



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:54 AM BST

PDB ID : 3K71
Title : Structure of integrin alphaX beta2 ectodomain
Authors : Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.
Deposited on : 2009-10-11
Resolution : 3.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

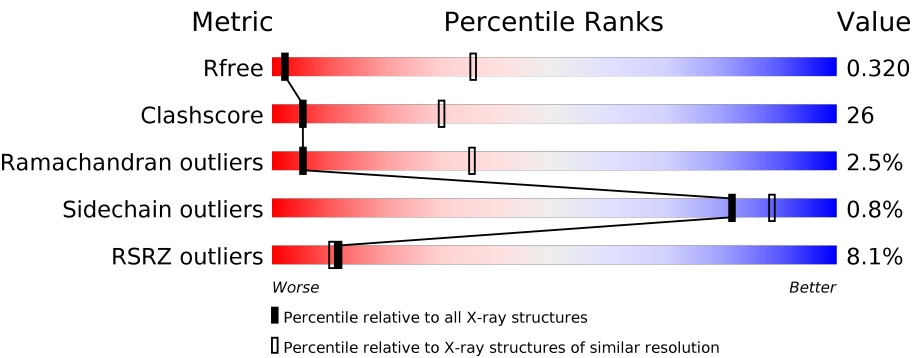
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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 on 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	1095	<div><div>3%</div><div>42%35%20%</div></div>
1	C	1095	<div><div>3%</div><div>44%35%19%</div></div>
1	E	1095	<div><div>4%</div><div>42%36%19%</div></div>
1	G	1095	<div><div>8%</div><div>54%42%</div></div>
2	B	687	<div><div>12%</div><div>64%33%</div></div>
2	D	687	<div><div>12%</div><div>62%34%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	687	
2	H	687	
3	I	2	
3	M	2	
3	N	2	
3	P	2	
3	S	2	
4	J	3	
4	K	3	
4	L	3	
4	O	3	
4	Q	3	
4	R	3	
4	U	3	
5	T	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	J	1	X	-	-	-
4	MAN	J	3	X	-	-	-
4	MAN	K	3	X	-	-	-
4	MAN	L	3	X	-	-	-
4	MAN	O	3	X	-	-	-
4	NAG	Q	1	-	-	X	-
4	NAG	Q	2	-	-	-	X
4	MAN	Q	3	X	-	-	X
4	MAN	R	3	X	-	-	-
4	MAN	U	3	X	-	-	-
5	MAN	T	3	X	-	-	-
6	NAG	D	3479	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	F	3094	-	-	-	X
8	MG	G	2009	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 50191 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	880	Total	C	N	O	S	0	0	0
			6782	4284	1173	1291	34			
1	C	884	Total	C	N	O	S	0	0	0
			6814	4305	1178	1297	34			
1	E	882	Total	C	N	O	S	0	0	0
			6802	4299	1176	1293	34			
1	G	1082	Total	C	N	O	S	0	0	0
			8392	5304	1454	1596	38			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	expression tag	UNP P20702
A	1086	CYS	-	expression tag	UNP P20702
A	1087	GLY	-	expression tag	UNP P20702
A	1088	GLY	-	expression tag	UNP P20702
A	1089	LEU	-	expression tag	UNP P20702
A	1090	GLU	-	expression tag	UNP P20702
A	1091	ASN	-	expression tag	UNP P20702
A	1092	LEU	-	expression tag	UNP P20702
A	1093	TYR	-	expression tag	UNP P20702
A	1094	PHE	-	expression tag	UNP P20702
A	1095	GLN	-	expression tag	UNP P20702
C	1085	GLY	-	expression tag	UNP P20702
C	1086	CYS	-	expression tag	UNP P20702
C	1087	GLY	-	expression tag	UNP P20702
C	1088	GLY	-	expression tag	UNP P20702
C	1089	LEU	-	expression tag	UNP P20702
C	1090	GLU	-	expression tag	UNP P20702
C	1091	ASN	-	expression tag	UNP P20702
C	1092	LEU	-	expression tag	UNP P20702
C	1093	TYR	-	expression tag	UNP P20702
C	1094	PHE	-	expression tag	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	expression tag	UNP P20702
E	1085	GLY	-	expression tag	UNP P20702
E	1086	CYS	-	expression tag	UNP P20702
E	1087	GLY	-	expression tag	UNP P20702
E	1088	GLY	-	expression tag	UNP P20702
E	1089	LEU	-	expression tag	UNP P20702
E	1090	GLU	-	expression tag	UNP P20702
E	1091	ASN	-	expression tag	UNP P20702
E	1092	LEU	-	expression tag	UNP P20702
E	1093	TYR	-	expression tag	UNP P20702
E	1094	PHE	-	expression tag	UNP P20702
E	1095	GLN	-	expression tag	UNP P20702
G	1085	GLY	-	expression tag	UNP P20702
G	1086	CYS	-	expression tag	UNP P20702
G	1087	GLY	-	expression tag	UNP P20702
G	1088	GLY	-	expression tag	UNP P20702
G	1089	LEU	-	expression tag	UNP P20702
G	1090	GLU	-	expression tag	UNP P20702
G	1091	ASN	-	expression tag	UNP P20702
G	1092	LEU	-	expression tag	UNP P20702
G	1093	TYR	-	expression tag	UNP P20702
G	1094	PHE	-	expression tag	UNP P20702
G	1095	GLN	-	expression tag	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	D	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	F	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	H	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	expression tag	UNP P05107
B	679	GLY	-	expression tag	UNP P05107
B	680	CYS	-	expression tag	UNP P05107

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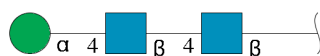
Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	expression tag	UNP P05107
B	682	GLU	-	expression tag	UNP P05107
B	684	LEU	-	expression tag	UNP P05107
B	685	TYR	-	expression tag	UNP P05107
B	686	PHE	-	expression tag	UNP P05107
B	687	GLN	-	expression tag	UNP P05107
D	678	ASP	-	expression tag	UNP P05107
D	679	GLY	-	expression tag	UNP P05107
D	680	CYS	-	expression tag	UNP P05107
D	681	GLY	-	expression tag	UNP P05107
D	682	GLU	-	expression tag	UNP P05107
D	684	LEU	-	expression tag	UNP P05107
D	685	TYR	-	expression tag	UNP P05107
D	686	PHE	-	expression tag	UNP P05107
D	687	GLN	-	expression tag	UNP P05107
F	678	ASP	-	expression tag	UNP P05107
F	679	GLY	-	expression tag	UNP P05107
F	680	CYS	-	expression tag	UNP P05107
F	681	GLY	-	expression tag	UNP P05107
F	682	GLU	-	expression tag	UNP P05107
F	684	LEU	-	expression tag	UNP P05107
F	685	TYR	-	expression tag	UNP P05107
F	686	PHE	-	expression tag	UNP P05107
F	687	GLN	-	expression tag	UNP P05107
H	678	ASP	-	expression tag	UNP P05107
H	679	GLY	-	expression tag	UNP P05107
H	680	CYS	-	expression tag	UNP P05107
H	681	GLY	-	expression tag	UNP P05107
H	682	GLU	-	expression tag	UNP P05107
H	684	LEU	-	expression tag	UNP P05107
H	685	TYR	-	expression tag	UNP P05107
H	686	PHE	-	expression tag	UNP P05107
H	687	GLN	-	expression tag	UNP P05107

- Molecule 3 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
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



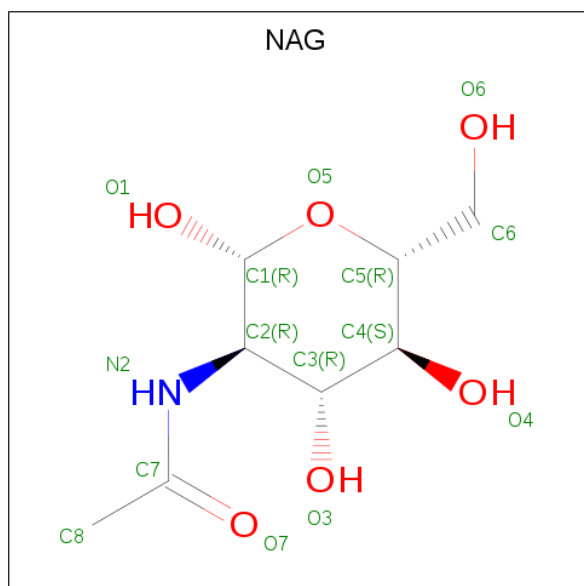
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	3	Total	Ca	0	0
			3	3		
7	D	1	Total	Ca	0	0
			1	1		
7	E	3	Total	Ca	0	0
			3	3		
7	H	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	3	Total	Ca	0	0
			3	3		
7	A	3	Total	Ca	0	0
			3	3		
7	F	1	Total	Ca	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Mg	0	0
			1	1		

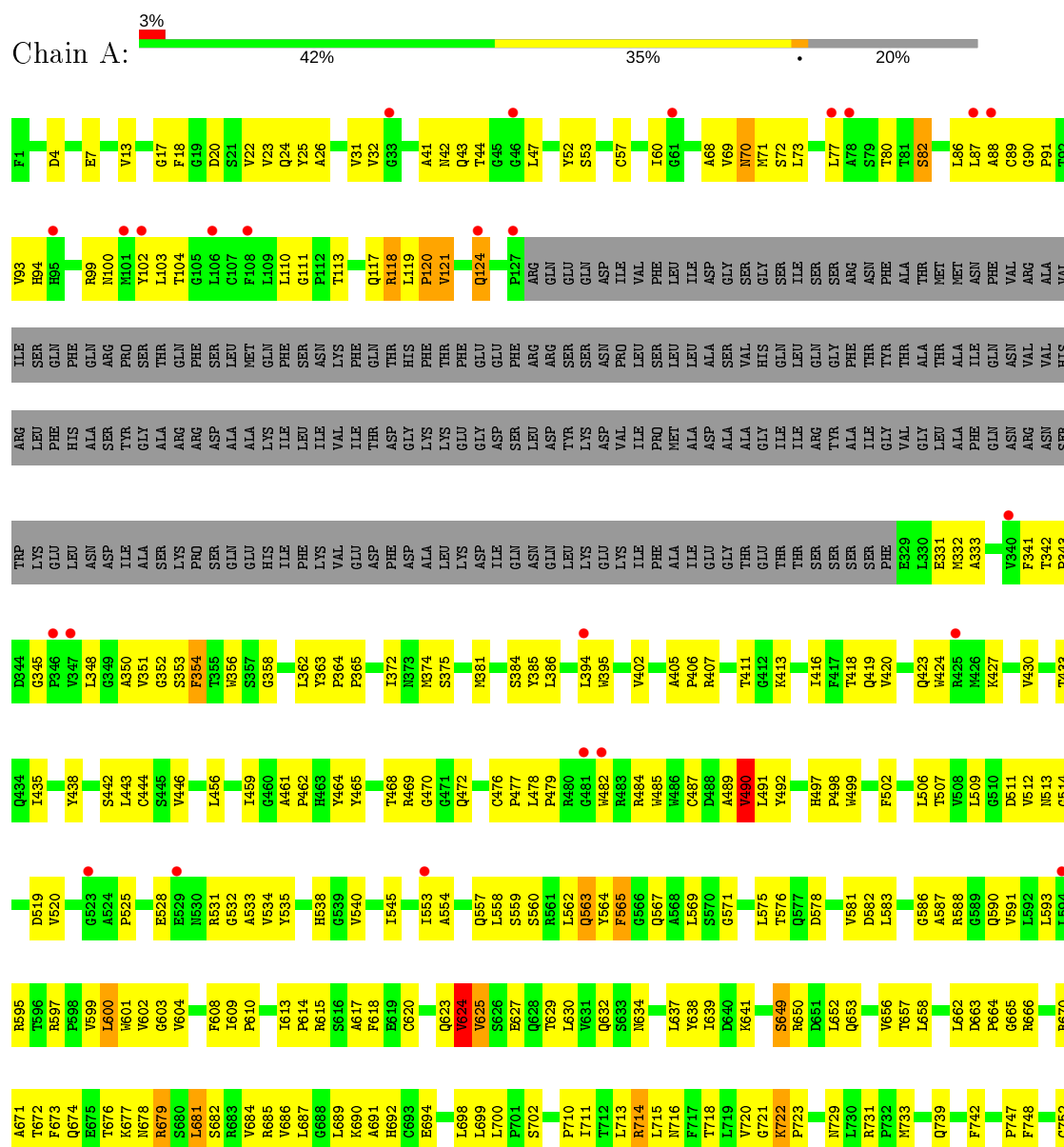
- Molecule 9 is water.

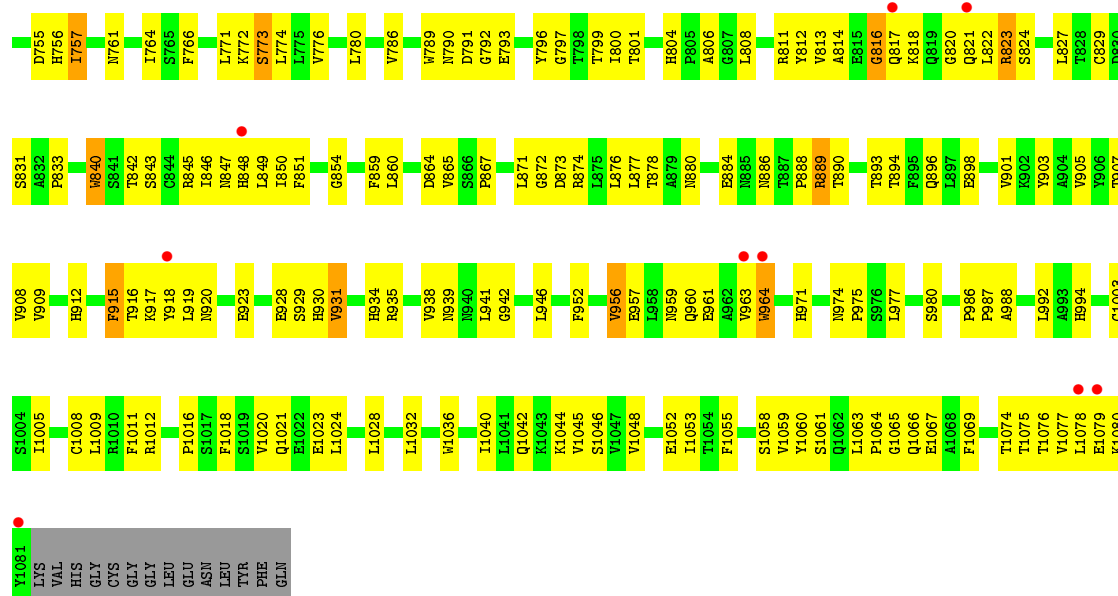
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	3	Total	O	0	0
			3	3		

3 Residue-property plots

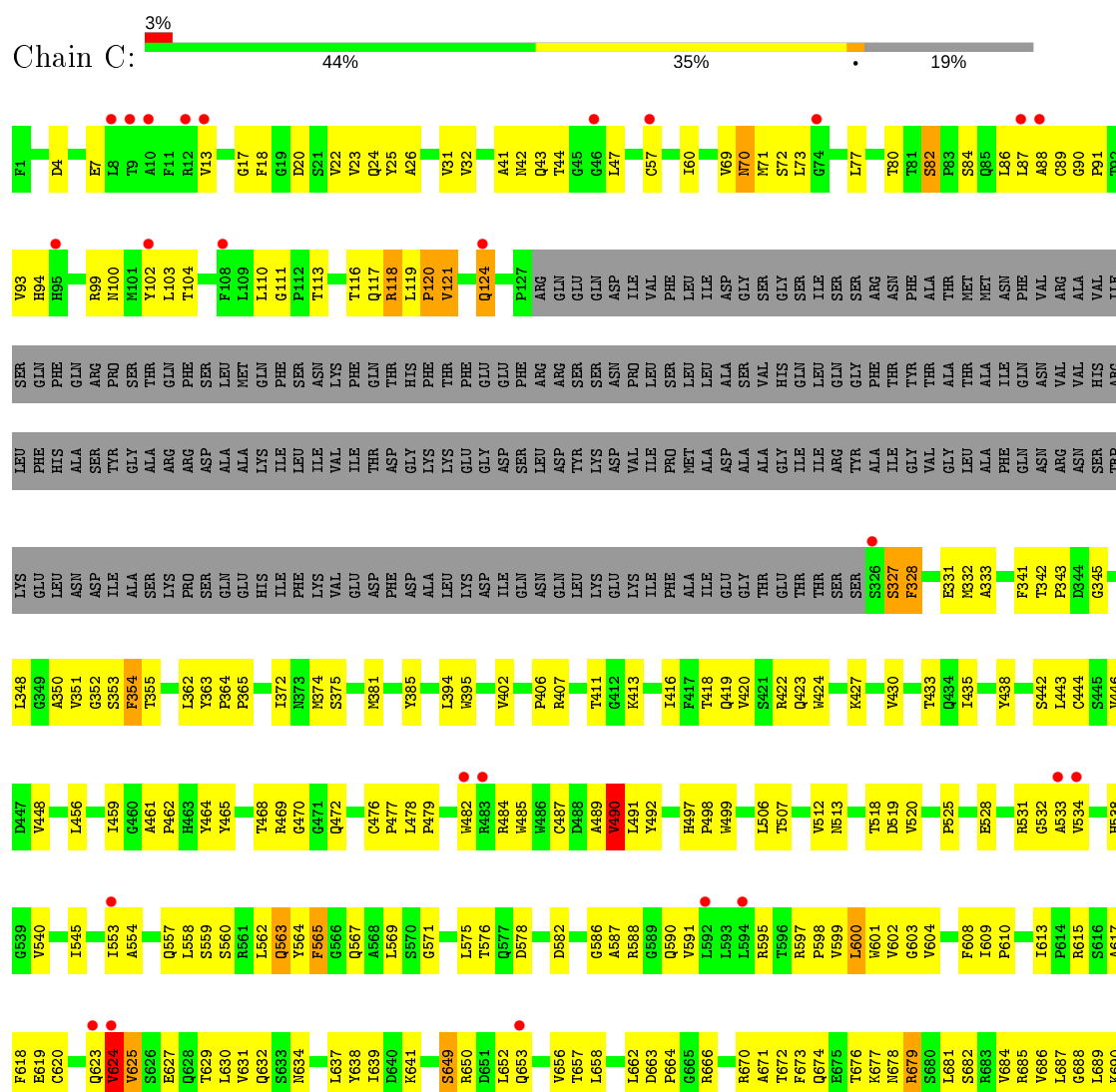
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

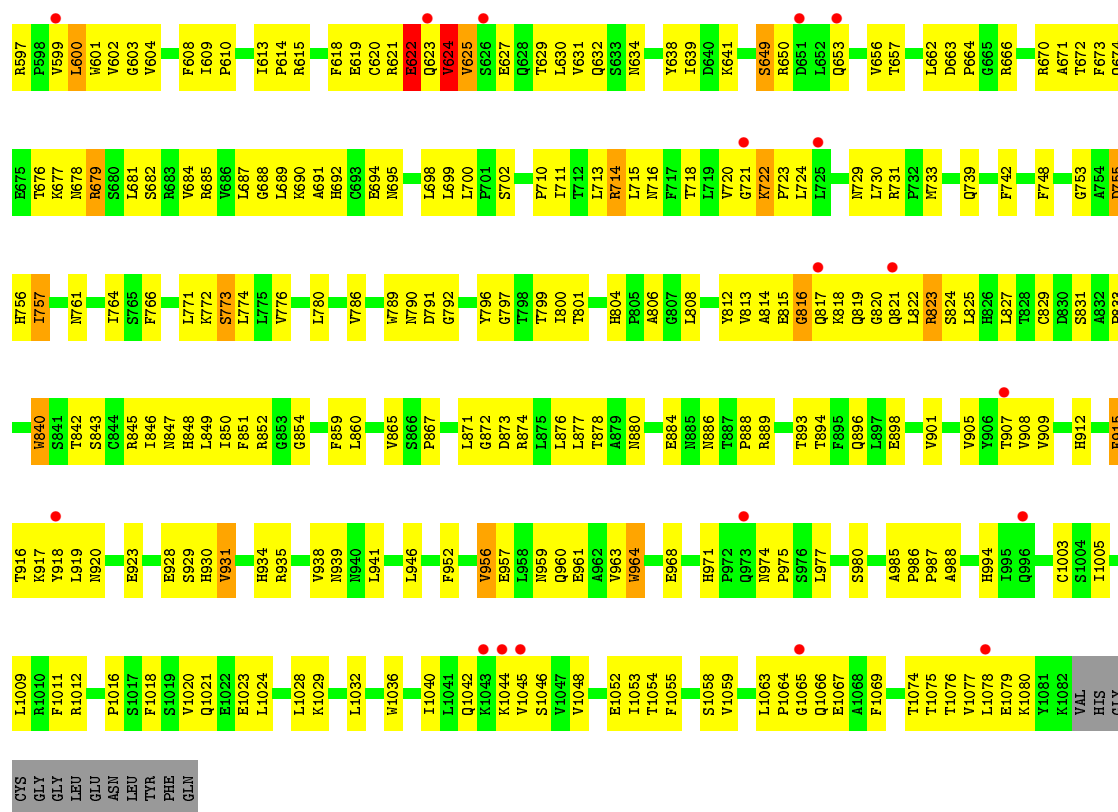
• Molecule 1: Integrin alpha-X



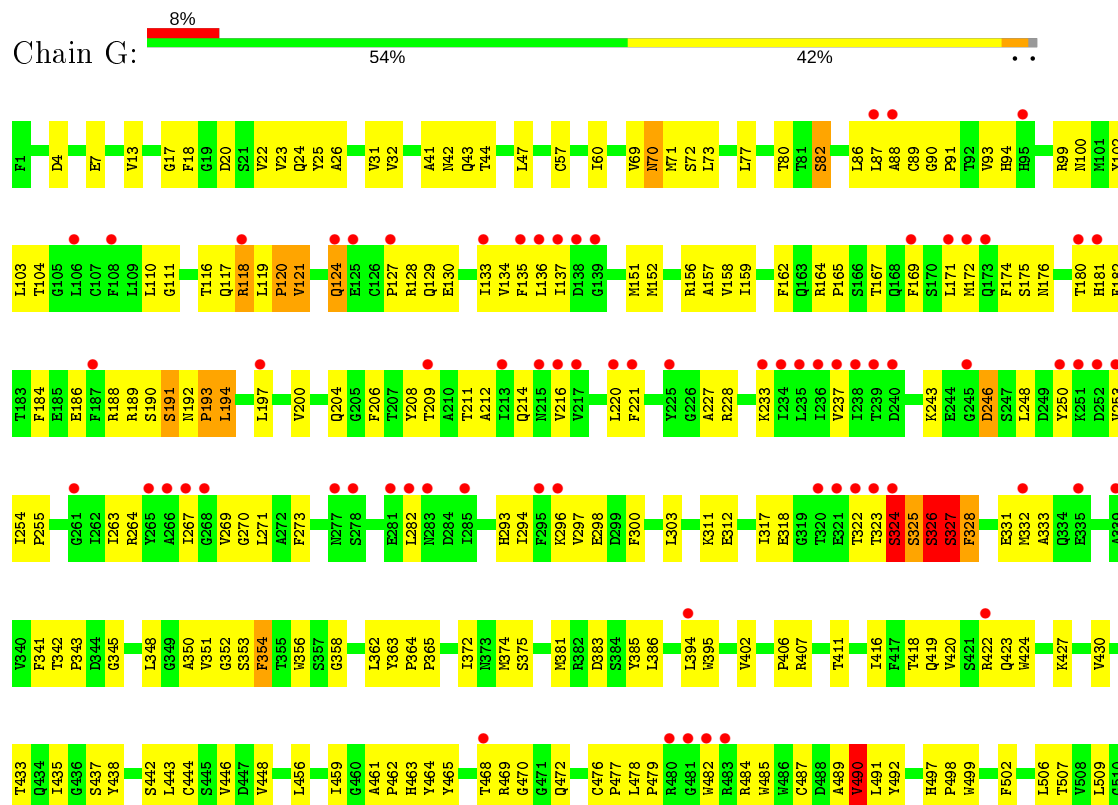


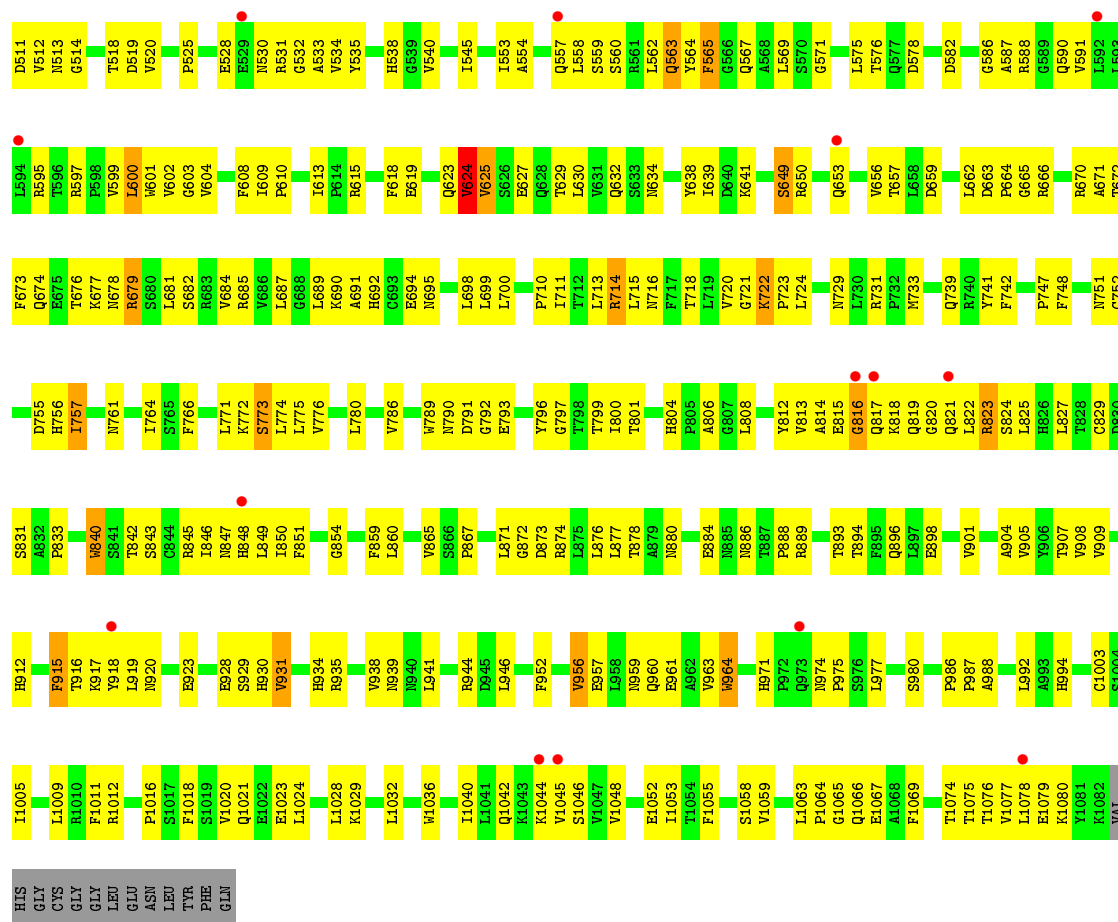
• Molecule 1: Integrin alpha-X



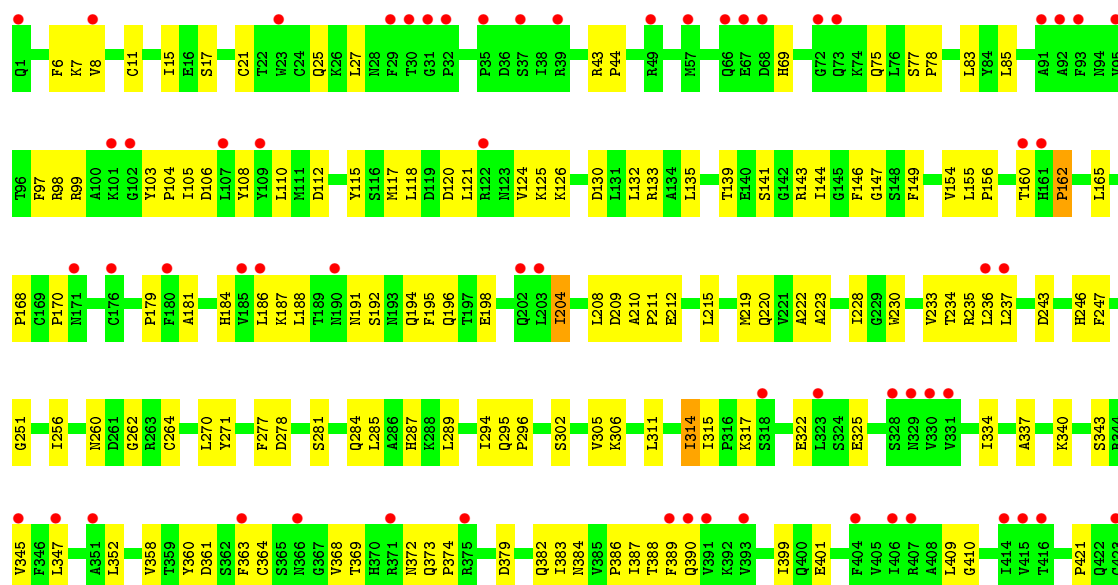


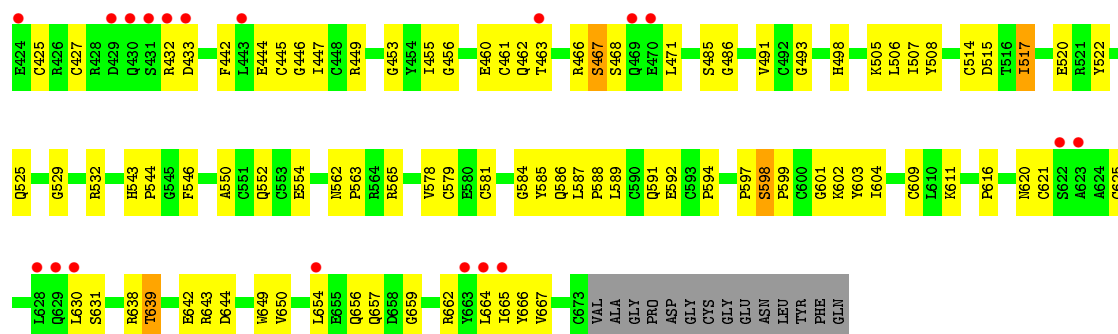
• Molecule 1: Integrin alpha-X



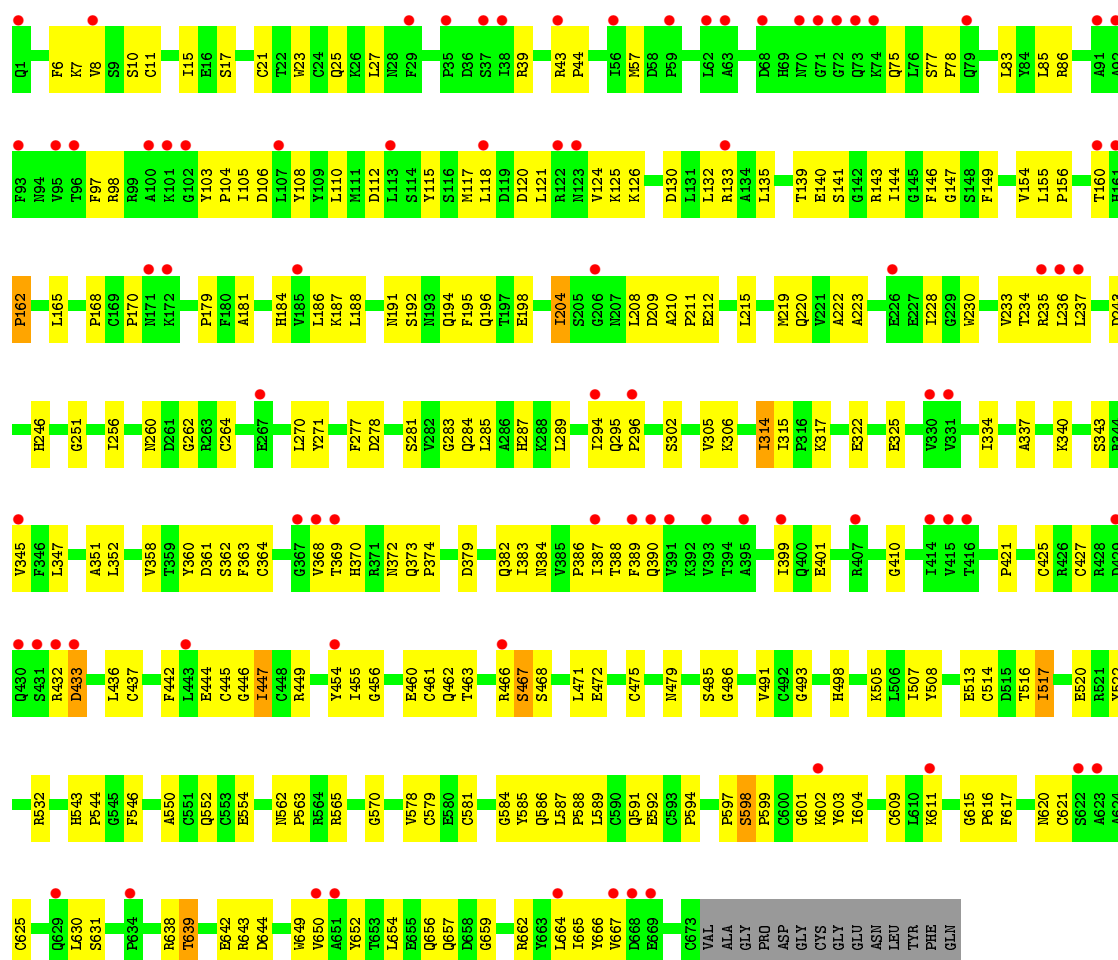


• Molecule 2: Integrin beta-2

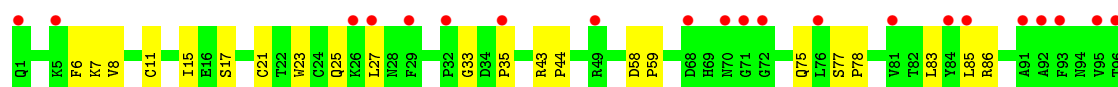


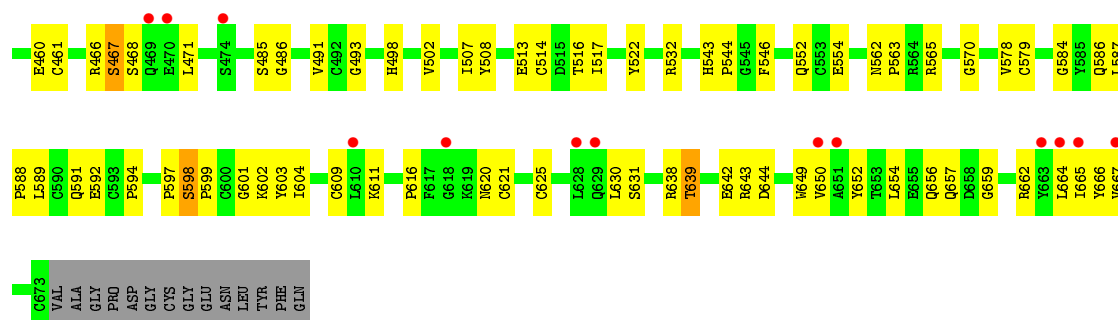


• Molecule 2: Integrin beta-2



• Molecule 2: Integrin beta-2





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

Chain I: 50% 50%

UAG1
UAG2

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

Chain M: 50% 50%

UAG1
UAG2

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

Chain N: 100%

UAG1
UAG2

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

Chain P: 50% 50%

UAG1
UAG2

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

Chain S: 50% 50%

UAG1
UAG2

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

Chain J:  100%

NA01
NA02
NA03

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

Chain K:  100%

NA01
NA02
NA03

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

Chain L:  33% 67%

NA01
NA02
NA03

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

Chain O:  100%

NA01
NA02
NA03

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

Chain Q:  33% 67%

NA01
NA02
NA03

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

Chain R:  100%

NA01
NA02
NA03

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

Chain U:  67% 33%



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.66Å 165.75Å 537.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.95 49.67 – 3.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.67-3.95) 99.4 (49.67-3.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.350 , 0.373 0.310 , 0.320	Depositor DCC
R_{free} test set	1022 reflections (0.87%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 130.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50191	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MAN, CA, 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	0.24	0/6936	0.45	0/9437
1	C	0.24	0/6969	0.45	0/9480
1	E	0.27	1/6957 (0.0%)	0.46	0/9464
1	G	0.26	0/8579	0.46	0/11652
2	B	0.25	0/5273	0.41	0/7119
2	D	0.24	0/5273	0.41	0/7119
2	F	0.25	0/5273	0.42	0/7119
2	H	0.24	0/5273	0.40	0/7119
All	All	0.25	1/50533 (0.0%)	0.44	0/68509

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	C	0	10
1	E	0	10
1	G	0	14
2	B	0	1
2	D	0	1
2	F	0	2
2	H	0	1
All	All	0	48

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	622	GLU	CG-CD	-8.81	1.38	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	490	VAL	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
1	A	889	ARG	Peptide
2	B	425	CYS	Peptide
1	C	118	ARG	Peptide
1	C	327	SER	Peptide
1	C	490	VAL	Peptide
1	C	624	VAL	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	82	SER	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
1	C	889	ARG	Peptide
2	D	425	CYS	Peptide
1	E	118	ARG	Peptide
1	E	490	VAL	Peptide
1	E	622	GLU	Peptide
1	E	624	VAL	Peptide
1	E	625	VAL	Peptide
1	E	816	GLY	Peptide
1	E	82	SER	Peptide
1	E	821	GLN	Peptide
1	E	824	SER	Peptide
1	E	889	ARG	Peptide
2	F	100	ALA	Peptide
2	F	425	CYS	Peptide
1	G	118	ARG	Peptide
1	G	127	PRO	Peptide
1	G	324	SER	Peptide
1	G	325	SER	Peptide
1	G	326	SER	Peptide
1	G	327	SER	Peptide

