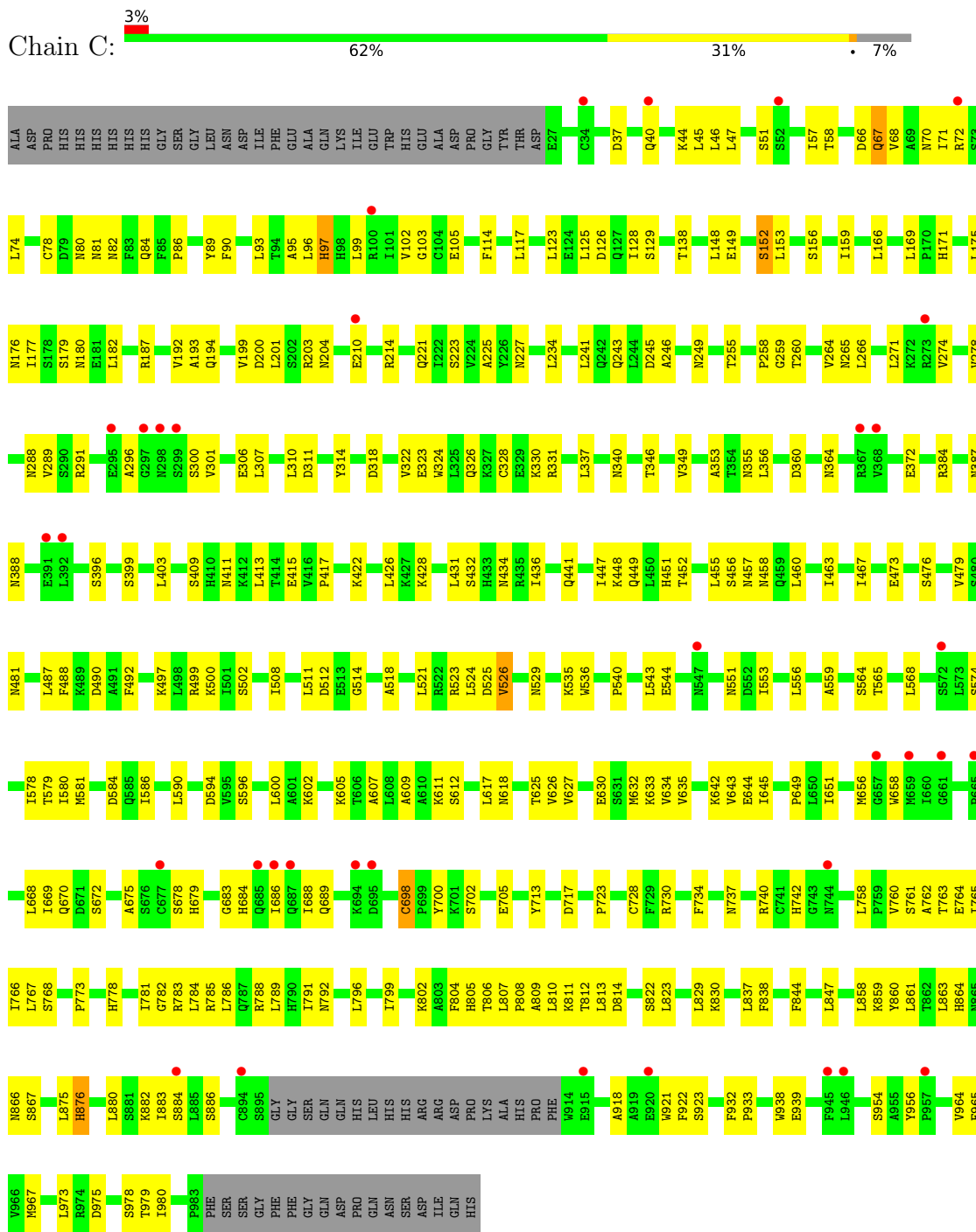
3 Residue-property plots i

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.

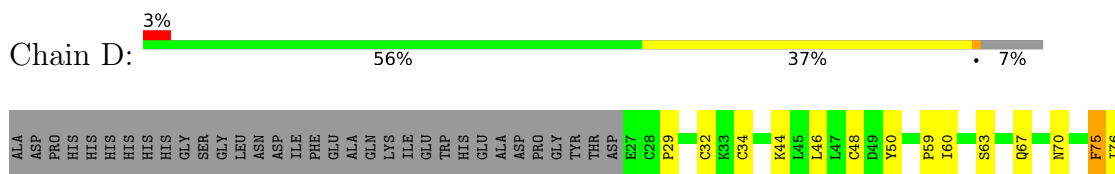
- Molecule 1: TIR domain-containing protein

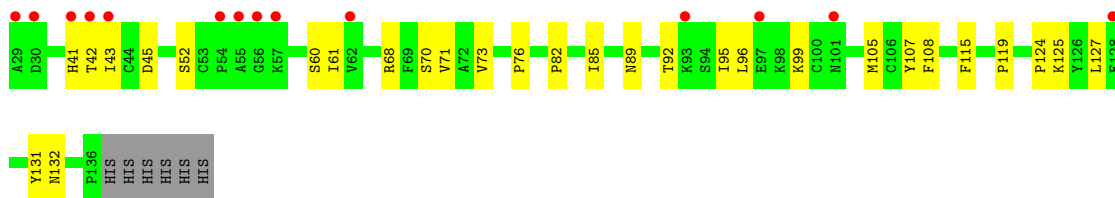


- Molecule 1: TIR domain-containing protein

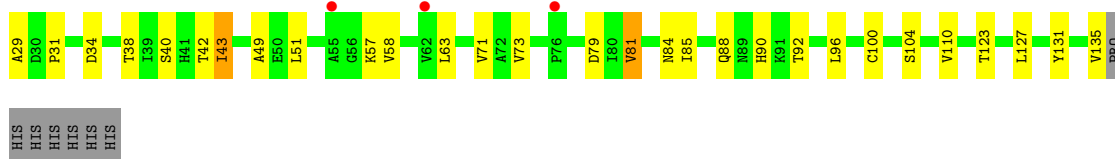


- Molecule 1: TIR domain-containing protein

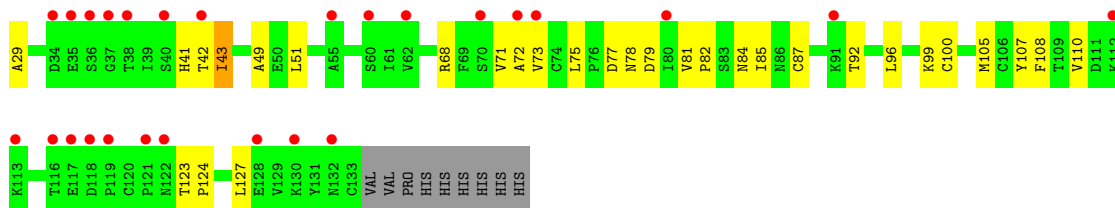




- Molecule 2: Latrophilin-like protein 1



- Molecule 2: Latrophilin-like protein 1



- 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



- 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



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

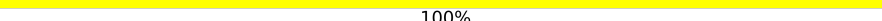


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%


MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain R:  100%


MAG1
MAG2

- 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:  25% 75%

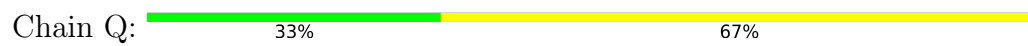
MAG1
MAG2
BMA3
MAN4

- 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:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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



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 74.15 – 4.00	Depositor EDS
% Data completeness (in resolution range)	55.5 (74.15-4.00) 55.6 (74.15-4.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 4.02Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.288 , 0.338 0.289 , 0.340	Depositor DCC
R_{free} test set	1861 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	139.9	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 594.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	32993	wwPDB-VP
Average B, all atoms (Å ²)	220.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/7436	0.59	0/10087
1	B	0.31	0/7405	0.60	0/10042
1	C	0.32	0/7436	0.61	0/10087
1	D	0.31	0/7436	0.60	0/10087
2	E	0.25	0/831	0.47	0/1131
2	F	0.19	0/831	0.42	0/1131
2	G	0.23	0/823	0.51	0/1119
2	H	0.23	0/809	0.47	0/1099
All	All	0.30	0/33007	0.59	0/44783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7315	0	7381	272	0
1	B	7286	0	7348	261	1
1	C	7315	0	7383	225	1
1	D	7315	0	7385	294	0
2	E	815	0	786	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	815	0	786	17	0
2	G	808	0	779	22	0
2	H	794	0	761	34	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	1111	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 17.