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Mol	Chain	Res	Type	Group
1	G	490	VAL	Peptide
1	G	624	VAL	Peptide
1	G	625	VAL	Peptide
1	G	816	GLY	Peptide
1	G	82	SER	Peptide
1	G	821	GLN	Peptide
1	G	824	SER	Peptide
1	G	889	ARG	Peptide
2	H	425	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6782	0	6641	427	0
1	C	6814	0	6672	418	0
1	E	6802	0	6662	428	2
1	G	8392	0	8229	492	2
2	B	5177	0	4966	214	0
2	D	5177	0	4966	246	0
2	F	5177	0	4966	249	0
2	H	5177	0	4966	234	0
3	I	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	P	28	0	25	0	0
3	S	28	0	25	0	0
4	J	39	0	34	3	0
4	K	39	0	34	0	0
4	L	39	0	34	0	0
4	O	39	0	34	0	0
4	Q	39	0	34	8	0
4	R	39	0	34	0	0
4	U	39	0	34	1	0
5	T	50	0	43	2	0
6	A	14	0	13	0	0
6	B	28	0	26	0	0
6	C	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	28	0	26	8	0
6	E	28	0	26	1	0
6	F	28	0	26	3	0
6	G	28	0	26	0	0
6	H	28	0	26	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	E	3	0	0	0	0
7	F	1	0	0	0	0
7	G	3	0	0	0	0
7	H	1	0	0	0	0
8	G	1	0	0	0	0
9	G	3	0	0	0	0
All	All	50191	0	48669	2584	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (2584) 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)
2:F:317:LYS:HE3	2:F:410:GLY:HA3	1.42	1.01
1:G:103:LEU:HD11	2:H:155:LEU:HD13	1.49	0.95
1:C:119:LEU:N	1:C:120:PRO:HA	1.83	0.94
1:A:119:LEU:N	1:A:120:PRO:HA	1.84	0.93
2:H:27:LEU:HG	2:H:446:GLY:HA2	1.51	0.93
1:E:103:LEU:HD11	2:F:155:LEU:HD13	1.51	0.92
1:C:94:HIS:NE2	2:D:155:LEU:HD21	1.84	0.92
1:E:119:LEU:N	1:E:120:PRO:HA	1.84	0.92
1:E:623:GLN:O	1:E:624:VAL:HG22	1.69	0.92
2:F:15:ILE:HG23	2:F:86:ARG:NH2	1.85	0.92
2:F:35:PRO:HG2	2:F:510:GLN:CD	1.90	0.92
1:G:119:LEU:N	1:G:120:PRO:HA	1.83	0.90
1:A:484:ARG:NH1	2:B:586:GLN:HG3	1.88	0.87
2:F:15:ILE:HD12	2:F:86:ARG:HH22	1.39	0.87
1:A:756:HIS:HA	1:C:1052:GLU:OE1	1.75	0.87
1:A:772:LYS:HA	1:C:789:TRP:CZ2	2.10	0.86
1:A:789:TRP:CZ2	1:C:772:LYS:HA	2.11	0.86
2:F:317:LYS:HE3	2:F:410:GLY:CA	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ARG:HH12	1:G:318:GLU:HG3	1.41	0.86
1:C:103:LEU:HD11	2:D:155:LEU:HD13	1.57	0.84
2:D:479:ASN:HD21	6:D:3479:NAG:H82	1.40	0.84
2:F:15:ILE:HD12	2:F:86:ARG:NH2	1.92	0.84
2:H:25:GLN:OE1	2:H:427:CYS:SG	2.36	0.83
2:H:532:ARG:HD3	2:H:554:GLU:CD	1.97	0.83
2:F:570:GLY:HA2	2:F:659:GLY:HA2	1.61	0.83
1:A:94:HIS:NE2	2:B:155:LEU:HD21	1.93	0.83
2:F:293:ASN:OD1	2:F:412:THR:HG22	1.79	0.82
1:G:99:ARG:NH1	1:G:318:GLU:HG3	1.94	0.82
1:C:625:VAL:HG21	1:C:627:GLU:HG3	1.59	0.82
1:C:113:THR:HG22	1:E:1029:LYS:CE	2.10	0.82
1:A:625:VAL:HG21	1:A:627:GLU:HG3	1.61	0.81
1:E:625:VAL:HG21	1:E:627:GLU:HG3	1.60	0.81
1:G:625:VAL:HG21	1:G:627:GLU:HG3	1.62	0.81
2:D:479:ASN:ND2	6:D:3479:NAG:C7	2.44	0.81
1:E:1064:PRO:HG3	1:E:1067:GLU:CD	2.01	0.81
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.01	0.81
2:D:570:GLY:HA2	2:D:659:GLY:HA2	1.64	0.80
1:E:1063:LEU:HD12	1:E:1064:PRO:CA	2.12	0.80
1:E:1063:LEU:HD12	1:E:1064:PRO:N	1.96	0.80
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.01	0.80
2:D:532:ARG:HD3	2:D:554:GLU:CD	2.02	0.80
2:F:479:ASN:HD22	6:F:3479:NAG:C1	1.95	0.80
1:G:1063:LEU:HD12	1:G:1064:PRO:CA	2.12	0.80
1:A:923:GLU:HB2	1:A:1080:LYS:HB3	1.63	0.80
1:C:1063:LEU:HD12	1:C:1064:PRO:N	1.96	0.80
1:C:1063:LEU:HD12	1:C:1064:PRO:CA	2.12	0.80
2:H:570:GLY:HA2	2:H:659:GLY:HA2	1.64	0.79
1:E:1052:GLU:OE1	1:G:756:HIS:HA	1.83	0.79
1:E:923:GLU:HB2	1:E:1080:LYS:HB3	1.63	0.79
1:G:1063:LEU:HD12	1:G:1064:PRO:N	1.97	0.79
1:A:1063:LEU:HD12	1:A:1064:PRO:CA	2.12	0.79
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.03	0.79
1:C:923:GLU:HB2	1:C:1080:LYS:HB3	1.64	0.79
1:G:923:GLU:HB2	1:G:1080:LYS:HB3	1.63	0.78
1:A:1063:LEU:HD12	1:A:1064:PRO:N	1.97	0.78
1:E:772:LYS:HA	1:G:789:TRP:CZ2	2.18	0.78
1:G:1064:PRO:HG3	1:G:1067:GLU:CD	2.04	0.78
1:G:623:GLN:O	1:G:624:VAL:HG22	1.84	0.78
1:G:99:ARG:NH1	1:G:318:GLU:CG	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:789:TRP:CZ2	1:G:772:LYS:HA	2.20	0.77
2:F:155:LEU:HB2	2:F:156:PRO:HA	1.67	0.77
2:B:155:LEU:HB2	2:B:156:PRO:HA	1.67	0.77
1:E:756:HIS:HA	1:G:1052:GLU:OE1	1.84	0.77
1:G:119:LEU:H	1:G:120:PRO:HA	1.50	0.76
2:D:155:LEU:HB2	2:D:156:PRO:HA	1.67	0.75
1:C:623:GLN:O	1:C:624:VAL:HG22	1.87	0.75
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.69	0.75
2:H:155:LEU:HB2	2:H:156:PRO:HA	1.67	0.75
1:C:113:THR:HG22	1:E:1029:LYS:HE3	1.67	0.74
1:E:94:HIS:NE2	2:F:155:LEU:HD21	2.02	0.74
1:G:756:HIS:O	1:G:757:ILE:HG22	1.87	0.74
1:A:623:GLN:O	1:A:624:VAL:HG22	1.87	0.74
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.69	0.74
2:D:10:SER:CB	2:D:449:ARG:CZ	2.65	0.74
2:H:27:LEU:CG	2:H:446:GLY:HA2	2.17	0.74
2:F:461:CYS:HB3	2:F:466:ARG:HD2	1.68	0.74
2:F:15:ILE:HG23	2:F:86:ARG:CZ	2.17	0.74
2:H:210:ALA:HB3	2:H:211:PRO:HD3	1.69	0.73
1:G:662:LEU:HD11	1:G:673:PHE:CZ	2.24	0.73
1:C:756:HIS:O	1:C:757:ILE:HG22	1.89	0.73
2:D:10:SER:HB3	2:D:449:ARG:CZ	2.18	0.73
1:E:848:HIS:HB2	2:F:485:SER:HB3	1.70	0.73
1:E:119:LEU:H	1:E:120:PRO:HA	1.50	0.73
1:A:119:LEU:H	1:A:120:PRO:HA	1.50	0.73
1:A:756:HIS:O	1:A:757:ILE:HG22	1.89	0.73
1:C:662:LEU:HD11	1:C:673:PHE:CZ	2.24	0.73
2:F:210:ALA:HB3	2:F:211:PRO:HD3	1.69	0.72
1:A:662:LEU:HD11	1:A:673:PHE:CZ	2.24	0.72
1:C:119:LEU:H	1:C:120:PRO:HA	1.50	0.72
2:D:25:GLN:HB3	2:D:445:CYS:HB3	1.72	0.72
1:G:484:ARG:NH1	2:H:586:GLN:HG3	2.03	0.72
1:E:756:HIS:O	1:E:757:ILE:HG22	1.90	0.72
1:G:273:PHE:HB2	1:G:296:LYS:HD2	1.72	0.72
2:F:461:CYS:SG	2:F:466:ARG:CD	2.78	0.72
1:E:721:GLY:C	1:E:723:PRO:HD3	2.10	0.72
1:E:1064:PRO:CG	1:E:1067:GLU:HG3	2.20	0.71
1:E:662:LEU:HD11	1:E:673:PHE:CZ	2.24	0.71
4:Q:1:NAG:H3	4:Q:2:NAG:N2	2.05	0.71
1:G:1064:PRO:CG	1:G:1067:GLU:HG3	2.20	0.71
2:D:25:GLN:CB	2:D:445:CYS:HB3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:817:GLN:N	1:E:818:LYS:HA	2.05	0.71
1:G:721:GLY:C	1:G:723:PRO:HD3	2.10	0.71
1:C:653:GLN:HB2	1:G:630:LEU:HD21	1.72	0.71
1:C:1064:PRO:CG	1:C:1067:GLU:HG3	2.20	0.71
1:A:721:GLY:C	1:A:723:PRO:HD3	2.11	0.71
2:H:27:LEU:HD21	2:H:446:GLY:O	1.91	0.71
1:A:1064:PRO:CG	1:A:1067:GLU:HG3	2.20	0.71
1:C:817:GLN:N	1:C:818:LYS:HA	2.06	0.70
1:C:94:HIS:CD2	2:D:155:LEU:HD21	2.25	0.70
1:C:721:GLY:C	1:C:723:PRO:HD3	2.11	0.70
1:A:731:ARG:O	1:A:731:ARG:HG3	1.92	0.70
1:C:731:ARG:O	1:C:731:ARG:HG3	1.92	0.70
1:G:328:PHE:O	1:G:354:PHE:HA	1.91	0.70
1:C:332:MET:SD	2:D:208:LEU:HD13	2.32	0.69
1:E:623:GLN:O	1:E:624:VAL:CG2	2.39	0.69
2:B:460:GLU:HG2	2:B:461:CYS:SG	2.32	0.69
1:C:484:ARG:NH1	2:D:586:GLN:HG3	2.08	0.69
1:E:491:LEU:HD11	1:E:545:ILE:HG12	1.75	0.69
1:C:812:TYR:CD2	1:C:814:ALA:HB2	2.28	0.69
2:D:25:GLN:OE1	2:D:427:CYS:SG	2.50	0.69
1:A:812:TYR:CD2	1:A:814:ALA:HB2	2.27	0.69
1:A:817:GLN:N	1:A:818:LYS:HA	2.07	0.69
1:E:43:GLN:HA	1:E:70:ASN:H	1.58	0.69
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	1.75	0.69
1:C:491:LEU:HD11	1:C:545:ILE:HG12	1.75	0.69
1:E:919:LEU:HB2	1:E:1079:GLU:HB3	1.75	0.69
1:C:43:GLN:HA	1:C:70:ASN:H	1.58	0.69
2:F:455:ILE:HG13	2:F:463:THR:HG23	1.74	0.69
1:A:653:GLN:HB2	1:E:630:LEU:HD21	1.75	0.68
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	1.75	0.68
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.75	0.68
2:B:317:LYS:HE3	2:B:410:GLY:HA3	1.74	0.68
2:F:546:PHE:HA	2:F:554:GLU:O	1.93	0.68
1:E:1032:LEU:HD21	1:E:1078:LEU:HD21	1.75	0.68
1:A:491:LEU:HD11	1:A:545:ILE:HG12	1.76	0.68
2:D:39:ARG:NE	2:D:447:ILE:CG2	2.57	0.68
2:F:317:LYS:CE	2:F:410:GLY:HA3	2.21	0.68
1:G:919:LEU:HB2	1:G:1079:GLU:HB3	1.75	0.68
1:A:912:HIS:ND1	1:A:935:ARG:HD2	2.09	0.68
1:A:513:ASN:HA	1:A:599:VAL:CG2	2.23	0.68
1:C:406:PRO:HB3	1:C:438:TYR:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:731:ARG:O	1:E:731:ARG:HG3	1.91	0.68
1:G:1032:LEU:HD21	1:G:1078:LEU:HD21	1.76	0.68
2:D:103:TYR:HB3	2:D:104:PRO:HD2	1.76	0.68
1:G:374:MET:HG3	1:G:381:MET:SD	2.34	0.68
1:G:491:LEU:HD11	1:G:545:ILE:HG12	1.75	0.68
1:C:328:PHE:O	1:C:354:PHE:HA	1.94	0.67
1:E:912:HIS:ND1	1:E:935:ARG:HD2	2.09	0.67
1:G:912:HIS:ND1	1:G:935:ARG:HD2	2.08	0.67
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.29	0.67
2:B:220:GLN:HA	2:B:264:CYS:HB3	1.76	0.67
1:E:374:MET:HG3	1:E:381:MET:SD	2.34	0.67
2:F:479:ASN:ND2	6:F:3479:NAG:C1	2.56	0.67
1:G:731:ARG:O	1:G:731:ARG:HG3	1.92	0.67
1:G:817:GLN:N	1:G:818:LYS:HA	2.08	0.67
1:A:374:MET:HG3	1:A:381:MET:SD	2.35	0.67
1:C:912:HIS:ND1	1:C:935:ARG:HD2	2.09	0.67
2:D:220:GLN:HA	2:D:264:CYS:HB3	1.76	0.67
2:H:597:PRO:O	2:H:598:SER:HB2	1.95	0.67
2:B:103:TYR:HB3	2:B:104:PRO:HD2	1.76	0.67
1:G:406:PRO:HB3	1:G:438:TYR:CE2	2.29	0.67
1:E:406:PRO:HB3	1:E:438:TYR:CE2	2.29	0.67
1:G:164:ARG:HB2	1:G:165:PRO:HA	1.76	0.67
1:C:1032:LEU:HD21	1:C:1078:LEU:HD21	1.75	0.67
2:D:27:LEU:HG	2:D:446:GLY:HA2	1.75	0.67
2:H:25:GLN:CB	2:H:445:CYS:HB3	2.25	0.67
1:C:812:TYR:CE2	1:C:814:ALA:HB2	2.29	0.67
2:H:27:LEU:CD2	2:H:446:GLY:HA2	2.25	0.67
2:H:220:GLN:HA	2:H:264:CYS:HB3	1.76	0.67
1:E:812:TYR:CE2	1:E:814:ALA:HB2	2.31	0.66
2:F:35:PRO:CG	2:F:510:GLN:CD	2.63	0.66
1:C:374:MET:HG3	1:C:381:MET:SD	2.35	0.66
2:F:220:GLN:HA	2:F:264:CYS:HB3	1.77	0.66
1:G:43:GLN:HA	1:G:70:ASN:H	1.58	0.66
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.77	0.66
1:E:812:TYR:CD2	1:E:814:ALA:HB2	2.29	0.66
1:G:513:ASN:HA	1:G:599:VAL:HG21	1.77	0.66
1:G:364:PRO:CB	1:G:365:PRO:HD2	2.26	0.66
2:H:103:TYR:HB3	2:H:104:PRO:HD2	1.77	0.66
2:H:15:ILE:HG23	2:H:86:ARG:CZ	2.25	0.66
1:A:484:ARG:NH1	2:B:586:GLN:CG	2.59	0.66
2:F:23:TRP:HE1	2:F:445:CYS:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:522:TYR:CD1	2:H:552:GLN:HA	2.31	0.66
1:A:43:GLN:HA	1:A:70:ASN:H	1.59	0.66
1:C:1064:PRO:HG2	1:C:1067:GLU:HG3	1.78	0.66
1:C:848:HIS:HB2	2:D:485:SER:HB3	1.78	0.65
1:E:562:LEU:HD11	1:E:590:GLN:HG2	1.79	0.65
1:G:181:HIS:CE1	1:G:200:VAL:HG13	2.31	0.65
1:G:322:THR:O	1:G:325:SER:HB2	1.96	0.65
1:G:513:ASN:HA	1:G:599:VAL:CG2	2.25	0.65
1:G:562:LEU:HD11	1:G:590:GLN:HG2	1.78	0.65
1:G:609:ILE:HB	1:G:610:PRO:HD3	1.77	0.65
1:G:194:LEU:HD22	1:G:197:LEU:HD12	1.77	0.65
1:A:1064:PRO:HG2	1:A:1067:GLU:HG3	1.79	0.65
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.78	0.65
2:D:479:ASN:HD21	6:D:3479:NAG:C8	2.08	0.65
1:E:364:PRO:CB	1:E:365:PRO:HD2	2.26	0.65
2:H:39:ARG:NE	2:H:447:ILE:CG2	2.59	0.65
1:A:599:VAL:O	1:A:599:VAL:HG23	1.95	0.65
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.26	0.65
1:A:630:LEU:HD21	1:E:653:GLN:HB2	1.77	0.65
1:A:364:PRO:CB	1:A:365:PRO:HD2	2.26	0.65
1:C:562:LEU:HD11	1:C:590:GLN:HG2	1.79	0.65
2:D:23:TRP:CZ2	2:D:447:ILE:HD13	2.31	0.65
1:A:562:LEU:HD11	1:A:590:GLN:HG2	1.79	0.65
2:F:103:TYR:HB3	2:F:104:PRO:HD2	1.77	0.65
2:F:27:LEU:HD21	2:F:443:LEU:HD11	1.78	0.65
1:E:609:ILE:HB	1:E:610:PRO:HD3	1.77	0.65
1:C:103:LEU:CD1	2:D:155:LEU:HD13	2.26	0.64
1:G:812:TYR:CD2	1:G:814:ALA:HB2	2.32	0.64
1:G:1064:PRO:HG2	1:G:1067:GLU:HG3	1.79	0.64
1:G:94:HIS:NE2	2:H:155:LEU:HD21	2.13	0.64
1:G:103:LEU:CD1	2:H:155:LEU:HD13	2.25	0.64
1:A:513:ASN:HA	1:A:599:VAL:HG21	1.78	0.64
1:E:1064:PRO:HG2	1:E:1067:GLU:HG3	1.78	0.64
2:F:101:LYS:HG2	2:F:102:GLY:H	1.62	0.64
1:G:659:ASP:OD2	4:U:1:NAG:H82	1.97	0.64
2:B:104:PRO:HD2	2:B:233:VAL:HG11	1.78	0.64
2:F:104:PRO:HD2	2:F:233:VAL:HG11	1.78	0.64
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.33	0.64
2:D:104:PRO:HD2	2:D:233:VAL:HG11	1.78	0.64
2:B:471:LEU:O	2:B:493:GLY:HA2	1.98	0.64
1:E:599:VAL:HG23	1:E:599:VAL:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:VAL:O	1:E:121:VAL:HG12	1.98	0.64
1:G:194:LEU:CD2	1:G:197:LEU:HD12	2.28	0.64
1:G:871:LEU:HD11	1:G:901:VAL:HG21	1.80	0.64
1:A:673:PHE:CG	1:A:681:LEU:HD23	2.33	0.64
1:A:871:LEU:HD11	1:A:901:VAL:HG21	1.80	0.64
2:D:10:SER:HB3	2:D:449:ARG:NE	2.13	0.64
1:C:118:ARG:HA	1:C:120:PRO:HA	1.80	0.63
1:E:332:MET:SD	2:F:208:LEU:HD13	2.38	0.63
1:E:673:PHE:CG	1:E:681:LEU:HD23	2.33	0.63
1:G:121:VAL:HG12	1:G:121:VAL:O	1.98	0.63
2:H:104:PRO:HD2	2:H:233:VAL:HG11	1.78	0.63
2:H:39:ARG:NE	2:H:447:ILE:HG23	2.13	0.63
2:B:597:PRO:O	2:B:598:SER:HB2	1.98	0.63
1:C:673:PHE:CG	1:C:681:LEU:HD23	2.33	0.63
1:G:269:VAL:HG11	1:G:300:PHE:CE2	2.34	0.63
1:C:513:ASN:HA	1:C:599:VAL:CG2	2.29	0.63
1:A:121:VAL:O	1:A:121:VAL:HG12	1.98	0.63
1:A:722:LYS:N	1:A:723:PRO:CD	2.62	0.63
2:F:35:PRO:HG2	2:F:510:GLN:NE2	2.12	0.63
1:G:673:PHE:CG	1:G:681:LEU:HD23	2.33	0.63
2:F:35:PRO:HG2	2:F:510:GLN:OE1	1.98	0.63
1:A:118:ARG:HA	1:A:120:PRO:HA	1.81	0.63
1:A:797:GLY:CA	1:A:884:GLU:HB2	2.29	0.63
2:B:27:LEU:HG	2:B:446:GLY:HA2	1.81	0.63
2:F:461:CYS:CB	2:F:466:ARG:HD2	2.29	0.63
1:G:662:LEU:HD11	1:G:673:PHE:CE1	2.34	0.62
1:G:797:GLY:CA	1:G:884:GLU:HB2	2.29	0.62
1:A:662:LEU:HD11	1:A:673:PHE:CE1	2.34	0.62
1:C:662:LEU:HD11	1:C:673:PHE:CE1	2.34	0.62
2:F:461:CYS:HB3	2:F:466:ARG:CD	2.29	0.62
2:D:597:PRO:O	2:D:598:SER:HB2	1.98	0.62
1:C:119:LEU:HD21	1:C:124:GLN:HE21	1.64	0.62
1:C:121:VAL:HG12	1:C:121:VAL:O	1.98	0.62
1:C:722:LYS:N	1:C:723:PRO:CD	2.63	0.62
1:C:797:GLY:CA	1:C:884:GLU:HB2	2.30	0.62
1:E:797:GLY:CA	1:E:884:GLU:HB2	2.29	0.62
1:C:599:VAL:O	1:C:599:VAL:HG23	1.99	0.62
1:C:625:VAL:CG2	1:C:627:GLU:HG3	2.28	0.62
1:C:871:LEU:HD11	1:C:901:VAL:HG21	1.82	0.62
1:C:1064:PRO:HG3	1:C:1067:GLU:CG	2.30	0.62
1:E:625:VAL:CG2	1:E:627:GLU:HG3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:LYS:N	1:E:723:PRO:CD	2.62	0.62
2:F:546:PHE:CE2	2:F:554:GLU:HG2	2.35	0.62
1:G:599:VAL:O	1:G:599:VAL:HG23	1.99	0.62
1:E:662:LEU:HD11	1:E:673:PHE:CE1	2.34	0.62
1:G:327:SER:O	1:G:328:PHE:O	2.18	0.62
1:G:722:LYS:N	1:G:723:PRO:CD	2.62	0.62
1:A:739:GLN:HB2	1:A:742:PHE:CZ	2.35	0.62
1:A:971:HIS:CE1	1:A:974:ASN:HB2	2.35	0.62
1:A:519:ASP:CG	1:A:538:HIS:HD1	2.03	0.61
2:F:460:GLU:HG2	2:F:461:CYS:SG	2.40	0.61
1:G:119:LEU:HD21	1:G:124:GLN:HE21	1.64	0.61
1:C:364:PRO:HB3	1:C:365:PRO:HD2	1.83	0.61
1:G:118:ARG:HA	1:G:120:PRO:HA	1.81	0.61
1:E:871:LEU:HD11	1:E:901:VAL:HG21	1.80	0.61
1:C:630:LEU:HD21	1:G:653:GLN:HB2	1.82	0.61
1:C:513:ASN:HA	1:C:599:VAL:HG21	1.82	0.61
1:E:364:PRO:HB3	1:E:365:PRO:HD2	1.83	0.61
2:H:295:GLN:HG3	2:H:317:LYS:HE2	1.82	0.61
2:B:295:GLN:HG3	2:B:317:LYS:HE2	1.82	0.61
1:E:963:VAL:HA	1:E:1036:TRP:CD1	2.35	0.61
2:B:597:PRO:O	2:B:598:SER:CB	2.48	0.61
2:D:597:PRO:O	2:D:598:SER:CB	2.48	0.61
1:E:739:GLN:HB2	1:E:742:PHE:CZ	2.35	0.61
2:D:295:GLN:HG3	2:D:317:LYS:HE2	1.82	0.61
1:E:1064:PRO:HG3	1:E:1067:GLU:CG	2.30	0.61
1:E:971:HIS:CE1	1:E:974:ASN:HB2	2.35	0.61
1:A:80:THR:HB	1:A:341:PHE:CG	2.35	0.61
2:F:27:LEU:CD2	2:F:446:GLY:HA2	2.30	0.61
1:G:364:PRO:HB3	1:G:365:PRO:HD2	1.82	0.61
1:G:625:VAL:CG2	1:G:627:GLU:HG3	2.30	0.61
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	1.83	0.61
1:A:119:LEU:HD21	1:A:124:GLN:HE21	1.65	0.61
1:A:364:PRO:HB3	1:A:365:PRO:HD2	1.83	0.61
2:B:154:VAL:HA	2:B:160:THR:HG22	1.83	0.61
1:E:118:ARG:HA	1:E:120:PRO:HA	1.81	0.61
1:E:119:LEU:HD21	1:E:124:GLN:HE21	1.64	0.61
1:A:1064:PRO:HG3	1:A:1067:GLU:CG	2.31	0.61
1:C:44:THR:HG22	1:C:71:MET:HG2	1.83	0.61
2:F:260:ASN:HA	2:F:277:PHE:CE2	2.36	0.61
1:C:739:GLN:HB2	1:C:742:PHE:CZ	2.36	0.60
1:A:928:GLU:HG3	1:A:929:SER:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:VAL:HA	1:A:1036:TRP:CD1	2.36	0.60
1:C:80:THR:HB	1:C:341:PHE:CG	2.36	0.60
2:D:479:ASN:ND2	6:D:3479:NAG:H82	2.15	0.60
1:E:80:THR:HB	1:E:341:PHE:CG	2.36	0.60
1:E:103:LEU:CD1	2:F:155:LEU:HD13	2.26	0.60
1:G:1064:PRO:HG3	1:G:1067:GLU:CG	2.31	0.60
1:G:80:THR:HB	1:G:341:PHE:CG	2.36	0.60
2:B:260:ASN:HA	2:B:277:PHE:CE2	2.37	0.60
1:C:928:GLU:HG3	1:C:929:SER:N	2.17	0.60
2:D:546:PHE:CD2	2:D:554:GLU:O	2.54	0.60
1:G:623:GLN:O	1:G:624:VAL:CG2	2.49	0.60
1:G:656:VAL:HG21	1:G:687:LEU:CD1	2.32	0.60
1:G:739:GLN:HB2	1:G:742:PHE:CZ	2.35	0.60
1:C:971:HIS:CE1	1:C:974:ASN:HB2	2.36	0.60
1:A:119:LEU:N	1:A:120:PRO:CA	2.60	0.60
1:A:513:ASN:CA	1:A:599:VAL:HG21	2.31	0.60
1:E:373:ASN:OD1	4:Q:1:NAG:H2	2.02	0.60
1:G:468:THR:HG23	1:G:498:PRO:HG3	1.84	0.60
2:H:597:PRO:O	2:H:598:SER:CB	2.49	0.60
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.36	0.60
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.83	0.60
1:C:519:ASP:CG	1:C:538:HIS:HD1	2.05	0.60
1:E:928:GLU:HG3	1:E:929:SER:N	2.17	0.60
1:G:1064:PRO:HG3	1:G:1067:GLU:HG3	1.83	0.60
1:G:971:HIS:CE1	1:G:974:ASN:HB2	2.36	0.60
2:D:462:GLN:HG2	2:D:463:THR:N	2.17	0.60
2:D:471:LEU:O	2:D:493:GLY:HA2	2.01	0.60
2:D:505:LYS:HA	2:D:517:ILE:HG21	1.84	0.60
2:D:587:LEU:HB3	2:D:588:PRO:HA	1.84	0.60
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.01	0.60
2:B:115:TYR:CD1	2:B:170:PRO:HD2	2.37	0.60
2:D:25:GLN:HA	2:D:445:CYS:O	2.02	0.60
2:F:295:GLN:HG3	2:F:317:LYS:HE2	1.82	0.60
2:F:587:LEU:HB3	2:F:588:PRO:HA	1.84	0.60
1:G:963:VAL:HA	1:G:1036:TRP:CD1	2.37	0.60
2:H:154:VAL:HA	2:H:160:THR:HG22	1.83	0.60
1:E:44:THR:HG22	1:E:71:MET:HG2	1.83	0.60
1:A:656:VAL:HG21	1:A:687:LEU:CD1	2.32	0.60
1:E:519:ASP:CG	1:E:538:HIS:HD1	2.05	0.60
1:E:469:ARG:NH2	2:F:287:HIS:HB2	2.15	0.60
1:G:519:ASP:CG	1:G:538:HIS:HD1	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:562:ASN:HB2	2:H:563:PRO:HD2	1.84	0.60
1:A:625:VAL:CG2	1:A:627:GLU:HG3	2.29	0.59
1:C:604:VAL:HG11	1:C:742:PHE:CD2	2.37	0.59
1:C:833:PRO:HA	1:C:840:TRP:HB2	1.84	0.59
2:D:154:VAL:HA	2:D:160:THR:HG22	1.83	0.59
2:F:115:TYR:CD1	2:F:170:PRO:HD2	2.37	0.59
2:F:546:PHE:CD2	2:F:554:GLU:HG2	2.36	0.59
2:D:260:ASN:HA	2:D:277:PHE:CE2	2.37	0.59
2:H:260:ASN:HA	2:H:277:PHE:CE2	2.37	0.59
2:D:562:ASN:HB2	2:D:563:PRO:HD2	1.84	0.59
1:E:615:ARG:HA	1:E:618:PHE:HB2	1.85	0.59
2:F:154:VAL:HA	2:F:160:THR:HG22	1.83	0.59
2:F:562:ASN:HB2	2:F:563:PRO:HD2	1.84	0.59
2:B:184:HIS:CE1	2:B:228:ILE:HG23	2.37	0.59
2:B:347:LEU:HD22	2:B:389:PHE:CD1	2.38	0.59
1:E:604:VAL:HG11	1:E:742:PHE:CD2	2.38	0.59
2:F:289:LEU:HD21	2:F:296:PRO:CD	2.33	0.59
1:G:615:ARG:HA	1:G:618:PHE:HB2	1.83	0.59
1:C:653:GLN:CB	1:G:630:LEU:HD21	2.32	0.59
2:H:184:HIS:CE1	2:H:228:ILE:HG23	2.38	0.59
2:H:289:LEU:HD21	2:H:296:PRO:CD	2.33	0.59
1:A:118:ARG:HG2	1:A:120:PRO:HB3	1.85	0.59
1:A:468:THR:HG23	1:A:498:PRO:HG3	1.84	0.59
1:C:490:VAL:HG12	1:C:491:LEU:N	2.18	0.59
2:F:27:LEU:HD23	2:F:446:GLY:HA2	1.83	0.59
1:G:362:LEU:HD23	1:G:363:TYR:N	2.18	0.59
1:G:44:THR:HG22	1:G:71:MET:HG2	1.83	0.59
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.37	0.59
1:G:118:ARG:HG2	1:G:120:PRO:HB3	1.85	0.59
1:G:812:TYR:CE2	1:G:814:ALA:HB2	2.38	0.59
2:H:587:LEU:HB3	2:H:588:PRO:HA	1.85	0.59
1:A:362:LEU:HD23	1:A:363:TYR:N	2.18	0.59
1:A:623:GLN:O	1:A:624:VAL:CG2	2.50	0.59
2:D:115:TYR:HA	2:D:204:ILE:HD13	1.85	0.59
2:D:289:LEU:HD21	2:D:296:PRO:CD	2.33	0.59
2:F:532:ARG:HD3	2:F:554:GLU:CD	2.22	0.59
2:B:317:LYS:HE3	2:B:410:GLY:CA	2.33	0.59
1:E:813:VAL:HB	1:E:823:ARG:HH21	1.66	0.59
2:F:571:ARG:HH21	2:F:660:MET:CG	2.16	0.59
1:G:137:ILE:HD13	1:G:152:MET:SD	2.42	0.59
1:G:928:GLU:HG3	1:G:929:SER:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:471:LEU:O	2:H:493:GLY:HA2	2.03	0.59
1:A:444:CYS:HB2	1:A:506:LEU:CD1	2.33	0.59
1:C:119:LEU:N	1:C:120:PRO:CA	2.60	0.59
1:E:362:LEU:HD23	1:E:363:TYR:N	2.18	0.59
1:E:656:VAL:HG21	1:E:687:LEU:CD1	2.32	0.59
1:G:721:GLY:C	1:G:723:PRO:CD	2.72	0.59
2:H:115:TYR:HA	2:H:204:ILE:HD13	1.85	0.59
2:B:592:GLU:O	2:B:594:PRO:HD3	2.02	0.58
2:F:15:ILE:HG23	2:F:86:ARG:HH21	1.66	0.58
1:G:490:VAL:HG12	1:G:491:LEU:N	2.18	0.58
1:A:490:VAL:HG12	1:A:491:LEU:N	2.18	0.58
2:B:289:LEU:HD21	2:B:296:PRO:CD	2.33	0.58
1:E:446:VAL:HG21	1:E:520:VAL:CG1	2.33	0.58
2:F:562:ASN:HB3	2:F:589:LEU:HD13	1.86	0.58
2:H:115:TYR:CD1	2:H:170:PRO:HD2	2.37	0.58
1:A:18:PHE:CE2	1:A:32:VAL:HG21	2.38	0.58
1:A:44:THR:HG22	1:A:71:MET:HG2	1.83	0.58
2:B:115:TYR:HA	2:B:204:ILE:HD13	1.85	0.58
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.85	0.58
1:C:18:PHE:CE2	1:C:32:VAL:HG21	2.38	0.58
1:C:362:LEU:HD23	1:C:363:TYR:N	2.18	0.58
2:F:184:HIS:CE1	2:F:228:ILE:HG23	2.38	0.58
1:G:385:TYR:CZ	2:H:253:LEU:HD11	2.39	0.58
1:A:822:LEU:HG	1:A:823:ARG:H	1.69	0.58
2:B:295:GLN:CG	2:B:317:LYS:HE2	2.34	0.58
1:C:444:CYS:HB2	1:C:506:LEU:CD1	2.34	0.58
2:D:442:PHE:CZ	2:D:449:ARG:HB2	2.39	0.58
1:E:1064:PRO:HG3	1:E:1067:GLU:HG3	1.83	0.58
2:F:442:PHE:CZ	2:F:449:ARG:HB2	2.39	0.58
2:F:597:PRO:O	2:F:598:SER:HB2	2.04	0.58
2:B:562:ASN:HB2	2:B:563:PRO:HD2	1.84	0.58
1:E:118:ARG:HG2	1:E:120:PRO:HB3	1.85	0.58
1:G:710:PRO:HG3	1:G:884:GLU:OE2	2.02	0.58
1:G:813:VAL:HB	1:G:823:ARG:HH21	1.68	0.58
2:D:184:HIS:CE1	2:D:228:ILE:HG23	2.38	0.58
1:A:604:VAL:HG11	1:A:742:PHE:CD2	2.39	0.58
1:C:468:THR:HG23	1:C:498:PRO:HG3	1.85	0.58
1:C:623:GLN:O	1:C:624:VAL:CG2	2.51	0.58
1:C:656:VAL:HG21	1:C:687:LEU:CD1	2.32	0.58
1:C:721:GLY:C	1:C:723:PRO:CD	2.72	0.58
1:E:468:THR:HG23	1:E:498:PRO:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:621:ARG:HG2	1:E:622:GLU:H	1.68	0.58
2:F:115:TYR:HA	2:F:204:ILE:HD13	1.85	0.58
1:G:604:VAL:HG11	1:G:742:PHE:CD2	2.38	0.58
1:A:666:ARG:HB3	2:B:498:HIS:CD2	2.39	0.58
1:C:446:VAL:HG21	1:C:520:VAL:CG1	2.33	0.58
1:G:986:PRO:CB	1:G:987:PRO:HD2	2.34	0.58
2:B:442:PHE:CZ	2:B:449:ARG:HB2	2.39	0.57
2:B:461:CYS:HB3	2:B:466:ARG:HD3	1.85	0.57
1:C:994:HIS:CG	1:C:1005:ILE:HD11	2.39	0.57
1:E:18:PHE:CE2	1:E:32:VAL:HG21	2.39	0.57
1:E:444:CYS:HB2	1:E:506:LEU:CD1	2.34	0.57
2:F:295:GLN:CG	2:F:317:LYS:HE2	2.34	0.57
1:G:332:MET:SD	2:H:208:LEU:HD13	2.44	0.57
2:D:347:LEU:HD22	2:D:389:PHE:CD1	2.39	0.57
1:E:833:PRO:HA	1:E:840:TRP:HB2	1.84	0.57
2:D:15:ILE:HG23	2:D:86:ARG:CZ	2.34	0.57
2:D:295:GLN:CG	2:D:317:LYS:HE2	2.34	0.57
1:E:364:PRO:CB	1:E:365:PRO:CD	2.83	0.57
1:E:721:GLY:C	1:E:723:PRO:CD	2.72	0.57
1:G:446:VAL:HG21	1:G:520:VAL:CG1	2.34	0.57
1:A:575:LEU:HD12	1:A:576:THR:N	2.20	0.57
1:A:721:GLY:C	1:A:723:PRO:CD	2.72	0.57
2:H:562:ASN:HB3	2:H:589:LEU:HD13	1.86	0.57
1:A:446:VAL:HG21	1:A:520:VAL:CG1	2.34	0.57
1:C:822:LEU:HG	1:C:823:ARG:H	1.69	0.57
1:E:986:PRO:CB	1:E:987:PRO:HD2	2.34	0.57
1:G:364:PRO:CB	1:G:365:PRO:CD	2.82	0.57
2:B:562:ASN:HB3	2:B:589:LEU:HD13	1.86	0.57
1:G:186:GLU:HA	1:G:189:ARG:HG2	1.85	0.57
1:G:444:CYS:HB2	1:G:506:LEU:CD1	2.34	0.57
2:D:23:TRP:CZ2	2:D:447:ILE:CD1	2.88	0.57
1:G:18:PHE:CE2	1:G:32:VAL:HG21	2.39	0.57
2:H:442:PHE:CZ	2:H:449:ARG:HB2	2.39	0.57
2:H:592:GLU:O	2:H:594:PRO:HD3	2.04	0.57
2:D:39:ARG:CD	2:D:447:ILE:CG2	2.82	0.57
2:D:562:ASN:HB3	2:D:589:LEU:HD13	1.86	0.57
1:E:407:ARG:HG2	2:F:247:PHE:CZ	2.40	0.57
1:E:490:VAL:HG12	1:E:491:LEU:N	2.18	0.57
2:F:444:GLU:OE2	2:F:445:CYS:SG	2.63	0.57
1:A:32:VAL:HG11	1:A:591:VAL:HG11	1.87	0.56
1:A:653:GLN:CB	1:E:630:LEU:HD21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:LEU:O	2:B:289:LEU:HB3	2.06	0.56
2:D:340:LYS:HD2	2:D:379:ASP:OD1	2.05	0.56
1:E:479:PRO:HD2	1:E:485:TRP:CD1	2.40	0.56
2:H:295:GLN:CG	2:H:317:LYS:HE2	2.34	0.56
1:A:364:PRO:CB	1:A:365:PRO:CD	2.83	0.56
1:A:833:PRO:HA	1:A:840:TRP:HB2	1.85	0.56
1:A:986:PRO:CB	1:A:987:PRO:HD2	2.35	0.56
2:D:460:GLU:HG2	2:D:461:CYS:SG	2.46	0.56
1:G:666:ARG:HB3	2:H:498:HIS:NE2	2.20	0.56
1:C:575:LEU:HD12	1:C:576:THR:N	2.21	0.56
2:D:479:ASN:HD22	6:D:3479:NAG:C1	2.19	0.56
1:G:513:ASN:CA	1:G:599:VAL:HG21	2.34	0.56
4:J:2:NAG:O3	4:J:3:MAN:H2	2.05	0.56
1:C:364:PRO:CB	1:C:365:PRO:CD	2.83	0.56
1:C:602:VAL:HG23	1:C:638:TYR:O	2.06	0.56
2:D:479:ASN:ND2	6:D:3479:NAG:C8	2.69	0.56
1:G:833:PRO:HA	1:G:840:TRP:HB2	1.86	0.56
1:C:118:ARG:HG2	1:C:120:PRO:HB3	1.85	0.56
1:E:831:SER:CB	1:E:842:THR:HG22	2.36	0.56
2:F:340:LYS:HA	2:F:343:SER:HB2	1.85	0.56
2:F:399:ILE:HG13	2:F:421:PRO:HG3	1.88	0.56
1:G:831:SER:CB	1:G:842:THR:HG22	2.36	0.56
1:A:602:VAL:HG23	1:A:638:TYR:O	2.05	0.56
1:A:831:SER:CB	1:A:842:THR:HG22	2.35	0.56
1:A:578:ASP:OD2	1:A:595:ARG:HD2	2.06	0.56
2:B:162:PRO:O	2:B:165:LEU:HB3	2.06	0.56
1:E:575:LEU:HD12	1:E:576:THR:N	2.21	0.56
1:G:47:LEU:HD11	1:G:88:ALA:CB	2.36	0.56
1:G:602:VAL:HG23	1:G:638:TYR:O	2.04	0.56
1:A:479:PRO:HD2	1:A:485:TRP:CD1	2.41	0.56
1:C:103:LEU:HD13	2:D:156:PRO:HG3	1.87	0.56
1:C:831:SER:CB	1:C:842:THR:HG22	2.36	0.56
2:D:162:PRO:O	2:D:165:LEU:HB3	2.06	0.56
2:D:285:LEU:O	2:D:289:LEU:HB3	2.06	0.56
2:H:399:ILE:HG13	2:H:421:PRO:HG3	1.88	0.56
2:B:609:CYS:SG	2:B:616:PRO:HB3	2.46	0.56
1:C:479:PRO:HD2	1:C:485:TRP:CD1	2.41	0.56
2:D:479:ASN:ND2	6:D:3479:NAG:N2	2.54	0.56
1:E:602:VAL:HG23	1:E:638:TYR:O	2.05	0.56
1:E:907:THR:CG2	1:E:1053:ILE:HD13	2.36	0.56
2:F:592:GLU:O	2:F:594:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:597:PRO:O	2:F:598:SER:CB	2.54	0.56
1:G:662:LEU:CD1	1:G:673:PHE:CE1	2.89	0.56
2:H:27:LEU:HD11	2:H:443:LEU:HD11	1.88	0.56
2:H:609:CYS:SG	2:H:616:PRO:HB3	2.46	0.56
1:A:928:GLU:HG3	1:A:929:SER:H	1.71	0.56
2:D:592:GLU:O	2:D:594:PRO:HD3	2.05	0.56
2:D:609:CYS:SG	2:D:616:PRO:HB3	2.46	0.56
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.88	0.56
1:G:214:GLN:CD	1:G:253:VAL:HG12	2.27	0.56
1:G:575:LEU:HD12	1:G:576:THR:N	2.20	0.56
1:G:907:THR:CG2	1:G:1053:ILE:HD13	2.36	0.56
1:C:565:PHE:HB2	1:C:587:ALA:HB2	1.88	0.55
1:E:578:ASP:OD2	1:E:595:ARG:HD2	2.06	0.55
2:F:616:PRO:HB2	2:F:620:ASN:HA	1.88	0.55
1:G:32:VAL:HG11	1:G:591:VAL:HG11	1.88	0.55
1:G:747:PRO:HB3	1:G:884:GLU:HG2	1.88	0.55
1:E:32:VAL:HG11	1:E:591:VAL:HG11	1.87	0.55
1:E:876:LEU:C	1:E:876:LEU:HD12	2.26	0.55
2:F:508:TYR:CZ	2:F:514:CYS:HB3	2.41	0.55
1:G:876:LEU:HD12	1:G:876:LEU:C	2.27	0.55
2:H:460:GLU:HG2	2:H:461:CYS:SG	2.47	0.55
1:A:876:LEU:HD12	1:A:876:LEU:C	2.27	0.55
2:B:103:TYR:HB3	2:B:104:PRO:CD	2.36	0.55
2:B:399:ILE:HG13	2:B:421:PRO:HG3	1.88	0.55
2:B:616:PRO:HB2	2:B:620:ASN:HA	1.88	0.55
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.89	0.55
1:C:666:ARG:HB3	2:D:498:HIS:CD2	2.41	0.55
1:E:418:THR:HG21	1:E:482:TRP:CZ2	2.42	0.55
2:F:285:LEU:O	2:F:289:LEU:HB3	2.06	0.55
2:H:591:GLN:HG2	2:H:592:GLU:N	2.22	0.55
2:H:616:PRO:HB2	2:H:620:ASN:HA	1.88	0.55
1:A:565:PHE:HB2	1:A:587:ALA:HB2	1.89	0.55
1:E:103:LEU:CD1	2:F:156:PRO:HG3	2.37	0.55
1:E:662:LEU:CD1	1:E:673:PHE:CE1	2.90	0.55
2:F:461:CYS:SG	2:F:466:ARG:NE	2.79	0.55
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.90	0.55
1:C:484:ARG:NH1	2:D:586:GLN:CG	2.69	0.55
1:C:876:LEU:HD12	1:C:876:LEU:C	2.27	0.55
2:H:162:PRO:O	2:H:165:LEU:HB3	2.06	0.55
1:A:907:THR:CG2	1:A:1053:ILE:HD13	2.36	0.55
1:E:822:LEU:HG	1:E:823:ARG:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:HIS:CD2	2:F:155:LEU:HD21	2.41	0.55
1:G:479:PRO:HD2	1:G:485:TRP:CD1	2.41	0.55
1:G:578:ASP:OD2	1:G:595:ARG:HD2	2.06	0.55
1:G:822:LEU:HG	1:G:823:ARG:H	1.70	0.55
2:B:6:PHE:O	2:B:8:VAL:HG23	2.07	0.55
1:C:907:THR:CG2	1:C:1053:ILE:HD13	2.36	0.55
1:C:941:LEU:HD12	1:C:941:LEU:N	2.22	0.55
1:C:986:PRO:CB	1:C:987:PRO:HD2	2.36	0.55
2:D:103:TYR:HB3	2:D:104:PRO:CD	2.36	0.55
2:D:399:ILE:HG13	2:D:421:PRO:HG3	1.88	0.55
1:E:47:LEU:HD11	1:E:88:ALA:CB	2.37	0.55
1:G:418:THR:HG21	1:G:482:TRP:CZ2	2.41	0.55
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.27	0.55
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.89	0.55
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.88	0.55
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.89	0.55
1:E:435:ILE:HD13	2:F:311:LEU:HB2	1.87	0.55
2:F:103:TYR:HB3	2:F:104:PRO:CD	2.37	0.55
2:H:285:LEU:O	2:H:289:LEU:HB3	2.06	0.55
1:A:47:LEU:HD11	1:A:88:ALA:CB	2.37	0.55
1:C:32:VAL:HG11	1:C:591:VAL:HG11	1.87	0.55
1:E:905:VAL:HG11	1:E:946:LEU:HD21	1.89	0.55
1:E:941:LEU:N	1:E:941:LEU:HD12	2.22	0.55
2:F:162:PRO:O	2:F:165:LEU:HB3	2.06	0.55
1:G:119:LEU:N	1:G:120:PRO:CA	2.60	0.55
1:A:639:ILE:HG13	1:A:689:LEU:HA	1.88	0.55
1:A:772:LYS:HG3	1:A:772:LYS:O	2.07	0.55
1:A:822:LEU:CG	1:A:823:ARG:H	2.20	0.55
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.27	0.55
1:C:418:THR:HG21	1:C:482:TRP:CZ2	2.42	0.55
1:C:578:ASP:OD2	1:C:595:ARG:HD2	2.06	0.55
1:C:47:LEU:HD11	1:C:88:ALA:CB	2.37	0.55
1:E:47:LEU:HB2	1:E:60:ILE:HG21	1.89	0.55
1:E:565:PHE:HB2	1:E:587:ALA:HB2	1.89	0.55
1:E:639:ILE:HG13	1:E:689:LEU:HA	1.88	0.55
1:E:786:VAL:HG11	1:E:859:PHE:CZ	2.42	0.55
2:F:347:LEU:HD22	2:F:389:PHE:CD1	2.42	0.55
1:E:513:ASN:HA	1:E:599:VAL:CG2	2.36	0.54
1:G:1065:GLY:C	1:G:1066:GLN:HG3	2.28	0.54
1:G:639:ILE:HG13	1:G:689:LEU:HA	1.89	0.54
1:G:941:LEU:HD12	1:G:941:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:444:GLU:OE2	2:H:445:CYS:SG	2.65	0.54
1:A:418:THR:HG21	1:A:482:TRP:CZ2	2.41	0.54
2:H:103:TYR:HB3	2:H:104:PRO:CD	2.37	0.54
2:H:6:PHE:O	2:H:8:VAL:HG23	2.07	0.54
1:A:905:VAL:HG11	1:A:946:LEU:HD21	1.89	0.54
2:F:604:ILE:HD11	2:F:642:GLU:HB2	1.89	0.54
2:F:609:CYS:SG	2:F:616:PRO:HB3	2.48	0.54
2:H:522:TYR:CE1	2:H:552:GLN:HA	2.42	0.54
2:D:6:PHE:O	2:D:8:VAL:HG23	2.07	0.54
1:G:136:LEU:HD13	1:G:216:VAL:HG21	1.89	0.54
1:G:174:PHE:CE1	1:G:209:THR:HA	2.42	0.54
1:G:311:LYS:HG3	1:G:312:GLU:N	2.20	0.54
1:G:772:LYS:O	1:G:772:LYS:HG3	2.08	0.54
1:A:941:LEU:HD12	1:A:941:LEU:N	2.22	0.54
1:C:327:SER:O	1:C:328:PHE:O	2.26	0.54
1:C:103:LEU:HD21	2:D:155:LEU:CD2	2.38	0.54
2:D:23:TRP:HZ2	2:D:447:ILE:CD1	2.21	0.54
1:E:928:GLU:HG3	1:E:929:SER:H	1.72	0.54
1:G:47:LEU:HB2	1:G:60:ILE:HG21	1.89	0.54
1:C:113:THR:HG22	1:E:1029:LYS:HE2	1.89	0.54
1:C:815:GLU:HB3	1:C:819:GLN:NE2	2.23	0.54
1:G:565:PHE:HB2	1:G:587:ALA:HB2	1.88	0.54
1:G:928:GLU:HG3	1:G:929:SER:H	1.72	0.54
1:A:615:ARG:HA	1:A:618:PHE:HB2	1.89	0.54
2:B:444:GLU:OE2	2:B:445:CYS:SG	2.66	0.54
2:B:468:SER:HB2	2:B:471:LEU:HG	1.90	0.54
2:B:591:GLN:HG2	2:B:592:GLU:N	2.22	0.54
2:B:599:PRO:HB2	2:B:603:TYR:HE2	1.73	0.54
1:C:905:VAL:HG11	1:C:946:LEU:HD21	1.90	0.54
1:G:333:ALA:HB1	1:G:350:ALA:HB1	1.90	0.54
1:G:766:PHE:CZ	1:G:877:LEU:CD1	2.91	0.54
1:G:786:VAL:HG11	1:G:859:PHE:CZ	2.43	0.54
1:G:905:VAL:HG11	1:G:946:LEU:HD21	1.90	0.54
1:G:665:GLY:HA3	2:H:498:HIS:HB3	1.88	0.54
2:B:112:ASP:O	2:B:117:MET:HG3	2.07	0.54
1:C:93:VAL:O	1:C:103:LEU:HA	2.08	0.54
1:C:531:ARG:HA	1:C:563:GLN:O	2.08	0.54
1:C:615:ARG:HA	1:C:618:PHE:HB2	1.90	0.54
1:E:1065:GLY:C	1:E:1066:GLN:HG3	2.27	0.54
1:A:652:LEU:HD21	1:E:609:ILE:HG22	1.89	0.54
1:E:772:LYS:HG3	1:E:772:LYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:ASP:O	2:F:117:MET:HG3	2.07	0.54
2:B:212:GLU:HG2	2:B:243:ASP:HB2	1.89	0.54
2:B:455:ILE:HG22	2:B:456:GLY:N	2.23	0.54
1:C:928:GLU:HG3	1:C:929:SER:H	1.72	0.54
1:E:964:TRP:CB	1:E:1032:LEU:HA	2.38	0.54
1:E:93:VAL:O	1:E:103:LEU:HA	2.08	0.54
1:G:506:LEU:HA	1:G:569:LEU:HD11	1.90	0.54
1:G:681:LEU:HD12	1:G:682:SER:N	2.23	0.54
2:H:468:SER:HB2	2:H:471:LEU:HG	1.90	0.54
1:C:420:VAL:HB	1:C:423:GLN:HB2	1.91	0.54
1:C:755:ASP:O	1:C:756:HIS:HB3	2.07	0.54
1:C:822:LEU:CG	1:C:823:ARG:H	2.20	0.54
2:D:112:ASP:O	2:D:117:MET:HG3	2.07	0.54
2:D:212:GLU:HG2	2:D:243:ASP:HB2	1.89	0.54
2:D:444:GLU:OE2	2:D:445:CYS:SG	2.66	0.54
1:E:671:ALA:O	1:E:672:THR:HG23	2.08	0.54
2:F:35:PRO:HB3	2:F:510:GLN:HG2	1.90	0.54
2:F:471:LEU:O	2:F:493:GLY:HA2	2.08	0.54
2:F:58:ASP:N	2:F:59:PRO:HD3	2.23	0.54
1:G:243:LYS:HD3	1:G:250:TYR:CE2	2.43	0.54
2:H:212:GLU:HG2	2:H:243:ASP:HB2	1.89	0.54
2:B:295:GLN:CD	2:B:317:LYS:HE2	2.28	0.53
1:C:506:LEU:HA	1:C:569:LEU:HD11	1.90	0.53
1:C:772:LYS:O	1:C:772:LYS:HG3	2.08	0.53
1:C:813:VAL:HB	1:C:823:ARG:HH21	1.72	0.53
2:D:591:GLN:HG2	2:D:592:GLU:N	2.23	0.53
1:E:994:HIS:CG	1:E:1005:ILE:HD11	2.43	0.53
2:F:295:GLN:CD	2:F:317:LYS:HE2	2.28	0.53
2:F:468:SER:HB2	2:F:471:LEU:HG	1.90	0.53
2:F:546:PHE:CD2	2:F:554:GLU:CG	2.91	0.53
2:F:6:PHE:O	2:F:8:VAL:HG23	2.07	0.53
1:G:184:PHE:CD2	1:G:227:ALA:HB2	2.43	0.53
1:G:600:LEU:O	1:G:600:LEU:HD12	2.08	0.53
2:H:112:ASP:O	2:H:117:MET:HG3	2.08	0.53
2:H:289:LEU:HD21	2:H:296:PRO:HD3	1.89	0.53
2:H:295:GLN:CD	2:H:317:LYS:HE2	2.29	0.53
1:A:964:TRP:CB	1:A:1032:LEU:HA	2.39	0.53
1:C:47:LEU:HB2	1:C:60:ILE:HG21	1.89	0.53
1:C:639:ILE:HG13	1:C:689:LEU:HA	1.89	0.53
1:C:786:VAL:HG11	1:C:859:PHE:CZ	2.44	0.53
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:468:SER:HB2	2:D:471:LEU:HG	1.90	0.53
2:D:604:ILE:HD11	2:D:642:GLU:HB2	1.90	0.53
1:E:103:LEU:HD13	2:F:156:PRO:HG3	1.90	0.53
2:H:317:LYS:HE3	2:H:410:GLY:HA3	1.90	0.53
1:A:506:LEU:HA	1:A:569:LEU:HD11	1.90	0.53
1:C:465:TYR:HB3	1:C:469:ARG:HA	1.91	0.53
1:E:491:LEU:HD11	1:E:545:ILE:CG1	2.38	0.53
2:H:347:LEU:HD22	2:H:389:PHE:CD1	2.43	0.53
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.91	0.53
1:A:94:HIS:CD2	2:B:155:LEU:HD21	2.43	0.53
1:G:93:VAL:O	1:G:103:LEU:HA	2.08	0.53
1:G:666:ARG:HB3	2:H:498:HIS:CD2	2.44	0.53
2:B:562:ASN:HB2	2:B:563:PRO:CD	2.39	0.53
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.38	0.53
1:C:103:LEU:CD1	2:D:156:PRO:HG3	2.39	0.53
1:E:476:CYS:CB	1:E:487:CYS:HA	2.38	0.53
2:H:604:ILE:HD11	2:H:642:GLU:HB2	1.90	0.53
1:A:681:LEU:HD12	1:A:682:SER:N	2.23	0.53
1:A:766:PHE:CZ	1:A:877:LEU:CD1	2.92	0.53
1:C:833:PRO:HA	1:C:840:TRP:CB	2.39	0.53
2:D:121:LEU:O	2:D:125:LYS:HB3	2.09	0.53
1:E:465:TYR:HB3	1:E:469:ARG:HA	1.91	0.53
2:F:212:GLU:HG2	2:F:243:ASP:HB2	1.89	0.53
2:F:289:LEU:HD21	2:F:296:PRO:HD3	1.89	0.53
1:G:174:PHE:HB2	1:G:212:ALA:HB2	1.91	0.53
1:G:243:LYS:O	1:G:243:LYS:HG3	2.08	0.53
1:G:531:ARG:HA	1:G:563:GLN:O	2.09	0.53
2:H:289:LEU:HD23	2:H:315:ILE:HD11	1.91	0.53
1:A:761:ASN:ND2	1:A:791:ASP:HB2	2.24	0.53
1:A:823:ARG:HD3	1:A:860:LEU:H	1.74	0.53
1:A:93:VAL:O	1:A:103:LEU:HA	2.08	0.53
2:B:289:LEU:HD21	2:B:296:PRO:HD3	1.89	0.53
1:C:761:ASN:ND2	1:C:791:ASP:HB2	2.24	0.53
1:G:964:TRP:CB	1:G:1032:LEU:HA	2.38	0.53
1:G:211:THR:HA	1:G:248:LEU:HD12	1.91	0.53
2:H:121:LEU:O	2:H:125:LYS:HB3	2.09	0.53
4:Q:1:NAG:C3	4:Q:2:NAG:N2	2.72	0.53
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.44	0.53
2:B:604:ILE:HD11	2:B:642:GLU:HB2	1.90	0.53
1:E:766:PHE:CZ	1:E:877:LEU:CD1	2.92	0.53
2:F:121:LEU:O	2:F:125:LYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:562:ASN:HB2	2:F:563:PRO:CD	2.39	0.53
1:G:476:CYS:CB	1:G:487:CYS:HA	2.38	0.53
1:G:491:LEU:HD12	1:G:492:TYR:N	2.24	0.53
1:A:531:ARG:HA	1:A:563:GLN:O	2.09	0.53
1:C:1063:LEU:HD12	1:C:1064:PRO:HA	1.90	0.53
1:C:766:PHE:CZ	1:C:877:LEU:CD1	2.92	0.53
2:D:57:MET:SD	2:D:427:CYS:SG	3.07	0.53
1:E:436:GLY:C	2:F:282:VAL:HG11	2.30	0.53
1:A:692:HIS:ND1	1:E:694:GLU:HA	2.24	0.53
1:E:952:PHE:HB2	1:E:1011:PHE:HB2	1.91	0.53
1:A:416:ILE:HD11	1:A:485:TRP:CZ2	2.45	0.52
1:A:499:TRP:CZ2	2:B:284:GLN:HG3	2.43	0.52
1:A:786:VAL:HG11	1:A:859:PHE:CZ	2.44	0.52
2:B:508:TYR:CZ	2:B:514:CYS:HB3	2.44	0.52
1:C:917:LYS:HE3	1:C:1077:VAL:CG2	2.39	0.52
2:D:289:LEU:HD21	2:D:296:PRO:HD3	1.90	0.52
1:C:652:LEU:HD21	1:G:609:ILE:HG22	1.90	0.52
1:A:671:ALA:O	1:A:672:THR:HG23	2.08	0.52
1:C:952:PHE:HB2	1:C:1011:PHE:HB2	1.91	0.52
1:E:420:VAL:HB	1:E:423:GLN:HB2	1.91	0.52
1:E:848:HIS:O	1:E:849:LEU:HB3	2.10	0.52
1:G:325:SER:OG	1:G:326:SER:N	2.42	0.52
1:G:491:LEU:HD12	1:G:491:LEU:C	2.30	0.52
1:G:952:PHE:HB2	1:G:1011:PHE:HB2	1.91	0.52
1:A:25:TYR:CD1	1:A:86:LEU:HB2	2.45	0.52
1:A:476:CYS:CB	1:A:487:CYS:HA	2.38	0.52
1:A:994:HIS:CG	1:A:1005:ILE:HD11	2.45	0.52
1:C:25:TYR:CD1	1:C:86:LEU:HB2	2.44	0.52
1:C:600:LEU:HD12	1:C:600:LEU:O	2.10	0.52
2:D:289:LEU:HD23	2:D:315:ILE:HD11	1.91	0.52
2:D:562:ASN:HB2	2:D:563:PRO:CD	2.39	0.52
1:G:159:ILE:HD12	1:G:197:LEU:HD11	1.89	0.52
2:H:546:PHE:CD2	2:H:554:GLU:O	2.62	0.52
1:A:333:ALA:HA	1:A:352:GLY:H	1.74	0.52
1:A:813:VAL:HB	1:A:823:ARG:HH21	1.75	0.52
1:C:476:CYS:CB	1:C:487:CYS:HA	2.39	0.52
1:C:634:ASN:ND2	1:G:690:LYS:HG3	2.24	0.52
1:C:681:LEU:HD12	1:C:682:SER:N	2.24	0.52
1:E:333:ALA:HB1	1:E:350:ALA:HB1	1.90	0.52
1:E:761:ASN:ND2	1:E:791:ASP:HB2	2.24	0.52
2:F:432:ARG:O	2:F:433:ASP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1063:LEU:HD12	1:G:1064:PRO:HA	1.90	0.52
1:G:221:PHE:CD1	1:G:233:LYS:HD2	2.44	0.52
1:G:465:TYR:HB3	1:G:469:ARG:HA	1.91	0.52
1:G:671:ALA:O	1:G:672:THR:HG23	2.10	0.52
2:H:135:LEU:HD11	2:H:139:THR:HB	1.90	0.52
1:G:484:ARG:NH1	2:H:586:GLN:CG	2.73	0.52
1:A:491:LEU:HD12	1:A:492:TYR:N	2.24	0.52
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.92	0.52
2:B:289:LEU:HD23	2:B:315:ILE:HD11	1.91	0.52
1:G:180:THR:CG2	1:G:220:LEU:HD21	2.39	0.52
1:G:420:VAL:HB	1:G:423:GLN:HB2	1.90	0.52
1:G:761:ASN:ND2	1:G:791:ASP:HB2	2.24	0.52
1:G:848:HIS:O	1:G:849:LEU:HB3	2.09	0.52
2:H:562:ASN:HB2	2:H:563:PRO:CD	2.39	0.52
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.39	0.52
1:A:18:PHE:CZ	1:A:32:VAL:HG21	2.45	0.52
1:C:491:LEU:HD12	1:C:492:TYR:N	2.24	0.52
1:E:333:ALA:HA	1:E:352:GLY:H	1.74	0.52
1:E:600:LEU:HD12	1:E:600:LEU:O	2.09	0.52
1:E:833:PRO:HA	1:E:840:TRP:CB	2.40	0.52
1:G:595:ARG:HB2	1:G:597:ARG:HH12	1.75	0.52
1:A:103:LEU:HD11	2:B:155:LEU:HD13	1.91	0.52
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	1.90	0.52
1:A:491:LEU:HD12	1:A:491:LEU:C	2.30	0.52
1:A:600:LEU:O	1:A:600:LEU:HD12	2.09	0.52
2:B:364:CYS:HB2	2:B:368:VAL:HB	1.92	0.52
1:C:513:ASN:CA	1:C:599:VAL:HG21	2.39	0.52
2:D:135:LEU:HD11	2:D:139:THR:HB	1.90	0.52
2:D:25:GLN:HB2	2:D:445:CYS:CA	2.39	0.52
1:E:917:LYS:HE3	1:E:1077:VAL:CG2	2.39	0.52
1:E:119:LEU:HD21	1:E:124:GLN:NE2	2.25	0.52
2:F:591:GLN:HG2	2:F:592:GLU:N	2.23	0.52
2:F:644:ASP:HB3	2:F:650:VAL:HG23	1.92	0.52
1:G:532:GLY:HA3	1:G:565:PHE:HD2	1.75	0.52
1:C:491:LEU:HD12	1:C:491:LEU:C	2.30	0.52
2:D:155:LEU:H	2:D:160:THR:CG2	2.23	0.52
1:E:531:ARG:HA	1:E:563:GLN:O	2.09	0.52
2:F:155:LEU:H	2:F:160:THR:CG2	2.23	0.52
2:F:638:ARG:HB2	2:F:654:LEU:O	2.10	0.52
1:G:873:ASP:C	1:G:901:VAL:HG12	2.30	0.52
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:LEU:H	2:B:160:THR:CG2	2.23	0.52
2:B:27:LEU:CD2	2:B:446:GLY:HA2	2.39	0.52
1:C:117:GLN:CB	1:C:121:VAL:HG21	2.40	0.52
1:C:525:PRO:HA	1:C:532:GLY:HA2	1.92	0.52
1:C:595:ARG:HB2	1:C:597:ARG:HH12	1.75	0.52
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.44	0.52
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.45	0.52
2:D:23:TRP:CH2	2:D:447:ILE:HD13	2.45	0.52
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.44	0.52
1:E:1063:LEU:HD12	1:E:1064:PRO:HA	1.90	0.52
1:E:815:GLU:HB3	1:E:819:GLN:NE2	2.25	0.52
2:F:83:LEU:HD13	2:F:85:LEU:HB2	1.92	0.52
1:G:18:PHE:CZ	1:G:32:VAL:HG21	2.45	0.52
1:G:25:TYR:CD1	1:G:86:LEU:HB2	2.44	0.52
2:H:155:LEU:H	2:H:160:THR:CG2	2.23	0.52
2:H:532:ARG:CD	2:H:554:GLU:HG3	2.40	0.52
1:A:525:PRO:HA	1:A:532:GLY:HA2	1.92	0.52
1:A:532:GLY:HA3	1:A:565:PHE:HD2	1.75	0.52
1:C:333:ALA:HA	1:C:352:GLY:H	1.74	0.52
1:C:416:ILE:HD11	1:C:485:TRP:CZ2	2.45	0.52
2:D:644:ASP:HB3	2:D:650:VAL:HG23	1.92	0.52
1:E:71:MET:HG3	1:E:90:GLY:HA3	1.92	0.52
1:G:917:LYS:HE3	1:G:1077:VAL:CG2	2.39	0.52
1:G:333:ALA:HA	1:G:352:GLY:H	1.74	0.52
1:G:99:ARG:NH1	1:G:318:GLU:CD	2.63	0.52
5:T:2:NAG:O3	5:T:3:MAN:H2	2.10	0.52
1:A:528:GLU:HB2	1:A:531:ARG:HB2	1.92	0.51
1:A:755:ASP:O	1:A:756:HIS:HB3	2.10	0.51
2:B:121:LEU:O	2:B:125:LYS:HB3	2.09	0.51
2:B:211:PRO:HB2	2:B:246:HIS:CE1	2.45	0.51
2:B:468:SER:HB2	2:B:471:LEU:CG	2.41	0.51
1:C:685:ARG:NH2	1:G:685:ARG:CZ	2.73	0.51
1:C:71:MET:HG3	1:C:90:GLY:HA3	1.92	0.51
1:E:528:GLU:HB2	1:E:531:ARG:HB2	1.92	0.51
1:G:25:TYR:CE1	1:G:86:LEU:HB2	2.44	0.51
2:D:546:PHE:CE2	2:D:554:GLU:HG2	2.44	0.51
2:D:638:ARG:HB2	2:D:654:LEU:O	2.10	0.51
1:E:430:VAL:HG21	1:E:487:CYS:SG	2.50	0.51
1:E:766:PHE:CZ	1:E:877:LEU:HD12	2.46	0.51
1:G:71:MET:HG3	1:G:90:GLY:HA3	1.92	0.51
1:G:766:PHE:CZ	1:G:877:LEU:HD12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ASP:C	1:A:901:VAL:HG12	2.30	0.51
1:C:430:VAL:HG21	1:C:487:CYS:SG	2.50	0.51
1:C:848:HIS:O	1:C:849:LEU:HB3	2.10	0.51
1:E:25:TYR:CD1	1:E:86:LEU:HB2	2.44	0.51
1:E:491:LEU:HD12	1:E:491:LEU:C	2.30	0.51
1:E:506:LEU:HA	1:E:569:LEU:HD11	1.90	0.51
2:F:25:GLN:OE1	2:F:427:CYS:SG	2.68	0.51
1:G:394:LEU:HD23	1:G:395:TRP:N	2.26	0.51
1:G:430:VAL:HG21	1:G:487:CYS:SG	2.51	0.51
1:G:491:LEU:HD11	1:G:545:ILE:CG1	2.39	0.51
1:G:822:LEU:CG	1:G:823:ARG:H	2.22	0.51
2:H:83:LEU:HD13	2:H:85:LEU:HB2	1.93	0.51
1:C:671:ALA:O	1:C:672:THR:HG23	2.11	0.51
1:E:117:GLN:CB	1:E:121:VAL:HG21	2.41	0.51
1:E:18:PHE:CZ	1:E:32:VAL:HG21	2.45	0.51
1:E:532:GLY:HA3	1:E:565:PHE:HD2	1.75	0.51
1:E:852:ARG:HD2	2:F:480:ASN:CG	2.30	0.51
2:F:211:PRO:HB2	2:F:246:HIS:CE1	2.45	0.51
1:G:254:ILE:N	1:G:255:PRO:CD	2.73	0.51
1:G:469:ARG:NH2	2:H:287:HIS:HB2	2.26	0.51
2:H:638:ARG:HB2	2:H:654:LEU:O	2.11	0.51
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.39	0.51
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.45	0.51
2:B:363:PHE:CE2	2:B:369:THR:HG23	2.46	0.51
1:C:394:LEU:HD23	1:C:395:TRP:N	2.26	0.51
1:E:822:LEU:CG	1:E:823:ARG:H	2.24	0.51
2:F:364:CYS:HB2	2:F:368:VAL:HB	1.92	0.51
1:G:117:GLN:CB	1:G:121:VAL:HG21	2.40	0.51
1:G:133:ILE:O	1:G:169:PHE:HA	2.09	0.51
1:G:416:ILE:HD11	1:G:485:TRP:CZ2	2.45	0.51
1:G:986:PRO:HB3	1:G:987:PRO:HD2	1.92	0.51
2:H:343:SER:HA	2:H:381:VAL:O	2.11	0.51
1:A:117:GLN:CB	1:A:121:VAL:HG21	2.40	0.51
1:A:394:LEU:HD23	1:A:395:TRP:N	2.26	0.51
1:A:848:HIS:O	1:A:849:LEU:HB3	2.10	0.51
2:F:466:ARG:O	2:F:467:SER:HB3	2.11	0.51
1:G:119:LEU:HD21	1:G:124:GLN:NE2	2.25	0.51
1:G:553:ILE:HG23	1:G:557:GLN:HG3	1.92	0.51
1:G:815:GLU:HB3	1:G:819:GLN:NE2	2.26	0.51
2:H:364:CYS:HB2	2:H:368:VAL:HB	1.93	0.51
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:ILE:HG23	1:C:557:GLN:HG3	1.93	0.51
1:C:873:ASP:C	1:C:901:VAL:HG12	2.31	0.51
2:D:364:CYS:HB2	2:D:368:VAL:HB	1.93	0.51
2:D:466:ARG:O	2:D:467:SER:HB3	2.11	0.51
2:D:468:SER:HB2	2:D:471:LEU:CG	2.40	0.51
2:D:587:LEU:N	2:D:587:LEU:HD12	2.26	0.51
1:E:907:THR:HG21	1:E:1053:ILE:HD13	1.93	0.51
1:E:755:ASP:O	1:E:756:HIS:HB3	2.10	0.51
1:E:383:ASP:OD2	2:F:211:PRO:HD3	2.11	0.51
2:F:347:LEU:HD22	2:F:389:PHE:CG	2.46	0.51
1:G:833:PRO:HA	1:G:840:TRP:CB	2.40	0.51
1:G:77:LEU:HD23	1:G:88:ALA:HA	1.93	0.51
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.91	0.51
2:B:644:ASP:HB3	2:B:650:VAL:HG23	1.92	0.51
1:C:766:PHE:CZ	1:C:877:LEU:HD12	2.46	0.51
1:E:394:LEU:HD23	1:E:395:TRP:N	2.26	0.51
1:E:416:ILE:HD11	1:E:485:TRP:CZ2	2.45	0.51
1:E:491:LEU:HD12	1:E:492:TYR:N	2.25	0.51
1:E:698:LEU:N	1:E:698:LEU:HD12	2.26	0.51
2:F:363:PHE:CE2	2:F:369:THR:HG23	2.46	0.51
1:G:994:HIS:CG	1:G:1005:ILE:HD11	2.45	0.51
2:H:466:ARG:O	2:H:467:SER:HB3	2.11	0.51
2:H:468:SER:HB2	2:H:471:LEU:CG	2.41	0.51
1:A:77:LEU:HD23	1:A:88:ALA:HA	1.93	0.51
2:B:347:LEU:HD22	2:B:389:PHE:CG	2.45	0.51
2:B:638:ARG:HB2	2:B:654:LEU:O	2.11	0.51
1:C:465:TYR:CG	1:C:469:ARG:HG3	2.46	0.51
2:D:347:LEU:HD22	2:D:389:PHE:CG	2.46	0.51
1:E:25:TYR:CE1	1:E:86:LEU:HB2	2.45	0.51
2:H:211:PRO:HB2	2:H:246:HIS:CE1	2.45	0.51
2:H:508:TYR:HE2	2:H:516:THR:HG23	1.75	0.51
1:A:766:PHE:CZ	1:A:877:LEU:HD12	2.46	0.51
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.93	0.51
1:C:491:LEU:HD11	1:C:545:ILE:CG1	2.39	0.51
2:D:83:LEU:HD13	2:D:85:LEU:HB2	1.92	0.51
1:E:465:TYR:CG	1:E:469:ARG:HG3	2.46	0.51
1:G:1044:LYS:HA	1:G:1079:GLU:HB2	1.93	0.51
1:G:499:TRP:CZ2	2:H:284:GLN:HG3	2.46	0.51
1:G:698:LEU:HD12	1:G:698:LEU:N	2.26	0.51
1:G:848:HIS:O	1:G:848:HIS:ND1	2.44	0.51
1:G:385:TYR:CE1	2:H:253:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.93	0.50
1:A:833:PRO:HA	1:A:840:TRP:CB	2.40	0.50
1:C:907:THR:HG21	1:C:1053:ILE:HD13	1.93	0.50
1:E:553:ILE:HG23	1:E:557:GLN:HG3	1.92	0.50
2:F:468:SER:HB2	2:F:471:LEU:CG	2.41	0.50
2:H:212:GLU:HG2	2:H:243:ASP:CB	2.41	0.50
1:A:634:ASN:ND2	1:E:690:LYS:HG3	2.26	0.50
1:A:89:CYS:O	1:A:91:PRO:HD3	2.11	0.50
1:C:119:LEU:HD21	1:C:124:GLN:NE2	2.25	0.50
2:D:154:VAL:HG23	2:D:160:THR:HG21	1.94	0.50
2:D:432:ARG:O	2:D:433:ASP:HB2	2.11	0.50
2:F:289:LEU:HD23	2:F:315:ILE:HD11	1.91	0.50
1:G:528:GLU:HB2	1:G:531:ARG:HB2	1.93	0.50
2:H:587:LEU:HD12	2:H:587:LEU:N	2.26	0.50
2:H:644:ASP:HB3	2:H:650:VAL:HG23	1.92	0.50
1:A:430:VAL:HG21	1:A:487:CYS:SG	2.50	0.50
2:B:154:VAL:HG23	2:B:160:THR:HG21	1.94	0.50
1:C:18:PHE:CZ	1:C:32:VAL:HG21	2.45	0.50
1:C:31:VAL:HG21	1:C:86:LEU:HD13	1.94	0.50
1:C:692:HIS:ND1	1:G:694:GLU:HA	2.27	0.50
1:C:77:LEU:HD23	1:C:88:ALA:HA	1.93	0.50
1:E:77:LEU:HD23	1:E:88:ALA:HA	1.93	0.50
1:E:385:TYR:CE1	2:F:253:LEU:HD11	2.46	0.50
1:E:436:GLY:HA3	2:F:282:VAL:CB	2.41	0.50
2:H:363:PHE:CE2	2:H:369:THR:HG23	2.46	0.50
2:B:466:ARG:O	2:B:467:SER:HB3	2.11	0.50
2:D:146:PHE:HB2	2:D:195:PHE:CZ	2.47	0.50
1:E:436:GLY:HA3	2:F:282:VAL:HB	1.93	0.50
1:E:525:PRO:HA	1:E:532:GLY:HA2	1.92	0.50
1:E:681:LEU:HD12	1:E:682:SER:N	2.26	0.50
1:E:848:HIS:ND1	1:E:848:HIS:O	2.45	0.50
1:G:674:GLN:HB2	1:G:699:LEU:HD11	1.94	0.50
1:G:715:LEU:O	1:G:715:LEU:HD12	2.12	0.50
1:G:801:THR:HG22	1:G:843:SER:CB	2.41	0.50
2:H:10:SER:HB3	2:H:449:ARG:CZ	2.41	0.50
1:A:681:LEU:C	1:A:681:LEU:HD12	2.32	0.50
1:C:446:VAL:HG12	1:C:456:LEU:CD1	2.42	0.50
1:C:532:GLY:HA3	1:C:565:PHE:HD2	1.75	0.50
1:C:764:ILE:CD1	1:C:800:ILE:HD11	2.41	0.50
2:D:77:SER:HA	2:D:78:PRO:C	2.32	0.50
1:E:595:ARG:HB2	1:E:597:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:987:PRO:O	1:G:988:ALA:HB3	2.11	0.50
1:A:820:GLY:N	1:A:822:LEU:HB3	2.26	0.50
2:B:505:LYS:HA	2:B:517:ILE:HG21	1.92	0.50
1:C:698:LEU:N	1:C:698:LEU:HD12	2.25	0.50
1:C:89:CYS:O	1:C:91:PRO:HD3	2.12	0.50
1:E:908:VAL:O	1:E:938:VAL:HG23	2.12	0.50
1:E:986:PRO:HB3	1:E:987:PRO:HD2	1.92	0.50
2:F:222:ALA:CB	2:F:294:ILE:HD12	2.42	0.50
1:G:656:VAL:HG21	1:G:687:LEU:HD11	1.94	0.50
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.12	0.50
1:A:553:ILE:HG23	1:A:557:GLN:HG3	1.93	0.50
1:A:907:THR:HG21	1:A:1053:ILE:HD13	1.93	0.50
2:B:462:GLN:HG2	2:B:463:THR:N	2.26	0.50
2:B:587:LEU:N	2:B:587:LEU:HD12	2.26	0.50
1:E:373:ASN:OD1	4:Q:1:NAG:C2	2.58	0.50
1:E:89:CYS:O	1:E:91:PRO:HD3	2.12	0.50
1:G:4:ASP:CG	1:G:597:ARG:NH2	2.65	0.50
1:G:525:PRO:HA	1:G:532:GLY:HA2	1.92	0.50
1:G:89:CYS:O	1:G:91:PRO:HD3	2.12	0.50
1:A:656:VAL:HG21	1:A:687:LEU:HD11	1.94	0.50
1:A:597:ARG:HB3	1:A:731:ARG:O	2.12	0.50
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.42	0.50
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.42	0.50
2:F:587:LEU:HD12	2:F:587:LEU:N	2.27	0.50
1:C:685:ARG:CZ	1:G:685:ARG:NH2	2.75	0.50
1:A:465:TYR:CG	1:A:469:ARG:HG3	2.46	0.50
2:B:546:PHE:HA	2:B:554:GLU:O	2.12	0.50
1:C:461:ALA:N	1:C:462:PRO:HD3	2.27	0.50
1:C:908:VAL:O	1:C:938:VAL:HG23	2.11	0.50
2:D:363:PHE:CE2	2:D:369:THR:HG23	2.46	0.50
1:E:461:ALA:N	1:E:462:PRO:HD3	2.27	0.50
1:E:873:ASP:C	1:E:901:VAL:HG12	2.32	0.50
2:F:77:SER:HA	2:F:78:PRO:C	2.32	0.50
1:G:267:ILE:HG21	1:G:303:LEU:HD11	1.93	0.50
1:G:465:TYR:CG	1:G:469:ARG:HG3	2.46	0.50
1:G:569:LEU:HD12	1:G:569:LEU:O	2.12	0.50
1:A:119:LEU:HD21	1:A:124:GLN:NE2	2.25	0.49
2:B:340:LYS:HA	2:B:343:SER:HB2	1.92	0.49
1:C:886:ASN:O	1:C:888:PRO:HD3	2.12	0.49
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.42	0.49
1:E:1044:LYS:HA	1:E:1079:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:GLU:HG2	2:F:243:ASP:CB	2.42	0.49
2:H:546:PHE:CE2	2:H:554:GLU:HG2	2.47	0.49
2:H:77:SER:HA	2:H:78:PRO:C	2.32	0.49
1:A:461:ALA:N	1:A:462:PRO:HD3	2.27	0.49
1:A:886:ASN:O	1:A:888:PRO:HD3	2.12	0.49
1:C:920:ASN:OD1	1:C:1080:LYS:HE2	2.13	0.49
2:D:75:GLN:O	2:D:97:PHE:CD1	2.65	0.49
1:E:674:GLN:HB2	1:E:699:LEU:HD11	1.94	0.49
1:G:4:ASP:HB2	1:G:597:ARG:CZ	2.42	0.49
1:G:886:ASN:O	1:G:888:PRO:HD3	2.12	0.49
1:G:908:VAL:O	1:G:938:VAL:HG23	2.12	0.49
1:G:70:ASN:HB3	1:G:94:HIS:ND1	2.27	0.49
2:H:222:ALA:CB	2:H:294:ILE:HD12	2.42	0.49
1:A:513:ASN:HA	1:A:599:VAL:HG22	1.92	0.49
1:A:908:VAL:O	1:A:938:VAL:HG23	2.12	0.49
1:G:174:PHE:O	1:G:174:PHE:CG	2.65	0.49
1:G:755:ASP:O	1:G:756:HIS:HB3	2.12	0.49
1:A:31:VAL:HG21	1:A:86:LEU:HD13	1.95	0.49
1:A:595:ARG:HB2	1:A:597:ARG:HH12	1.77	0.49
1:A:848:HIS:O	1:A:848:HIS:ND1	2.45	0.49
1:C:848:HIS:O	1:C:848:HIS:ND1	2.45	0.49
2:F:33:GLY:O	2:F:474:SER:CB	2.59	0.49
1:G:461:ALA:N	1:G:462:PRO:HD3	2.27	0.49
1:A:446:VAL:HG12	1:A:456:LEU:CD1	2.43	0.49
1:A:698:LEU:HD12	1:A:698:LEU:N	2.26	0.49
1:A:715:LEU:HD12	1:A:715:LEU:O	2.12	0.49
1:A:780:LEU:O	1:A:865:VAL:HG12	2.12	0.49
1:A:801:THR:HG22	1:A:843:SER:CB	2.42	0.49
1:A:893:THR:O	1:A:893:THR:HG23	2.12	0.49
1:A:666:ARG:HB3	2:B:498:HIS:NE2	2.28	0.49
2:D:110:LEU:HD11	2:D:237:LEU:HD23	1.95	0.49
1:E:513:ASN:HA	1:E:599:VAL:HG21	1.93	0.49
1:G:325:SER:O	1:G:326:SER:HB3	2.13	0.49
1:G:446:VAL:HG12	1:G:456:LEU:CD1	2.42	0.49
2:H:146:PHE:HB2	2:H:195:PHE:CZ	2.47	0.49
1:A:362:LEU:C	1:A:362:LEU:HD23	2.33	0.49
1:A:674:GLN:HB2	1:A:699:LEU:HD11	1.95	0.49
1:A:797:GLY:HA3	1:A:884:GLU:HB2	1.95	0.49
2:B:212:GLU:HG2	2:B:243:ASP:CB	2.42	0.49
2:D:135:LEU:CD1	2:D:139:THR:HB	2.43	0.49
2:D:39:ARG:NE	2:D:447:ILE:HG23	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:886:ASN:O	1:E:888:PRO:HD3	2.12	0.49
2:F:132:LEU:HA	2:F:135:LEU:HB3	1.95	0.49
1:G:938:VAL:HG12	1:G:1024:LEU:O	2.13	0.49
2:B:75:GLN:O	2:B:97:PHE:CD1	2.66	0.49
1:C:1063:LEU:HG	1:C:1064:PRO:HD3	1.95	0.49
1:C:801:THR:HG22	1:C:843:SER:CB	2.42	0.49
1:C:938:VAL:HG12	1:C:1024:LEU:O	2.12	0.49
1:E:446:VAL:HG12	1:E:456:LEU:CD1	2.42	0.49
1:E:801:THR:HG22	1:E:843:SER:CB	2.43	0.49
2:F:105:ILE:HG21	2:F:135:LEU:HD13	1.95	0.49
2:F:186:LEU:HD13	2:F:195:PHE:CD1	2.48	0.49
1:G:920:ASN:OD1	1:G:1080:LYS:HE2	2.13	0.49
2:H:105:ILE:HG21	2:H:135:LEU:HD13	1.95	0.49
2:H:186:LEU:HD13	2:H:195:PHE:CD1	2.48	0.49
1:C:1058:SER:O	1:C:1059:VAL:HB	2.13	0.49
1:C:362:LEU:C	1:C:362:LEU:HD23	2.33	0.49
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.00	0.49
1:E:827:LEU:CD1	1:E:829:CYS:SG	3.01	0.49
2:F:251:GLY:HA3	2:F:278:ASP:OD1	2.13	0.49
2:F:75:GLN:O	2:F:97:PHE:CD1	2.66	0.49
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.43	0.49
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.93	0.49
1:C:681:LEU:HD12	1:C:681:LEU:C	2.33	0.49
2:F:146:PHE:HB2	2:F:195:PHE:CZ	2.47	0.49
1:G:776:VAL:HG12	1:G:867:PRO:O	2.13	0.49
1:A:484:ARG:HH11	2:B:594:PRO:HG2	1.77	0.49
1:A:986:PRO:CB	1:A:987:PRO:CD	2.90	0.49
1:A:469:ARG:NH2	2:B:287:HIS:HB2	2.27	0.49
1:C:47:LEU:HB2	1:C:60:ILE:CG2	2.43	0.49
1:A:771:LEU:O	1:C:789:TRP:CZ2	2.66	0.49
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.48	0.49
1:E:1058:SER:O	1:E:1059:VAL:HB	2.13	0.49
1:E:47:LEU:HB2	1:E:60:ILE:CG2	2.43	0.49
1:G:137:ILE:HB	1:G:151:MET:HE1	1.95	0.49
1:G:681:LEU:HD12	1:G:681:LEU:C	2.32	0.49
2:H:154:VAL:HG23	2:H:160:THR:HG21	1.94	0.49
1:A:764:ILE:CD1	1:A:800:ILE:HD11	2.43	0.48
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.01	0.48
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.47	0.48
2:B:110:LEU:HD11	2:B:237:LEU:HD23	1.95	0.48
1:E:70:ASN:HB3	1:E:94:HIS:ND1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:VAL:HG21	1:E:86:LEU:HD13	1.94	0.48
1:E:920:ASN:OD1	1:E:1080:LYS:HE2	2.13	0.48
1:G:827:LEU:CD1	1:G:829:CYS:SG	3.01	0.48
2:H:110:LEU:HD11	2:H:237:LEU:HD23	1.95	0.48
1:A:411:THR:HG22	1:A:435:ILE:HA	1.96	0.48
1:A:657:THR:HG23	1:A:720:VAL:HB	1.95	0.48
1:A:70:ASN:HB3	1:A:94:HIS:ND1	2.28	0.48
2:B:656:GLN:HG2	2:B:657:GLN:N	2.28	0.48
2:D:251:GLY:HA3	2:D:278:ASP:OD1	2.13	0.48
1:E:780:LEU:O	1:E:865:VAL:HG12	2.14	0.48
1:E:385:TYR:CZ	2:F:253:LEU:HD11	2.48	0.48
1:G:907:THR:HG21	1:G:1053:ILE:HD13	1.93	0.48
1:G:780:LEU:O	1:G:865:VAL:HG12	2.13	0.48
1:A:47:LEU:HB2	1:A:60:ILE:CG2	2.43	0.48
2:B:186:LEU:HD13	2:B:195:PHE:CD1	2.48	0.48
2:B:77:SER:HA	2:B:78:PRO:C	2.32	0.48
1:C:986:PRO:HB3	1:C:987:PRO:HD2	1.95	0.48
1:E:1063:LEU:HG	1:E:1064:PRO:HD3	1.95	0.48
1:E:797:GLY:HA3	1:E:884:GLU:HB2	1.94	0.48
1:E:986:PRO:HG3	1:E:1003:CYS:O	2.13	0.48
2:F:121:LEU:HD23	2:F:121:LEU:O	2.14	0.48
1:G:657:THR:HG23	1:G:720:VAL:HB	1.95	0.48
2:H:135:LEU:CD1	2:H:139:THR:HB	2.43	0.48
2:H:132:LEU:HA	2:H:135:LEU:HB3	1.95	0.48
1:A:576:THR:HG23	1:A:582:ASP:OD2	2.14	0.48
1:A:776:VAL:HG12	1:A:867:PRO:O	2.13	0.48
1:A:894:THR:O	1:C:874:ARG:NH2	2.47	0.48
1:C:477:PRO:HG2	1:C:489:ALA:HB2	1.96	0.48
2:D:270:LEU:HD23	2:D:271:TYR:O	2.14	0.48
2:D:656:GLN:HG2	2:D:657:GLN:N	2.28	0.48
1:E:362:LEU:HD23	1:E:362:LEU:C	2.34	0.48
1:E:569:LEU:HD12	1:E:569:LEU:O	2.14	0.48
1:E:715:LEU:HD12	1:E:715:LEU:O	2.13	0.48
1:E:657:THR:HG23	1:E:720:VAL:HB	1.94	0.48
2:F:154:VAL:HG23	2:F:160:THR:HG21	1.93	0.48
2:F:656:GLN:HG2	2:F:657:GLN:N	2.28	0.48
1:G:47:LEU:HB2	1:G:60:ILE:CG2	2.43	0.48
1:G:31:VAL:HG21	1:G:86:LEU:HD13	1.95	0.48
2:H:532:ARG:HD3	2:H:554:GLU:CG	2.43	0.48
2:H:75:GLN:O	2:H:97:PHE:CD1	2.66	0.48
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.28	0.48
1:E:470:GLY:HA2	1:E:497:HIS:O	2.13	0.48
1:G:362:LEU:HD23	1:G:362:LEU:C	2.33	0.48
2:B:105:ILE:HG21	2:B:135:LEU:HD13	1.95	0.48
1:C:657:THR:HG23	1:C:720:VAL:HB	1.95	0.48
1:C:797:GLY:HA3	1:C:884:GLU:HB2	1.95	0.48
1:E:1009:LEU:HD22	1:E:1011:PHE:CE1	2.49	0.48
1:E:656:VAL:HG21	1:E:687:LEU:HD11	1.95	0.48
1:G:477:PRO:HG2	1:G:489:ALA:HB2	1.96	0.48
1:G:676:THR:HG23	1:G:678:ASN:H	1.79	0.48
1:G:797:GLY:HA3	1:G:884:GLU:HB2	1.95	0.48
1:G:806:ALA:HA	1:G:840:TRP:NE1	2.29	0.48
1:A:1009:LEU:HD22	1:A:1011:PHE:CE1	2.48	0.48
2:B:105:ILE:HG12	2:B:106:ASP:N	2.29	0.48
2:B:251:GLY:HA3	2:B:278:ASP:OD1	2.14	0.48
1:C:117:GLN:HB2	1:C:121:VAL:HG21	1.95	0.48
1:C:25:TYR:CG	1:C:26:ALA:N	2.82	0.48
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.95	0.48
2:D:105:ILE:HG12	2:D:106:ASP:N	2.29	0.48
2:D:105:ILE:HG21	2:D:135:LEU:HD13	1.95	0.48
2:D:39:ARG:CD	2:D:447:ILE:HG23	2.42	0.48
1:E:938:VAL:HG12	1:E:1024:LEU:O	2.13	0.48
1:E:119:LEU:N	1:E:120:PRO:CA	2.60	0.48
1:E:477:PRO:HG2	1:E:489:ALA:HB2	1.96	0.48
1:E:827:LEU:HD13	1:E:829:CYS:SG	2.54	0.48
1:E:986:PRO:CB	1:E:987:PRO:CD	2.90	0.48
2:F:105:ILE:HG12	2:F:106:ASP:N	2.29	0.48
1:G:656:VAL:HG13	1:G:718:THR:O	2.14	0.48
2:H:270:LEU:HD23	2:H:271:TYR:O	2.13	0.48
1:A:1063:LEU:HG	1:A:1064:PRO:HD3	1.96	0.48
1:A:470:GLY:HA2	1:A:497:HIS:O	2.14	0.48
1:A:4:ASP:CG	1:A:597:ARG:NH2	2.67	0.48
1:A:575:LEU:HD12	1:A:576:THR:CG2	2.44	0.48
1:A:880:ASN:OD1	1:A:894:THR:HG22	2.14	0.48
1:C:656:VAL:HG21	1:C:687:LEU:HD11	1.95	0.48
1:C:986:PRO:CB	1:C:987:PRO:CD	2.92	0.48
2:D:43:ARG:HB3	2:D:44:PRO:HD3	1.96	0.48
2:F:546:PHE:HD2	2:F:554:GLU:HG3	1.78	0.48
2:H:105:ILE:HG12	2:H:106:ASP:N	2.28	0.48
1:A:477:PRO:HG2	1:A:489:ALA:HB2	1.96	0.48
1:A:569:LEU:HD12	1:A:569:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.96	0.48
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.49	0.48
1:C:569:LEU:O	1:C:569:LEU:HD12	2.14	0.48
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.44	0.48
1:C:715:LEU:HD12	1:C:715:LEU:O	2.13	0.48
2:D:363:PHE:HB2	2:D:388:THR:HB	1.96	0.48
1:E:117:GLN:HB2	1:E:121:VAL:HG21	1.95	0.48
1:E:716:ASN:OD1	1:E:716:ASN:C	2.52	0.48
1:E:764:ILE:CD1	1:E:800:ILE:HD11	2.43	0.48
2:F:43:ARG:HB3	2:F:44:PRO:HD3	1.96	0.48
2:F:532:ARG:HD3	2:F:554:GLU:OE1	2.14	0.48
2:H:659:GLY:O	2:H:662:ARG:HG2	2.14	0.48
2:B:132:LEU:HA	2:B:135:LEU:HB3	1.95	0.48
1:C:806:ALA:HA	1:C:840:TRP:NE1	2.29	0.48
1:C:827:LEU:HD13	1:C:829:CYS:SG	2.53	0.48
2:D:222:ALA:HB2	2:D:294:ILE:CD1	2.44	0.48
1:G:908:VAL:HG13	1:G:1069:PHE:HB3	1.96	0.48
1:G:575:LEU:HD12	1:G:576:THR:CG2	2.44	0.48
1:G:986:PRO:CB	1:G:987:PRO:CD	2.91	0.48
1:A:110:LEU:N	1:A:110:LEU:HD12	2.29	0.47
1:A:25:TYR:CG	1:A:26:ALA:N	2.82	0.47
1:A:731:ARG:NH2	1:A:733:MET:SD	2.87	0.47
2:B:135:LEU:HD11	2:B:139:THR:HB	1.95	0.47
1:E:86:LEU:HD23	1:E:87:LEU:N	2.29	0.47
2:F:461:CYS:SG	2:F:466:ARG:HD2	2.54	0.47
1:G:986:PRO:HG3	1:G:1003:CYS:O	2.13	0.47
1:G:121:VAL:CG1	1:G:121:VAL:O	2.62	0.47
1:G:478:LEU:HA	1:G:485:TRP:HE1	1.79	0.47
1:G:71:MET:CG	1:G:90:GLY:HA3	2.44	0.47
1:G:739:GLN:HB2	1:G:742:PHE:CE1	2.49	0.47
1:A:4:ASP:HB2	1:A:597:ARG:CZ	2.44	0.47
1:A:739:GLN:HB2	1:A:742:PHE:CE1	2.49	0.47
1:A:827:LEU:HD13	1:A:829:CYS:SG	2.54	0.47
1:A:73:LEU:HA	1:A:90:GLY:HA2	1.96	0.47
2:B:27:LEU:CG	2:B:446:GLY:HA2	2.43	0.47
2:D:132:LEU:HA	2:D:135:LEU:HB3	1.95	0.47
1:E:650:ARG:HD3	1:E:729:ASN:HB3	1.96	0.47
1:E:739:GLN:HB2	1:E:742:PHE:CE1	2.50	0.47
1:E:893:THR:O	1:E:893:THR:HG23	2.13	0.47
2:F:110:LEU:HD11	2:F:237:LEU:HD23	1.95	0.47
2:F:270:LEU:HD23	2:F:271:TYR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:222:ALA:HB2	2:F:294:ILE:CD1	2.45	0.47
1:G:1009:LEU:HD22	1:G:1011:PHE:CE1	2.49	0.47
1:G:25:TYR:CG	1:G:26:ALA:N	2.82	0.47
1:G:470:GLY:HA2	1:G:497:HIS:O	2.14	0.47
1:G:565:PHE:HB2	1:G:587:ALA:CB	2.44	0.47
1:G:961:GLU:HG2	1:G:1036:TRP:HA	1.96	0.47
1:G:741:TYR:CD2	2:H:502:VAL:HG22	2.49	0.47
1:A:565:PHE:HB2	1:A:587:ALA:CB	2.44	0.47
1:A:831:SER:HB3	1:A:842:THR:HG22	1.95	0.47
1:A:876:LEU:HB3	1:A:898:GLU:HG3	1.96	0.47
1:A:905:VAL:CG1	1:A:946:LEU:HD21	2.44	0.47
1:A:986:PRO:HB3	1:A:987:PRO:HD2	1.94	0.47
1:C:478:LEU:HA	1:C:485:TRP:HE1	1.80	0.47
1:C:780:LEU:O	1:C:865:VAL:HG12	2.14	0.47
1:C:893:THR:HG23	1:C:893:THR:O	2.14	0.47
1:C:905:VAL:HG21	1:C:946:LEU:HD22	1.97	0.47
2:D:340:LYS:HA	2:D:343:SER:HB2	1.96	0.47
2:D:616:PRO:HB3	2:D:621:CYS:SG	2.54	0.47
1:E:444:CYS:CB	1:E:506:LEU:CD1	2.93	0.47
1:E:73:LEU:HA	1:E:90:GLY:HA2	1.96	0.47
1:E:905:VAL:CG1	1:E:946:LEU:HD21	2.44	0.47
1:E:908:VAL:HG13	1:E:1069:PHE:HB3	1.96	0.47
2:F:630:LEU:HD12	2:F:665:ILE:HB	1.97	0.47
1:G:293:HIS:O	1:G:294:ILE:HG13	2.14	0.47
1:G:273:PHE:CB	1:G:296:LYS:HD2	2.42	0.47
1:G:724:LEU:HD12	1:G:729:ASN:ND2	2.30	0.47
1:G:764:ILE:CD1	1:G:800:ILE:HD11	2.44	0.47
2:H:121:LEU:O	2:H:121:LEU:HD23	2.14	0.47
2:H:251:GLY:HA3	2:H:278:ASP:OD1	2.14	0.47
1:A:1058:SER:O	1:A:1059:VAL:HB	2.14	0.47
2:B:616:PRO:HB3	2:B:621:CYS:SG	2.54	0.47
1:C:110:LEU:N	1:C:110:LEU:HD12	2.30	0.47
1:A:789:TRP:CZ2	1:C:771:LEU:O	2.66	0.47
2:D:11:CYS:O	2:D:15:ILE:HG12	2.14	0.47
1:E:980:SER:HB3	1:E:1012:ARG:HB3	1.96	0.47
1:E:478:LEU:HA	1:E:485:TRP:HE1	1.79	0.47
1:E:961:GLU:HG2	1:E:1036:TRP:HA	1.96	0.47
2:F:135:LEU:HD11	2:F:139:THR:HB	1.95	0.47
1:G:117:GLN:HB2	1:G:121:VAL:HG21	1.95	0.47
1:G:831:SER:HB3	1:G:842:THR:HG22	1.96	0.47
1:G:86:LEU:HD23	1:G:87:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:630:LEU:HD12	2:H:665:ILE:HB	1.96	0.47
1:A:975:PRO:HG2	1:A:977:LEU:HD11	1.97	0.47
2:B:149:PHE:HA	2:B:181:ALA:O	2.14	0.47
2:B:222:ALA:HB2	2:B:294:ILE:CD1	2.44	0.47
1:C:961:GLU:HG2	1:C:1036:TRP:HA	1.96	0.47
1:C:609:ILE:CB	1:C:610:PRO:HD3	2.44	0.47
1:C:676:THR:HG23	1:C:678:ASN:H	1.79	0.47
1:C:776:VAL:HG12	1:C:867:PRO:O	2.14	0.47
1:E:465:TYR:CG	1:E:469:ARG:CG	2.98	0.47
1:E:731:ARG:NH2	1:E:733:MET:SD	2.87	0.47
1:E:89:CYS:C	1:E:91:PRO:HD3	2.35	0.47
1:G:609:ILE:CB	1:G:610:PRO:HD3	2.42	0.47
2:H:165:LEU:HD12	2:H:179:PRO:HG2	1.96	0.47
2:H:508:TYR:CE2	2:H:516:THR:HG23	2.50	0.47
1:A:657:THR:HG22	1:A:684:VAL:HG22	1.97	0.47
2:B:121:LEU:O	2:B:121:LEU:HD23	2.14	0.47
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.96	0.47
1:C:980:SER:HB3	1:C:1012:ARG:HB3	1.96	0.47
1:C:411:THR:HG22	1:C:435:ILE:HA	1.97	0.47
1:C:575:LEU:HD12	1:C:576:THR:CG2	2.44	0.47
1:C:71:MET:CG	1:C:90:GLY:HA3	2.44	0.47
1:C:731:ARG:NH2	1:C:733:MET:SD	2.88	0.47
2:D:39:ARG:NE	2:D:447:ILE:HG22	2.30	0.47
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.49	0.47
1:E:806:ALA:HA	1:E:840:TRP:NE1	2.30	0.47
1:E:831:SER:HA	1:E:842:THR:HG22	1.97	0.47
1:E:905:VAL:HG21	1:E:946:LEU:HD22	1.96	0.47
1:G:1058:SER:O	1:G:1059:VAL:HB	2.13	0.47
1:G:822:LEU:HG	1:G:823:ARG:N	2.30	0.47
1:G:893:THR:O	1:G:893:THR:HG23	2.15	0.47
2:H:39:ARG:CZ	2:H:447:ILE:HG23	2.43	0.47
1:A:117:GLN:HB2	1:A:121:VAL:HG21	1.95	0.47
1:A:121:VAL:CG1	1:A:121:VAL:O	2.62	0.47
1:A:478:LEU:HA	1:A:485:TRP:HE1	1.80	0.47
1:A:676:THR:HG23	1:A:678:ASN:H	1.79	0.47
1:A:89:CYS:C	1:A:91:PRO:HD3	2.34	0.47
2:B:270:LEU:HD23	2:B:271:TYR:O	2.14	0.47
2:B:382:GLN:HG3	2:B:383:ILE:H	1.80	0.47
1:C:470:GLY:HA2	1:C:497:HIS:O	2.14	0.47
1:C:512:VAL:HG23	1:C:513:ASN:N	2.30	0.47
2:D:659:GLY:O	2:D:662:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:ASP:CG	1:E:597:ARG:NH2	2.68	0.47
1:E:831:SER:HB3	1:E:842:THR:HG22	1.96	0.47
2:F:277:PHE:CE1	2:F:278:ASP:O	2.68	0.47
2:F:424:GLU:HA	2:F:424:GLU:OE1	2.14	0.47
2:F:43:ARG:N	2:F:44:PRO:CD	2.78	0.47
1:G:110:LEU:N	1:G:110:LEU:HD12	2.29	0.47
1:G:827:LEU:HD13	1:G:829:CYS:SG	2.54	0.47
1:G:831:SER:HA	1:G:842:THR:HG22	1.96	0.47
2:H:656:GLN:HG2	2:H:657:GLN:N	2.29	0.47
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.96	0.47
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.14	0.47
1:A:13:VAL:HG21	1:A:57:CYS:HB2	1.96	0.47
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.97	0.47
1:C:121:VAL:O	1:C:121:VAL:CG1	2.62	0.47
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.93	0.47
1:C:465:TYR:CG	1:C:469:ARG:CG	2.98	0.47
1:C:650:ARG:HD3	1:C:729:ASN:HB3	1.97	0.47
1:C:831:SER:HB3	1:C:842:THR:HG22	1.96	0.47
2:D:23:TRP:HZ2	2:D:447:ILE:HD13	1.76	0.47
2:D:43:ARG:N	2:D:44:PRO:CD	2.78	0.47
2:D:630:LEU:HD12	2:D:665:ILE:HB	1.97	0.47
2:H:222:ALA:HB2	2:H:294:ILE:CD1	2.45	0.47
2:H:43:ARG:HB3	2:H:44:PRO:HD3	1.96	0.47
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.14	0.47
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.96	0.47
2:B:363:PHE:HB2	2:B:388:THR:HB	1.97	0.47
1:C:86:LEU:HD23	1:C:87:LEU:N	2.30	0.47
1:C:89:CYS:C	1:C:91:PRO:HD3	2.35	0.47
1:E:25:TYR:CG	1:E:26:ALA:N	2.82	0.47
1:E:565:PHE:HB2	1:E:587:ALA:CB	2.44	0.47
2:F:372:ASN:O	2:F:373:GLN:HG3	2.15	0.47
2:F:382:GLN:HG3	2:F:383:ILE:H	1.79	0.47
2:F:461:CYS:CB	2:F:466:ARG:CD	2.92	0.47
1:G:444:CYS:CB	1:G:506:LEU:CD1	2.92	0.47
1:G:444:CYS:HB2	1:G:506:LEU:HD12	1.97	0.47
1:G:657:THR:HG22	1:G:684:VAL:HG22	1.97	0.47
2:H:155:LEU:HD12	2:H:155:LEU:C	2.35	0.47
2:H:363:PHE:HB2	2:H:388:THR:HB	1.96	0.47
1:A:630:LEU:HD21	1:E:653:GLN:CB	2.44	0.47
1:A:822:LEU:HG	1:A:823:ARG:N	2.29	0.47
1:C:657:THR:HG22	1:C:684:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:ASN:C	1:C:716:ASN:OD1	2.54	0.47
2:D:121:LEU:O	2:D:121:LEU:HD23	2.14	0.47
2:D:345:VAL:HG11	2:D:387:ILE:CD1	2.45	0.47
2:D:372:ASN:O	2:D:373:GLN:HG3	2.15	0.47
2:F:135:LEU:CD1	2:F:139:THR:HB	2.45	0.47
2:F:616:PRO:HB3	2:F:621:CYS:SG	2.55	0.47
1:G:181:HIS:CE1	1:G:200:VAL:CG1	2.97	0.47
1:G:411:THR:HG22	1:G:435:ILE:HA	1.96	0.47
1:G:876:LEU:HB3	1:G:898:GLU:HG3	1.97	0.47
2:H:372:ASN:O	2:H:373:GLN:HG3	2.15	0.47
1:A:444:CYS:HB2	1:A:506:LEU:HD12	1.97	0.47
2:B:155:LEU:C	2:B:155:LEU:HD12	2.35	0.47
2:B:118:LEU:HD21	2:B:204:ILE:CD1	2.45	0.47
1:C:576:THR:HG23	1:C:582:ASP:OD2	2.15	0.47
1:C:656:VAL:HG13	1:C:718:THR:O	2.15	0.47
1:C:752:CYS:O	1:C:752:CYS:SG	2.72	0.47
1:C:761:ASN:HB3	1:C:792:GLY:HA3	1.97	0.47
1:C:822:LEU:HG	1:C:823:ARG:N	2.29	0.47
2:D:143:ARG:C	2:D:144:ILE:HD12	2.36	0.47
2:D:165:LEU:HD12	2:D:179:PRO:HG2	1.97	0.47
2:D:362:SER:HB2	2:D:370:HIS:HB2	1.97	0.47
2:D:466:ARG:HB2	2:D:491:VAL:HG13	1.96	0.47
1:E:110:LEU:HD12	1:E:110:LEU:N	2.30	0.47
1:E:512:VAL:HG23	1:E:513:ASN:N	2.30	0.47
1:E:609:ILE:CB	1:E:610:PRO:HD3	2.43	0.47
1:E:776:VAL:HG12	1:E:867:PRO:O	2.14	0.47
2:F:155:LEU:HD12	2:F:155:LEU:C	2.35	0.47
1:G:1063:LEU:HG	1:G:1064:PRO:HD3	1.95	0.47
1:G:156:ARG:HB3	1:G:197:LEU:HD13	1.97	0.47
1:G:89:CYS:C	1:G:91:PRO:HD3	2.34	0.47
2:H:347:LEU:HD22	2:H:389:PHE:CG	2.49	0.47
2:H:455:ILE:HG22	2:H:456:GLY:N	2.30	0.47
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.45	0.46
1:A:41:ALA:O	1:A:42:ASN:C	2.54	0.46
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.92	0.46
1:A:512:VAL:HG23	1:A:513:ASN:N	2.31	0.46
1:A:650:ARG:HD3	1:A:729:ASN:HB3	1.97	0.46
1:A:806:ALA:HA	1:A:840:TRP:NE1	2.29	0.46
2:B:340:LYS:HD2	2:B:379:ASP:OD1	2.15	0.46
1:C:714:ARG:C	1:C:714:ARG:HD2	2.36	0.46
1:C:71:MET:SD	1:C:90:GLY:HA3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:PHE:HA	2:D:181:ALA:O	2.14	0.46
1:E:681:LEU:HD12	1:E:681:LEU:C	2.35	0.46
1:E:71:MET:SD	1:E:90:GLY:HA3	2.55	0.46
2:H:118:LEU:HD21	2:H:204:ILE:CD1	2.45	0.46
1:G:385:TYR:CZ	2:H:253:LEU:CD1	2.98	0.46
1:A:71:MET:CG	1:A:90:GLY:HA3	2.44	0.46
1:C:739:GLN:HB2	1:C:742:PHE:CE1	2.50	0.46
2:D:6:PHE:CG	2:D:7:LYS:N	2.84	0.46
1:A:685:ARG:NH2	1:E:685:ARG:CZ	2.78	0.46
1:E:850:ILE:HG22	1:E:851:PHE:N	2.30	0.46
2:F:118:LEU:HD21	2:F:204:ILE:CD1	2.46	0.46
2:F:345:VAL:HG11	2:F:387:ILE:CD1	2.45	0.46
2:F:659:GLY:O	2:F:662:ARG:HG2	2.15	0.46
1:G:135:PHE:HZ	1:G:158:VAL:HB	1.80	0.46
1:G:714:ARG:C	1:G:714:ARG:HD2	2.36	0.46
1:G:905:VAL:CG1	1:G:946:LEU:HD21	2.45	0.46
2:H:149:PHE:HA	2:H:181:ALA:O	2.14	0.46
2:H:43:ARG:N	2:H:44:PRO:CD	2.78	0.46
1:A:86:LEU:HD23	1:A:87:LEU:N	2.30	0.46
2:B:165:LEU:HD12	2:B:179:PRO:HG2	1.97	0.46
2:B:453:GLY:O	2:B:462:GLN:HG3	2.16	0.46
1:C:13:VAL:HG21	1:C:57:CYS:HB2	1.96	0.46
1:C:73:LEU:HA	1:C:90:GLY:HA2	1.97	0.46
1:C:975:PRO:HG2	1:C:977:LEU:HD11	1.97	0.46
2:D:334:ILE:HA	2:D:337:ALA:CB	2.45	0.46
2:D:382:GLN:HG3	2:D:383:ILE:H	1.79	0.46
2:D:532:ARG:CD	2:D:554:GLU:HG3	2.45	0.46
2:D:659:GLY:O	2:D:662:ARG:CG	2.63	0.46
1:E:13:VAL:HG21	1:E:57:CYS:HB2	1.96	0.46
1:E:575:LEU:HD12	1:E:576:THR:CG2	2.44	0.46
1:E:71:MET:CG	1:E:90:GLY:HA3	2.44	0.46
1:E:876:LEU:HB3	1:E:898:GLU:HG3	1.97	0.46
2:F:11:CYS:O	2:F:15:ILE:HG12	2.15	0.46
2:F:460:GLU:OE2	2:F:461:CYS:SG	2.74	0.46
1:G:13:VAL:HG21	1:G:57:CYS:HB2	1.96	0.46
1:G:406:PRO:HB3	1:G:438:TYR:CZ	2.51	0.46
1:G:905:VAL:HG21	1:G:946:LEU:HD22	1.98	0.46
2:H:616:PRO:HB3	2:H:621:CYS:SG	2.54	0.46
1:A:93:VAL:HB	1:A:104:THR:CG2	2.45	0.46
2:B:143:ARG:C	2:B:144:ILE:HD12	2.36	0.46
1:A:103:LEU:HD13	2:B:156:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:780:LEU:HD23	1:E:780:LEU:C	2.36	0.46
1:G:93:VAL:HB	1:G:104:THR:CG2	2.45	0.46
1:G:41:ALA:O	1:G:42:ASN:C	2.54	0.46
2:H:277:PHE:CE1	2:H:278:ASP:O	2.68	0.46
2:H:6:PHE:CG	2:H:7:LYS:N	2.83	0.46
1:A:714:ARG:C	1:A:714:ARG:HD2	2.36	0.46
2:B:25:GLN:OE1	2:B:427:CYS:SG	2.73	0.46
1:C:597:ARG:HB3	1:C:731:ARG:O	2.15	0.46
1:C:780:LEU:C	1:C:780:LEU:HD23	2.36	0.46
2:D:277:PHE:CE1	2:D:278:ASP:O	2.68	0.46
1:E:576:THR:HG23	1:E:582:ASP:OD2	2.15	0.46
1:E:823:ARG:HD3	1:E:860:LEU:H	1.80	0.46
1:E:93:VAL:HB	1:E:104:THR:CG2	2.44	0.46
2:F:363:PHE:HB2	2:F:388:THR:HB	1.96	0.46
1:G:576:THR:HG23	1:G:582:ASP:OD2	2.14	0.46
1:G:71:MET:SD	1:G:90:GLY:HA3	2.55	0.46
1:G:731:ARG:NH2	1:G:733:MET:SD	2.88	0.46
1:G:73:LEU:HA	1:G:90:GLY:HA2	1.97	0.46
1:A:649:SER:O	1:A:650:ARG:HB3	2.16	0.46
1:A:831:SER:HA	1:A:842:THR:HG22	1.96	0.46
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.50	0.46
1:C:663:ASP:N	1:C:664:PRO:HD3	2.31	0.46
1:E:676:THR:HG23	1:E:678:ASN:H	1.79	0.46
2:F:149:PHE:HA	2:F:181:ALA:O	2.15	0.46
1:G:175:SER:CB	1:G:204:GLN:O	2.64	0.46
2:H:362:SER:HB2	2:H:370:HIS:HB2	1.98	0.46
2:H:659:GLY:O	2:H:662:ARG:CG	2.63	0.46
1:A:406:PRO:HB3	1:A:438:TYR:CZ	2.51	0.46
1:A:71:MET:SD	1:A:90:GLY:HA3	2.55	0.46
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.97	0.46
2:B:43:ARG:N	2:B:44:PRO:CD	2.78	0.46
1:C:93:VAL:HB	1:C:104:THR:CG2	2.45	0.46
2:D:118:LEU:HD21	2:D:204:ILE:CD1	2.46	0.46
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.51	0.46
1:E:411:THR:HG22	1:E:435:ILE:HA	1.96	0.46
2:F:98:ARG:HG2	2:F:98:ARG:O	2.15	0.46
1:G:850:ILE:HG22	1:G:851:PHE:N	2.30	0.46
2:H:143:ARG:C	2:H:144:ILE:HD12	2.36	0.46
2:H:507:ILE:HG22	2:H:508:TYR:N	2.31	0.46
1:A:22:VAL:HG22	1:A:23:VAL:N	2.31	0.46
1:A:465:TYR:CG	1:A:469:ARG:CG	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:ILE:HA	2:B:337:ALA:CB	2.46	0.46
2:B:659:GLY:O	2:B:662:ARG:HG2	2.15	0.46
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.97	0.46
1:C:601:TRP:HZ2	1:C:641:LYS:HD3	1.81	0.46
2:D:155:LEU:C	2:D:155:LEU:HD12	2.36	0.46
1:E:41:ALA:O	1:E:42:ASN:C	2.54	0.46
1:E:975:PRO:HG2	1:E:977:LEU:HD11	1.98	0.46
1:G:980:SER:HB3	1:G:1012:ARG:HB3	1.97	0.46
1:G:221:PHE:CE1	1:G:233:LYS:HD2	2.51	0.46
1:G:465:TYR:CG	1:G:469:ARG:CG	2.98	0.46
1:G:716:ASN:OD1	1:G:716:ASN:C	2.53	0.46
1:G:772:LYS:O	1:G:773:SER:HB3	2.16	0.46
2:H:345:VAL:HG11	2:H:387:ILE:CD1	2.46	0.46
4:Q:1:NAG:O3	4:Q:2:NAG:C7	2.64	0.46
1:A:345:GLY:HA3	1:A:363:TYR:O	2.16	0.46
2:B:11:CYS:O	2:B:15:ILE:HG12	2.16	0.46
2:B:432:ARG:O	2:B:433:ASP:HB2	2.16	0.46
2:B:659:GLY:O	2:B:662:ARG:CG	2.63	0.46
1:E:657:THR:HG22	1:E:684:VAL:HG22	1.97	0.46
1:E:710:PRO:HG3	1:E:884:GLU:OE2	2.16	0.46
1:E:656:VAL:HG13	1:E:718:THR:O	2.16	0.46
1:E:823:ARG:NH1	1:E:825:LEU:O	2.49	0.46
2:F:143:ARG:C	2:F:144:ILE:HD12	2.36	0.46
2:F:6:PHE:CG	2:F:7:LYS:N	2.83	0.46
1:G:878:THR:HG22	1:G:896:GLN:HB3	1.98	0.46
2:H:219:MET:HE2	2:H:262:GLY:HA2	1.98	0.46
1:A:656:VAL:HG13	1:A:718:THR:O	2.15	0.46
2:B:135:LEU:CD1	2:B:139:THR:HB	2.45	0.46
2:B:6:PHE:CG	2:B:7:LYS:N	2.83	0.46
1:C:406:PRO:HB3	1:C:438:TYR:CD2	2.51	0.46
2:D:479:ASN:HD21	6:D:3479:NAG:C7	2.21	0.46
1:E:406:PRO:HB3	1:E:438:TYR:CZ	2.51	0.46
1:E:790:ASN:O	1:E:854:GLY:HA2	2.15	0.46
2:F:165:LEU:HD12	2:F:179:PRO:HG2	1.97	0.46
1:G:939:ASN:HB3	1:G:1023:GLU:HA	1.98	0.46
1:G:99:ARG:HG3	1:G:100:ASN:OD1	2.16	0.46
2:H:334:ILE:HA	2:H:337:ALA:CB	2.46	0.46
2:H:643:ARG:NH2	2:H:649:TRP:CZ2	2.84	0.46
4:Q:1:NAG:H3	4:Q:2:NAG:HN2	1.77	0.46
1:A:939:ASN:HB3	1:A:1023:GLU:HA	1.98	0.45
1:A:878:THR:HG22	1:A:896:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:ASN:HB3	1:C:1023:GLU:HA	1.98	0.45
1:C:575:LEU:HD12	1:C:576:THR:HG23	1.99	0.45
2:D:168:PRO:CG	2:D:179:PRO:HG3	2.47	0.45
2:D:209:ASP:OD2	2:D:246:HIS:CE1	2.70	0.45
2:D:652:TYR:HB3	2:D:667:VAL:HA	1.98	0.45
1:E:465:TYR:HB3	1:E:469:ARG:HG2	1.98	0.45
2:F:659:GLY:O	2:F:662:ARG:CG	2.64	0.45
1:G:130:GLU:HB3	1:G:228:ARG:CZ	2.45	0.45
1:G:533:ALA:HA	1:G:554:ALA:HA	1.98	0.45
1:G:649:SER:O	1:G:650:ARG:HB3	2.15	0.45
2:H:27:LEU:CD2	2:H:446:GLY:CA	2.93	0.45
2:H:98:ARG:O	2:H:98:ARG:HG2	2.15	0.45
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.98	0.45
1:A:23:VAL:HG22	1:A:24:GLN:N	2.31	0.45
1:A:575:LEU:HD12	1:A:576:THR:HG23	1.99	0.45
1:A:597:ARG:HD2	1:A:731:ARG:O	2.16	0.45
2:B:98:ARG:HB2	2:B:386:PRO:HG3	1.98	0.45
1:C:345:GLY:HA3	1:C:363:TYR:O	2.16	0.45
1:E:444:CYS:HB2	1:E:506:LEU:HD12	1.98	0.45
1:E:601:TRP:HZ2	1:E:641:LYS:HD3	1.82	0.45
2:F:191:ASN:ND2	2:F:194:GLN:HB3	2.31	0.45
2:F:571:ARG:HH21	2:F:660:MET:HG3	1.81	0.45
1:G:820:GLY:N	1:G:822:LEU:HB3	2.31	0.45
2:H:432:ARG:O	2:H:433:ASP:HB2	2.16	0.45
2:H:461:CYS:HB3	2:H:466:ARG:HD3	1.98	0.45
1:A:716:ASN:OD1	1:A:716:ASN:C	2.54	0.45
1:A:850:ILE:HG22	1:A:851:PHE:N	2.32	0.45
1:A:710:PRO:HG3	1:A:884:GLU:OE2	2.17	0.45
2:B:305:VAL:HG13	2:B:306:LYS:N	2.32	0.45
1:C:525:PRO:HB3	1:C:564:TYR:HB2	1.99	0.45
1:C:649:SER:O	1:C:650:ARG:HB3	2.16	0.45
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.52	0.45
1:E:446:VAL:CG1	1:E:456:LEU:HD11	2.47	0.45
1:E:4:ASP:HB2	1:E:597:ARG:CZ	2.46	0.45
1:E:820:GLY:N	1:E:822:LEU:HB3	2.31	0.45
1:E:822:LEU:HG	1:E:823:ARG:N	2.31	0.45
1:E:790:ASN:HB2	1:E:851:PHE:CE1	2.52	0.45
2:F:643:ARG:NH2	2:F:649:TRP:CZ2	2.85	0.45
1:G:282:LEU:O	1:G:294:ILE:HD11	2.17	0.45
1:G:766:PHE:HZ	1:G:877:LEU:HD12	1.80	0.45
1:G:804:HIS:CE1	1:G:840:TRP:NE1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:118:LEU:HD21	2:H:204:ILE:HD13	1.98	0.45
2:H:382:GLN:HG3	2:H:383:ILE:H	1.79	0.45
1:A:676:THR:O	1:A:677:LYS:CB	2.64	0.45
2:B:372:ASN:O	2:B:373:GLN:HG3	2.16	0.45
2:B:546:PHE:CD2	2:B:554:GLU:HG2	2.50	0.45
2:B:631:SER:HB3	2:B:664:LEU:HD11	1.97	0.45
2:B:98:ARG:HG2	2:B:98:ARG:O	2.15	0.45
1:C:41:ALA:O	1:C:42:ASN:C	2.55	0.45
1:C:446:VAL:CG1	1:C:456:LEU:HD11	2.47	0.45
1:C:619:GLU:O	1:C:620:CYS:SG	2.74	0.45
1:C:850:ILE:HG22	1:C:851:PHE:N	2.31	0.45
1:C:880:ASN:OD1	1:C:894:THR:HG22	2.17	0.45
1:C:905:VAL:CG1	1:C:946:LEU:HD21	2.45	0.45
2:D:39:ARG:HD2	2:D:447:ILE:HG21	1.98	0.45
1:E:1020:VAL:HG12	1:E:1021:GLN:HG3	1.98	0.45
1:A:685:ARG:CZ	1:E:685:ARG:NH2	2.79	0.45
1:E:987:PRO:O	1:E:988:ALA:HB3	2.16	0.45
2:F:652:TYR:HB3	2:F:667:VAL:HA	1.99	0.45
1:G:323:THR:O	1:G:324:SER:C	2.54	0.45
1:G:780:LEU:C	1:G:780:LEU:HD23	2.36	0.45
1:G:823:ARG:HD3	1:G:860:LEU:H	1.81	0.45
4:Q:1:NAG:N2	4:Q:2:NAG:H82	2.31	0.45
1:A:406:PRO:HB3	1:A:438:TYR:CD2	2.52	0.45
1:A:772:LYS:O	1:A:773:SER:HB3	2.16	0.45
1:C:670:ARG:HG2	1:C:711:ILE:CG2	2.46	0.45
1:C:790:ASN:HB2	1:C:851:PHE:CE1	2.51	0.45
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.52	0.45
2:D:98:ARG:HG2	2:D:98:ARG:O	2.15	0.45
1:E:533:ALA:HA	1:E:554:ALA:HA	1.99	0.45
1:E:575:LEU:HD12	1:E:576:THR:HG23	1.99	0.45
2:F:334:ILE:HA	2:F:337:ALA:CB	2.46	0.45
2:F:479:ASN:ND2	6:F:3479:NAG:N2	2.62	0.45
1:G:916:THR:O	1:G:1076:THR:HG23	2.17	0.45
1:G:663:ASP:N	1:G:664:PRO:HD3	2.32	0.45
1:G:919:LEU:O	2:H:643:ARG:NH1	2.47	0.45
2:H:11:CYS:O	2:H:15:ILE:HG12	2.15	0.45
2:H:98:ARG:HB2	2:H:386:PRO:HG3	1.98	0.45
2:H:631:SER:HB3	2:H:664:LEU:HD11	1.97	0.45
1:A:772:LYS:HB3	1:C:789:TRP:NE1	2.32	0.45
1:A:780:LEU:HD23	1:A:780:LEU:C	2.36	0.45
1:A:848:HIS:O	1:A:849:LEU:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:PRO:CG	2:B:179:PRO:HG3	2.47	0.45
2:B:277:PHE:CE1	2:B:278:ASP:O	2.69	0.45
1:C:652:LEU:HD21	1:G:609:ILE:CG2	2.47	0.45
1:C:876:LEU:HB3	1:C:898:GLU:HG3	1.98	0.45
1:C:964:TRP:HB3	1:C:1032:LEU:HA	1.98	0.45
2:D:455:ILE:HG22	2:D:456:GLY:N	2.32	0.45
1:C:919:LEU:HD11	2:D:643:ARG:NH1	2.32	0.45
1:E:121:VAL:O	1:E:121:VAL:CG1	2.62	0.45
2:F:631:SER:HB3	2:F:664:LEU:HD11	1.97	0.45
1:G:17:GLY:O	1:G:20:ASP:HB2	2.17	0.45
1:G:419:GLN:HA	1:G:424:TRP:HA	1.99	0.45
1:G:465:TYR:HB3	1:G:469:ARG:HG2	1.98	0.45
1:G:975:PRO:HG2	1:G:977:LEU:HD11	1.97	0.45
1:A:1003:CYS:HB3	1:A:1008:CYS:HB2	1.85	0.45
1:A:446:VAL:CG1	1:A:456:LEU:HD11	2.47	0.45
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.46	0.45
1:A:662:LEU:HD21	1:A:698:LEU:HD23	1.99	0.45
1:A:804:HIS:CE1	1:A:840:TRP:NE1	2.85	0.45
2:B:665:ILE:HD12	2:B:665:ILE:N	2.32	0.45
1:C:1064:PRO:HG3	1:C:1067:GLU:OE2	2.16	0.45
1:C:23:VAL:HG22	1:C:24:GLN:N	2.31	0.45
1:C:22:VAL:HG22	1:C:23:VAL:N	2.32	0.45
1:C:69:VAL:HG12	1:C:70:ASN:N	2.32	0.45
2:D:345:VAL:HG11	2:D:387:ILE:HD11	1.98	0.45
1:E:964:TRP:HB3	1:E:1032:LEU:HA	1.99	0.45
1:E:23:VAL:HG22	1:E:24:GLN:N	2.32	0.45
1:E:345:GLY:HA3	1:E:363:TYR:O	2.16	0.45
1:A:686:VAL:CG1	1:E:695:ASN:O	2.64	0.45
1:E:714:ARG:HD2	1:E:714:ARG:C	2.36	0.45
1:E:724:LEU:HD12	1:E:729:ASN:ND2	2.32	0.45
2:F:168:PRO:CG	2:F:179:PRO:HG3	2.47	0.45
2:F:305:VAL:HG13	2:F:306:LYS:N	2.32	0.45
2:F:99:ARG:O	2:F:383:ILE:O	2.35	0.45
1:G:243:LYS:HD2	1:G:246:ASP:OD2	2.17	0.45
1:G:317:ILE:HG23	1:G:317:ILE:O	2.17	0.45
1:G:345:GLY:HA3	1:G:363:TYR:O	2.15	0.45
1:G:416:ILE:HG22	1:G:427:LYS:HD3	1.99	0.45
1:G:456:LEU:HA	1:G:477:PRO:HA	1.99	0.45
1:G:476:CYS:HB3	1:G:487:CYS:HA	1.98	0.45
1:G:670:ARG:HG2	1:G:711:ILE:CG2	2.47	0.45
2:H:181:ALA:HB3	2:H:271:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:2:NAG:C3	4:J:3:MAN:H2	2.46	0.45
1:A:99:ARG:HG3	1:A:100:ASN:OD1	2.17	0.45
1:A:419:GLN:HA	1:A:424:TRP:HA	1.99	0.45
1:A:713:LEU:HD23	1:A:713:LEU:C	2.38	0.45
1:A:790:ASN:HB2	1:A:851:PHE:CE1	2.51	0.45
1:A:961:GLU:HG2	1:A:1036:TRP:HA	1.97	0.45
2:B:181:ALA:HB3	2:B:271:TYR:CZ	2.52	0.45
2:B:215:LEU:HD12	2:B:246:HIS:O	2.17	0.45
2:B:506:LEU:O	2:B:515:ASP:HA	2.17	0.45
2:B:83:LEU:O	2:B:83:LEU:HD12	2.16	0.45
1:C:99:ARG:HG3	1:C:100:ASN:OD1	2.17	0.45
1:C:676:THR:O	1:C:677:LYS:CB	2.65	0.45
1:C:599:VAL:HG12	1:C:733:MET:HG3	1.99	0.45
1:C:831:SER:HA	1:C:842:THR:HG22	1.98	0.45
1:C:804:HIS:CE1	1:C:840:TRP:NE1	2.85	0.45
1:C:766:PHE:HZ	1:C:877:LEU:HD12	1.82	0.45
1:E:435:ILE:O	2:F:282:VAL:HG21	2.16	0.45
1:G:406:PRO:HB3	1:G:438:TYR:CD2	2.52	0.45
2:H:466:ARG:HB2	2:H:491:VAL:HG13	1.98	0.45
2:H:665:ILE:N	2:H:665:ILE:HD12	2.32	0.45
1:A:652:LEU:HD21	1:E:609:ILE:CG2	2.46	0.45
1:A:971:HIS:CE1	1:A:974:ASN:CB	3.00	0.45
2:B:219:MET:HE2	2:B:262:GLY:HA2	1.99	0.45
2:B:383:ILE:HG22	2:B:384:ASN:N	2.32	0.45
1:C:1024:LEU:C	1:C:1024:LEU:HD23	2.37	0.45
1:C:686:VAL:CG1	1:G:695:ASN:O	2.65	0.45
1:C:772:LYS:O	1:C:773:SER:HB3	2.16	0.45
2:D:118:LEU:HD21	2:D:204:ILE:HD13	1.98	0.45
2:D:644:ASP:HB3	2:D:650:VAL:CG2	2.47	0.45
1:E:416:ILE:HG22	1:E:427:LYS:HD3	1.99	0.45
1:E:649:SER:O	1:E:650:ARG:HB3	2.16	0.45
1:E:599:VAL:HG12	1:E:733:MET:HG3	1.98	0.45
1:G:158:VAL:O	1:G:158:VAL:HG12	2.17	0.45
1:G:171:LEU:HB3	1:G:182:PHE:CE1	2.51	0.45
1:G:446:VAL:CG1	1:G:456:LEU:HD11	2.47	0.45
1:G:507:THR:HG21	1:G:571:GLY:N	2.32	0.45
1:G:69:VAL:HG12	1:G:70:ASN:N	2.32	0.45
1:G:848:HIS:O	1:G:849:LEU:CB	2.65	0.45
1:A:69:VAL:HG12	1:A:70:ASN:N	2.32	0.45
1:A:992:LEU:C	1:A:992:LEU:HD23	2.37	0.45
2:B:120:ASP:O	2:B:124:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:ASN:ND2	2:B:277:PHE:HZ	2.15	0.45
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.85	0.45
2:D:191:ASN:ND2	2:D:194:GLN:HB3	2.32	0.45
2:D:305:VAL:HG13	2:D:306:LYS:N	2.32	0.45
2:D:665:ILE:HG22	2:D:666:TYR:N	2.32	0.45
1:E:1064:PRO:HG3	1:E:1067:GLU:OE2	2.16	0.45
1:E:348:LEU:HD12	1:E:348:LEU:N	2.32	0.45
1:E:525:PRO:HB3	1:E:564:TYR:HB2	1.99	0.45
1:A:694:GLU:HA	1:E:692:HIS:ND1	2.32	0.45
1:E:772:LYS:O	1:E:773:SER:HB3	2.17	0.45
2:F:215:LEU:HD12	2:F:246:HIS:O	2.17	0.45
2:F:665:ILE:HD12	2:F:665:ILE:N	2.32	0.45
1:G:137:ILE:CD1	1:G:152:MET:SD	3.05	0.45
1:G:174:PHE:O	1:G:174:PHE:CD1	2.70	0.45
1:G:188:ARG:NH2	1:G:228:ARG:HD3	2.32	0.45
1:G:212:ALA:O	1:G:216:VAL:HG23	2.16	0.45
1:G:297:VAL:HG12	1:G:298:GLU:N	2.32	0.45
2:H:305:VAL:HG13	2:H:306:LYS:N	2.32	0.45
2:H:383:ILE:HG22	2:H:384:ASN:N	2.32	0.45
1:A:1045:VAL:HG22	1:A:1046:SER:N	2.32	0.44
1:A:25:TYR:OH	1:A:111:GLY:HA2	2.17	0.44
1:A:456:LEU:HA	1:A:477:PRO:HA	1.99	0.44
1:A:613:ILE:HD12	1:A:748:PHE:CD2	2.52	0.44
1:A:987:PRO:O	1:A:988:ALA:HB3	2.17	0.44
1:A:435:ILE:HD13	2:B:311:LEU:HB2	1.98	0.44
1:C:118:ARG:HA	1:C:120:PRO:CA	2.47	0.44
1:C:533:ALA:HA	1:C:554:ALA:HA	1.99	0.44
1:C:4:ASP:HB2	1:C:597:ARG:CZ	2.46	0.44
1:C:662:LEU:HD21	1:C:698:LEU:HD23	1.98	0.44
2:D:25:GLN:HB2	2:D:445:CYS:HA	1.99	0.44
2:D:508:TYR:HE2	2:D:516:THR:HG23	1.82	0.44
2:D:631:SER:HB3	2:D:664:LEU:HD11	1.97	0.44
1:E:476:CYS:HB3	1:E:487:CYS:HA	1.98	0.44
2:F:209:ASP:OD2	2:F:246:HIS:CE1	2.70	0.44
2:F:219:MET:HE2	2:F:262:GLY:HA2	1.99	0.44
2:F:644:ASP:HB3	2:F:650:VAL:CG2	2.47	0.44
2:F:665:ILE:HG22	2:F:666:TYR:N	2.32	0.44
1:G:512:VAL:HG23	1:G:513:ASN:N	2.31	0.44
1:G:575:LEU:HD12	1:G:576:THR:HG23	1.99	0.44
2:H:168:PRO:CG	2:H:179:PRO:HG3	2.47	0.44
2:H:209:ASP:OD2	2:H:246:HIS:CE1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.99	0.44
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.99	0.44
1:C:419:GLN:HA	1:C:424:TRP:HA	1.99	0.44
1:C:4:ASP:CG	1:C:597:ARG:NH2	2.70	0.44
1:C:761:ASN:O	1:C:762:LEU:HD23	2.17	0.44
2:D:360:TYR:HD1	2:D:374:PRO:HA	1.82	0.44
1:E:406:PRO:HB3	1:E:438:TYR:CD2	2.52	0.44
1:E:507:THR:HG21	1:E:571:GLY:N	2.33	0.44
1:E:878:THR:HG22	1:E:896:GLN:HB3	1.98	0.44
2:F:120:ASP:O	2:F:124:VAL:HB	2.17	0.44
2:H:108:TYR:CE2	2:H:147:GLY:HA3	2.52	0.44
1:A:752:CYS:HB2	1:A:793:GLU:OE2	2.18	0.44
2:B:209:ASP:OD2	2:B:246:HIS:CE1	2.70	0.44
1:C:1003:CYS:HB3	1:C:1008:CYS:HB2	1.85	0.44
1:C:348:LEU:HD12	1:C:348:LEU:N	2.32	0.44
1:C:456:LEU:HA	1:C:477:PRO:HA	1.99	0.44
2:D:219:MET:CE	2:D:262:GLY:HA2	2.47	0.44
2:D:215:LEU:HD12	2:D:246:HIS:O	2.17	0.44
1:E:1024:LEU:HD23	1:E:1024:LEU:C	2.38	0.44
2:F:108:TYR:CE2	2:F:147:GLY:HA3	2.52	0.44