All (1111) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:52:SER:HB3	2:F:105:MET:HE3	1.63	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:B:309:MET:HE2	3:M:1:NAG:H83	1.67	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
2:H:105:MET:HE3	2:H:107:TYR:HE2	1.50	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
1:C:86:PRO:HG2	1:C:89:TYR:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:650:LEU:HD13	1:B:659:MET:HE1	1.77	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:258:PRO:C	1:C:260:THR:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:OE2	3:M:1:NAG:O6	2.12	0.63
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: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:A:632:MET:HE1	1:A:643:VAL:HG21	1.81	0.62
1:C:965:PHE:HE2	1:C:967:MET:HE3	1.64	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:503:MET:HE2	1:A:524:LEU:HD11	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:43:SER:OG	1:B:44:LYS:N	2.34	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:H:105:MET:HE3	2:H:107:TYR:CE2	2.36	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:D:312:ALA:C	1:D:315:ASN:HD22	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:731:ASP:CG	1:D:736:ILE:H	2.12	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:A:503:MET:HE3	1:A:526:VAL:HG12	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:664:LYS:HA	1:A:665:PRO:C	2.29	0.55
1:B:241:LEU:HD21	1:B:244:LEU:HD22	1.88	0.55
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:D:806:THR:HG21	2:H:78:ASN:C	2.31	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:C:632:MET:HE1	1:C:643:VAL:HG21	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:632:MET:HE1	1:D:643:VAL:HG11	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: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:C:965:PHE:CE2	1:C:967:MET:HE3	2.42	0.53
1:A:97:HIS:ND1	1:A:119:ALA:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:350:LEU:C	1:D:352:ASN:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:146:ALA:C	1:B:148:LEU:H	2.18	0.51
1:D:75:PHE:CD2	1:D:100:ARG:HD3	2.45	0.51
1:A:632:MET:HE2	1:A:658:TRP:CH2	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
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:B:536:TRP:CD1	1:B:557:THR:HG1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:632:MET:HE1	1:D:643:VAL:HG21	1.93	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:C:773:PRO:C	1:C:796:LEU:HD12	2.36	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:140:ASP:HB3	1:B:143:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:864:HIS:CG	1:C:884:SER:HG	2.27	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:D:114:PHE:HD1	1:D:117:LEU:HD12	1.77	0.49
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:324:TRP:C	1:D:326:GLN:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:SER:HA	1:A:102:VAL:O	2.12	0.49
1:A:581:MET:HE2	1:A:603:LEU:HD11	1.95	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
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
3:I:2:NAG:O6	3:I:3:BMA:O5	2.29	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:A:170:PRO:C	1:A:172:LEU:H	2.22	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:681:VAL:HG13	1:D:729:PHE:CE2	2.49	0.48
1:C:626:VAL:HA	1:C:656:MET:HE1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:536:TRP:CD1	1:D:557:THR:H	2.30	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:D:75:PHE:CD1	1:D:75:PHE:C	2.91	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:78:CYS:HB2	1:C:103:GLY:C	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:105:MET:HE1	2:F:107:TYR:HH	1.80	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
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:A:137:MET:HE3	1:A:151:PHE:HZ	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:627:VAL:N	1:C:656:MET:HE1	2.30	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:778:HIS:HB3	2:H:77:ASP:CG	2.41	0.46
1:D:941:VAL:HG11	1:D:958:PRO:HD3	1.97	0.46
1:A:600:LEU:HB2	1:A:622:ASN:CG	2.40	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:D:568:LEU:C	1:D:590:LEU:HD23	2.41	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: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
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: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:A:717:ASP:CG	2:E:70:SER:HA	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:616:ARG:HH21	1:D:642:LYS:HZ1	1.65	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:258:PRO:C	1:A:260:THR:H	2.25	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
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
1:D:932:PHE:C	1:D:934:LYS:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:743:GLY:C	1:A:745:SER:H	2.24	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
1:A:312:ALA:C	1:A:315:ASN:HD22	2.26	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:488:PHE:HA	1:B:115:GLU:CD	2.43	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:522:ARG:C	1:B:543:LEU:HD12	2.43	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:549:ASP:OD1	1:D:574:SER:OG	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:PRO:C	1:C:260:THR:N	2.73	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: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:378:SER:C	1:B:380:ILE:H	2.26	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:309:MET:CE	3:M:1:NAG:H83	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LYS:HG2	1:B:31:PHE:CE1	2.54	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
1:A:385:LEU:O	1:A:408:LEU:HA	2.19	0.42
1:A:632:MET:HE3	1:A:667:VAL:HG11	2.00	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: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:B:619:LEU:C	1:B:622:ASN:HD22	2.28	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:D:632:MET:CE	1:D:643:VAL:HG21	2.49	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
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:75:PHE:CD1	1:A:75:PHE:C	2.98	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:658:TRP:CD1	1:B:658:TRP:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:872:PRO:C	1:D:874:VAL:H	2.27	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:D:743:GLY:C	1:D:745:SER:H	2.28	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
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:C:457:ASN:CG	1:C:481:ASN:HD22	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:ALA:HB3	1:B:573:LEU:HD23	2.02	0.41
1:B:717:ASP:CG	2:F:70:SER:HA	2.44	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: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:581:MET:HE3	1:C:586:ILE:HD11	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:75:PHE:C	1:D:75:PHE:HD1	2.27	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:D:632:MET:HE2	1:D:658:TRP:CZ3	2.56	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
1:C:324:TRP:C	1:C:326:GLN:H	2.28	0.41
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:A:845:SER:C	1:A:868:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:556:LEU:HB2	1:D:585:GLN:CD	2.46	0.40
1:D:608:LEU:HB2	1:D:631:SER:O	2.21	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
1:D:717:ASP:CG	1:D:760:VAL:HG11	2.46	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%)	48	81
1	C	935/1007 (93%)	802 (86%)	132 (14%)	1 (0%)	48	81
1	D	935/1007 (93%)	812 (87%)	122 (13%)	1 (0%)	48	81
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%)	48	81

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%)	838 (98%)	13 (2%)	57	70
1	B	847/908 (93%)	830 (98%)	17 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	851/908 (94%)	835 (98%)	16 (2%)	50	67
1	D	851/908 (94%)	839 (99%)	12 (1%)	59	71
2	E	97/103 (94%)	97 (100%)	0	100	100
2	F	97/103 (94%)	97 (100%)	0	100	100
2	G	96/103 (93%)	94 (98%)	2 (2%)	47	65
2	H	94/103 (91%)	92 (98%)	2 (2%)	47	65
All	All	3784/4044 (94%)	3722 (98%)	62 (2%)	55	70

All (62) 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	141	VAL
1	A	152	SER
1	A	346	THR
1	A	416	VAL
1	A	486	LEU
1	A	490	ASP
1	A	603	LEU
1	A	608	LEU
1	A	791	ILE
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	141	VAL
1	B	289	VAL
1	B	322	VAL
1	B	483	GLU
1	B	490	ASP

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Mol	Chain	Res	Type
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	97	HIS
1	C	138	THR
1	C	152	SER
1	C	255	THR
1	C	322	VAL
1	C	372	GLU
1	C	490	ASP
1	C	526	VAL
1	C	698	CYS
1	C	791	ILE
1	C	876	HIS
1	D	75	PHE
1	D	111	VAL
1	D	138	THR
1	D	322	VAL
1	D	564	SER
1	D	608	LEU
1	D	629	THR
1	D	666	LYS
1	D	668	LEU
1	D	770	VAL
1	D	865	ASN
1	D	916	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 (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	355	ASN
1	A	382	ASN
1	A	475	HIS
1	A	576	ASN

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Mol	Chain	Res	Type
1	A	582	ASN
1	A	655	GLN
1	A	684	HIS
1	A	774	GLN
1	A	916	HIS
1	B	82	ASN
1	B	336	HIS
1	B	355	ASN
1	B	377	ASN
1	B	655	GLN
1	B	836	GLN
1	B	940	ASN
1	C	173	GLN
1	C	292	ASN
1	C	340	ASN
1	C	355	ASN
1	C	388	ASN
1	C	410	HIS
1	C	458	ASN
1	C	582	ASN
1	C	873	GLN
1	D	108	HIS
1	D	127	GLN
1	D	171	HIS
1	D	340	ASN
1	D	410	HIS
1	D	433	HIS
1	D	458	ASN
1	D	542	ASN
1	D	550	ASN
1	D	575	ASN
1	D	582	ASN
1	D	585	GLN
1	D	597	ASN
1	D	778	HIS
1	D	916	HIS
1	D	925	HIS
2	E	41	HIS
2	G	101	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.50	0	17,19,21	0.46	0
3	NAG	I	2	3	14,14,15	0.76	1 (7%)	17,19,21	0.92	1 (5%)
3	BMA	I	3	3	11,11,12	0.95	1 (9%)	15,15,17	1.14	1 (6%)
3	MAN	I	4	3	11,11,12	1.01	0	15,15,17	1.00	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	0.41	0
4	NAG	K	1	4,1	14,14,15	0.35	0	17,19,21	0.56	0
4	NAG	K	2	4	14,14,15	0.43	0	17,19,21	0.41	0
5	NAG	L	1	1,5	14,14,15	0.69	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	L	2	5	14,14,15	0.18	0	17,19,21	0.65	0
5	BMA	L	3	5	11,11,12	1.56	2 (18%)	15,15,17	1.22	2 (13%)
5	MAN	L	4	5	11,11,12	1.54	3 (27%)	15,15,17	1.20	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.31	0	17,19,21	1.11	2 (11%)
3	NAG	M	2	3	14,14,15	0.55	0	17,19,21	0.43	0
3	BMA	M	3	3	11,11,12	0.88	0	15,15,17	0.83	0
3	MAN	M	4	3	11,11,12	0.99	0	15,15,17	1.31	1 (6%)
4	NAG	N	1	4,1	14,14,15	0.21	0	17,19,21	0.97	1 (5%)
4	NAG	N	2	4	14,14,15	0.90	1 (7%)	17,19,21	0.50	0
4	NAG	O	1	4,1	14,14,15	0.64	0	17,19,21	0.74	1 (5%)
4	NAG	O	2	4	14,14,15	0.69	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	P	1	1,6	14,14,15	0.32	0	17,19,21	0.65	0
6	NAG	P	2	6	14,14,15	0.51	0	17,19,21	0.87	1 (5%)
6	BMA	P	3	6	11,11,12	1.67	3 (27%)	15,15,17	1.95	5 (33%)
6	MAN	P	4	6	11,11,12	1.53	2 (18%)	15,15,17	1.21	1 (6%)
6	MAN	P	5	6	11,11,12	2.03	3 (27%)	15,15,17	1.56	1 (6%)
7	NAG	Q	1	7,1	14,14,15	0.79	1 (7%)	17,19,21	0.53	0
7	NAG	Q	2	7	14,14,15	0.31	0	17,19,21	0.64	0
7	BMA	Q	3	7	11,11,12	1.29	2 (18%)	15,15,17	1.03	0
4	NAG	R	1	4,1	14,14,15	0.62	0	17,19,21	0.78	1 (5%)
4	NAG	R	2	4	14,14,15	0.98	1 (7%)	17,19,21	0.75	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	-	2/6/23/26	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	-	3/6/23/26	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	7,1	-	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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	5	MAN	O5-C5	3.87	1.51	1.43
6	P	3	BMA	C1-C2	3.69	1.61	1.52
6	P	5	MAN	C2-C3	3.57	1.58	1.52
4	R	2	NAG	C1-C2	3.48	1.57	1.52
6	P	4	MAN	C1-C2	3.25	1.60	1.52
5	L	3	BMA	O3-C3	2.93	1.50	1.43
7	Q	3	BMA	O5-C1	-2.89	1.38	1.43
5	L	4	MAN	O5-C5	2.87	1.49	1.43
4	N	2	NAG	C1-C2	2.86	1.56	1.52
6	P	5	MAN	C1-C2	2.79	1.58	1.52
5	L	4	MAN	C2-C3	2.73	1.56	1.52
6	P	4	MAN	C2-C3	2.66	1.56	1.52
5	L	3	BMA	C2-C3	2.54	1.56	1.52
3	I	3	BMA	C1-C2	2.41	1.58	1.52
6	P	3	BMA	O5-C1	2.34	1.47	1.43
7	Q	3	BMA	C4-C5	2.30	1.57	1.53
7	Q	1	NAG	C1-C2	2.28	1.55	1.52
5	L	1	NAG	C1-C2	2.27	1.55	1.52
6	P	3	BMA	C2-C3	2.27	1.56	1.52
5	L	4	MAN	C1-C2	2.27	1.57	1.52
3	I	2	NAG	C1-C2	2.13	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	5	MAN	C1-O5-C5	4.97	118.84	112.19
6	P	3	BMA	C1-O5-C5	4.51	118.23	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	4	MAN	C1-O5-C5	4.08	117.66	112.19
5	L	4	MAN	C1-O5-C5	3.68	117.12	112.19
6	P	3	BMA	C3-C4-C5	-2.97	104.85	110.23
3	M	1	NAG	C2-N2-C7	2.92	126.81	122.90
3	I	4	MAN	C1-O5-C5	2.90	116.08	112.19
3	I	3	BMA	C1-O5-C5	2.88	116.04	112.19
6	P	3	BMA	O3-C3-C2	2.79	115.74	110.05
5	L	3	BMA	O3-C3-C2	2.71	115.58	110.05
6	P	4	MAN	C1-O5-C5	2.63	115.71	112.19
4	N	1	NAG	C1-O5-C5	2.60	115.66	112.19
5	L	1	NAG	C1-O5-C5	2.54	115.59	112.19
4	J	1	NAG	C1-O5-C5	2.52	115.56	112.19
3	I	2	NAG	C1-O5-C5	2.43	115.44	112.19
6	P	2	NAG	C2-N2-C7	2.40	126.11	122.90
4	R	1	NAG	C1-O5-C5	2.30	115.26	112.19
6	P	3	BMA	O2-C2-C1	2.24	114.35	109.22
5	L	3	BMA	C1-O5-C5	2.15	115.06	112.19
3	M	1	NAG	C1-C2-N2	2.13	113.79	110.43
4	O	1	NAG	O4-C4-C5	2.08	114.46	109.32
6	P	3	BMA	O5-C5-C4	-2.04	105.87	110.83

There are no chirality outliers.