2:F:654:LEU:HD13	2:F:665:ILE:HG13	2.00	0.44
1:G:102:TYR:CG	1:G:331:GLU:HB3	2.53	0.44
1:G:603:GLY:O	1:G:638:TYR:CD2	2.71	0.44
1:G:666:ARG:CZ	1:G:670:ARG:HH21	2.31	0.44
1:A:507:THR:HG21	1:A:571:GLY:N	2.33	0.44
1:A:533:ALA:HA	1:A:554:ALA:HA	1.99	0.44
2:B:108:TYR:CE2	2:B:147:GLY:HA3	2.52	0.44
2:B:118:LEU:HD21	2:B:204:ILE:HD13	1.98	0.44
2:B:222:ALA:HB2	2:B:294:ILE:HD12	2.00	0.44
1:C:916:THR:O	1:C:1076:THR:HG23	2.17	0.44
1:C:406:PRO:HB3	1:C:438:TYR:CZ	2.51	0.44
1:C:499:TRP:CZ2	2:D:284:GLN:HG3	2.53	0.44
1:C:823:ARG:HD3	1:C:860:LEU:H	1.82	0.44
1:C:971:HIS:CE1	1:C:974:ASN:CB	3.01	0.44
2:D:120:ASP:O	2:D:124:VAL:HB	2.17	0.44
2:D:222:ALA:HB2	2:D:294:ILE:HD12	2.00	0.44
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.98	0.44
2:D:507:ILE:HG22	2:D:508:TYR:N	2.32	0.44
2:D:532:ARG:O	2:D:543:HIS:HB2	2.18	0.44
2:D:565:ARG:HD3	2:D:565:ARG:HA	1.83	0.44
1:E:662:LEU:HD21	1:E:698:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:880:ASN:OD1	1:E:894:THR:HG22	2.17	0.44
2:F:118:LEU:HD21	2:F:204:ILE:HD13	1.98	0.44
2:F:219:MET:CE	2:F:262:GLY:HA2	2.47	0.44
2:F:98:ARG:HB2	2:F:386:PRO:HG3	1.98	0.44
1:A:113:THR:HG22	1:G:1029:LYS:CE	2.48	0.44
1:G:25:TYR:OH	1:G:111:GLY:HA2	2.17	0.44
1:G:348:LEU:N	1:G:348:LEU:HD12	2.32	0.44
1:G:790:ASN:HB2	1:G:851:PHE:CE1	2.52	0.44
2:H:25:GLN:HB2	2:H:445:CYS:HB3	1.99	0.44
1:A:766:PHE:HZ	1:A:877:LEU:HD12	1.81	0.44
1:A:790:ASN:O	1:A:854:GLY:HA2	2.17	0.44
2:B:191:ASN:ND2	2:B:194:GLN:HB3	2.32	0.44
1:C:17:GLY:O	1:C:20:ASP:HB2	2.18	0.44
1:C:476:CYS:HB3	1:C:487:CYS:HA	1.98	0.44
1:C:444:CYS:HB2	1:C:506:LEU:HD12	1.97	0.44
1:C:507:THR:HG21	1:C:571:GLY:N	2.33	0.44
2:D:83:LEU:O	2:D:83:LEU:HD12	2.17	0.44
1:E:22:VAL:HG22	1:E:23:VAL:N	2.32	0.44
1:E:663:ASP:N	1:E:664:PRO:HD3	2.32	0.44
1:E:971:HIS:NE2	1:E:974:ASN:CB	2.81	0.44
2:F:181:ALA:HB3	2:F:271:TYR:CZ	2.52	0.44
2:F:260:ASN:ND2	2:F:277:PHE:HZ	2.15	0.44
2:F:532:ARG:O	2:F:543:HIS:HB2	2.17	0.44
1:G:23:VAL:HG22	1:G:24:GLN:N	2.31	0.44
1:G:323:THR:O	1:G:324:SER:O	2.36	0.44
2:H:25:GLN:HB3	2:H:445:CYS:HB3	1.98	0.44
2:H:644:ASP:HB3	2:H:650:VAL:CG2	2.48	0.44
1:A:1028:LEU:O	1:A:1028:LEU:HD12	2.17	0.44
1:A:118:ARG:HA	1:A:120:PRO:CA	2.47	0.44
1:A:351:VAL:HG23	1:A:352:GLY:N	2.33	0.44
2:B:237:LEU:HD13	2:B:294:ILE:HG23	1.99	0.44
2:B:507:ILE:HG22	2:B:508:TYR:N	2.32	0.44
1:C:790:ASN:O	1:C:854:GLY:HA2	2.17	0.44
1:E:102:TYR:CG	1:E:331:GLU:HB3	2.53	0.44
1:E:670:ARG:HG2	1:E:711:ILE:CG2	2.47	0.44
1:E:789:TRP:CZ2	1:G:771:LEU:O	2.71	0.44
1:G:1020:VAL:HG12	1:G:1021:GLN:HG3	1.98	0.44
1:G:934:HIS:ND1	1:G:1074:THR:CG2	2.80	0.44
1:G:676:THR:O	1:G:677:LYS:CB	2.65	0.44
1:G:761:ASN:HB3	1:G:792:GLY:HA3	1.99	0.44
2:H:120:ASP:O	2:H:124:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:285:LEU:C	2:H:287:HIS:N	2.71	0.44
2:H:222:ALA:HB2	2:H:294:ILE:HD12	2.00	0.44
2:H:454:TYR:O	2:H:455:ILE:HD13	2.18	0.44
2:H:652:TYR:HB3	2:H:667:VAL:HA	1.99	0.44
1:A:525:PRO:HB3	1:A:564:TYR:HB2	1.99	0.44
1:A:601:TRP:HZ2	1:A:641:LYS:HD3	1.82	0.44
2:B:6:PHE:CD2	2:B:7:LYS:N	2.86	0.44
1:C:103:LEU:HD21	2:D:155:LEU:HD22	1.99	0.44
1:C:25:TYR:OH	1:C:111:GLY:HA2	2.18	0.44
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.98	0.44
1:C:992:LEU:HD23	1:C:992:LEU:C	2.38	0.44
2:D:154:VAL:HG22	2:D:155:LEU:N	2.33	0.44
1:E:25:TYR:OH	1:E:111:GLY:HA2	2.18	0.44
1:E:534:VAL:HG23	1:E:565:PHE:CZ	2.53	0.44
2:F:83:LEU:O	2:F:83:LEU:HD12	2.17	0.44
1:G:964:TRP:HB3	1:G:1032:LEU:HA	1.99	0.44
1:G:180:THR:HG21	1:G:220:LEU:HD21	2.00	0.44
1:G:342:THR:OG1	1:G:343:PRO:HD2	2.18	0.44
1:G:534:VAL:HG23	1:G:565:PHE:CE2	2.53	0.44
2:H:191:ASN:ND2	2:H:194:GLN:HB3	2.32	0.44
2:H:219:MET:CE	2:H:262:GLY:HA2	2.48	0.44
2:H:256:ILE:HG13	2:H:256:ILE:O	2.17	0.44
2:H:260:ASN:ND2	2:H:277:PHE:HZ	2.15	0.44
2:H:120:ASP:OD1	2:H:325:GLU:O	2.36	0.44
1:A:102:TYR:CG	1:A:331:GLU:HB3	2.52	0.44
1:A:916:THR:O	1:A:1076:THR:HG23	2.17	0.44
1:C:799:THR:HA	1:C:845:ARG:HA	2.00	0.44
2:D:120:ASP:OD1	2:D:325:GLU:O	2.36	0.44
2:D:505:LYS:HA	2:D:517:ILE:CG2	2.47	0.44
1:E:676:THR:O	1:E:677:LYS:CB	2.65	0.44
1:E:69:VAL:HG12	1:E:70:ASN:N	2.32	0.44
1:E:848:HIS:O	1:E:849:LEU:CB	2.65	0.44
2:F:186:LEU:HD21	2:F:198:GLU:CB	2.48	0.44
1:G:1020:VAL:O	1:G:1021:GLN:HB2	2.17	0.44
1:G:1028:LEU:O	1:G:1028:LEU:HD12	2.18	0.44
1:G:766:PHE:CE1	1:G:877:LEU:HD11	2.53	0.44
1:G:964:TRP:HB3	1:G:1032:LEU:HG	2.00	0.44
2:H:532:ARG:O	2:H:543:HIS:HB2	2.17	0.44
2:H:654:LEU:HD13	2:H:665:ILE:HG13	2.00	0.44
2:H:83:LEU:O	2:H:83:LEU:HD12	2.17	0.44
1:A:964:TRP:HB2	1:A:1032:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:C	1:A:73:LEU:HD12	2.38	0.44
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.99	0.44
2:B:219:MET:CE	2:B:262:GLY:HA2	2.48	0.44
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.32	0.44
1:C:102:TYR:CG	1:C:331:GLU:HB3	2.53	0.44
1:C:416:ILE:HG22	1:C:427:LYS:HD3	1.99	0.44
1:C:433:THR:HG23	1:C:464:TYR:CE1	2.53	0.44
1:C:804:HIS:HB2	1:C:808:LEU:HD11	1.99	0.44
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.85	0.44
1:E:419:GLN:HA	1:E:424:TRP:HA	1.99	0.44
1:E:916:THR:O	1:E:1076:THR:HG23	2.18	0.44
1:G:1048:VAL:HG22	1:G:1075:THR:HB	2.00	0.44
1:G:175:SER:HB2	1:G:204:GLN:O	2.18	0.44
1:G:513:ASN:HA	1:G:599:VAL:HG22	1.98	0.44
1:G:650:ARG:HD3	1:G:729:ASN:HB3	1.99	0.44
1:E:874:ARG:NH2	1:G:894:THR:O	2.51	0.44
1:G:992:LEU:C	1:G:992:LEU:HD23	2.37	0.44
1:A:971:HIS:NE2	1:A:974:ASN:CB	2.81	0.43
2:B:154:VAL:HG22	2:B:155:LEU:N	2.33	0.43
2:B:532:ARG:O	2:B:543:HIS:HB2	2.17	0.43
2:B:665:ILE:HG22	2:B:666:TYR:N	2.33	0.43
1:C:513:ASN:HA	1:C:599:VAL:HG22	2.00	0.43
1:C:534:VAL:HG23	1:C:565:PHE:CZ	2.53	0.43
2:D:654:LEU:HD13	2:D:665:ILE:HG13	2.00	0.43
1:E:87:LEU:HD21	1:E:348:LEU:HD11	2.00	0.43
1:E:678:ASN:ND2	6:E:3678:NAG:C7	2.78	0.43
1:E:456:LEU:HA	1:E:477:PRO:HA	1.99	0.43
1:E:959:ASN:O	1:E:960:GLN:HB3	2.18	0.43
2:F:154:VAL:HG22	2:F:155:LEU:N	2.33	0.43
2:F:345:VAL:HG11	2:F:387:ILE:HD11	2.00	0.43
2:F:507:ILE:HG22	2:F:508:TYR:N	2.33	0.43
1:G:964:TRP:HB2	1:G:1032:LEU:HA	2.00	0.43
1:G:136:LEU:HD23	1:G:237:VAL:HG22	1.99	0.43
1:G:22:VAL:HG22	1:G:23:VAL:N	2.31	0.43
1:G:525:PRO:HB3	1:G:564:TYR:HB2	1.99	0.43
1:G:790:ASN:O	1:G:854:GLY:HA2	2.17	0.43
1:G:383:ASP:OD2	2:H:211:PRO:HD3	2.18	0.43
2:H:215:LEU:HD12	2:H:246:HIS:O	2.17	0.43
2:H:665:ILE:HG22	2:H:666:TYR:N	2.32	0.43
1:A:766:PHE:CE1	1:A:877:LEU:HD11	2.54	0.43
2:B:345:VAL:HG11	2:B:387:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:ILE:CG2	2:B:456:GLY:N	2.80	0.43
2:D:186:LEU:HD21	2:D:198:GLU:CB	2.48	0.43
1:E:1020:VAL:O	1:E:1021:GLN:HB2	2.18	0.43
1:E:939:ASN:HB3	1:E:1023:GLU:HA	1.99	0.43
1:A:1048:VAL:HG22	1:A:1075:THR:HB	2.00	0.43
1:A:17:GLY:O	1:A:20:ASP:HB2	2.19	0.43
1:A:354:PHE:CG	4:J:1:NAG:H62	2.54	0.43
1:A:959:ASN:O	1:A:960:GLN:HB3	2.18	0.43
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.53	0.43
1:C:1028:LEU:HD12	1:C:1028:LEU:O	2.19	0.43
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.53	0.43
1:C:679:ARG:HD3	1:C:679:ARG:C	2.39	0.43
2:D:188:LEU:HD12	2:D:230:TRP:HA	2.00	0.43
2:D:260:ASN:ND2	2:D:277:PHE:HZ	2.15	0.43
2:D:401:GLU:HA	2:D:421:PRO:HD3	2.00	0.43
1:E:1048:VAL:HG22	1:E:1075:THR:HB	2.00	0.43
1:E:804:HIS:CE1	1:E:840:TRP:NE1	2.86	0.43
2:F:126:LYS:HG2	2:F:196:GLN:O	2.18	0.43
1:G:601:TRP:HZ2	1:G:641:LYS:HD3	1.82	0.43
1:G:94:HIS:CD2	2:H:155:LEU:HD21	2.53	0.43
1:G:959:ASN:O	1:G:960:GLN:HB3	2.18	0.43
2:H:186:LEU:HD21	2:H:198:GLU:CB	2.48	0.43
2:H:345:VAL:HG11	2:H:387:ILE:HD11	1.99	0.43
1:A:534:VAL:HG23	1:A:565:PHE:CE2	2.53	0.43
1:A:964:TRP:HB3	1:A:1032:LEU:HA	1.99	0.43
2:B:644:ASP:HB3	2:B:650:VAL:CG2	2.47	0.43
1:C:964:TRP:HB2	1:C:1032:LEU:HA	2.00	0.43
1:C:351:VAL:HG23	1:C:352:GLY:N	2.33	0.43
1:C:613:ILE:HD12	1:C:748:PHE:CD2	2.53	0.43
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.99	0.43
1:C:971:HIS:NE2	1:C:974:ASN:CB	2.82	0.43
2:D:219:MET:HE2	2:D:262:GLY:HA2	2.01	0.43
2:D:383:ILE:HG22	2:D:384:ASN:N	2.32	0.43
1:E:964:TRP:HB2	1:E:1032:LEU:HA	1.99	0.43
1:E:1065:GLY:O	1:E:1066:GLN:HG3	2.18	0.43
1:E:446:VAL:HG12	1:E:456:LEU:HD11	2.00	0.43
1:E:464:TYR:O	1:E:465:TYR:HB3	2.18	0.43
1:E:964:TRP:HB3	1:E:1032:LEU:HG	2.00	0.43
2:F:237:LEU:HD13	2:F:294:ILE:HG23	1.99	0.43
2:F:285:LEU:C	2:F:287:HIS:N	2.71	0.43
1:G:351:VAL:HG23	1:G:352:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:VAL:O	1:G:430:VAL:HG23	2.19	0.43
1:G:662:LEU:HD21	1:G:698:LEU:HD23	1.99	0.43
1:G:73:LEU:C	1:G:73:LEU:HD12	2.38	0.43
2:H:126:LYS:HG2	2:H:196:GLN:O	2.18	0.43
2:H:599:PRO:HB2	2:H:603:TYR:HE2	1.83	0.43
1:A:1065:GLY:O	1:A:1066:GLN:HG3	2.19	0.43
1:A:87:LEU:HD21	1:A:348:LEU:HD11	2.00	0.43
1:A:476:CYS:HB3	1:A:487:CYS:HA	1.98	0.43
1:A:666:ARG:CZ	1:A:670:ARG:HH21	2.31	0.43
1:A:964:TRP:HB3	1:A:1032:LEU:HG	2.00	0.43
2:B:120:ASP:OD1	2:B:325:GLU:O	2.37	0.43
2:B:584:GLY:O	2:B:586:GLN:HG2	2.18	0.43
1:C:964:TRP:HB3	1:C:1032:LEU:HG	2.01	0.43
1:C:465:TYR:CD1	1:C:469:ARG:HG2	2.54	0.43
1:C:534:VAL:HG23	1:C:565:PHE:CE2	2.53	0.43
1:C:663:ASP:HB3	1:C:666:ARG:HD3	2.00	0.43
2:D:317:LYS:HE3	2:D:410:GLY:HA3	2.00	0.43
2:D:611:LYS:CB	2:D:667:VAL:HB	2.49	0.43
1:E:17:GLY:O	1:E:20:ASP:HB2	2.18	0.43
1:E:534:VAL:HG23	1:E:565:PHE:CE2	2.53	0.43
1:A:686:VAL:HG11	1:E:695:ASN:O	2.18	0.43
2:F:611:LYS:CB	2:F:667:VAL:HB	2.49	0.43
1:G:713:LEU:C	1:G:713:LEU:HD23	2.38	0.43
1:G:804:HIS:HB2	1:G:808:LEU:HD11	1.99	0.43
1:G:956:VAL:HG12	1:G:957:GLU:N	2.34	0.43
2:H:188:LEU:HD12	2:H:230:TRP:HA	2.01	0.43
2:H:237:LEU:HD13	2:H:294:ILE:HG23	1.99	0.43
2:H:6:PHE:CD2	2:H:7:LYS:N	2.85	0.43
1:A:909:VAL:HG12	1:A:1069:PHE:O	2.19	0.43
1:A:348:LEU:N	1:A:348:LEU:HD12	2.33	0.43
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.99	0.43
1:A:920:ASN:O	1:A:1080:LYS:HG2	2.18	0.43
2:B:144:ILE:HG22	2:B:195:PHE:CZ	2.54	0.43
1:C:342:THR:OG1	1:C:343:PRO:HD2	2.17	0.43
1:C:464:TYR:O	1:C:465:TYR:HB3	2.18	0.43
1:C:848:HIS:O	1:C:849:LEU:CB	2.65	0.43
1:C:956:VAL:HG12	1:C:957:GLU:N	2.34	0.43
1:C:985:ALA:HA	1:C:986:PRO:HD3	1.86	0.43
2:D:126:LYS:HG2	2:D:196:GLN:O	2.18	0.43
1:E:1045:VAL:HG22	1:E:1046:SER:N	2.33	0.43
1:E:351:VAL:HG23	1:E:352:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLU:O	1:E:620:CYS:SG	2.76	0.43
1:E:804:HIS:HB2	1:E:808:LEU:HD11	1.99	0.43
2:F:360:TYR:HD1	2:F:374:PRO:HA	1.83	0.43
2:F:466:ARG:HB2	2:F:491:VAL:HG13	2.00	0.43
1:G:1020:VAL:O	1:G:1021:GLN:CB	2.67	0.43
1:G:87:LEU:HD21	1:G:348:LEU:HD11	2.00	0.43
1:G:446:VAL:HG12	1:G:456:LEU:HD11	2.00	0.43
2:H:25:GLN:HB2	2:H:445:CYS:CB	2.49	0.43
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.82	0.43
1:A:342:THR:OG1	1:A:343:PRO:HD2	2.18	0.43
1:A:534:VAL:HG23	1:A:565:PHE:CZ	2.53	0.43
1:A:608:PHE:O	1:A:609:ILE:C	2.57	0.43
1:A:663:ASP:N	1:A:664:PRO:HD3	2.32	0.43
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.19	0.43
1:C:472:GLN:NE2	1:C:492:TYR:HB2	2.33	0.43
1:C:73:LEU:C	1:C:73:LEU:HD12	2.38	0.43
1:C:930:HIS:O	1:C:931:VAL:C	2.57	0.43
2:D:237:LEU:HD13	2:D:294:ILE:HG23	1.99	0.43
2:D:6:PHE:CD2	2:D:7:LYS:N	2.87	0.43
1:E:1028:LEU:O	1:E:1028:LEU:HD12	2.19	0.43
1:E:465:TYR:CD1	1:E:469:ARG:HG2	2.54	0.43
1:E:472:GLN:NE2	1:E:492:TYR:HB2	2.34	0.43
1:E:609:ILE:HD12	1:E:632:GLN:OE1	2.19	0.43
2:F:144:ILE:HG22	2:F:195:PHE:CZ	2.54	0.43
2:F:6:PHE:CD2	2:F:7:LYS:N	2.86	0.43
1:G:134:VAL:HG11	1:G:216:VAL:HG13	2.01	0.43
1:G:254:ILE:HG23	1:G:264:ARG:NH2	2.33	0.43
1:G:418:THR:HB	1:G:427:LYS:CG	2.49	0.43
1:G:534:VAL:HG23	1:G:565:PHE:CZ	2.53	0.43
1:G:752:CYS:HB2	1:G:793:GLU:CD	2.39	0.43
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.19	0.43
1:A:464:TYR:O	1:A:465:TYR:HB3	2.19	0.43
1:A:663:ASP:HB3	1:A:666:ARG:HD3	2.01	0.43
1:A:722:LYS:N	1:A:723:PRO:HD2	2.33	0.43
1:A:796:TYR:CE2	1:A:850:ILE:HD13	2.54	0.43
2:B:256:ILE:HG13	2:B:256:ILE:O	2.19	0.43
2:B:654:LEU:HD13	2:B:665:ILE:HG13	2.00	0.43
1:C:442:SER:O	1:C:459:ILE:HA	2.19	0.43
1:C:666:ARG:CZ	1:C:670:ARG:HH21	2.31	0.43
1:C:713:LEU:C	1:C:713:LEU:HD23	2.39	0.43
1:E:613:ILE:HD12	1:E:748:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:761:ASN:HB3	1:E:792:GLY:HA3	2.01	0.43
1:E:956:VAL:HG12	1:E:957:GLU:N	2.34	0.43
2:F:256:ILE:HG13	2:F:256:ILE:O	2.18	0.43
2:F:383:ILE:HG22	2:F:384:ASN:N	2.32	0.43
2:F:601:GLY:O	2:F:602:LYS:HB2	2.19	0.43
2:F:621:CYS:SG	2:F:625:CYS:SG	3.17	0.43
1:G:172:MET:SD	1:G:216:VAL:CG2	3.07	0.43
1:E:771:LEU:O	1:G:789:TRP:CZ2	2.71	0.43
1:G:796:TYR:CE2	1:G:850:ILE:HD13	2.54	0.43
2:H:154:VAL:HA	2:H:160:THR:CG2	2.49	0.43
2:H:154:VAL:HG22	2:H:155:LEU:N	2.33	0.43
2:H:99:ARG:O	2:H:383:ILE:O	2.37	0.43
1:A:1024:LEU:C	1:A:1024:LEU:HD23	2.39	0.43
1:A:586:GLY:HA2	1:A:591:VAL:HG23	2.00	0.43
1:A:609:ILE:HD12	1:A:632:GLN:OE1	2.18	0.43
1:A:679:ARG:HD3	1:A:679:ARG:C	2.39	0.43
2:B:611:LYS:CB	2:B:667:VAL:HB	2.49	0.43
2:D:621:CYS:SG	2:D:625:CYS:SG	3.17	0.43
1:E:118:ARG:HA	1:E:120:PRO:CA	2.47	0.43
1:E:376:GLN:HB2	4:Q:1:NAG:H61	2.01	0.43
1:E:418:THR:HB	1:E:427:LYS:CG	2.49	0.43
1:E:499:TRP:CZ2	2:F:284:GLN:HG3	2.54	0.43
1:E:603:GLY:O	1:E:638:TYR:CD2	2.72	0.43
1:G:1064:PRO:HG3	1:G:1067:GLU:OE2	2.19	0.43
1:G:464:TYR:O	1:G:465:TYR:HB3	2.18	0.43
1:G:472:GLN:NE2	1:G:492:TYR:HB2	2.34	0.43
2:H:401:GLU:HA	2:H:421:PRO:HD3	2.01	0.43
2:H:601:GLY:O	2:H:602:LYS:HB2	2.19	0.43
2:B:281:SER:OG	2:B:284:GLN:HB2	2.19	0.43
2:B:360:TYR:HD1	2:B:374:PRO:HA	1.84	0.43
1:C:909:VAL:HG12	1:C:1069:PHE:O	2.19	0.43
1:C:676:THR:O	1:C:677:LYS:HB3	2.19	0.43
1:C:822:LEU:CG	1:C:823:ARG:N	2.82	0.43
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.82	0.43
2:D:144:ILE:HG22	2:D:195:PHE:CZ	2.54	0.43
2:D:334:ILE:HA	2:D:337:ALA:HB2	2.01	0.43
2:D:665:ILE:HD12	2:D:665:ILE:N	2.32	0.43
1:E:689:LEU:C	1:E:689:LEU:HD12	2.39	0.43
1:E:73:LEU:HD12	1:E:73:LEU:C	2.39	0.43
1:E:799:THR:HA	1:E:845:ARG:HA	2.01	0.43
1:E:766:PHE:CE1	1:E:877:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:971:HIS:CE1	1:E:974:ASN:CB	3.00	0.43
1:E:99:ARG:HG3	1:E:100:ASN:OD1	2.18	0.43
1:G:190:SER:O	1:G:193:PRO:HD3	2.19	0.43
1:G:243:LYS:HB2	1:G:246:ASP:HB2	2.01	0.43
1:G:385:TYR:CE2	1:G:407:ARG:HD3	2.54	0.43
1:G:433:THR:HG23	1:G:464:TYR:CE1	2.54	0.43
2:H:352:LEU:CD2	2:H:358:VAL:HG23	2.49	0.43
2:H:621:CYS:SG	2:H:625:CYS:SG	3.17	0.43
1:A:385:TYR:CE2	1:A:407:ARG:HD3	2.53	0.42
1:A:418:THR:HB	1:A:427:LYS:CG	2.49	0.42
2:B:188:LEU:HD12	2:B:230:TRP:HA	2.00	0.42
2:B:401:GLU:HA	2:B:421:PRO:HD3	2.00	0.42
1:C:920:ASN:O	1:C:1080:LYS:HG2	2.19	0.42
1:A:874:ARG:NH2	1:C:894:THR:O	2.52	0.42
2:D:256:ILE:O	2:D:256:ILE:HG13	2.18	0.42
2:D:352:LEU:CD2	2:D:358:VAL:HG23	2.49	0.42
2:F:222:ALA:HB2	2:F:294:ILE:HD12	2.00	0.42
1:G:103:LEU:CD1	2:H:156:PRO:HG3	2.49	0.42
1:G:971:HIS:CE1	1:G:974:ASN:CB	3.01	0.42
2:H:144:ILE:HG22	2:H:195:PHE:CZ	2.54	0.42
2:H:611:LYS:CB	2:H:667:VAL:HB	2.48	0.42
1:A:465:TYR:CD1	1:A:469:ARG:HG2	2.54	0.42
2:B:126:LYS:HG2	2:B:196:GLN:O	2.18	0.42
2:B:543:HIS:HB3	2:B:544:PRO:HD2	2.02	0.42
1:C:353:SER:C	1:C:354:PHE:CG	2.92	0.42
1:C:689:LEU:HD12	1:C:689:LEU:C	2.39	0.42
1:C:959:ASN:O	1:C:960:GLN:HB3	2.18	0.42
1:E:342:THR:OG1	1:E:343:PRO:HD2	2.18	0.42
1:E:766:PHE:HZ	1:E:877:LEU:HD12	1.81	0.42
1:E:796:TYR:CE2	1:E:850:ILE:HD13	2.54	0.42
1:C:84:SER:OG	1:E:968:GLU:OE1	2.32	0.42
2:F:401:GLU:HA	2:F:421:PRO:HD3	2.00	0.42
2:F:455:ILE:HG22	2:F:456:GLY:N	2.35	0.42
1:G:1024:LEU:HD23	1:G:1024:LEU:C	2.39	0.42
1:G:509:LEU:HB3	1:G:519:ASP:O	2.19	0.42
1:G:689:LEU:HD12	1:G:689:LEU:C	2.39	0.42
1:G:918:TYR:O	1:G:919:LEU:C	2.57	0.42
2:H:115:TYR:HA	2:H:204:ILE:CD1	2.50	0.42
1:A:464:TYR:HD2	1:A:472:GLN:HB2	1.85	0.42
1:A:676:THR:O	1:A:677:LYS:HB3	2.19	0.42
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:584:GLY:O	2:D:586:GLN:HG2	2.20	0.42
2:D:639:THR:O	2:D:639:THR:HG23	2.19	0.42
1:E:920:ASN:O	1:E:1080:LYS:HG2	2.19	0.42
1:E:433:THR:HG23	1:E:464:TYR:CE1	2.53	0.42
1:E:464:TYR:HD2	1:E:472:GLN:HB2	1.85	0.42
2:F:352:LEU:CD2	2:F:358:VAL:HG23	2.49	0.42
1:G:267:ILE:HG21	1:G:303:LEU:CD1	2.50	0.42
1:G:464:TYR:HD2	1:G:472:GLN:HB2	1.85	0.42
1:G:608:PHE:O	1:G:609:ILE:C	2.57	0.42
1:E:1054:THR:HG21	1:G:757:ILE:HG21	2.01	0.42
2:H:360:TYR:HD1	2:H:374:PRO:HA	1.83	0.42
2:H:584:GLY:O	2:H:586:GLN:HG2	2.19	0.42
2:H:639:THR:HG23	2:H:639:THR:O	2.19	0.42
1:A:442:SER:O	1:A:459:ILE:HA	2.20	0.42
1:A:433:THR:HG23	1:A:464:TYR:CE1	2.54	0.42
1:A:7:GLU:O	1:A:595:ARG:NH2	2.53	0.42
1:C:1065:GLY:O	1:C:1066:GLN:HG3	2.18	0.42
1:C:796:TYR:CE2	1:C:850:ILE:HD13	2.55	0.42
2:D:17:SER:HB2	2:D:21:CYS:SG	2.59	0.42
1:E:385:TYR:CE2	1:E:407:ARG:HD3	2.54	0.42
1:E:442:SER:O	1:E:459:ILE:HA	2.19	0.42
1:E:468:THR:HG23	1:E:498:PRO:CG	2.50	0.42
1:E:671:ALA:HB2	1:E:700:LEU:HD23	2.02	0.42
1:G:939:ASN:HA	1:G:1018:PHE:HZ	1.84	0.42
1:C:690:LYS:HG3	1:G:634:ASN:ND2	2.35	0.42
1:C:686:VAL:HG11	1:G:695:ASN:O	2.19	0.42
1:A:761:ASN:HB3	1:A:792:GLY:HA3	2.00	0.42
1:A:930:HIS:O	1:A:931:VAL:C	2.57	0.42
1:A:956:VAL:HG12	1:A:957:GLU:N	2.34	0.42
2:B:160:THR:O	2:B:165:LEU:HD22	2.20	0.42
2:B:186:LEU:HD21	2:B:198:GLU:CB	2.48	0.42
2:B:505:LYS:HA	2:B:517:ILE:CG2	2.49	0.42
2:B:639:THR:HG23	2:B:639:THR:O	2.19	0.42
1:C:117:GLN:HB3	1:C:121:VAL:CG2	2.50	0.42
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.84	0.42
1:E:676:THR:O	1:E:677:LYS:HB3	2.19	0.42
1:E:620:CYS:HB3	1:E:702:SER:O	2.19	0.42
1:E:748:PHE:N	1:E:748:PHE:CD1	2.88	0.42
1:E:939:ASN:HA	1:E:1018:PHE:HZ	1.85	0.42
2:F:543:HIS:HB3	2:F:544:PRO:HD2	2.01	0.42
1:G:162:PHE:HB3	1:G:167:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:ILE:HD12	1:G:317:ILE:CD1	2.49	0.42
1:G:912:HIS:ND1	1:G:935:ARG:CD	2.81	0.42
1:G:971:HIS:NE2	1:G:974:ASN:CB	2.82	0.42
1:A:446:VAL:HG12	1:A:456:LEU:HD11	2.01	0.42
1:A:472:GLN:NE2	1:A:492:TYR:HB2	2.34	0.42
1:A:671:ALA:O	1:A:672:THR:CG2	2.68	0.42
1:A:812:TYR:HD2	1:A:814:ALA:HB2	1.80	0.42
1:A:939:ASN:HA	1:A:1018:PHE:HZ	1.85	0.42
2:B:302:SER:HB3	2:B:322:GLU:CG	2.50	0.42
1:C:1040:ILE:CD1	1:C:1042:GLN:HB2	2.49	0.42
1:C:609:ILE:HD12	1:C:632:GLN:OE1	2.19	0.42
1:C:825:LEU:HD11	1:C:846:ILE:HG23	2.00	0.42
1:C:987:PRO:O	1:C:988:ALA:HB3	2.19	0.42
1:E:1040:ILE:CD1	1:E:1042:GLN:HB2	2.49	0.42
1:E:934:HIS:ND1	1:E:1074:THR:CG2	2.82	0.42
1:E:430:VAL:O	1:E:430:VAL:HG23	2.20	0.42
1:E:586:GLY:HA2	1:E:591:VAL:HG23	2.00	0.42
1:G:1045:VAL:HG22	1:G:1046:SER:N	2.33	0.42
1:G:353:SER:C	1:G:354:PHE:CG	2.92	0.42
1:G:465:TYR:CD1	1:G:469:ARG:HG2	2.54	0.42
1:G:609:ILE:HD12	1:G:632:GLN:OE1	2.19	0.42
1:G:663:ASP:HB3	1:G:666:ARG:HD3	2.01	0.42
1:G:772:LYS:O	1:G:773:SER:CB	2.68	0.42
1:A:1040:ILE:CD1	1:A:1042:GLN:HB2	2.50	0.42
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.55	0.42
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.49	0.42
1:C:1065:GLY:O	1:C:1066:GLN:CG	2.68	0.42
1:C:87:LEU:HD21	1:C:348:LEU:HD11	2.00	0.42
1:C:446:VAL:HG12	1:C:456:LEU:HD11	2.00	0.42
1:C:586:GLY:HA2	1:C:591:VAL:HG23	2.01	0.42
1:C:720:VAL:HG22	1:C:721:GLY:N	2.35	0.42
1:C:73:LEU:HA	1:C:89:CYS:O	2.20	0.42
2:D:281:SER:OG	2:D:284:GLN:HB2	2.20	0.42
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.02	0.42
1:E:679:ARG:HD3	1:E:679:ARG:C	2.40	0.42
1:E:871:LEU:CD1	1:E:901:VAL:HG11	2.50	0.42
1:E:73:LEU:HA	1:E:89:CYS:O	2.20	0.42
1:E:930:HIS:O	1:E:931:VAL:C	2.57	0.42
1:E:407:ARG:HD2	2:F:250:ASP:OD2	2.20	0.42
1:G:250:TYR:HA	1:G:253:VAL:HG22	2.01	0.42
1:G:586:GLY:HA2	1:G:591:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:920:ASN:O	1:G:1080:LYS:HG2	2.19	0.42
2:H:281:SER:OG	2:H:284:GLN:HB2	2.19	0.42
1:A:419:GLN:CG	1:A:424:TRP:CD1	3.03	0.42
1:A:698:LEU:C	1:A:699:LEU:HD12	2.40	0.42
1:A:752:CYS:HB2	1:A:793:GLU:CD	2.40	0.42
2:B:187:LYS:HG2	2:B:188:LEU:N	2.35	0.42
2:B:219:MET:SD	2:B:285:LEU:HD23	2.60	0.42
2:B:99:ARG:O	2:B:383:ILE:O	2.37	0.42
1:C:748:PHE:CD1	1:C:748:PHE:N	2.88	0.42
1:C:826:HIS:HB3	1:C:848:HIS:NE2	2.35	0.42
1:C:766:PHE:CE1	1:C:877:LEU:HD11	2.55	0.42
2:D:25:GLN:O	2:D:446:GLY:HA3	2.20	0.42
2:D:98:ARG:HD3	2:D:386:PRO:HG3	2.02	0.42
1:E:1020:VAL:O	1:E:1021:GLN:CB	2.68	0.42
1:E:909:VAL:HG12	1:E:1069:PHE:O	2.19	0.42
1:E:7:GLU:O	1:E:595:ARG:NH2	2.53	0.42
1:E:629:THR:CG2	1:E:630:LEU:N	2.83	0.42
2:F:315:ILE:HA	2:F:316:PRO:HD3	1.87	0.42
2:F:120:ASP:OD1	2:F:325:GLU:O	2.36	0.42
1:G:1065:GLY:O	1:G:1066:GLN:HG3	2.19	0.42
1:G:676:THR:O	1:G:677:LYS:HB3	2.19	0.42
1:G:679:ARG:C	1:G:679:ARG:HD3	2.40	0.42
1:G:774:LEU:O	1:G:774:LEU:HG	2.20	0.42
1:A:117:GLN:HB3	1:A:121:VAL:CG2	2.50	0.42
1:A:564:TYR:CZ	1:A:588:ARG:HD2	2.55	0.42
2:B:162:PRO:O	2:B:165:LEU:CB	2.67	0.42
1:C:678:ASN:ND2	6:C:3678:NAG:C7	2.78	0.42
1:C:7:GLU:O	1:C:595:ARG:NH2	2.53	0.42
2:D:302:SER:HB3	2:D:322:GLU:CG	2.50	0.42
2:D:361:ASP:HB2	2:D:390:GLN:HB3	2.02	0.42
2:D:508:TYR:CE2	2:D:516:THR:HG23	2.55	0.42
2:D:599:PRO:HB2	2:D:603:TYR:HE2	1.85	0.42
1:E:827:LEU:HD12	1:E:827:LEU:O	2.20	0.42
2:F:334:ILE:HA	2:F:337:ALA:HB2	2.02	0.42
2:F:639:THR:O	2:F:639:THR:HG23	2.19	0.42
1:G:629:THR:CG2	1:G:630:LEU:N	2.83	0.42
1:G:722:LYS:N	1:G:723:PRO:HD2	2.33	0.42
1:G:752:CYS:HB2	1:G:793:GLU:OE2	2.20	0.42
1:G:909:VAL:HG12	1:G:1069:PHE:O	2.19	0.42
1:G:956:VAL:O	1:G:963:VAL:HG23	2.20	0.42
2:H:132:LEU:HD22	2:H:192:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:SER:HB2	2:H:21:CYS:SG	2.60	0.42
2:B:334:ILE:HA	2:B:337:ALA:HB2	2.02	0.42
2:B:601:GLY:O	2:B:602:LYS:HB2	2.20	0.42
1:C:1048:VAL:HG22	1:C:1075:THR:HB	2.00	0.42
1:C:328:PHE:HB2	1:C:354:PHE:O	2.20	0.42
1:C:402:VAL:CG1	1:C:443:LEU:HD22	2.50	0.42
1:C:629:THR:CG2	1:C:630:LEU:N	2.82	0.42
2:D:454:TYR:O	2:D:455:ILE:HD13	2.20	0.42
1:E:117:GLN:HB3	1:E:121:VAL:CG2	2.50	0.42
1:E:753:GLY:C	1:E:755:ASP:H	2.22	0.42
1:E:971:HIS:NE2	1:E:974:ASN:HB2	2.35	0.42
2:F:115:TYR:HA	2:F:204:ILE:CD1	2.50	0.42
2:F:460:GLU:OE2	2:F:492:CYS:SG	2.78	0.42
1:G:1040:ILE:CD1	1:G:1042:GLN:HB2	2.49	0.42
1:G:118:ARG:HA	1:G:120:PRO:CA	2.47	0.42
1:G:442:SER:O	1:G:459:ILE:HA	2.19	0.42
1:G:609:ILE:HB	1:G:610:PRO:CD	2.46	0.42
1:G:698:LEU:C	1:G:699:LEU:HD12	2.40	0.42
1:G:930:HIS:O	1:G:931:VAL:C	2.57	0.42
2:H:314:ILE:HG22	2:H:315:ILE:N	2.35	0.42
2:H:532:ARG:HD3	2:H:554:GLU:OE1	2.19	0.42
1:A:908:VAL:HG12	1:A:909:VAL:N	2.35	0.41
1:C:603:GLY:O	1:C:638:TYR:CD2	2.73	0.41
2:D:532:ARG:HD3	2:D:554:GLU:CG	2.49	0.41
1:E:666:ARG:CZ	1:E:670:ARG:HH21	2.32	0.41
1:E:663:ASP:HB3	1:E:666:ARG:HD3	2.01	0.41
1:E:713:LEU:C	1:E:713:LEU:HD23	2.39	0.41
1:E:720:VAL:HG22	1:E:721:GLY:N	2.35	0.41
1:E:908:VAL:HG12	1:E:909:VAL:N	2.35	0.41
1:G:7:GLU:O	1:G:595:ARG:NH2	2.53	0.41
1:C:694:GLU:HA	1:G:692:HIS:ND1	2.35	0.41
1:G:799:THR:HA	1:G:845:ARG:HA	2.01	0.41
1:G:917:LYS:HE3	1:G:1077:VAL:HG23	2.02	0.41
2:H:162:PRO:O	2:H:165:LEU:CB	2.67	0.41
2:H:219:MET:SD	2:H:285:LEU:HD23	2.60	0.41
2:H:39:ARG:CD	2:H:447:ILE:HG23	2.49	0.41
1:A:511:ASP:OD1	1:A:514:GLY:HA2	2.21	0.41
1:A:689:LEU:C	1:A:689:LEU:HD12	2.40	0.41
1:A:71:MET:O	1:A:72:SER:C	2.58	0.41
1:A:747:PRO:HB3	1:A:884:GLU:HG2	2.02	0.41
2:B:17:SER:HB2	2:B:21:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:ASP:HB2	2:B:390:GLN:HB3	2.02	0.41
1:C:919:LEU:CB	1:C:1079:GLU:HB3	2.47	0.41
1:C:354:PHE:HB2	1:C:355:THR:H	1.68	0.41
1:C:418:THR:HB	1:C:427:LYS:CG	2.49	0.41
1:C:564:TYR:CZ	1:C:588:ARG:HD2	2.55	0.41
1:C:608:PHE:O	1:C:609:ILE:C	2.59	0.41
2:D:132:LEU:HD22	2:D:192:SER:HB3	2.01	0.41
2:D:160:THR:O	2:D:165:LEU:HD22	2.20	0.41
1:E:353:SER:C	1:E:354:PHE:CG	2.92	0.41
1:E:608:PHE:O	1:E:609:ILE:C	2.58	0.41
2:F:187:LYS:HG2	2:F:188:LEU:N	2.35	0.41
1:G:269:VAL:HG11	1:G:300:PHE:CZ	2.54	0.41
1:G:602:VAL:HB	1:G:639:ILE:CG2	2.51	0.41
1:G:73:LEU:HA	1:G:89:CYS:O	2.20	0.41
2:H:187:LYS:HG2	2:H:188:LEU:N	2.35	0.41
1:A:599:VAL:CG2	1:A:599:VAL:O	2.65	0.41
1:A:637:LEU:HD11	1:A:658:LEU:HD21	2.03	0.41
1:A:73:LEU:HA	1:A:89:CYS:O	2.20	0.41
1:A:766:PHE:HB3	1:A:786:VAL:HG23	2.02	0.41
1:A:971:HIS:NE2	1:A:974:ASN:HB2	2.35	0.41
2:B:98:ARG:HD3	2:B:386:PRO:HG3	2.02	0.41
1:A:848:HIS:HB2	2:B:485:SER:HB3	2.02	0.41
2:B:565:ARG:HD3	2:B:565:ARG:HA	1.84	0.41
1:C:419:GLN:CG	1:C:424:TRP:CD1	3.03	0.41
1:C:448:VAL:HA	1:C:518:THR:HG22	2.03	0.41
1:C:698:LEU:C	1:C:699:LEU:HD12	2.41	0.41
1:C:671:ALA:HB2	1:C:700:LEU:HD23	2.01	0.41
2:D:162:PRO:O	2:D:165:LEU:CB	2.67	0.41
2:D:543:HIS:HB3	2:D:544:PRO:HD2	2.02	0.41
1:E:71:MET:O	1:E:72:SER:C	2.58	0.41
1:E:918:TYR:O	1:E:919:LEU:C	2.58	0.41
1:E:985:ALA:HA	1:E:986:PRO:HD3	1.86	0.41
2:F:162:PRO:O	2:F:165:LEU:CB	2.67	0.41
2:F:132:LEU:HD22	2:F:192:SER:HB3	2.01	0.41
2:F:17:SER:HB2	2:F:21:CYS:SG	2.60	0.41
2:F:98:ARG:HD3	2:F:386:PRO:HG3	2.02	0.41
1:G:1065:GLY:O	1:G:1066:GLN:CG	2.68	0.41
1:G:372:ILE:HG13	1:G:372:ILE:O	2.20	0.41
1:G:437:SER:HA	1:G:463:HIS:O	2.20	0.41
1:G:871:LEU:CD1	1:G:901:VAL:HG11	2.50	0.41
1:G:385:TYR:CE1	2:H:253:LEU:CD1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:LEU:HD21	2:H:446:GLY:C	2.40	0.41
2:H:302:SER:HB3	2:H:322:GLU:CG	2.50	0.41
1:A:1060:TYR:O	1:A:1061:SER:HB3	2.21	0.41
1:A:353:SER:C	1:A:354:PHE:CG	2.92	0.41
1:A:559:SER:O	1:A:560:SER:C	2.59	0.41
1:A:720:VAL:HG22	1:A:721:GLY:N	2.35	0.41
1:A:772:LYS:O	1:A:773:SER:CB	2.68	0.41
1:A:822:LEU:CG	1:A:823:ARG:N	2.83	0.41
1:A:919:LEU:O	2:B:643:ARG:NH1	2.53	0.41
1:A:956:VAL:O	1:A:963:VAL:HG23	2.20	0.41
1:C:871:LEU:CD1	1:C:901:VAL:HG11	2.50	0.41
2:D:188:LEU:CD1	2:D:230:TRP:HA	2.51	0.41
2:D:285:LEU:C	2:D:287:HIS:N	2.71	0.41
2:D:513:GLU:HG2	2:D:514:CYS:N	2.35	0.41
2:D:601:GLY:O	2:D:602:LYS:HB2	2.19	0.41
1:E:1065:GLY:O	1:E:1066:GLN:CG	2.68	0.41
1:E:671:ALA:O	1:E:672:THR:CG2	2.68	0.41
2:F:584:GLY:O	2:F:586:GLN:HG2	2.20	0.41
1:G:915:PHE:CD1	1:G:1074:THR:CG2	3.03	0.41
1:G:117:GLN:HB3	1:G:121:VAL:CG2	2.50	0.41
1:G:564:TYR:CZ	1:G:588:ARG:HD2	2.55	0.41
2:H:160:THR:O	2:H:165:LEU:HD22	2.20	0.41
2:H:230:TRP:CE3	2:H:235:ARG:HD3	2.56	0.41
2:H:442:PHE:CE1	2:H:449:ARG:HD3	2.56	0.41
2:B:188:LEU:CD1	2:B:230:TRP:HA	2.51	0.41
2:B:234:THR:CG2	2:B:236:LEU:HD13	2.51	0.41
2:B:616:PRO:HB2	2:B:620:ASN:CA	2.50	0.41
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.69	0.41
1:C:710:PRO:HG3	1:C:884:GLU:OE2	2.20	0.41
1:C:917:LYS:HE3	1:C:1077:VAL:HG23	2.02	0.41
2:D:314:ILE:HG22	2:D:315:ILE:N	2.35	0.41
2:D:340:LYS:HD2	2:D:379:ASP:CG	2.41	0.41
2:D:352:LEU:HD22	2:D:358:VAL:HG23	2.03	0.41
2:F:160:THR:O	2:F:165:LEU:HD22	2.20	0.41
2:F:188:LEU:HD12	2:F:230:TRP:HA	2.01	0.41
2:F:281:SER:OG	2:F:284:GLN:HB2	2.20	0.41
2:F:545:GLY:O	2:F:555:ARG:HA	2.19	0.41
2:F:522:TYR:CE1	2:F:552:GLN:HA	2.54	0.41
1:G:797:GLY:N	1:G:884:GLU:HB2	2.36	0.41
2:H:15:ILE:HG23	2:H:86:ARG:NE	2.34	0.41
2:H:334:ILE:HA	2:H:337:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLN:HB3	1:A:121:VAL:HG21	2.02	0.41
1:A:372:ILE:HG13	1:A:372:ILE:O	2.21	0.41
1:A:430:VAL:HG23	1:A:430:VAL:O	2.20	0.41
1:A:603:GLY:O	1:A:638:TYR:CD2	2.73	0.41
1:A:774:LEU:O	1:A:774:LEU:HG	2.21	0.41
1:A:831:SER:CA	1:A:842:THR:HG22	2.51	0.41
1:A:917:LYS:HE3	1:A:1077:VAL:HG23	2.02	0.41
2:B:115:TYR:HA	2:B:204:ILE:CD1	2.50	0.41
2:B:621:CYS:SG	2:B:625:CYS:SG	3.18	0.41
1:C:597:ARG:HA	1:C:598:PRO:HD3	1.95	0.41
1:C:71:MET:O	1:C:72:SER:C	2.59	0.41
1:A:789:TRP:NE1	1:C:772:LYS:HB3	2.35	0.41
1:C:939:ASN:HA	1:C:1018:PHE:HZ	1.85	0.41
1:C:956:VAL:O	1:C:963:VAL:HG23	2.21	0.41
2:D:305:VAL:HG13	2:D:306:LYS:HG3	2.03	0.41
2:D:75:GLN:CD	2:D:98:ARG:O	2.59	0.41
1:E:402:VAL:CG1	1:E:443:LEU:HD22	2.51	0.41
1:E:797:GLY:N	1:E:884:GLU:HB2	2.36	0.41
2:F:155:LEU:HB2	2:F:156:PRO:CA	2.46	0.41
2:F:305:VAL:HG13	2:F:306:LYS:HG3	2.03	0.41
2:F:520:GLU:HB3	2:F:550:ALA:HB2	2.03	0.41
2:F:58:ASP:N	2:F:59:PRO:CD	2.84	0.41
1:G:206:PHE:HB2	1:G:208:TYR:HE2	1.85	0.41
1:G:671:ALA:HB2	1:G:700:LEU:HD23	2.02	0.41
1:G:971:HIS:NE2	1:G:974:ASN:HB2	2.35	0.41
1:A:1065:GLY:O	1:A:1066:GLN:CG	2.68	0.41
1:A:352:GLY:HA2	1:A:356:TRP:HA	2.03	0.41
1:A:413:LYS:HG3	1:A:430:VAL:O	2.21	0.41
2:B:132:LEU:HD22	2:B:192:SER:HB3	2.01	0.41
1:C:617:ALA:HB1	1:C:702:SER:HA	2.03	0.41
2:D:115:TYR:HA	2:D:204:ILE:CD1	2.50	0.41
2:D:472:GLU:HA	2:D:475:CYS:CB	2.50	0.41
1:E:372:ILE:HG13	1:E:372:ILE:O	2.21	0.41
1:E:413:LYS:HG3	1:E:430:VAL:O	2.21	0.41
1:E:448:VAL:HA	1:E:518:THR:HG22	2.03	0.41
2:F:169:CYS:HA	2:F:170:PRO:HD3	1.80	0.41
2:F:219:MET:SD	2:F:285:LEU:HD23	2.60	0.41
2:F:436:LEU:O	2:F:437:CYS:HB2	2.21	0.41
1:G:243:LYS:O	1:G:243:LYS:CG	2.69	0.41
1:G:720:VAL:HG22	1:G:721:GLY:N	2.35	0.41
1:G:823:ARG:NH1	1:G:825:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:848:HIS:HB2	2:H:485:SER:HB3	2.02	0.41
2:H:234:THR:CG2	2:H:236:LEU:HD13	2.51	0.41
2:H:361:ASP:HB2	2:H:390:GLN:HB3	2.02	0.41
2:H:98:ARG:HD3	2:H:386:PRO:HG3	2.02	0.41
5:T:2:NAG:C3	5:T:3:MAN:H2	2.50	0.41
1:A:25:TYR:O	1:A:26:ALA:C	2.59	0.41
1:A:629:THR:CG2	1:A:630:LEU:N	2.83	0.41
1:A:671:ALA:HB2	1:A:700:LEU:HD23	2.02	0.41
1:A:912:HIS:ND1	1:A:935:ARG:CD	2.82	0.41
2:B:130:ASP:HA	2:B:133:ARG:HB3	2.02	0.41
2:B:106:ASP:OD2	2:B:188:LEU:HD13	2.21	0.41
2:B:285:LEU:C	2:B:287:HIS:N	2.71	0.41
2:B:520:GLU:HB3	2:B:550:ALA:HB2	2.03	0.41
2:D:130:ASP:HA	2:D:133:ARG:HB3	2.03	0.41
2:D:462:GLN:HG2	2:D:463:THR:H	1.84	0.41
1:E:117:GLN:HB3	1:E:121:VAL:HG21	2.03	0.41
1:E:437:SER:HA	1:E:463:HIS:O	2.21	0.41
1:E:559:SER:O	1:E:560:SER:C	2.59	0.41
1:E:564:TYR:CZ	1:E:588:ARG:HD2	2.55	0.41
1:E:766:PHE:HB3	1:E:786:VAL:HG23	2.03	0.41
2:F:105:ILE:HG21	2:F:135:LEU:CD1	2.51	0.41
2:F:314:ILE:HG22	2:F:315:ILE:N	2.35	0.41
2:F:578:VAL:HG12	2:F:579:CYS:N	2.35	0.41
1:G:174:PHE:CB	1:G:212:ALA:HB2	2.50	0.41
1:G:270:GLY:O	1:G:271:LEU:HB3	2.20	0.41
1:G:419:GLN:CG	1:G:424:TRP:CD1	3.04	0.41
2:H:436:LEU:O	2:H:437:CYS:HB2	2.21	0.41
1:G:665:GLY:CA	2:H:498:HIS:HB3	2.50	0.41
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.03	0.41
1:A:797:GLY:N	1:A:884:GLU:HB2	2.35	0.41
1:A:871:LEU:HD12	1:A:903:TYR:OH	2.20	0.41
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.51	0.41
1:C:116:THR:HG22	1:C:117:GLN:N	2.36	0.41
1:C:117:GLN:HB3	1:C:121:VAL:HG21	2.02	0.41
1:C:507:THR:HG22	1:C:569:LEU:CD1	2.51	0.41
2:D:271:TYR:O	2:D:271:TYR:CG	2.74	0.41
2:D:581:CYS:HB3	2:D:585:TYR:HB2	2.03	0.41
1:E:422:ARG:HA	1:E:424:TRP:HZ3	1.86	0.41
1:E:698:LEU:C	1:E:699:LEU:HD12	2.41	0.41
1:E:819:GLN:HA	1:E:820:GLY:HA2	1.80	0.41
1:E:956:VAL:O	1:E:963:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:LEU:CD1	2:F:230:TRP:HA	2.51	0.41
2:F:461:CYS:SG	2:F:466:ARG:HD3	2.60	0.41
2:F:525:GLN:HB3	2:F:529:GLY:N	2.36	0.41
2:F:565:ARG:HA	2:F:565:ARG:HD3	1.83	0.41
1:G:562:LEU:HA	1:G:562:LEU:HD23	1.85	0.41
1:G:671:ALA:O	1:G:672:THR:CG2	2.69	0.41
2:H:352:LEU:HD22	2:H:358:VAL:HG23	2.03	0.41
2:H:565:ARG:HD3	2:H:565:ARG:HA	1.83	0.41
1:A:509:LEU:HB3	1:A:519:ASP:O	2.21	0.41
1:A:840:TRP:CD1	1:A:840:TRP:N	2.89	0.41
1:A:871:LEU:CD1	1:A:901:VAL:HG11	2.50	0.41
2:B:317:LYS:NZ	2:B:409:LEU:HB3	2.36	0.41
1:C:422:ARG:HA	1:C:424:TRP:HZ3	1.86	0.41
1:C:609:ILE:HB	1:C:610:PRO:CD	2.48	0.41
1:C:722:LYS:N	1:C:723:PRO:HD2	2.33	0.41
1:C:840:TRP:N	1:C:840:TRP:CD1	2.89	0.41
1:C:908:VAL:HG12	1:C:909:VAL:N	2.35	0.41
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.51	0.41
2:D:219:MET:SD	2:D:285:LEU:HD23	2.60	0.41
2:D:442:PHE:CE1	2:D:449:ARG:HD3	2.55	0.41
1:C:919:LEU:CD1	2:D:643:ARG:NH1	2.84	0.41
1:E:915:PHE:CD1	1:E:1074:THR:CG2	3.04	0.41
1:E:917:LYS:HE3	1:E:1077:VAL:HG23	2.02	0.41
1:E:919:LEU:CB	1:E:1079:GLU:HB3	2.47	0.41
1:E:358:GLY:HA3	1:E:386:LEU:HB3	2.03	0.41
1:E:436:GLY:HA3	2:F:282:VAL:HG21	2.03	0.41
1:E:722:LYS:N	1:E:723:PRO:HD2	2.33	0.41
2:F:154:VAL:HA	2:F:160:THR:CG2	2.49	0.41
1:G:352:GLY:HA2	1:G:356:TRP:HA	2.03	0.41
1:G:908:VAL:HG12	1:G:909:VAL:N	2.35	0.41
2:H:69:HIS:HB2	2:H:70:ASN:H	1.73	0.41
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.68	0.41
1:A:602:VAL:HB	1:A:639:ILE:CG2	2.51	0.41
2:B:230:TRP:CE3	2:B:235:ARG:HD3	2.56	0.41
2:B:314:ILE:HG22	2:B:315:ILE:N	2.35	0.41
1:C:413:LYS:HG3	1:C:430:VAL:O	2.21	0.41
1:C:610:PRO:HG2	1:C:631:VAL:HA	2.03	0.41
1:C:797:GLY:N	1:C:884:GLU:HB2	2.36	0.41
2:D:106:ASP:OD2	2:D:188:LEU:HD13	2.21	0.41
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.51	0.41
1:C:469:ARG:HD3	2:D:283:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:597:ARG:HD2	1:E:731:ARG:O	2.20	0.41
1:E:610:PRO:HG2	1:E:631:VAL:HA	2.03	0.41
1:E:772:LYS:O	1:E:773:SER:CB	2.69	0.41
1:E:812:TYR:HD2	1:E:814:ALA:HB2	1.84	0.41
1:E:840:TRP:CD1	1:E:840:TRP:N	2.88	0.41
2:F:302:SER:HB3	2:F:322:GLU:CG	2.50	0.41
2:F:442:PHE:CE1	2:F:449:ARG:HD3	2.56	0.41
1:G:358:GLY:HA3	1:G:386:LEU:HB3	2.03	0.41
1:G:448:VAL:HA	1:G:518:THR:HG22	2.03	0.41
1:G:559:SER:O	1:G:560:SER:C	2.59	0.41
1:G:613:ILE:HD12	1:G:748:PHE:CD2	2.55	0.41
1:G:880:ASN:OD1	1:G:894:THR:HG22	2.21	0.41
2:H:424:GLU:OE1	2:H:424:GLU:HA	2.21	0.41
2:H:578:VAL:HG12	2:H:579:CYS:N	2.35	0.41
1:A:1064:PRO:HG3	1:A:1067:GLU:OE2	2.18	0.40
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.56	0.40
1:A:690:LYS:HG3	1:E:634:ASN:ND2	2.36	0.40
1:A:799:THR:HA	1:A:845:ARG:HA	2.02	0.40
2:B:345:VAL:HG11	2:B:387:ILE:HD11	2.03	0.40
1:A:484:ARG:HH12	2:B:586:GLN:HG3	1.80	0.40
2:B:75:GLN:CD	2:B:98:ARG:O	2.59	0.40
1:C:25:TYR:O	1:C:26:ALA:C	2.59	0.40
1:C:430:VAL:HG23	1:C:430:VAL:O	2.20	0.40
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.40
2:D:285:LEU:O	2:D:287:HIS:N	2.55	0.40
2:D:520:GLU:HB3	2:D:550:ALA:HB2	2.03	0.40
1:E:43:GLN:O	1:E:70:ASN:HA	2.21	0.40
1:E:430:VAL:HG13	1:E:485:TRP:CE3	2.56	0.40
1:E:602:VAL:HB	1:E:639:ILE:CG2	2.51	0.40
1:E:894:THR:O	1:G:874:ARG:NH2	2.54	0.40
2:F:219:MET:O	2:F:223:ALA:HB2	2.21	0.40
2:F:230:TRP:CE3	2:F:235:ARG:HD3	2.56	0.40
2:F:361:ASP:HB2	2:F:390:GLN:HB3	2.02	0.40
2:F:616:PRO:HB2	2:F:620:ASN:CA	2.50	0.40
1:A:915:PHE:CD1	1:A:1074:THR:CG2	3.04	0.40
1:A:597:ARG:HG3	1:A:731:ARG:CG	2.51	0.40
1:A:889:ARG:HB3	1:A:890:THR:H	1.74	0.40
1:A:975:PRO:O	1:A:977:LEU:HD13	2.22	0.40
2:B:154:VAL:HA	2:B:160:THR:CG2	2.49	0.40
2:B:442:PHE:CE1	2:B:449:ARG:HD3	2.56	0.40
2:B:578:VAL:HG12	2:B:579:CYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:599:PRO:O	2:B:603:TYR:CD2	2.75	0.40
1:C:559:SER:O	1:C:560:SER:C	2.59	0.40
1:C:599:VAL:O	1:C:599:VAL:CG2	2.68	0.40
1:C:637:LEU:HD11	1:C:658:LEU:HD21	2.03	0.40
1:C:43:GLN:O	1:C:70:ASN:HA	2.22	0.40
1:C:772:LYS:O	1:C:773:SER:CB	2.68	0.40
1:C:764:ILE:HD12	1:C:800:ILE:HD13	2.03	0.40
2:D:317:LYS:HB2	2:D:317:LYS:HE2	1.93	0.40
1:E:507:THR:HG22	1:E:569:LEU:CD1	2.51	0.40
1:E:530:ASN:ND2	1:E:563:GLN:HG2	2.36	0.40
1:E:614:PRO:O	1:E:615:ARG:HB3	2.22	0.40
1:E:639:ILE:HG12	1:E:688:GLY:O	2.21	0.40
2:F:106:ASP:OD2	2:F:188:LEU:HD13	2.21	0.40
2:F:223:ALA:HB1	2:F:264:CYS:H	1.86	0.40
1:G:176:ASN:HB3	1:G:206:PHE:HD1	1.86	0.40
1:G:214:GLN:OE1	1:G:253:VAL:HG12	2.20	0.40
1:G:618:PHE:CE2	1:G:619:GLU:HG3	2.56	0.40
2:H:611:LYS:HG2	2:H:667:VAL:HB	2.03	0.40
2:H:75:GLN:CD	2:H:98:ARG:O	2.60	0.40
1:A:614:PRO:O	1:A:615:ARG:HB3	2.22	0.40
1:A:917:LYS:HE3	1:A:1077:VAL:HG21	2.03	0.40
1:A:332:MET:SD	2:B:208:LEU:HD13	2.61	0.40
2:B:466:ARG:HB2	2:B:491:VAL:HG13	2.02	0.40
2:B:525:GLN:HB3	2:B:529:GLY:N	2.36	0.40
2:B:581:CYS:HB3	2:B:585:TYR:HB2	2.03	0.40
1:C:944:ARG:N	1:C:1020:VAL:HG21	2.36	0.40
2:D:139:THR:HG22	2:D:140:GLU:N	2.36	0.40
2:D:223:ALA:HB1	2:D:264:CYS:H	1.86	0.40
1:E:116:THR:HG22	1:E:117:GLN:N	2.36	0.40
1:E:419:GLN:CG	1:E:424:TRP:CD1	3.03	0.40
1:E:623:GLN:C	1:E:624:VAL:HG22	2.39	0.40
2:F:304:MET:HE3	2:F:307:THR:HG21	2.03	0.40
2:F:611:LYS:HG2	2:F:667:VAL:HB	2.04	0.40
1:G:484:ARG:HH11	2:H:594:PRO:HG2	1.85	0.40
1:G:530:ASN:ND2	1:G:563:GLN:HG2	2.37	0.40
1:G:71:MET:O	1:G:72:SER:C	2.58	0.40
1:G:827:LEU:HD12	1:G:827:LEU:O	2.21	0.40
1:G:775:LEU:CD1	1:G:904:ALA:HB2	2.51	0.40
2:H:543:HIS:HB3	2:H:544:PRO:HD2	2.02	0.40
1:A:502:PHE:CE2	1:A:535:TYR:CD2	3.09	0.40
1:A:613:ILE:HA	1:A:614:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:HIS:O	1:A:756:HIS:CG	2.74	0.40
1:A:811:ARG:HD3	1:A:864:ASP:OD2	2.22	0.40
2:B:219:MET:O	2:B:223:ALA:HB2	2.21	0.40
2:B:611:LYS:HG2	2:B:667:VAL:HB	2.04	0.40
1:C:468:THR:HG23	1:C:498:PRO:CG	2.50	0.40
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.03	0.40
1:C:764:ILE:HD13	1:C:879:ALA:HB1	2.03	0.40
2:D:187:LYS:HG2	2:D:188:LEU:N	2.35	0.40
2:D:230:TRP:CE3	2:D:235:ARG:HD3	2.56	0.40
2:D:436:LEU:O	2:D:437:CYS:HB2	2.21	0.40
2:D:578:VAL:HG12	2:D:579:CYS:N	2.36	0.40
2:D:615:GLY:HA2	2:D:616:PRO:HD2	1.95	0.40
1:E:393:ALA:HB3	1:E:400:SER:HB2	2.04	0.40
1:E:562:LEU:HA	1:E:562:LEU:HD23	1.85	0.40
1:E:583:LEU:O	1:E:593:LEU:HD23	2.22	0.40
1:E:774:LEU:HG	1:E:774:LEU:O	2.21	0.40
2:F:440:LYS:HG3	2:F:454:TYR:CZ	2.56	0.40
1:G:191:SER:O	1:G:192:ASN:OD1	2.40	0.40
1:G:422:ARG:HA	1:G:424:TRP:HZ3	1.86	0.40
1:G:402:VAL:CG1	1:G:443:LEU:HD22	2.51	0.40
1:G:502:PHE:CE2	1:G:535:TYR:CD2	3.10	0.40
1:G:815:GLU:HB3	1:G:819:GLN:HE21	1.86	0.40
1:G:840:TRP:CD1	1:G:840:TRP:N	2.89	0.40
2:H:188:LEU:CD1	2:H:230:TRP:HA	2.51	0.40
2:H:176:CYS:HB2	2:H:204:ILE:O	2.22	0.40
2:H:234:THR:HG22	2:H:235:ARG:N	2.36	0.40
1:A:1023:GLU:O	1:A:1024:LEU:C	2.60	0.40
1:A:358:GLY:HA3	1:A:386:LEU:HB3	2.03	0.40
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.51	0.40
1:A:52:TYR:O	1:A:53:SER:C	2.60	0.40
1:A:507:THR:HG22	1:A:569:LEU:CD1	2.51	0.40
1:A:583:LEU:O	1:A:593:LEU:HD23	2.21	0.40
1:A:679:ARG:O	1:A:679:ARG:HD3	2.22	0.40
1:A:68:ALA:HA	1:A:93:VAL:HG13	2.04	0.40
1:A:617:ALA:HB1	1:A:702:SER:HA	2.03	0.40
1:A:748:PHE:CD1	1:A:748:PHE:N	2.88	0.40
1:A:757:ILE:HG21	1:C:1054:THR:HG21	2.03	0.40
2:B:118:LEU:HD23	2:B:204:ILE:HG21	2.04	0.40
2:B:285:LEU:O	2:B:287:HIS:N	2.55	0.40
1:C:372:ILE:O	1:C:372:ILE:HG13	2.21	0.40
1:C:639:ILE:HG12	1:C:688:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:917:LYS:HE3	1:C:1077:VAL:HG21	2.03	0.40
2:D:302:SER:O	2:D:305:VAL:HG12	2.22	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.03	0.40
1:E:609:ILE:HB	1:E:610:PRO:CD	2.47	0.40
2:F:130:ASP:HA	2:F:133:ARG:HB3	2.02	0.40
2:F:271:TYR:CG	2:F:271:TYR:O	2.74	0.40
1:G:1058:SER:O	1:G:1059:VAL:CB	2.70	0.40
1:G:116:THR:HG22	1:G:117:GLN:N	2.36	0.40
1:G:137:ILE:HG13	1:G:137:ILE:O	2.21	0.40
1:G:156:ARG:HG3	1:G:157:ALA:N	2.35	0.40
1:G:430:VAL:HG13	1:G:485:TRP:CE3	2.56	0.40
1:G:511:ASP:OD1	1:G:514:GLY:HA2	2.21	0.40
1:G:656:VAL:HG21	1:G:687:LEU:HD12	2.04	0.40
1:G:748:PHE:N	1:G:748:PHE:CD1	2.88	0.40
1:G:831:SER:CA	1:G:842:THR:HG22	2.51	0.40
1:G:944:ARG:N	1:G:1020:VAL:HG21	2.36	0.40
2:H:118:LEU:HD23	2:H:204:ILE:HG21	2.04	0.40
2:H:219:MET:O	2:H:223:ALA:HB2	2.21	0.40
2:H:243:ASP:O	2:H:304:MET:HE2	2.21	0.40
2:H:271:TYR:CG	2:H:271:TYR:O	2.74	0.40
2:H:305:VAL:HG13	2:H:306:LYS:HG3	2.03	0.40
2:H:315:ILE:HA	2:H:316:PRO:HD3	1.87	0.40
2:H:312:THR:CG2	2:H:344:ARG:HH22	2.34	0.40
2:H:513:GLU:HG2	2:H:514:CYS:N	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:622:GLU:OE1	1:G:194:LEU:N[4_455]	1.85	0.35
1:E:622:GLU:OE2	1:G:192:ASN:C[4_455]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	876/1095 (80%)	660 (75%)	190 (22%)	26 (3%)	4	32
1	C	880/1095 (80%)	662 (75%)	193 (22%)	25 (3%)	5	33
1	E	878/1095 (80%)	659 (75%)	192 (22%)	27 (3%)	4	31
1	G	1080/1095 (99%)	834 (77%)	214 (20%)	32 (3%)	4	32
2	B	671/687 (98%)	511 (76%)	149 (22%)	11 (2%)	9	44
2	D	671/687 (98%)	514 (77%)	144 (22%)	13 (2%)	8	40
2	F	671/687 (98%)	512 (76%)	145 (22%)	14 (2%)	7	38
2	H	671/687 (98%)	512 (76%)	147 (22%)	12 (2%)	8	41
All	All	6398/7128 (90%)	4864 (76%)	1374 (22%)	160 (2%)	5	35

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	757	ILE
2	B	162	PRO
2	B	598	SER
1	C	82	SER
1	C	328	PHE
1	C	757	ILE
2	D	162	PRO
2	D	598	SER
1	E	82	SER
1	E	757	ILE
2	F	162	PRO
2	F	598	SER
1	G	82	SER
1	G	324	SER
1	G	326	SER
1	G	328	PHE
1	G	757	ILE
2	H	162	PRO
2	H	598	SER
1	A	490	VAL
1	A	624	VAL
1	A	691	ALA
1	A	931	VAL

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Mol	Chain	Res	Type
1	A	956	VAL
2	B	314	ILE
1	C	490	VAL
1	C	624	VAL
1	C	691	ALA
1	C	931	VAL
1	C	956	VAL
2	D	314	ILE
1	E	490	VAL
1	E	624	VAL
1	E	691	ALA
1	E	931	VAL
1	E	956	VAL
2	F	314	ILE
1	G	194	LEU
1	G	490	VAL
1	G	624	VAL
1	G	691	ALA
1	G	931	VAL
1	G	956	VAL
2	H	314	ILE
1	A	70	ASN
1	A	563	GLN
1	A	649	SER
1	A	722	LYS
1	A	847	ASN
2	B	467	SER
2	B	639	THR
1	C	70	ASN
1	C	563	GLN
1	C	649	SER
1	C	722	LYS
1	C	847	ASN
2	D	467	SER
2	D	639	THR
1	E	70	ASN
1	E	563	GLN
1	E	649	SER
1	E	722	LYS
1	E	755	ASP
1	E	847	ASN
2	F	433	ASP