All (51) torsion outliers are listed below:

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

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

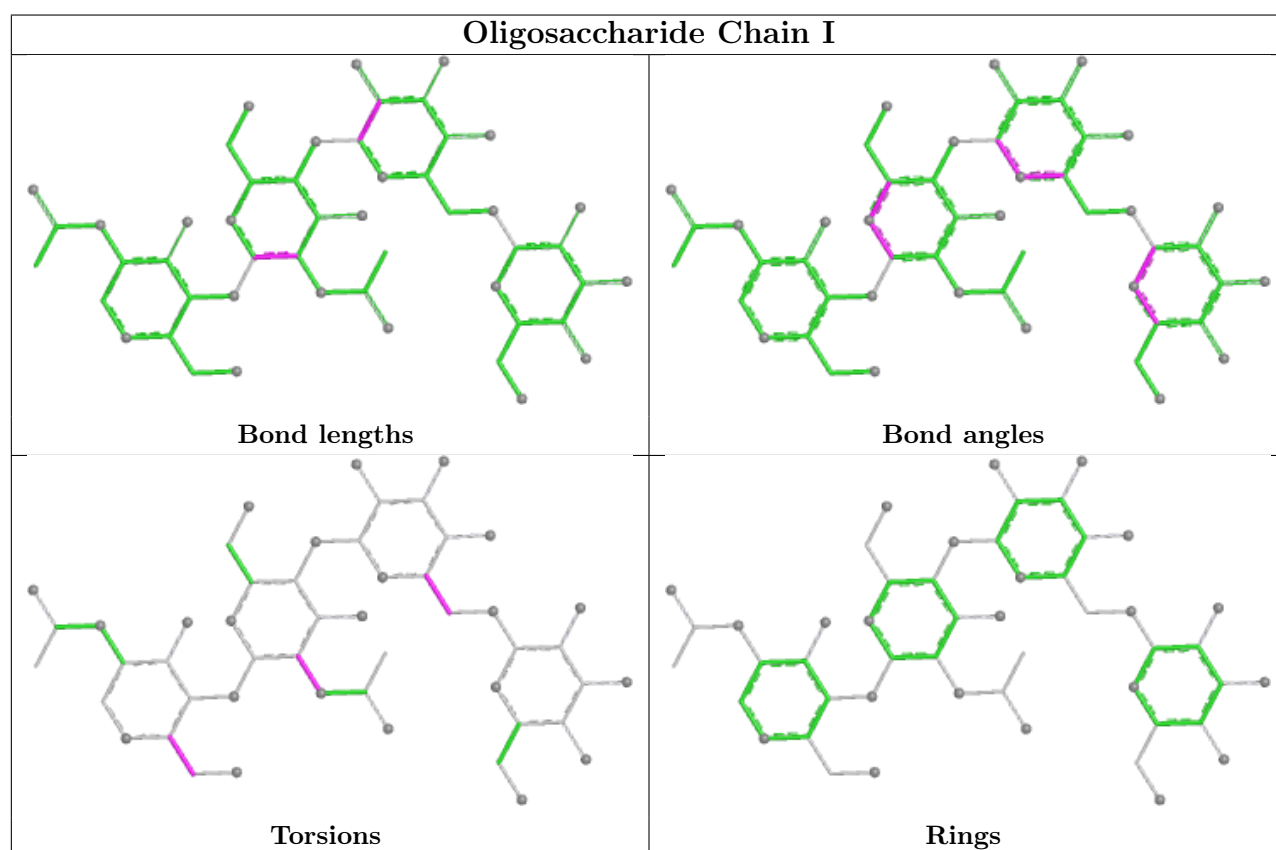
All (1) ring outliers are listed below:

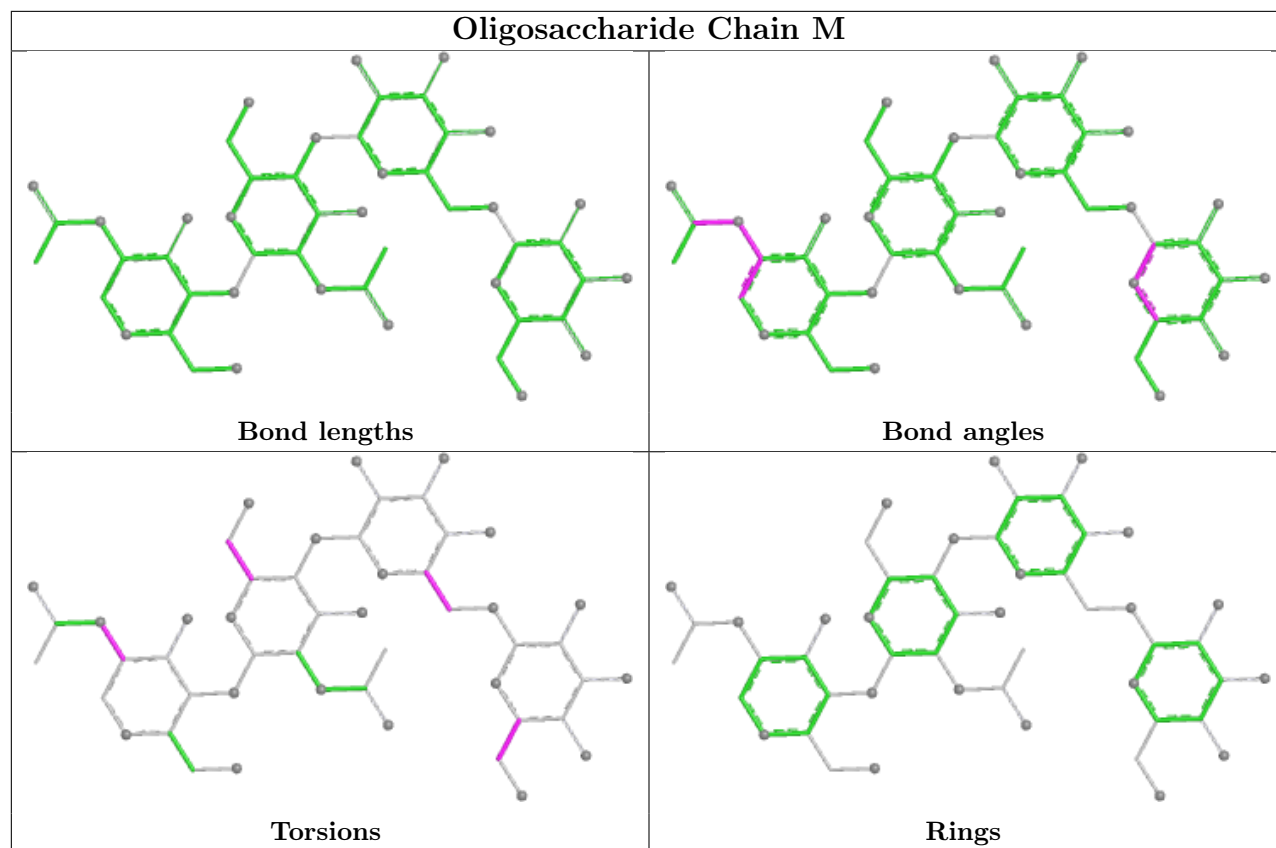
Mol	Chain	Res	Type	Atoms
5	L	4	MAN	C1-C2-C3-C4-C5-O5

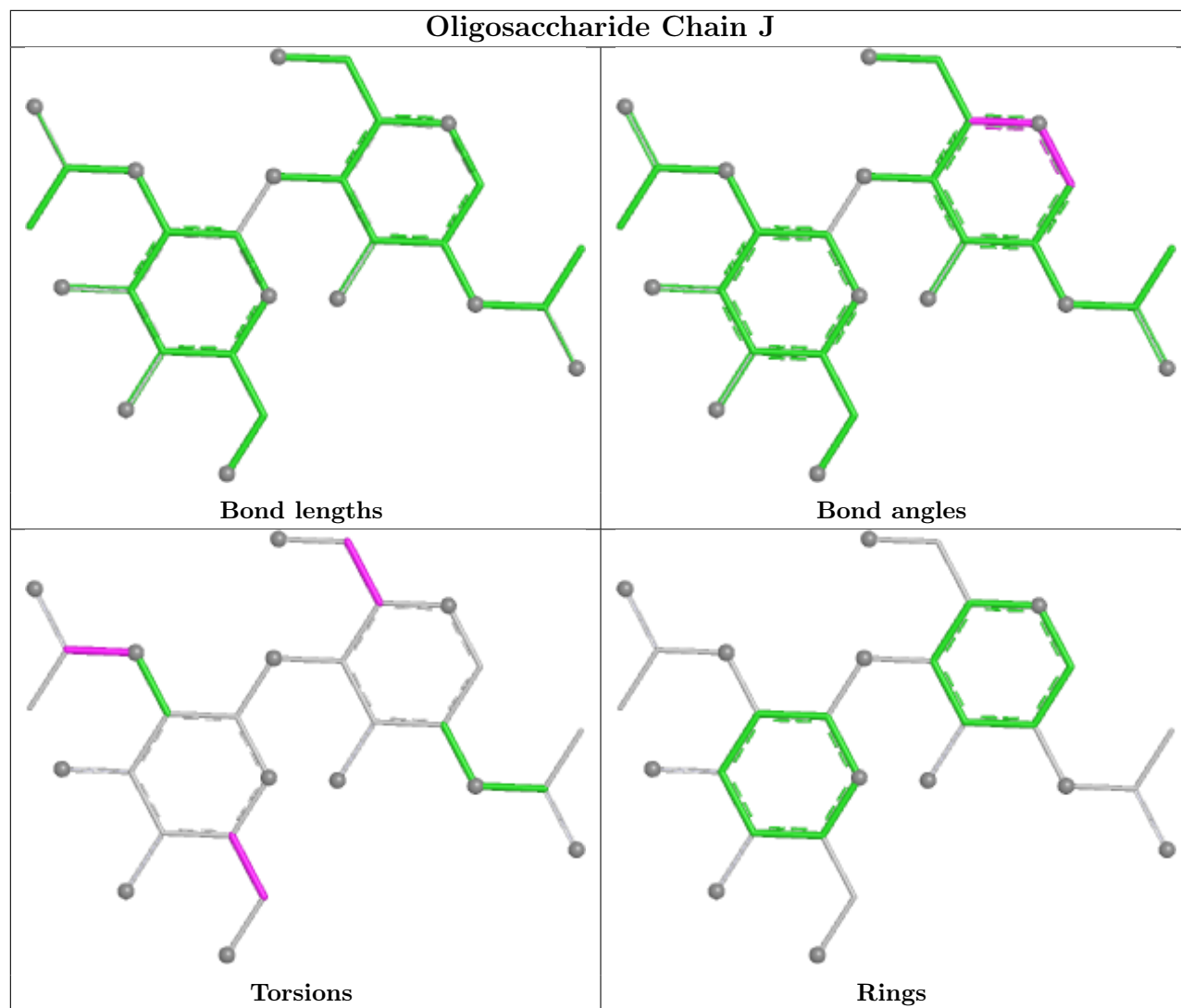
8 monomers are involved in 14 short contacts:

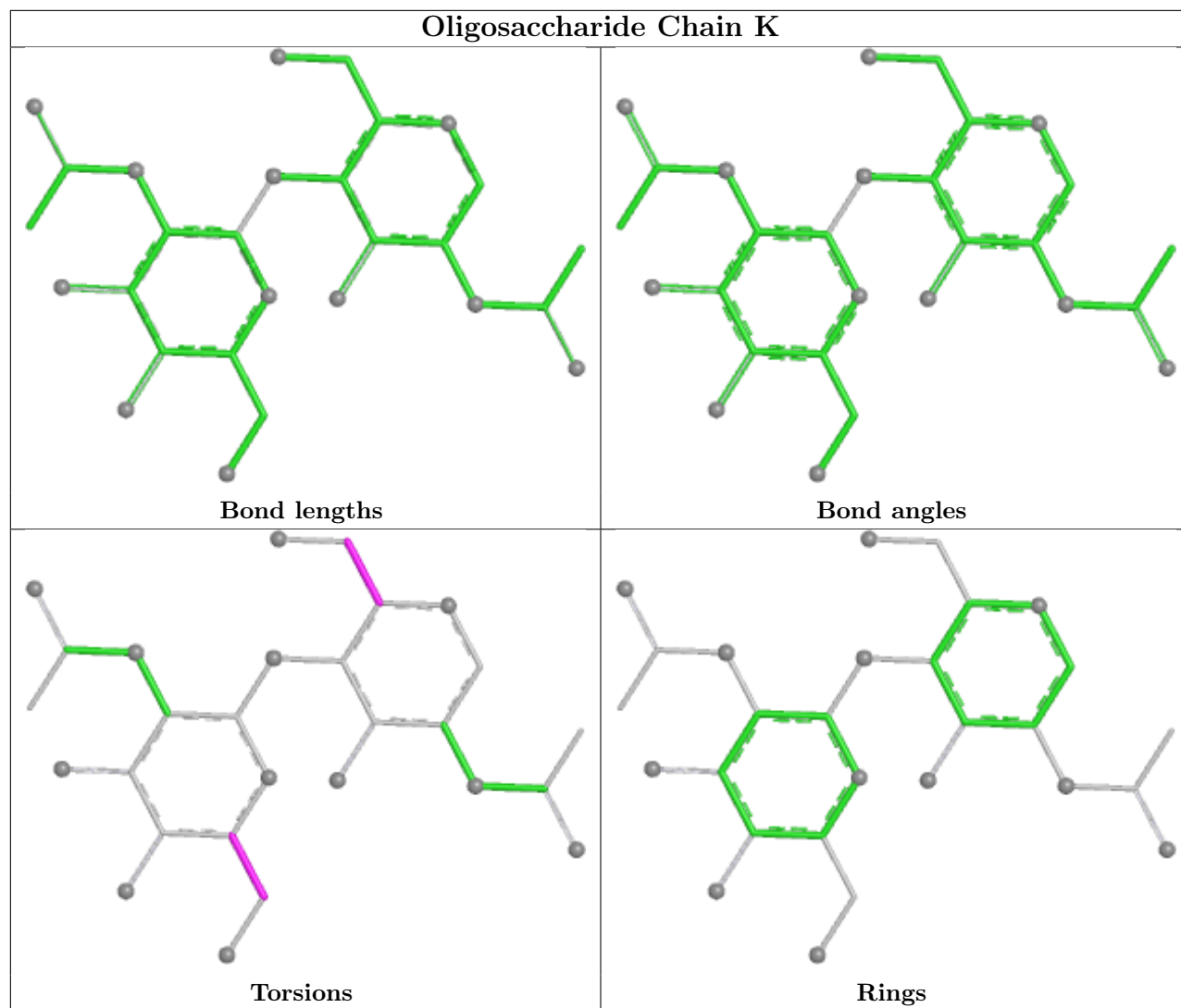
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	5	0
6	P	4	MAN	3	0
4	O	1	NAG	2	0
6	P	1	NAG	2	0
3	I	2	NAG	2	0
3	I	3	BMA	1	0
4	O	2	NAG	1	0
6	P	3	BMA	1	0

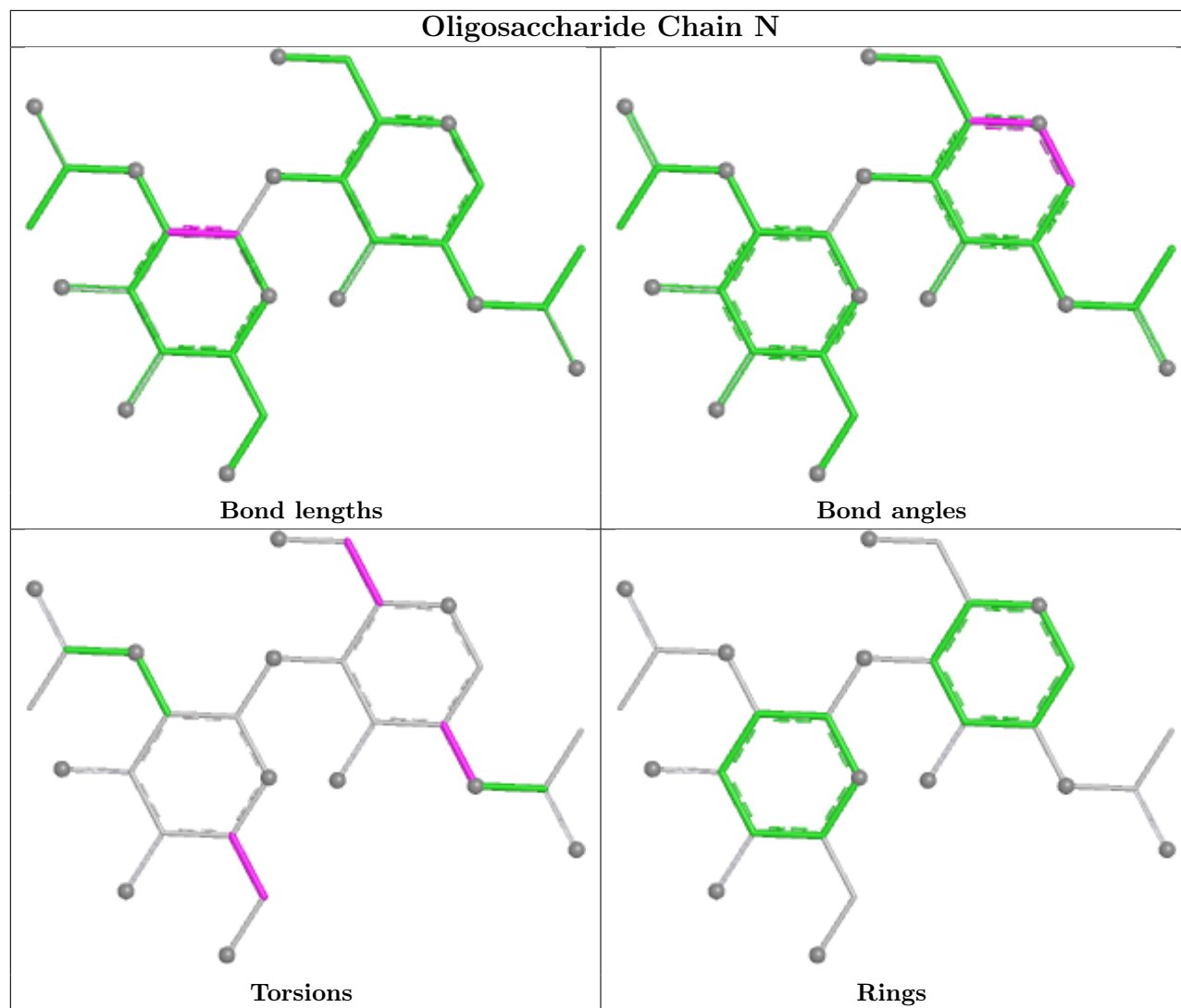
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