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Mol	Chain	Res	Type
2	F	467	SER
2	F	639	THR
1	G	70	ASN
1	G	563	GLN
1	G	649	SER
1	G	722	LYS
1	G	847	ASN
2	H	69	HIS
2	H	467	SER
2	H	639	THR
1	A	124	GLN
1	A	354	PHE
1	A	773	SER
1	A	816	GLY
2	B	141	SER
1	C	124	GLN
1	C	354	PHE
1	C	773	SER
2	D	141	SER
1	E	124	GLN
1	E	354	PHE
1	E	773	SER
2	F	101	LYS
2	F	141	SER
1	G	124	GLN
1	G	327	SER
1	G	354	PHE
1	G	558	LEU
1	G	773	SER
2	H	141	SER
1	A	375	SER
1	A	558	LEU
2	B	69	HIS
1	C	375	SER
1	C	558	LEU
1	C	816	GLY
2	D	433	ASP
1	E	375	SER
1	E	558	LEU
1	G	193	PRO
1	G	246	ASP
1	G	375	SER

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Mol	Chain	Res	Type
1	G	751	ASN
1	G	816	GLY
1	A	846	ILE
1	A	872	GLY
1	C	846	ILE
1	C	872	GLY
2	D	351	ALA
2	D	617	PHE
1	E	730	LEU
1	E	816	GLY
1	E	846	ILE
1	E	872	GLY
2	F	351	ALA
2	F	617	PHE
1	G	846	ILE
1	G	872	GLY
2	H	351	ALA
1	A	121	VAL
1	C	121	VAL
1	E	121	VAL
1	G	121	VAL
1	A	1016	PRO
2	B	204	ILE
2	B	517	ILE
1	C	1016	PRO
2	D	517	ILE
1	E	1016	PRO
2	F	517	ILE
1	G	1016	PRO
2	H	447	ILE
2	H	517	ILE
1	A	540	VAL
2	B	447	ILE
2	B	486	GLY
1	C	540	VAL
2	D	204	ILE
2	D	447	ILE
1	E	540	VAL
2	F	204	ILE
2	F	447	ILE
2	F	486	GLY
1	G	540	VAL

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Mol	Chain	Res	Type
2	H	204	ILE
2	H	486	GLY
1	A	942	GLY
2	D	486	GLY
1	E	581	VAL
1	A	581	VAL
1	A	120	PRO
1	C	120	PRO
1	E	120	PRO
1	G	120	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/934 (80%)	737 (98%)	12 (2%)	62	79
1	C	753/934 (81%)	743 (99%)	10 (1%)	69	81
1	E	751/934 (80%)	741 (99%)	10 (1%)	69	81
1	G	924/934 (99%)	911 (99%)	13 (1%)	67	80
2	B	582/592 (98%)	582 (100%)	0	100	100
2	D	582/592 (98%)	582 (100%)	0	100	100
2	F	582/592 (98%)	582 (100%)	0	100	100
2	H	582/592 (98%)	582 (100%)	0	100	100
All	All	5505/6104 (90%)	5460 (99%)	45 (1%)	81	88

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	PHE
1	A	567	GLN
1	A	600	LEU
1	A	620	CYS
1	A	679	ARG

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Mol	Chain	Res	Type
1	A	681	LEU
1	A	714	ARG
1	A	823	ARG
1	A	840	TRP
1	A	915	PHE
1	A	964	TRP
1	A	1055	PHE
1	C	565	PHE
1	C	567	GLN
1	C	600	LEU
1	C	679	ARG
1	C	714	ARG
1	C	823	ARG
1	C	840	TRP
1	C	915	PHE
1	C	964	TRP
1	C	1055	PHE
1	E	565	PHE
1	E	567	GLN
1	E	600	LEU
1	E	679	ARG
1	E	714	ARG
1	E	823	ARG
1	E	840	TRP
1	E	915	PHE
1	E	964	TRP
1	E	1055	PHE
1	G	128	ARG
1	G	129	GLN
1	G	191	SER
1	G	565	PHE
1	G	567	GLN
1	G	600	LEU
1	G	679	ARG
1	G	714	ARG
1	G	823	ARG
1	G	840	TRP
1	G	915	PHE
1	G	964	TRP
1	G	1055	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	472	GLN
1	A	495	GLN
1	A	567	GLN
1	A	692	HIS
1	A	819	GLN
2	B	159	ASN
2	B	295	GLN
1	C	334	GLN
1	C	434	GLN
1	C	472	GLN
1	C	495	GLN
1	C	567	GLN
1	C	692	HIS
1	C	819	GLN
2	D	159	ASN
2	D	295	GLN
2	D	479	ASN
1	E	334	GLN
1	E	472	GLN
1	E	495	GLN
1	E	567	GLN
1	E	692	HIS
1	E	819	GLN
2	F	159	ASN
2	F	295	GLN
2	F	479	ASN
1	G	334	GLN
1	G	472	GLN
1	G	495	GLN
1	G	567	GLN
1	G	692	HIS
1	G	819	GLN
2	H	159	ASN
2	H	295	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

35 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	1,3	14,14,15	0.58	0	17,19,21	0.60	0
3	NAG	I	2	3	14,14,15	0.65	0	17,19,21	1.15	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
4	NAG	J	2	4	14,14,15	0.51	0	17,19,21	2.15	2 (11%)
4	MAN	J	3	4	11,11,12	0.55	0	15,15,17	1.16	2 (13%)
4	NAG	K	1	1,4	14,14,15	0.72	0	17,19,21	1.17	2 (11%)
4	NAG	K	2	4	14,14,15	0.63	0	17,19,21	0.86	1 (5%)
4	MAN	K	3	4	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.71	0	17,19,21	2.14	5 (29%)
4	NAG	L	2	4	14,14,15	0.56	0	17,19,21	0.89	0
4	MAN	L	3	4	11,11,12	0.64	0	15,15,17	1.60	2 (13%)
3	NAG	M	1	1,3	14,14,15	0.49	0	17,19,21	0.80	0
3	NAG	M	2	3	14,14,15	0.62	0	17,19,21	1.19	1 (5%)
3	NAG	N	1	1,3	14,14,15	0.55	0	17,19,21	1.08	1 (5%)
3	NAG	N	2	3	14,14,15	0.62	0	17,19,21	2.00	2 (11%)
4	NAG	O	1	1,4	14,14,15	0.60	0	17,19,21	1.32	1 (5%)
4	NAG	O	2	4	14,14,15	0.59	0	17,19,21	1.01	1 (5%)
4	MAN	O	3	4	11,11,12	0.67	0	15,15,17	1.46	2 (13%)
3	NAG	P	1	1,3	14,14,15	0.51	0	17,19,21	0.87	0
3	NAG	P	2	3	14,14,15	0.63	0	17,19,21	1.17	1 (5%)
4	NAG	Q	1	1,4	14,14,15	0.37	0	17,19,21	1.07	1 (5%)
4	NAG	Q	2	4	14,14,15	0.73	0	17,19,21	1.70	3 (17%)
4	MAN	Q	3	4	11,11,12	0.65	0	15,15,17	1.29	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	1	1,4	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
4	NAG	R	2	4	14,14,15	0.60	0	17,19,21	0.96	1 (5%)
4	MAN	R	3	4	11,11,12	0.68	0	15,15,17	1.51	2 (13%)
3	NAG	S	1	1,3	14,14,15	0.57	0	17,19,21	0.70	0
3	NAG	S	2	3	14,14,15	0.60	0	17,19,21	1.14	2 (11%)
5	NAG	T	1	1,5	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
5	NAG	T	2	5	14,14,15	0.57	0	17,19,21	2.09	2 (11%)
5	MAN	T	3	5	11,11,12	0.56	0	15,15,17	0.87	0
5	MAN	T	4	5	11,11,12	0.64	0	15,15,17	0.62	0
4	NAG	U	1	1,4	14,14,15	0.64	0	17,19,21	1.80	3 (17%)
4	NAG	U	2	4	14,14,15	0.62	0	17,19,21	0.90	1 (5%)
4	MAN	U	3	4	11,11,12	0.68	0	15,15,17	1.40	2 (13%)

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	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	MAN	J	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	MAN	K	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	3/6/23/26	0/1/1/1
4	MAN	L	3	4	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
4	MAN	O	3	4	1/1/4/5	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-O5-C5	7.55	122.42	112.19
5	T	2	NAG	C1-O5-C5	7.41	122.23	112.19
3	N	2	NAG	C1-O5-C5	7.06	121.76	112.19
4	U	1	NAG	C1-O5-C5	5.99	120.31	112.19
4	L	1	NAG	C1-O5-C5	5.39	119.49	112.19
4	O	1	NAG	C1-O5-C5	4.47	118.25	112.19
4	Q	2	NAG	C1-O5-C5	4.45	118.22	112.19
4	Q	2	NAG	C4-C3-C2	4.14	117.08	111.02
4	L	3	MAN	C1-O5-C5	4.05	117.68	112.19
4	R	3	MAN	C1-C2-C3	3.81	114.35	109.67
4	O	3	MAN	C1-C2-C3	3.77	114.31	109.67
4	R	3	MAN	C1-O5-C5	3.76	117.28	112.19
4	L	3	MAN	C1-C2-C3	3.70	114.21	109.67
3	M	2	NAG	C1-O5-C5	3.49	116.92	112.19
4	L	1	NAG	C3-C4-C5	3.45	116.39	110.24
4	U	3	MAN	C1-C2-C3	3.40	113.84	109.67
4	K	3	MAN	C1-C2-C3	3.36	113.80	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	3	MAN	C1-O5-C5	3.22	116.55	112.19
4	K	3	MAN	C1-O5-C5	3.21	116.55	112.19
4	O	3	MAN	C1-O5-C5	3.17	116.49	112.19
4	K	1	NAG	C4-C3-C2	3.17	115.66	111.02
3	P	2	NAG	C1-O5-C5	3.14	116.45	112.19
4	J	2	NAG	O5-C1-C2	3.12	116.21	111.29
3	N	2	NAG	O5-C1-C2	3.12	116.21	111.29
4	L	1	NAG	O5-C5-C4	3.06	118.27	110.83
3	N	1	NAG	C1-O5-C5	2.99	116.25	112.19
3	I	2	NAG	C1-O5-C5	2.97	116.21	112.19
4	J	3	MAN	O5-C5-C6	2.95	111.83	107.20
5	T	2	NAG	O5-C1-C2	2.89	115.85	111.29
4	R	1	NAG	C4-C3-C2	2.82	115.16	111.02
3	S	2	NAG	C1-O5-C5	2.78	115.96	112.19
4	L	1	NAG	C4-C3-C2	2.74	115.04	111.02
4	J	1	NAG	C1-O5-C5	2.71	115.86	112.19
4	Q	3	MAN	O5-C5-C6	2.70	111.44	107.20
4	K	1	NAG	C1-O5-C5	2.58	115.68	112.19
4	U	1	NAG	O5-C1-C2	2.54	115.30	111.29
4	Q	1	NAG	O5-C1-C2	2.53	115.28	111.29
4	L	1	NAG	O5-C1-C2	2.49	115.21	111.29
4	U	1	NAG	C4-C3-C2	2.41	114.55	111.02
4	O	2	NAG	O4-C4-C3	2.33	115.72	110.35
3	S	2	NAG	O5-C5-C6	2.32	110.83	107.20
4	Q	3	MAN	C1-C2-C3	-2.30	106.84	109.67
4	Q	3	MAN	C1-O5-C5	-2.30	109.08	112.19
4	Q	2	NAG	C3-C4-C5	2.25	114.25	110.24
4	U	2	NAG	O4-C4-C3	2.24	115.54	110.35
4	J	3	MAN	C2-C3-C4	-2.21	107.08	110.89
5	T	1	NAG	C1-O5-C5	2.18	115.14	112.19
4	K	2	NAG	O4-C4-C3	2.05	115.09	110.35
4	R	2	NAG	O4-C4-C3	2.02	115.03	110.35

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	U	3	MAN	C1
4	K	3	MAN	C1
4	R	3	MAN	C1
4	Q	3	MAN	C1
5	T	3	MAN	C1
4	J	1	NAG	C1

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Mol	Chain	Res	Type	Atom
4	J	3	MAN	C1
4	O	3	MAN	C1
4	L	3	MAN	C1

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	U	2	NAG	C3-C2-N2-C7
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	O	2	NAG	C3-C2-N2-C7
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
5	T	3	MAN	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
4	Q	3	MAN	O5-C5-C6-O6
4	Q	1	NAG	C8-C7-N2-C2
4	J	3	MAN	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
5	T	3	MAN	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6

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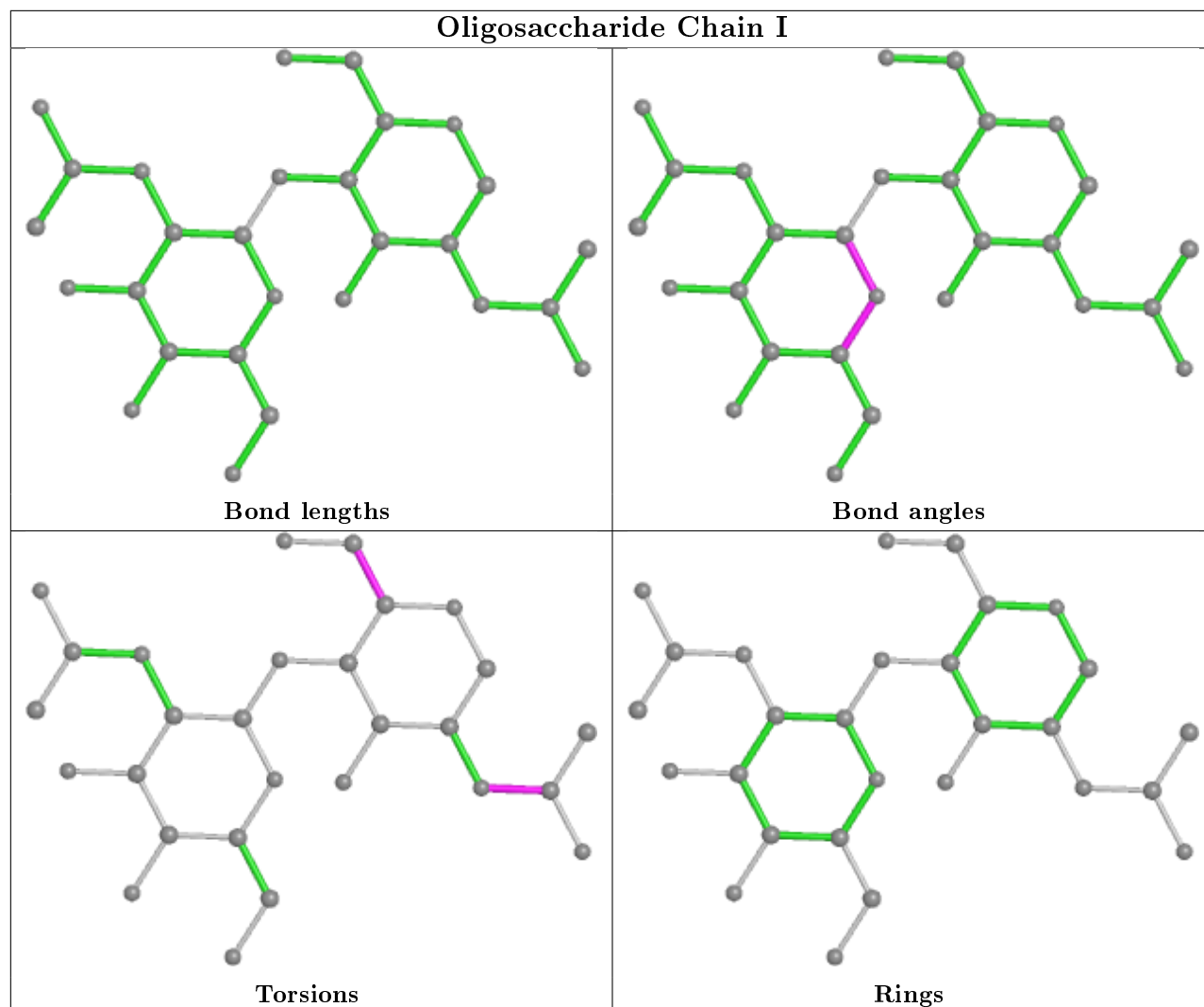
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	Q	3	MAN	C4-C5-C6-O6
4	J	3	MAN	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
4	J	1	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6

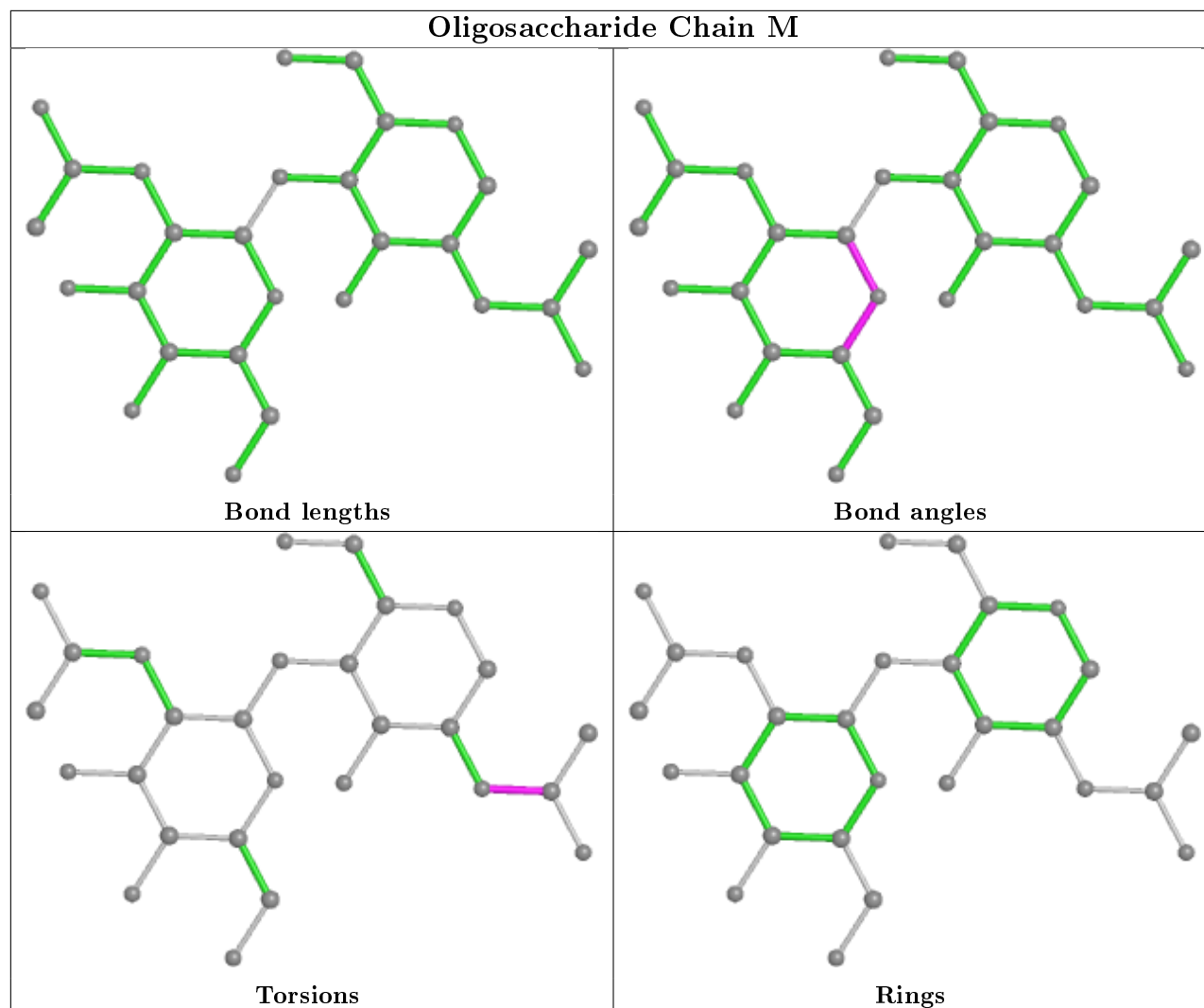
There are no ring outliers.