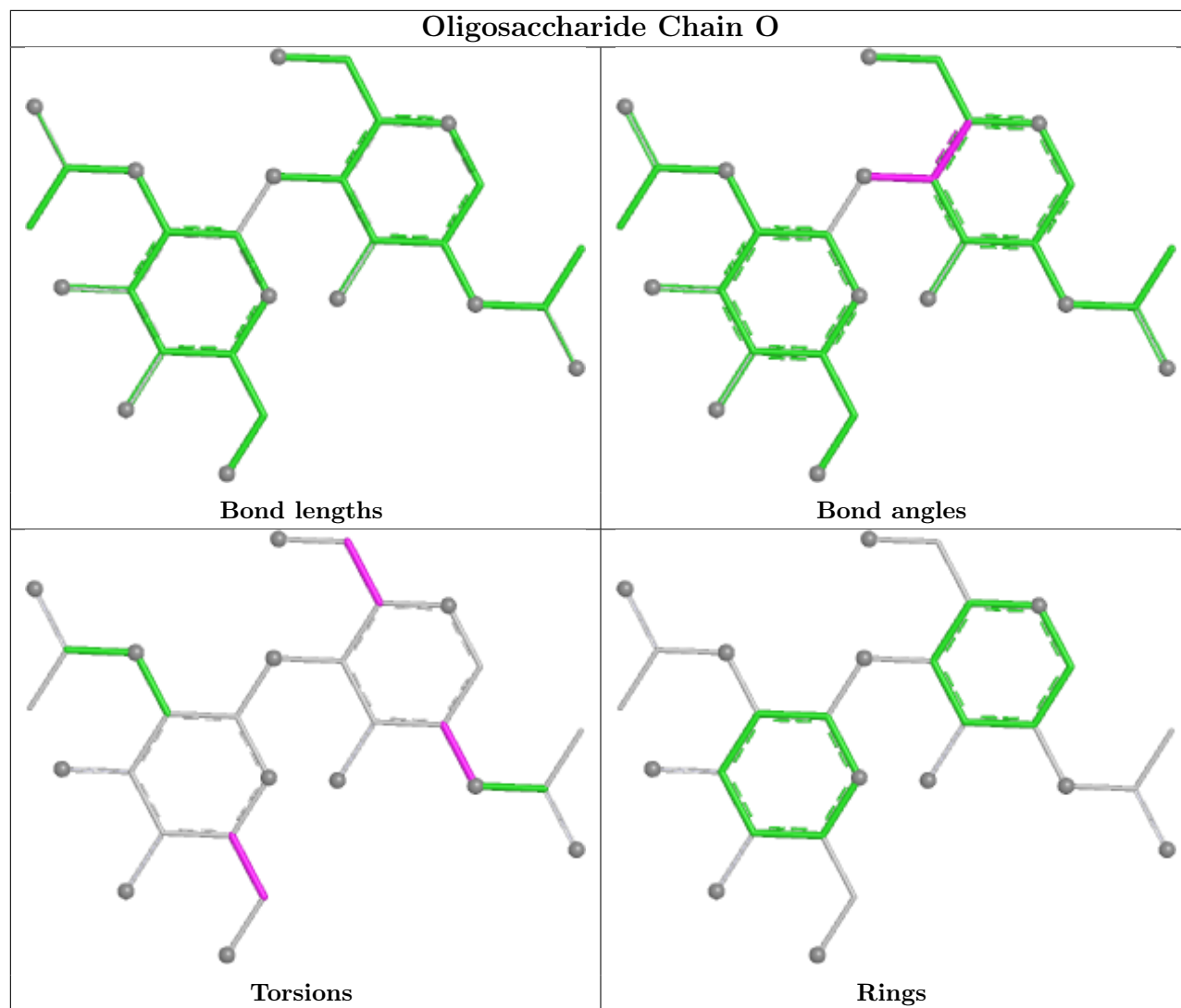


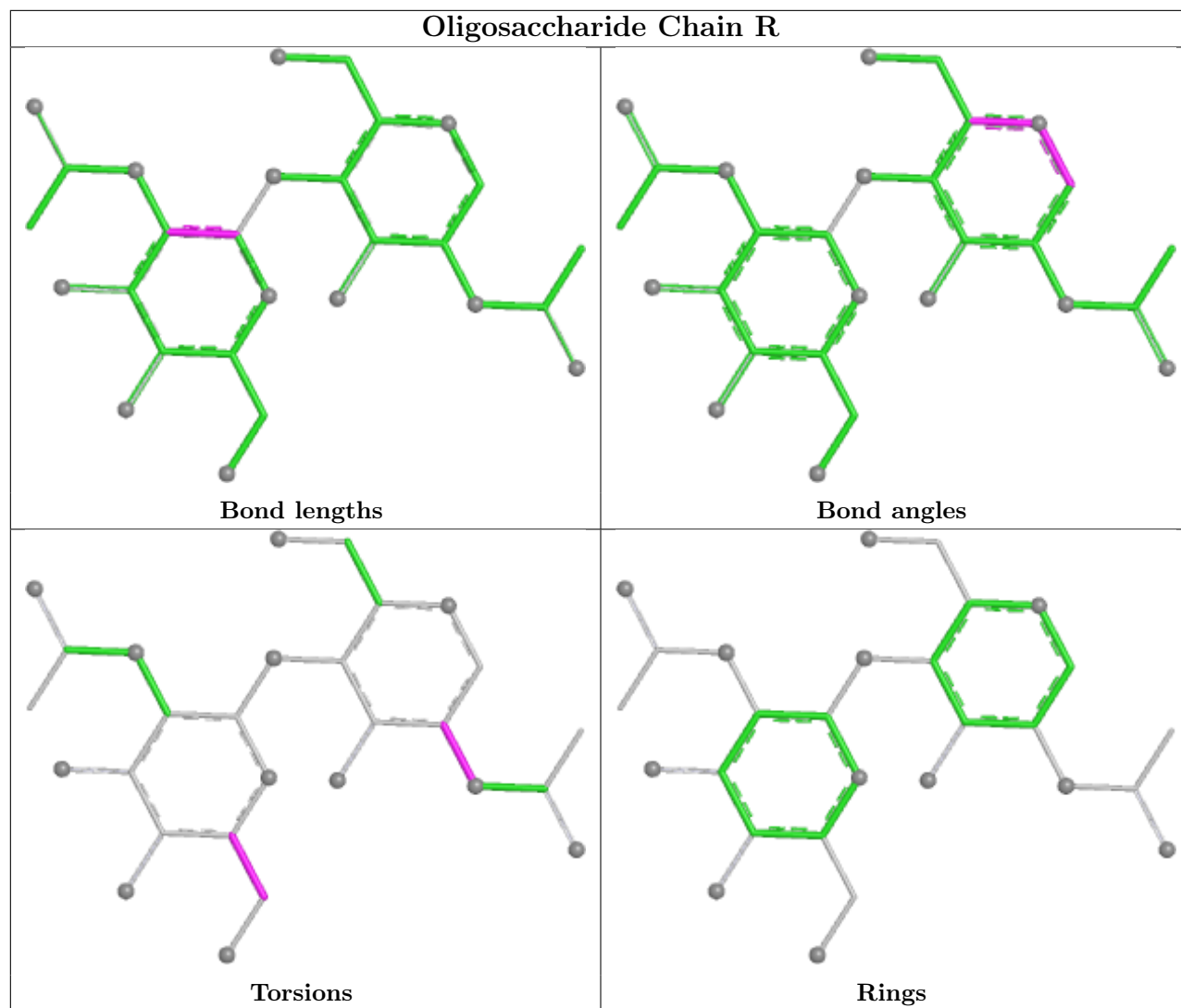


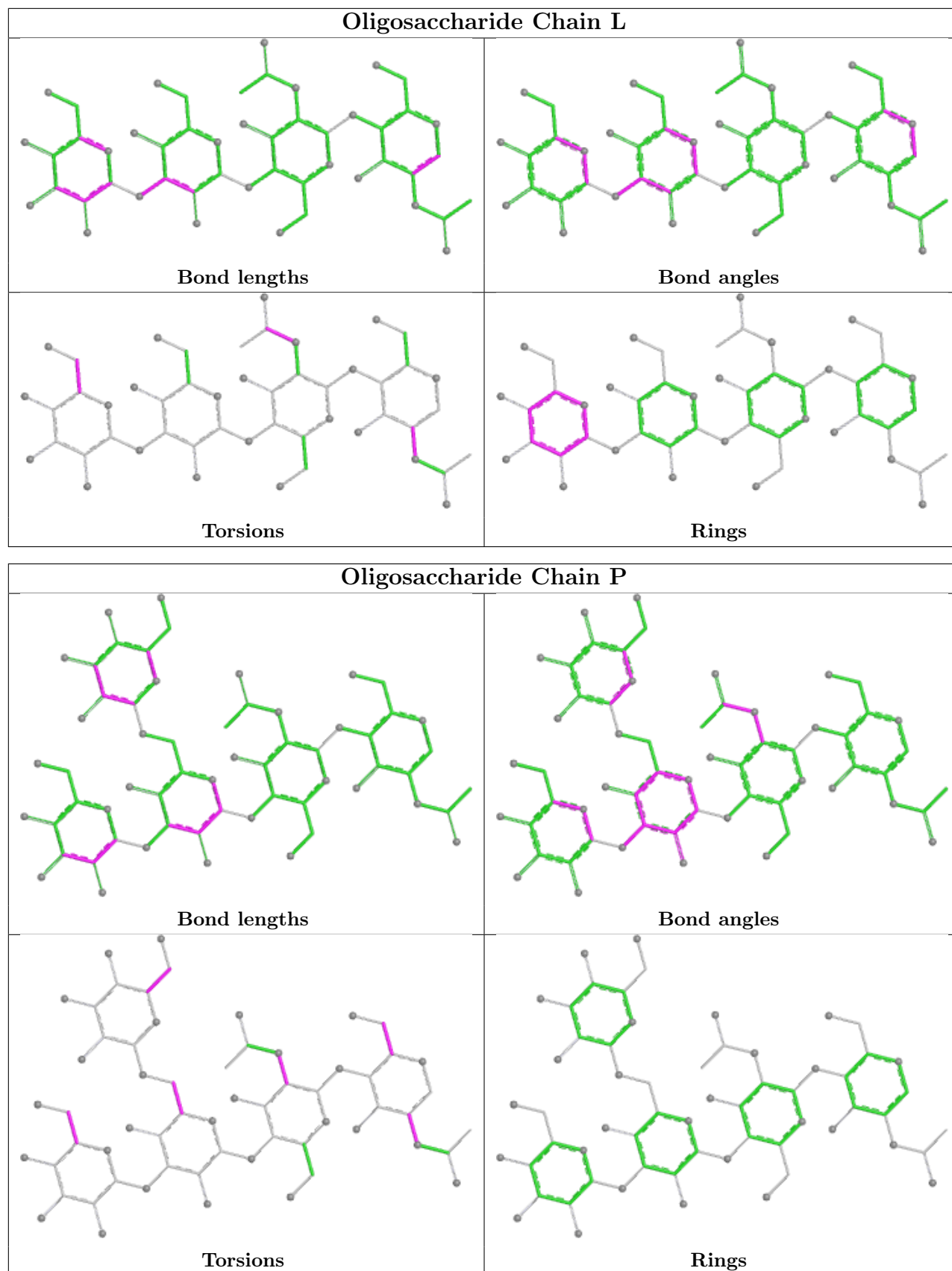


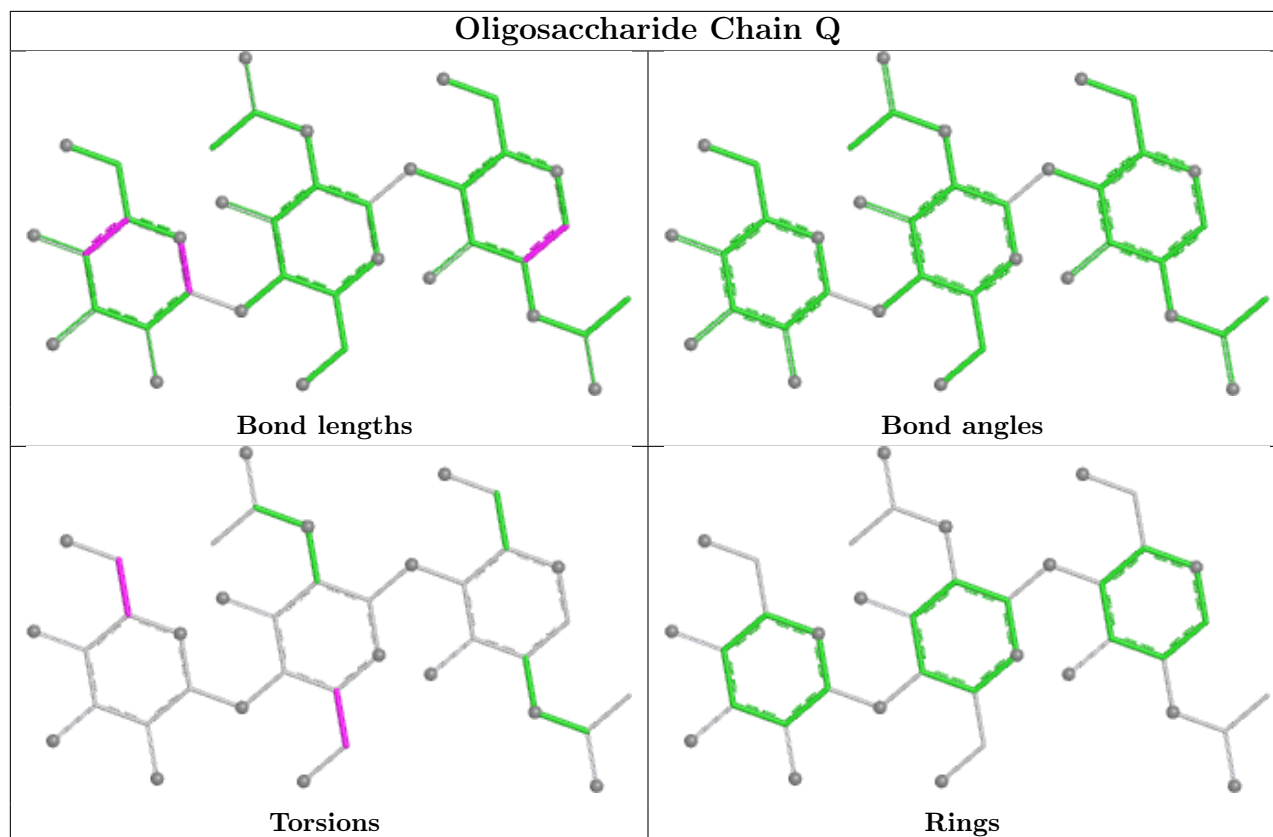












5.6 Ligand geometry [i](#)

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	A	1102	1	14,14,15	0.66	0	17,19,21	0.63	0
8	NAG	B	1101	1	14,14,15	0.83	1 (7%)	17,19,21	0.65	0
8	NAG	D	1101	1	14,14,15	0.47	0	17,19,21	0.66	1 (5%)
8	NAG	C	1102	1	14,14,15	0.50	0	17,19,21	0.48	0
8	NAG	B	1102	1	14,14,15	0.51	0	17,19,21	0.52	0
8	NAG	A	1101	1	14,14,15	0.59	0	17,19,21	0.54	0
8	NAG	B	1103	1	14,14,15	0.20	0	17,19,21	0.53	0
8	NAG	D	1102	1	14,14,15	0.65	1 (7%)	17,19,21	0.63	0
8	NAG	C	1101	1	14,14,15	0.67	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1103	1	14,14,15	0.65	1 (7%)	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	A	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1101	1	-	1/6/23/26	0/1/1/1
8	NAG	D	1101	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1102	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1101	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1103	1	-	2/6/23/26	0/1/1/1
8	NAG	D	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1101	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1103	1	-	1/6/23/26	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	2.25	1.47	1.43
8	A	1103	NAG	C1-C2	2.23	1.55	1.52
8	D	1102	NAG	C1-C2	2.22	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1101	NAG	C1-O5-C5	2.25	115.20	112.19

There are no chirality outliers.

All (19) 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

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

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1101	NAG	1	0
8	D	1101	NAG	1	0
8	A	1101	NAG	2	0
8	B	1103	NAG	1	0
8	D	1102	NAG	1	0
8	C	1101	NAG	1	0
8	A	1103	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	939/1007 (93%)	-0.33	22 (2%) 61 45	136, 195, 266, 306	0
1	B	935/1007 (92%)	-0.23	47 (5%) 34 28	156, 213, 258, 322	0
1	C	939/1007 (93%)	-0.25	35 (3%) 45 34	109, 198, 254, 299	0
1	D	939/1007 (93%)	-0.32	27 (2%) 53 39	123, 224, 290, 319	0
2	E	108/114 (94%)	0.11	8 (7%) 20 20	227, 296, 318, 335	0
2	F	108/114 (94%)	0.54	14 (12%) 7 11	277, 350, 369, 379	0
2	G	107/114 (93%)	-0.26	3 (2%) 55 40	221, 264, 284, 289	0
2	H	105/114 (92%)	1.03	26 (24%) 2 4	295, 346, 370, 382	0
All	All	4180/4484 (93%)	-0.22	182 (4%) 39 31	109, 213, 315, 382	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	55	ALA	11.0
2	H	37	GLY	9.5
1	C	298	ASN	8.5
1	B	948	ASN	8.0
2	F	54	PRO	8.0
1	D	710	CYS	7.7
2	H	132	ASN	7.2
2	F	56	GLY	7.2
2	F	97	GLU	7.1
1	D	673	GLU	6.9
1	B	293	GLU	6.6
2	H	113	LYS	6.5
2	H	55	ALA	6.4
1	B	461	GLN	6.4
2	H	36	SER	6.3
1	A	298	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	981	CYS	6.1
1	D	715	ASN	5.8
1	C	391	GLU	5.7
1	D	744	ASN	5.5
2	H	91	LYS	5.5
1	C	52	SER	5.4
1	A	38	PRO	5.3
1	C	295	GLU	5.3
1	D	716	CYS	5.2
1	B	263	HIS	4.9
2	E	55	ALA	4.9
1	C	957	PRO	4.9
1	D	709	ILE	4.8
1	C	694	LYS	4.8
1	D	960	MET	4.8
1	C	40	GLN	4.7
2	H	112	LYS	4.7
1	B	915	GLU	4.6
1	A	494	ARG	4.6
1	B	221	GLN	4.4
1	B	475	HIS	4.3
2	F	101	ASN	4.3
1	B	157	ARG	4.2
2	G	76	PRO	4.2
1	A	591	GLU	4.1
1	D	250	ARG	4.1
2	H	117	GLU	4.0
1	C	744	ASN	3.9
1	D	713	TYR	3.9
1	D	263	HIS	3.9
2	H	38	THR	3.9
2	H	118	ASP	3.8
2	E	35	GLU	3.8
2	H	72	ALA	3.8
1	C	677	CYS	3.7
1	C	695	ASP	3.7
1	D	708	CYS	3.6
1	C	368	VAL	3.6
1	B	977	ASN	3.6
2	F	29	ALA	3.6
1	B	158	ASN	3.6
2	H	60	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	674	THR	3.5
1	C	299	SER	3.5
1	B	131	ALA	3.4
1	B	982	VAL	3.4
2	E	50	GLU	3.4
2	H	128	GLU	3.4
1	A	733	GLN	3.4
1	A	39	VAL	3.4
1	D	414	THR	3.3
2	F	42	THR	3.3
1	B	286	ALA	3.3
1	C	210	GLU	3.3
1	D	245	ASP	3.3
1	C	884	SER	3.3
1	A	470	ASP	3.3
1	B	437	ALA	3.3
1	D	676	SER	3.3
1	B	295	GLU	3.2
1	A	589	SER	3.2
1	C	920	GLU	3.2
1	B	960	MET	3.2
2	H	40	SER	3.1
2	H	121	PRO	3.1
1	A	56	THR	3.1
1	B	520	GLY	3.1
1	B	507	LYS	3.1
2	H	62	VAL	3.0
1	C	661	GLY	3.0
1	B	242	GLN	3.0
1	B	483	GLU	3.0
2	H	35	GLU	3.0
1	A	472	SER	3.0
1	A	613	GLN	3.0
2	F	43	ILE	3.0
1	B	496	PRO	2.9
2	E	34	ASP	2.9
1	D	843	ARG	2.9
2	H	80	ILE	2.9
2	E	135	VAL	2.9
1	C	273	ARG	2.9
1	D	675	ALA	2.9
1	C	657	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	134	SER	2.8
2	H	70	SER	2.8
1	C	367	ARG	2.8
1	A	36	PRO	2.8
1	D	179	SER	2.8
1	D	243	GLN	2.8
1	D	441	GLN	2.8
1	B	499	ARG	2.8
2	H	122	ASN	2.8
1	C	915	GLU	2.7
1	B	945	PHE	2.7
1	D	306	GLU	2.7
1	B	522	ARG	2.7
2	F	93	LYS	2.7
2	G	62	VAL	2.7
2	H	119	PRO	2.7
1	C	685	GLN	2.6
1	D	415	GLU	2.6
1	A	402	LYS	2.6
2	H	73	VAL	2.6
1	A	732	ASP	2.6
2	F	57	LYS	2.5
1	B	262	VAL	2.5
1	C	34	CYS	2.5
1	A	523	ARG	2.5
1	A	94	THR	2.5
1	A	330	LYS	2.5
1	C	665	PRO	2.5
1	B	264	VAL	2.5
1	C	72	ARG	2.5
1	B	638	VAL	2.4
1	B	272	LYS	2.4
2	H	130	LYS	2.4
1	D	369	PHE	2.4
2	E	134	VAL	2.4
1	A	41	PRO	2.4
1	C	100	ARG	2.4
1	C	297	GLY	2.4
1	C	686	ILE	2.4
2	H	116	THR	2.4
2	H	34	ASP	2.4
1	B	497	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	62	VAL	2.3
1	C	687	GLN	2.3
1	C	894	CYS	2.3
2	E	76	PRO	2.3
1	A	544	GLU	2.3
1	B	274	VAL	2.3
1	A	615	ARG	2.3
1	A	592	SER	2.3
1	D	417	PRO	2.3
1	D	584	ASP	2.3
1	B	57	ILE	2.2
1	B	243	GLN	2.2
1	B	82	ASN	2.2
1	B	465	PRO	2.2
1	C	659	MET	2.2
1	C	392	LEU	2.2
1	C	945	PHE	2.2
2	H	42	THR	2.2
2	F	30	ASP	2.1
1	D	202	SER	2.1
1	B	983	PRO	2.1
1	B	459	GLN	2.1
1	B	714	GLY	2.1
1	B	730	ARG	2.1
2	F	41	HIS	2.1
1	C	572	SER	2.1
1	B	285	VAL	2.1
2	E	73	VAL	2.1
1	B	30	LYS	2.1
1	B	319	SER	2.1
1	C	946	LEU	2.1
1	B	56	THR	2.1
1	C	547	ASN	2.0
1	D	416	VAL	2.0
1	A	569	LYS	2.0
1	B	976	TYR	2.0
2	G	55	ALA	2.0
1	B	732	ASP	2.0
1	B	58	THR	2.0
2	F	128	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.

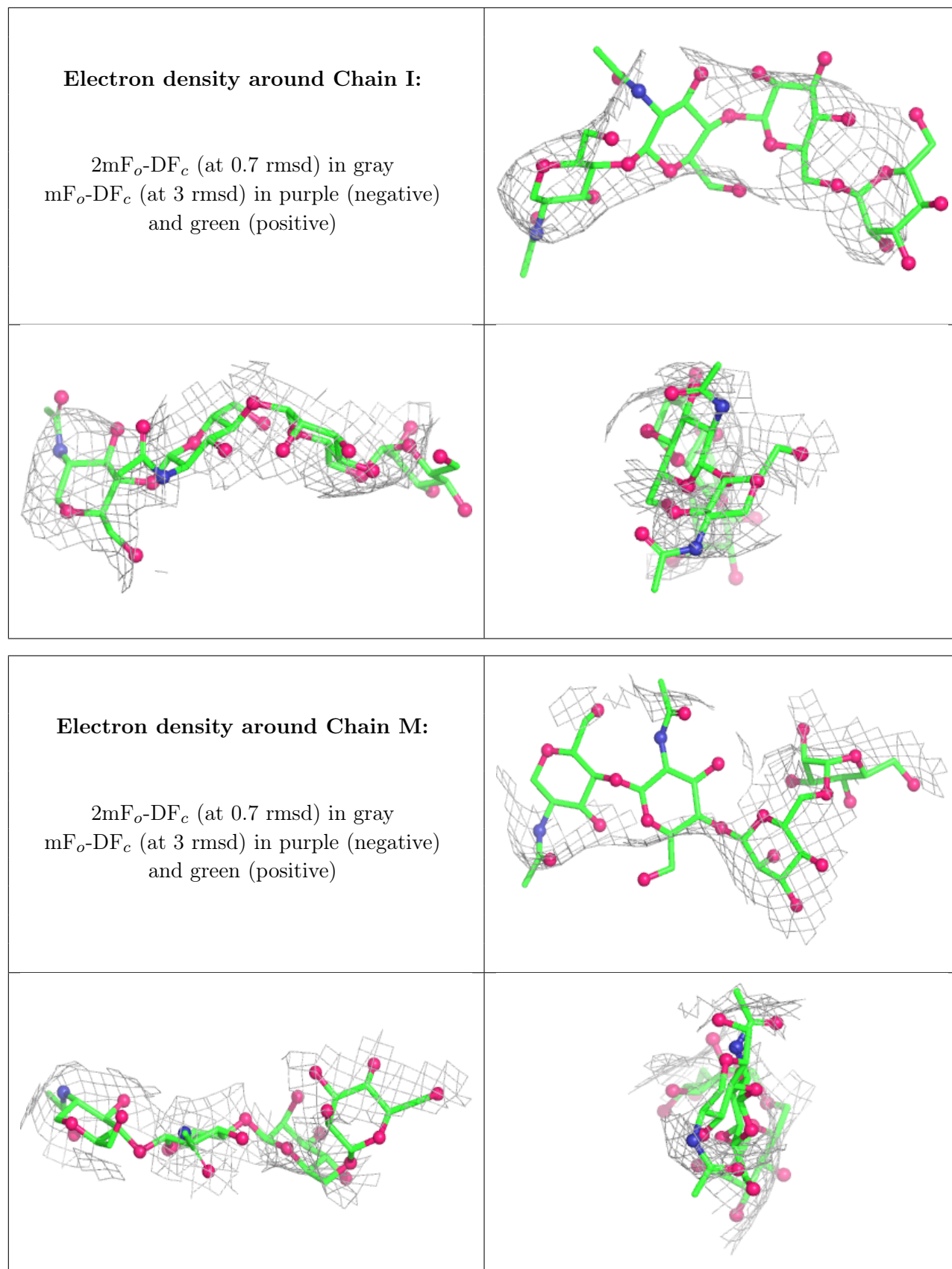
6.3 Carbohydrates [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	R	2	14/15	0.89	0.07	253,253,253,253	0
3	MAN	M	4	11/12	0.90	0.10	251,251,251,251	0
7	BMA	Q	3	11/12	0.90	0.06	234,234,234,234	0
6	MAN	P	5	11/12	0.92	0.11	229,229,229,229	0
4	NAG	N	2	14/15	0.93	0.15	226,226,226,226	0
5	BMA	L	3	11/12	0.95	0.07	234,234,234,234	0
6	MAN	P	4	11/12	0.95	0.11	222,222,222,222	0
4	NAG	J	2	14/15	0.95	0.21	239,239,239,239	0
4	NAG	K	2	14/15	0.95	0.07	246,246,246,246	0
5	MAN	L	4	11/12	0.96	0.10	257,257,257,257	0
4	NAG	O	1	14/15	0.96	0.07	202,202,202,202	0
4	NAG	J	1	14/15	0.96	0.13	211,211,211,211	0
7	NAG	Q	1	14/15	0.96	0.10	199,199,199,199	0
3	MAN	I	4	11/12	0.96	0.10	246,246,246,246	0
5	NAG	L	1	14/15	0.97	0.10	199,199,199,199	0
3	BMA	I	3	11/12	0.97	0.06	230,230,230,230	0
4	NAG	N	1	14/15	0.97	0.04	233,233,233,233	0
3	NAG	M	2	14/15	0.97	0.10	212,212,212,212	0
3	BMA	M	3	11/12	0.97	0.11	230,230,230,230	0
4	NAG	R	1	14/15	0.97	0.07	255,255,255,255	0
4	NAG	K	1	14/15	0.97	0.12	225,225,225,225	0
4	NAG	O	2	14/15	0.98	0.20	228,228,228,228	0
5	NAG	L	2	14/15	0.98	0.07	191,191,191,191	0
3	NAG	I	2	14/15	0.98	0.07	224,224,224,224	0
3	NAG	M	1	14/15	0.98	0.08	210,210,210,210	0
3	NAG	I	1	14/15	0.99	0.08	199,199,199,199	0
6	NAG	P	1	14/15	0.99	0.07	224,224,224,224	0
6	NAG	P	2	14/15	0.99	0.12	234,234,234,234	0
7	NAG	Q	2	14/15	0.99	0.10	221,221,221,221	0
6	BMA	P	3	11/12	0.99	0.12	233,233,233,233	0

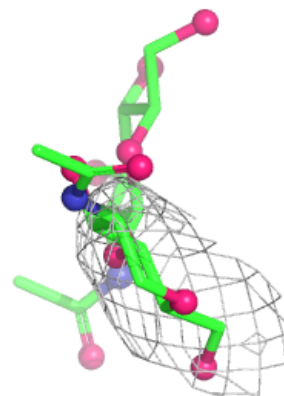
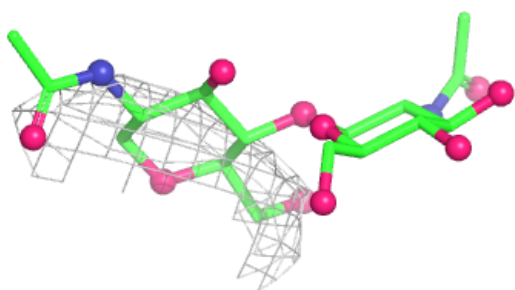
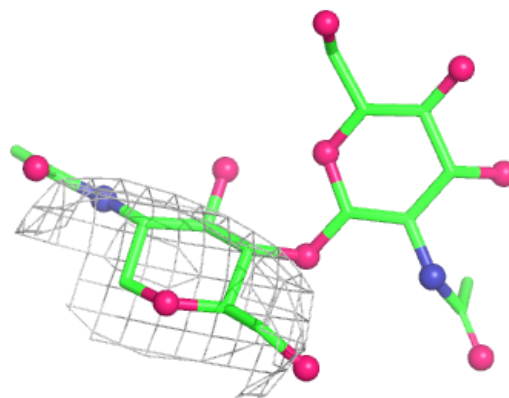
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

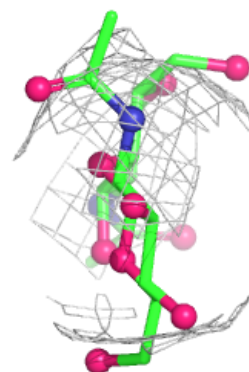
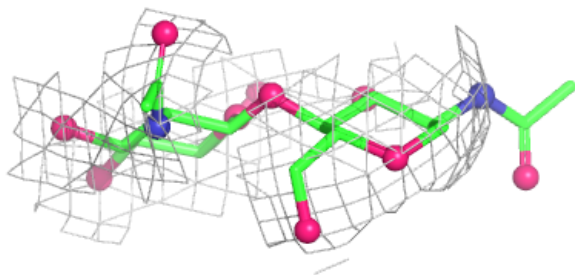
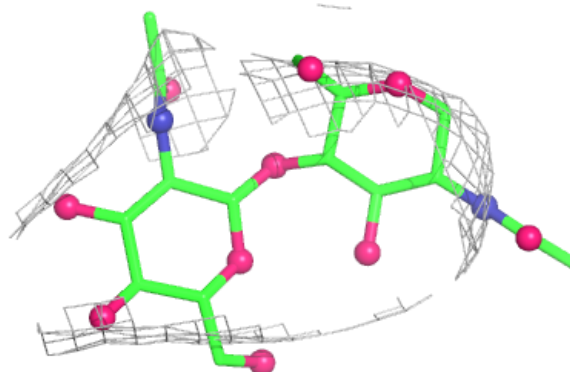


Electron density around Chain J:

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

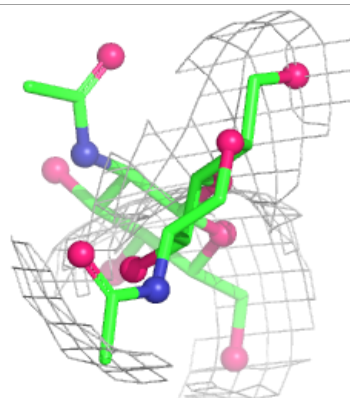
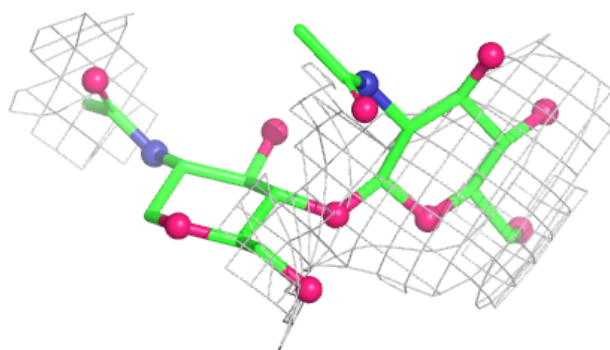
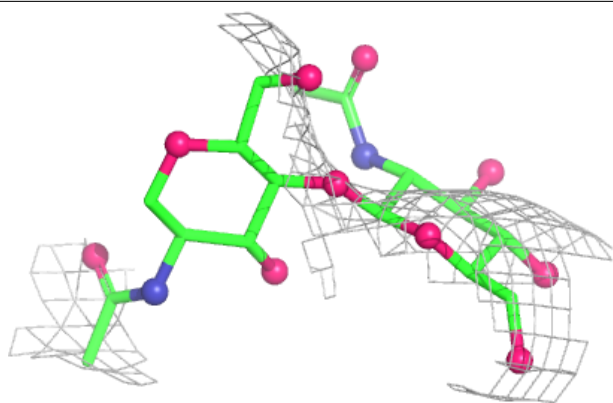
**Electron density around Chain K:**

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

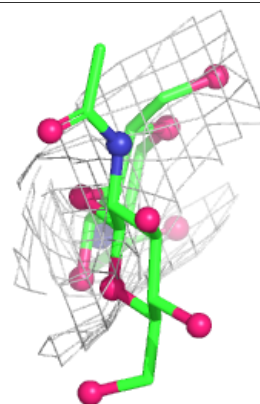
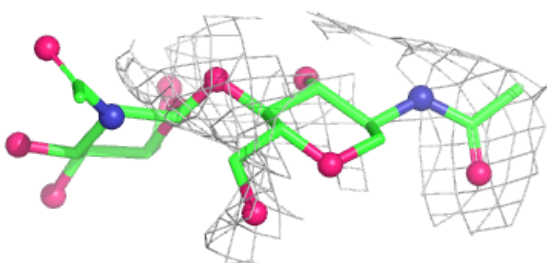
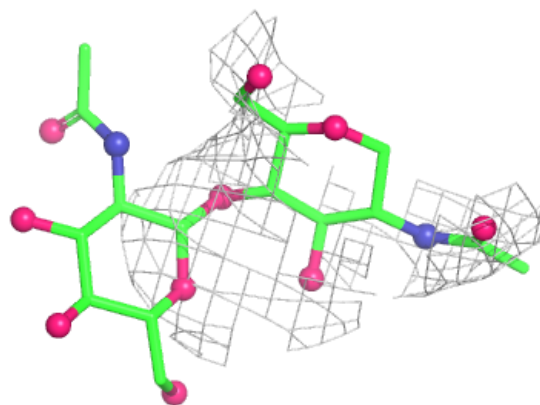


Electron density around Chain N:

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

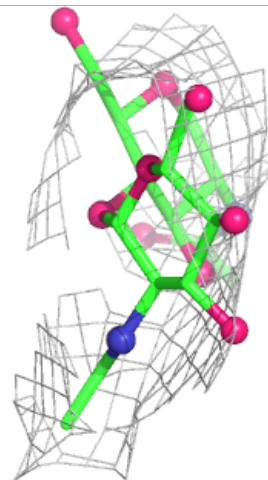
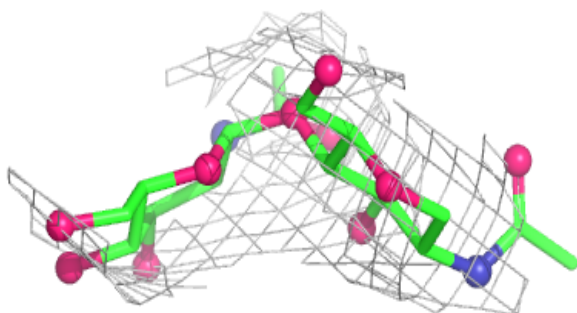
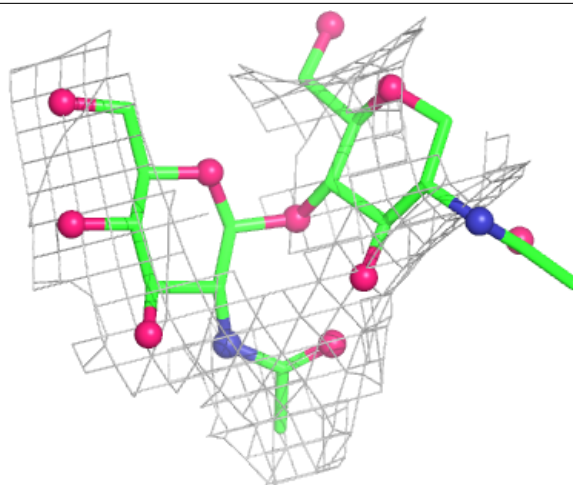
**Electron density around Chain O:**

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



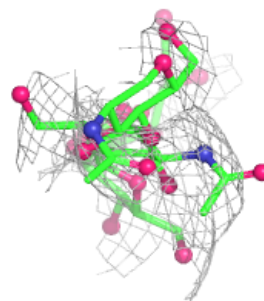
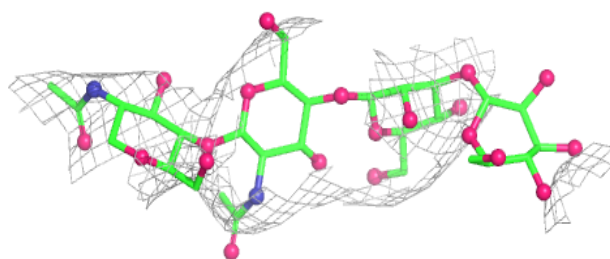
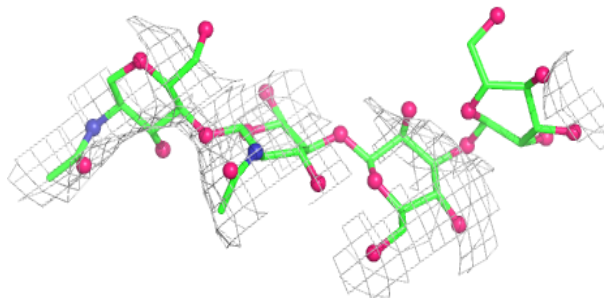
Electron density around Chain R:

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

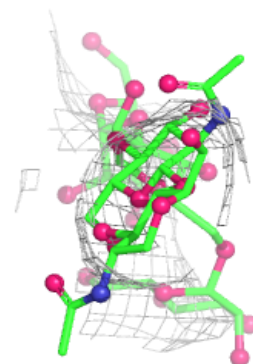
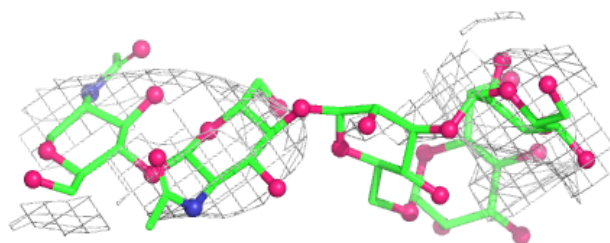
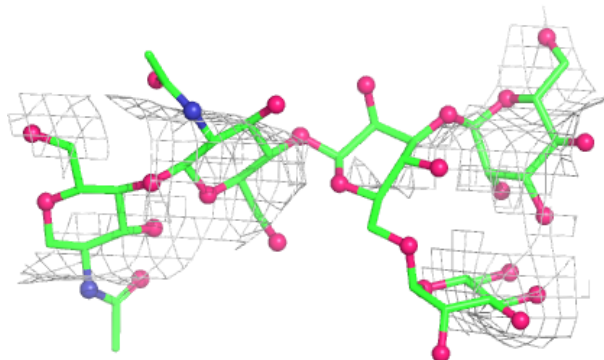


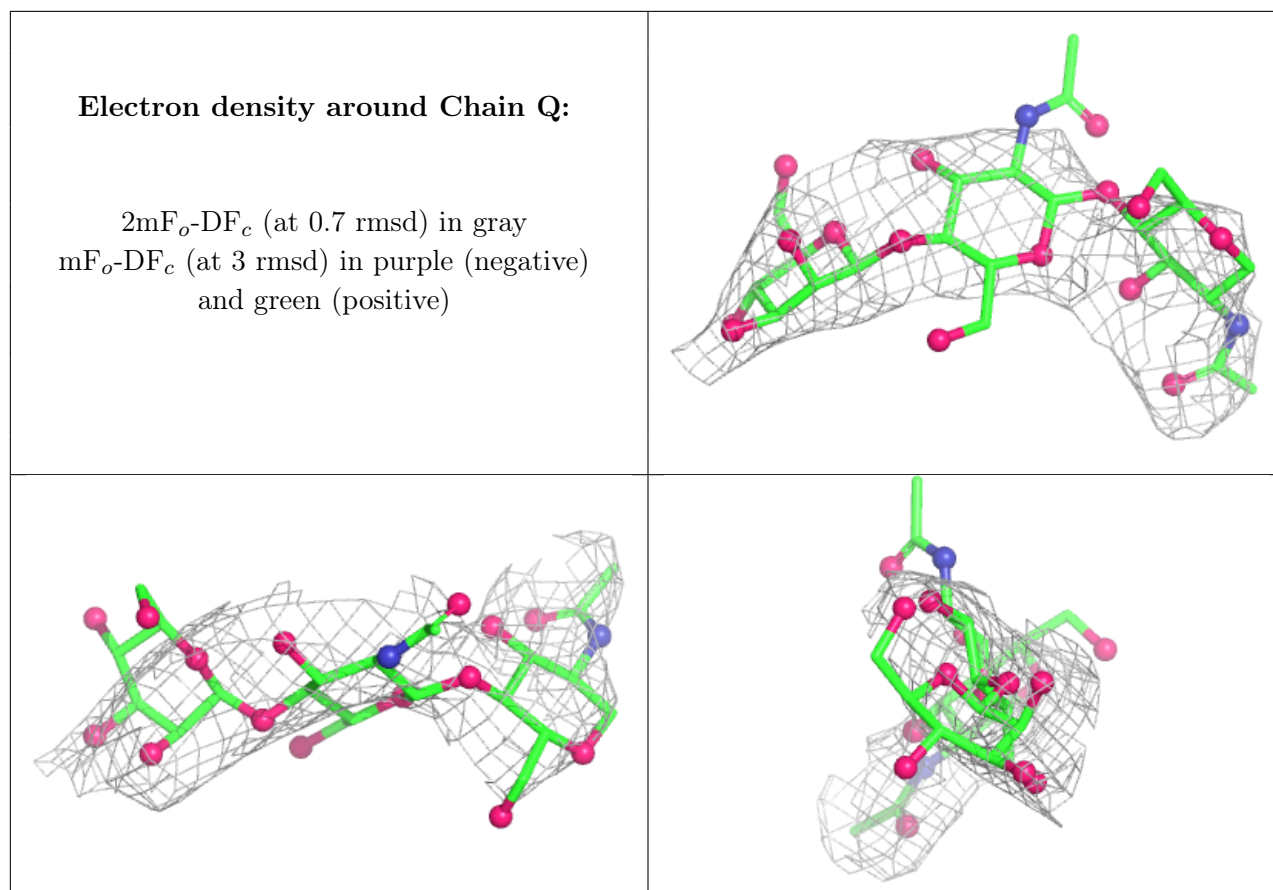
Electron density around Chain L:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	B	1101	14/15	0.86	0.10	264,264,264,264	0
8	NAG	B	1103	14/15	0.94	0.10	234,234,234,234	0
8	NAG	A	1101	14/15	0.95	0.11	209,209,209,209	0
8	NAG	C	1102	14/15	0.95	0.06	220,220,220,220	0
8	NAG	A	1102	14/15	0.97	0.10	254,254,254,254	0
8	NAG	D	1102	14/15	0.97	0.12	234,234,234,234	0
8	NAG	C	1101	14/15	0.98	0.07	175,175,175,175	0
8	NAG	B	1102	14/15	0.98	0.14	235,235,235,235	0
8	NAG	D	1101	14/15	0.98	0.09	246,246,246,246	0
8	NAG	A	1103	14/15	0.98	0.08	204,204,204,204	0

6.5 Other polymers [i](#)

There are no such residues in this entry.