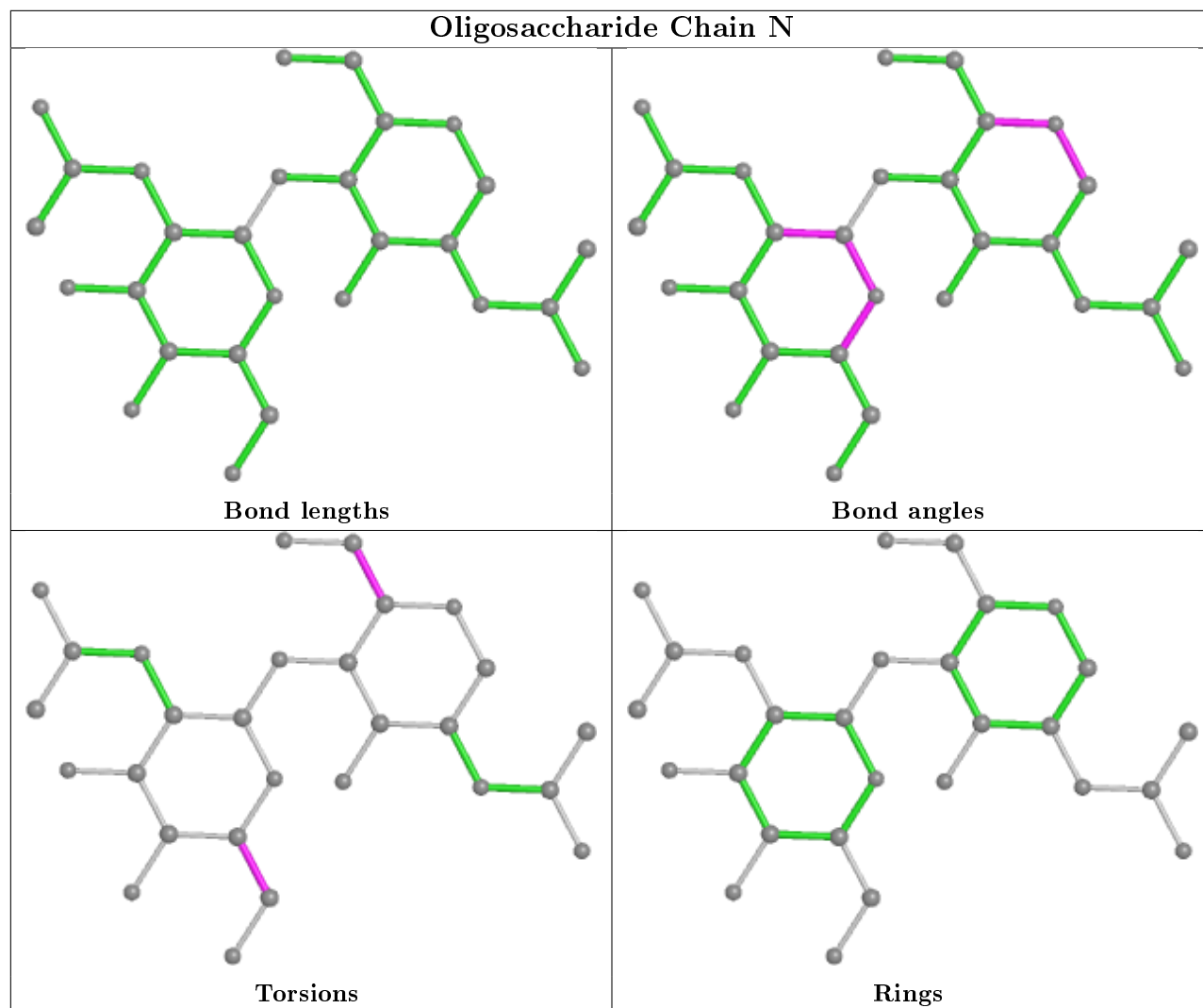
8 monomers are involved in 14 short contacts:

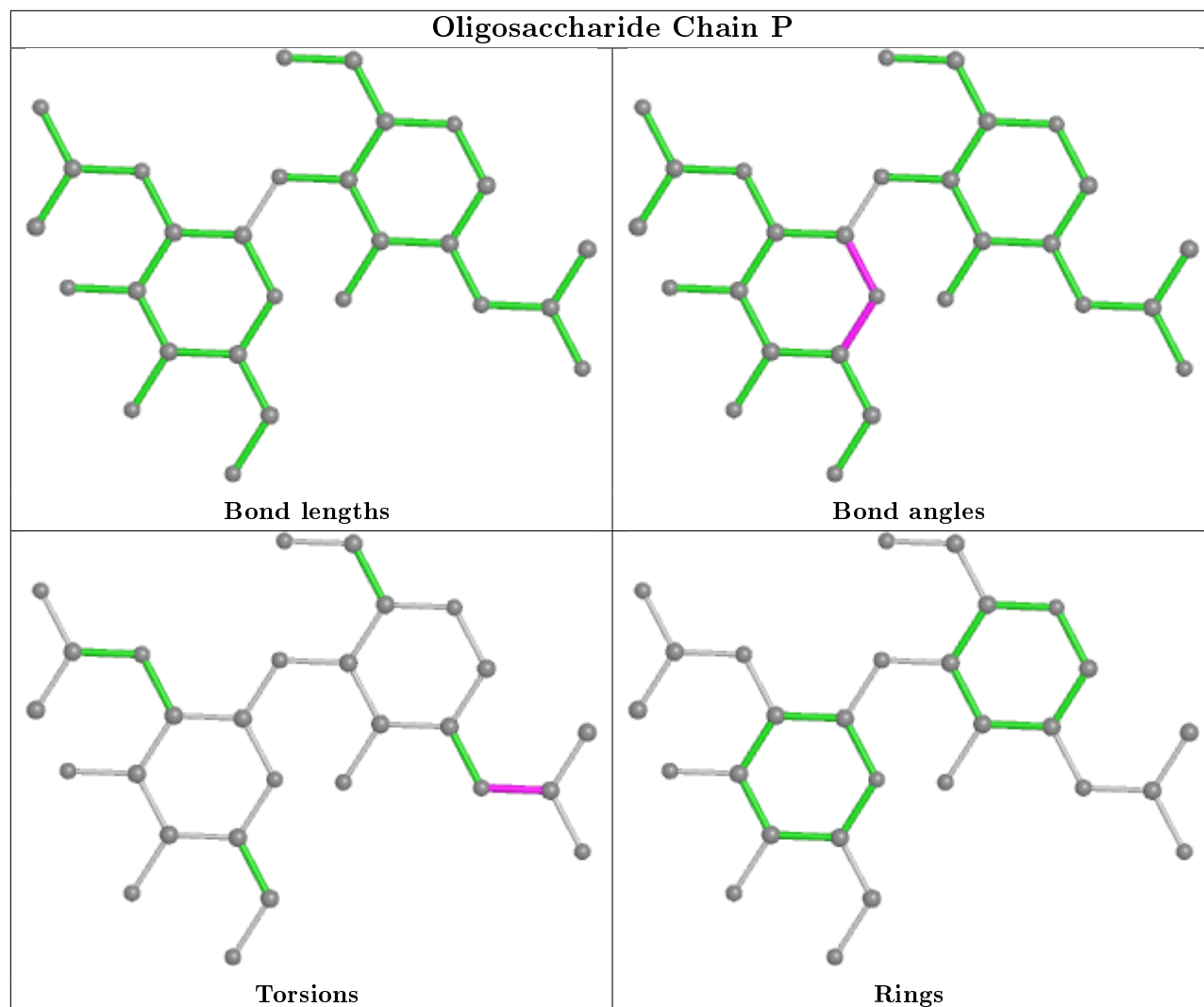
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	NAG	8	0
5	T	3	MAN	2	0
4	J	1	NAG	1	0
4	J	2	NAG	2	0
4	J	3	MAN	2	0
5	T	2	NAG	2	0
4	U	1	NAG	1	0
4	Q	2	NAG	5	0

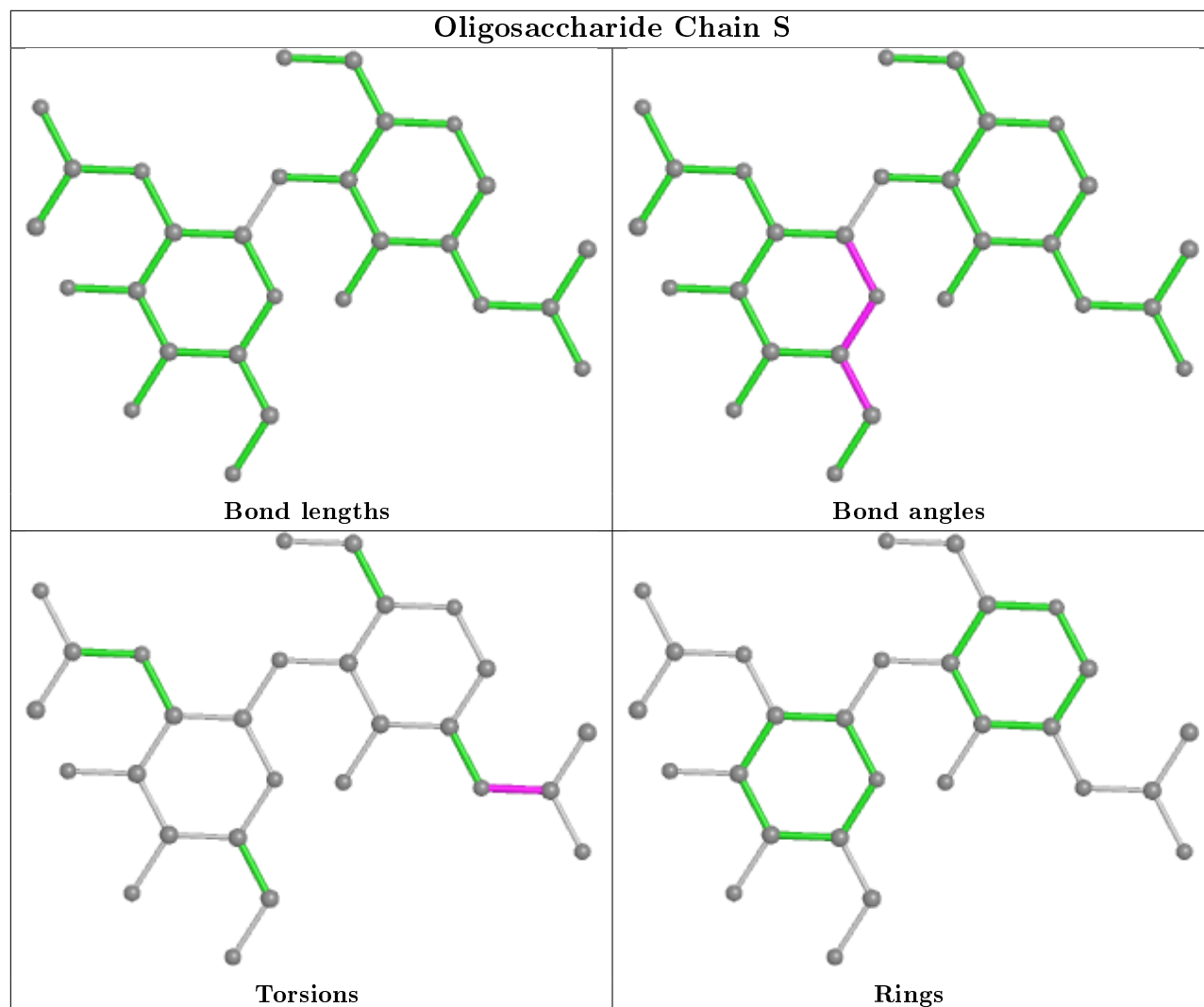
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

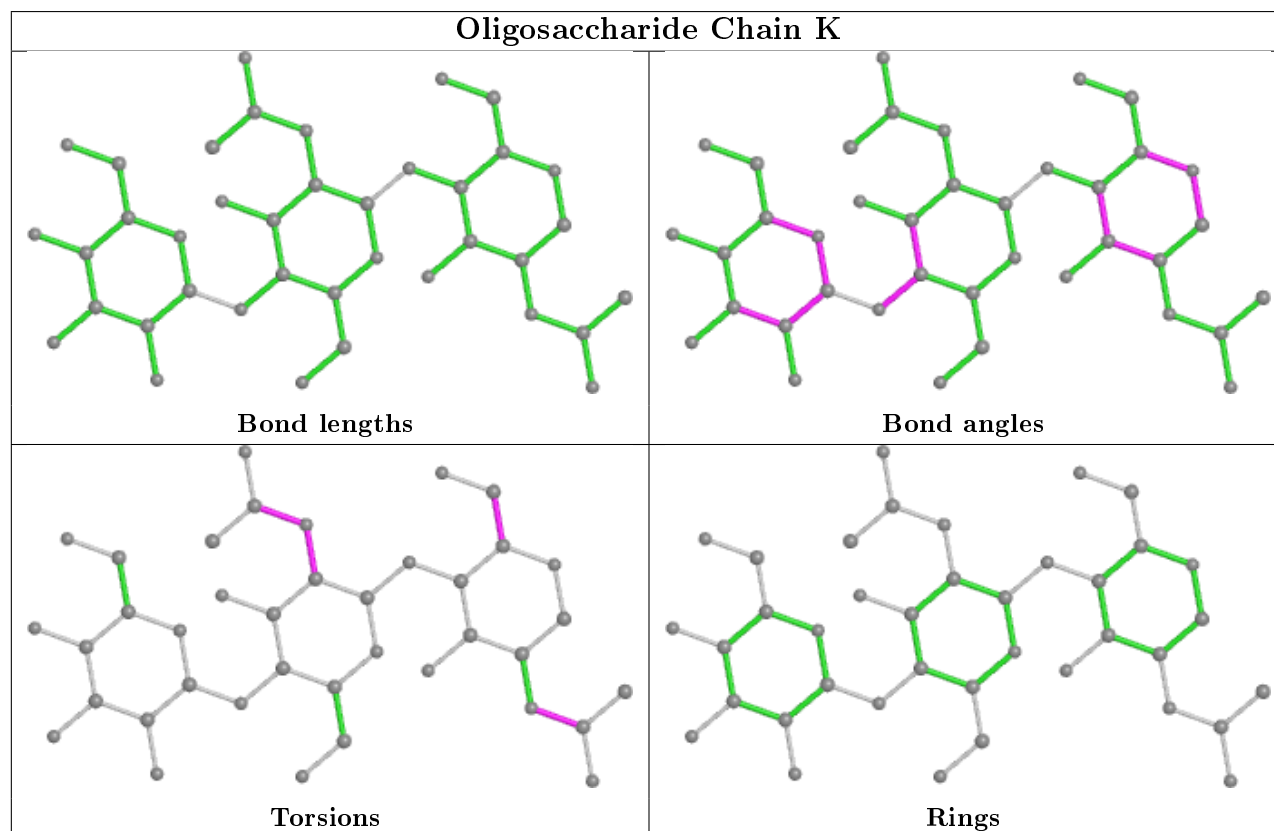
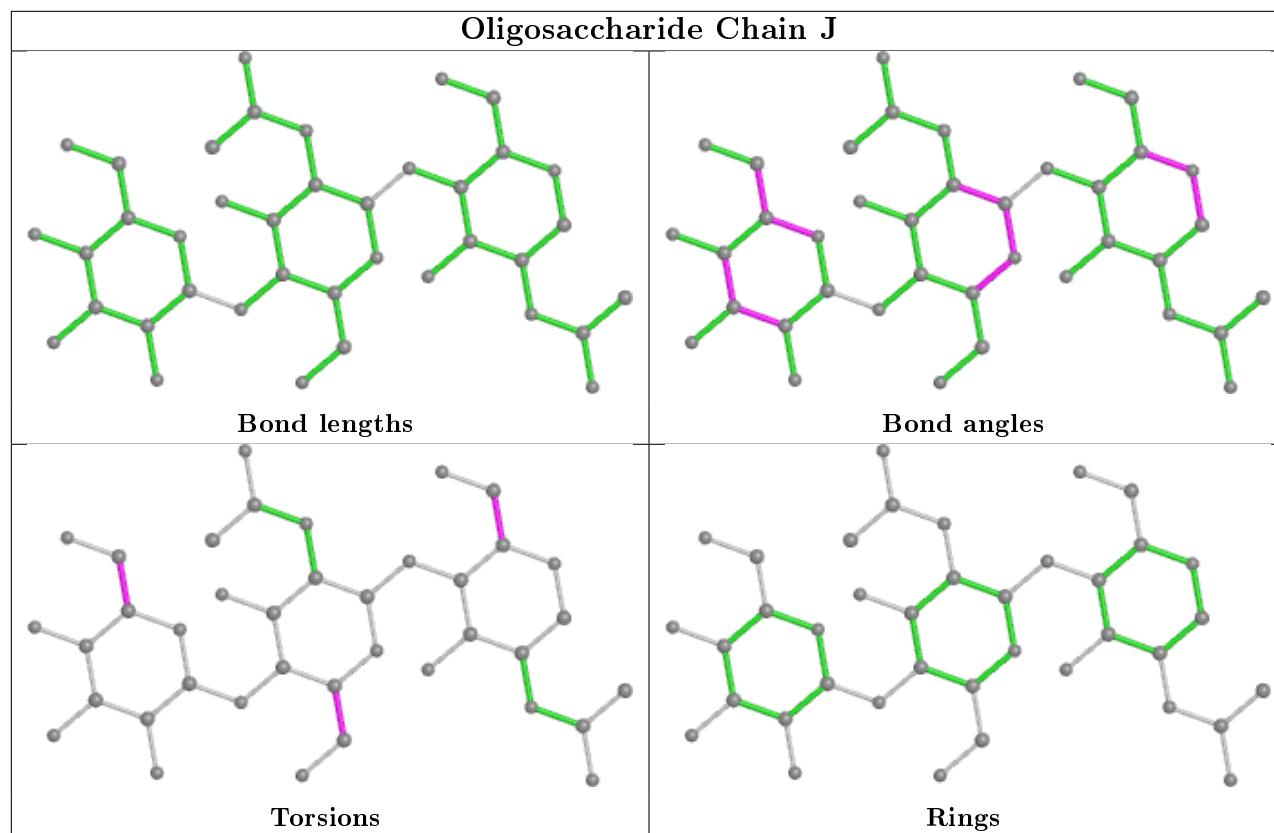


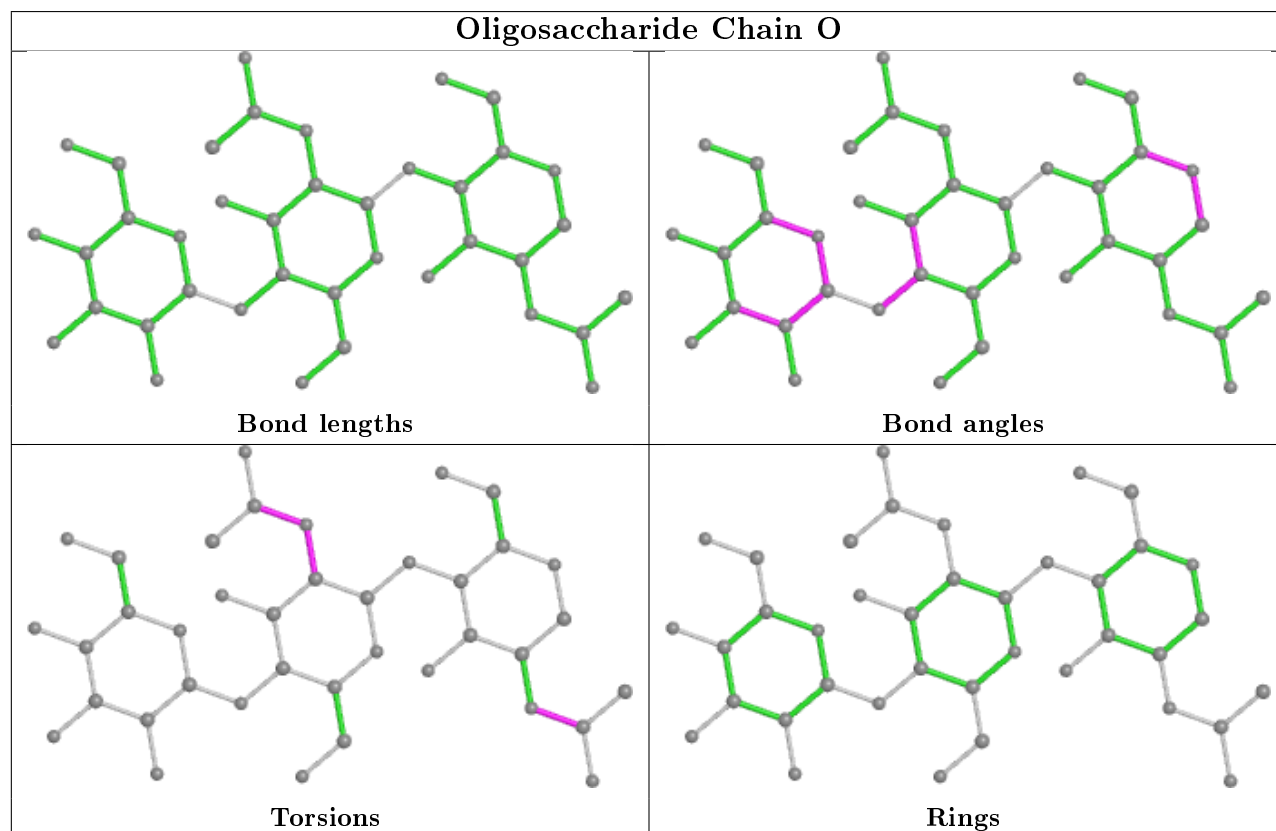
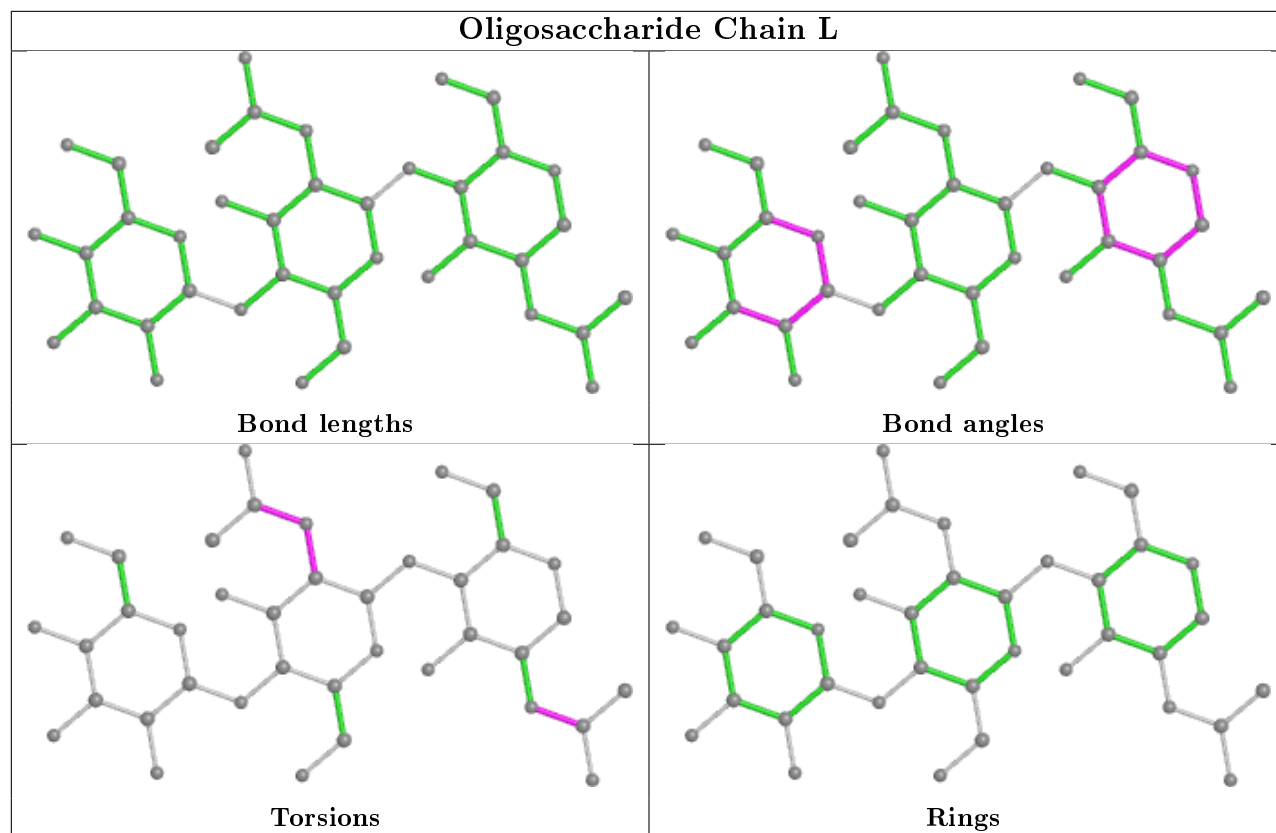


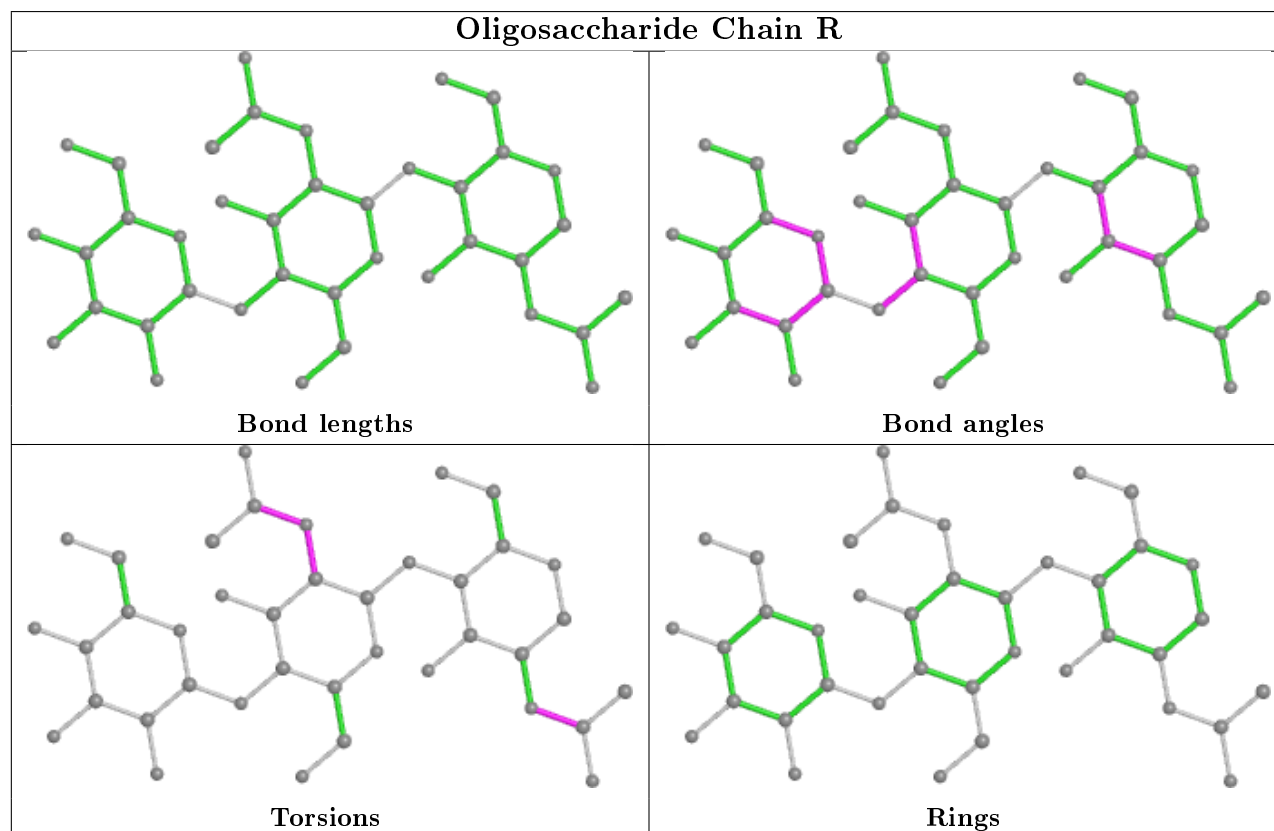
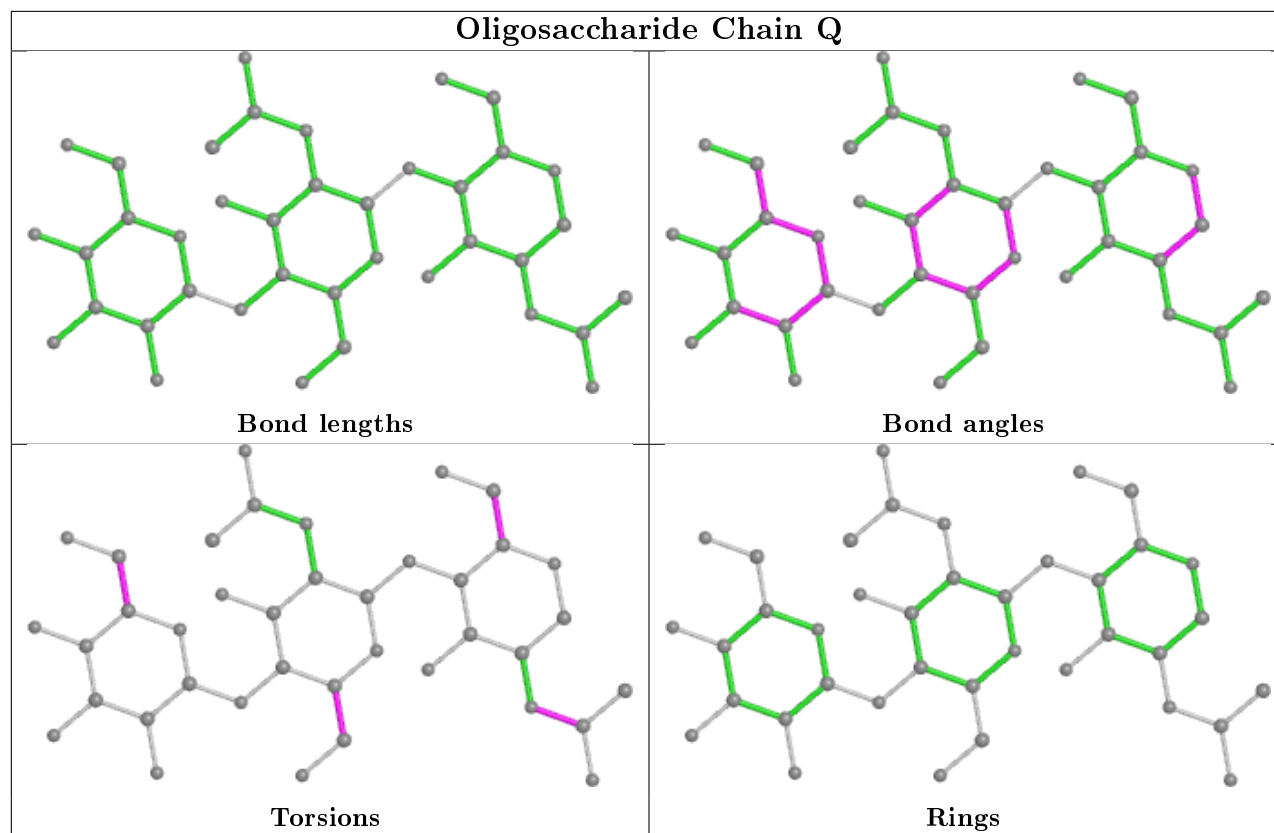


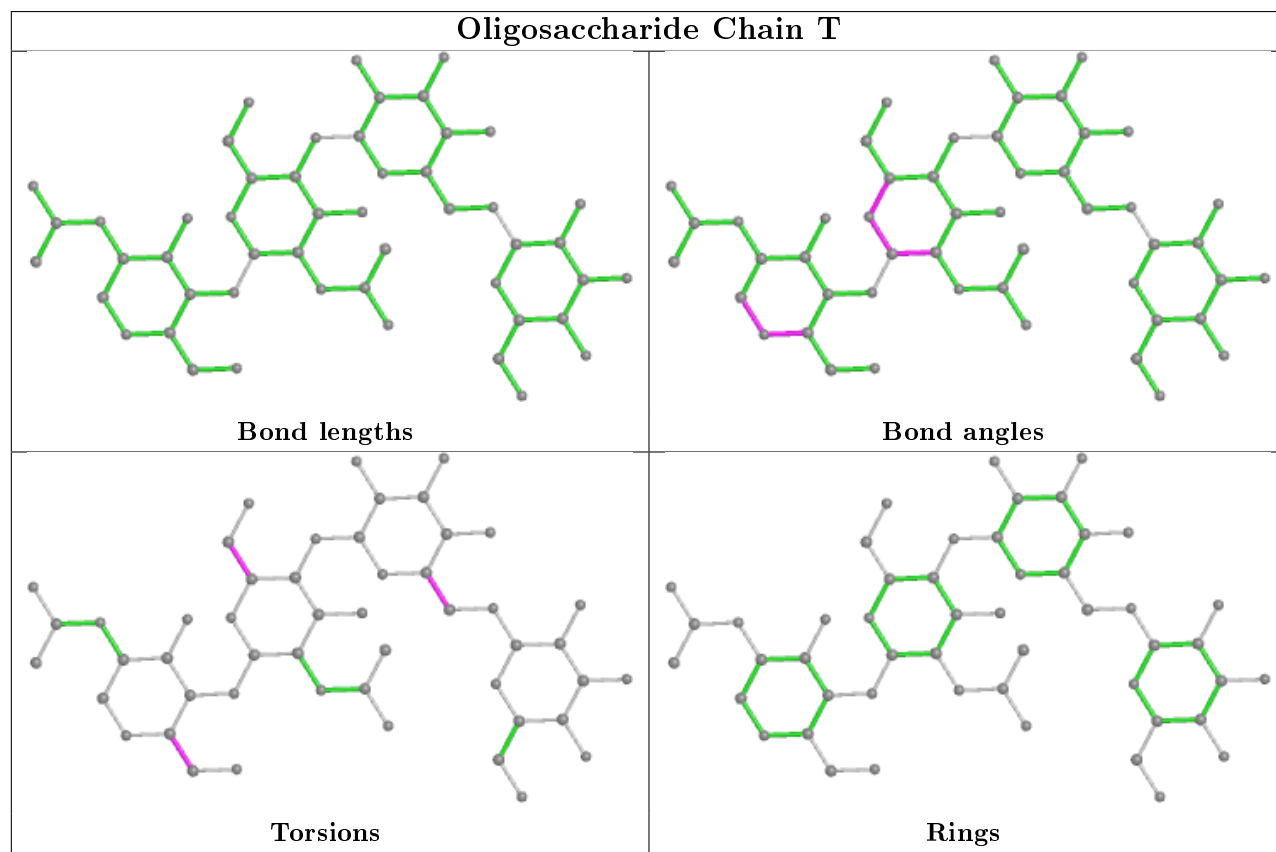
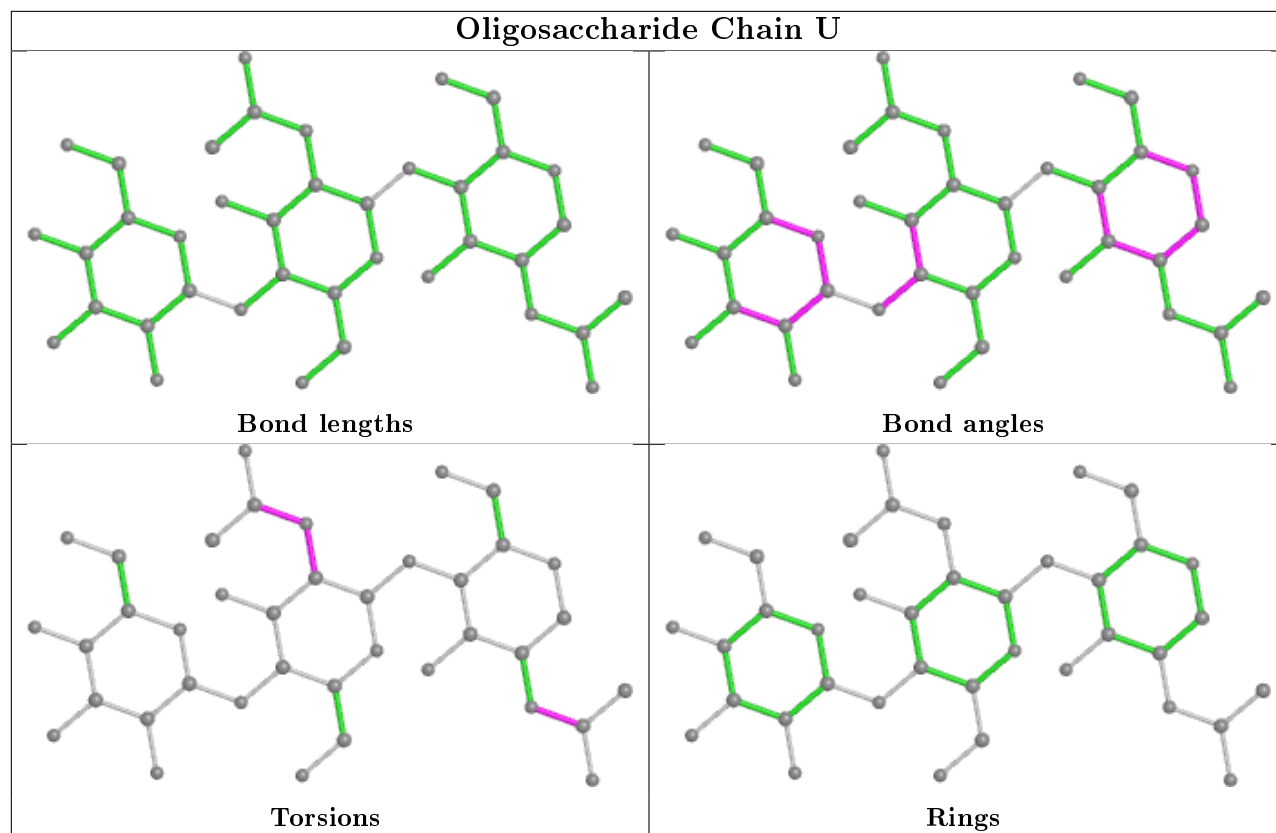












5.6 Ligand geometry

Of 32 ligands modelled in this entry, 17 are monoatomic - leaving 15 for Mogul analysis.

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
6	NAG	E	3880	1	14,14,15	0.44	0	17,19,21	1.68	1 (5%)
6	NAG	C	3880	1	14,14,15	0.47	0	17,19,21	1.49	1 (5%)
6	NAG	D	3094	2	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
6	NAG	G	3678	1	14,14,15	0.50	0	17,19,21	0.96	2 (11%)
6	NAG	F	3094	2	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
6	NAG	A	3678	1	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
6	NAG	B	3094	2	14,14,15	0.46	0	17,19,21	0.97	2 (11%)
6	NAG	B	3479	-	14,14,15	0.48	0	17,19,21	0.90	1 (5%)
6	NAG	E	3678	1	14,14,15	0.51	0	17,19,21	0.98	2 (11%)
6	NAG	H	3094	2	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
6	NAG	D	3479	-	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
6	NAG	C	3678	1	14,14,15	0.51	0	17,19,21	0.79	0
6	NAG	F	3479	-	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
6	NAG	G	3880	1	14,14,15	0.48	0	17,19,21	1.56	1 (5%)
6	NAG	H	3479	-	14,14,15	0.50	0	17,19,21	0.94	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
6	NAG	E	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	C	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	F	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	A	3678	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3479	-	-	0/6/23/26	0/1/1/1
6	NAG	E	3678	1	-	2/6/23/26	0/1/1/1
6	NAG	H	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	D	3479	-	-	0/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	2/6/23/26	0/1/1/1
6	NAG	F	3479	-	-	0/6/23/26	0/1/1/1
6	NAG	G	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	H	3479	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	3880	NAG	C1-O5-C5	5.87	120.14	112.19
6	G	3880	NAG	C1-O5-C5	5.54	119.70	112.19
6	C	3880	NAG	C1-O5-C5	5.06	119.05	112.19
6	D	3479	NAG	O5-C5-C6	2.73	111.48	107.20
6	H	3094	NAG	C1-O5-C5	2.50	115.58	112.19
6	B	3094	NAG	C1-O5-C5	2.48	115.55	112.19
6	F	3094	NAG	C1-O5-C5	2.43	115.49	112.19
6	D	3094	NAG	O5-C5-C6	2.37	110.93	107.20
6	F	3479	NAG	C1-O5-C5	2.34	115.36	112.19
6	G	3678	NAG	O5-C1-C2	2.27	114.88	111.29
6	E	3678	NAG	O5-C1-C2	2.23	114.81	111.29
6	G	3678	NAG	C1-O5-C5	2.22	115.20	112.19
6	B	3094	NAG	O5-C5-C6	2.21	110.66	107.20
6	E	3678	NAG	C1-O5-C5	2.16	115.11	112.19
6	B	3479	NAG	C2-N2-C7	-2.13	119.88	122.90
6	A	3678	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3880	NAG	C8-C7-N2-C2
6	C	3880	NAG	O7-C7-N2-C2
6	E	3880	NAG	C8-C7-N2-C2
6	E	3880	NAG	O7-C7-N2-C2
6	G	3880	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	G	3880	NAG	O7-C7-N2-C2
6	G	3880	NAG	O5-C5-C6-O6
6	C	3880	NAG	O5-C5-C6-O6
6	E	3880	NAG	O5-C5-C6-O6
6	C	3678	NAG	C4-C5-C6-O6
6	E	3678	NAG	C4-C5-C6-O6
6	E	3678	NAG	O5-C5-C6-O6
6	C	3678	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	3678	NAG	1	0
6	D	3479	NAG	8	0
6	C	3678	NAG	1	0
6	F	3479	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	880/1095 (80%)	0.25	34 (3%)	39	31	101, 200, 285, 359	0
1	C	884/1095 (80%)	0.22	35 (3%)	38	31	97, 199, 281, 348	0
1	E	882/1095 (80%)	0.28	48 (5%)	25	22	96, 199, 284, 352	0
1	G	1082/1095 (98%)	0.44	86 (7%)	12	11	99, 211, 324, 419	0
2	B	673/687 (97%)	0.46	81 (12%)	4	5	139, 249, 313, 389	2 (0%)
2	D	673/687 (97%)	0.64	82 (12%)	4	5	140, 249, 312, 366	2 (0%)
2	F	673/687 (97%)	0.64	90 (13%)	3	3	141, 250, 314, 382	2 (0%)
2	H	673/687 (97%)	0.39	61 (9%)	9	8	141, 249, 313, 371	2 (0%)
All	All	6420/7128 (90%)	0.40	517 (8%)	12	10	96, 225, 307, 419	8 (0%)

All (517) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	92	ALA	8.6
2	D	430	GLN	8.4
2	F	107	LEU	8.0
1	A	482	TRP	7.7
1	G	482	TRP	7.4
2	B	329	ASN	7.2
2	B	92	ALA	7.2
2	D	71	GLY	6.8
2	B	91	ALA	6.7
2	F	236	LEU	6.5
2	D	72	GLY	6.4
1	G	220	LEU	6.4
1	G	239	THR	6.4
1	G	321	GLU	6.3
1	G	322	THR	6.3
2	F	429	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
2	F	629	GLN	6.0
2	F	628	LEU	6.0
2	F	91	ALA	5.9
1	G	136	LEU	5.9
2	D	1	GLN	5.8
1	G	265	TYR	5.8
1	E	482	TRP	5.7
2	F	431	SER	5.7
1	G	238	ILE	5.6
1	G	817	GLN	5.6
2	B	469	GLN	5.4
2	F	393	VAL	5.4
1	G	323	THR	5.4
2	H	469	GLN	5.4
1	A	124	GLN	5.3
2	H	93	PHE	5.3
1	E	821	GLN	5.3
1	A	33	GLY	5.2
2	F	70	ASN	5.2
1	G	278	SER	5.2
1	C	482	TRP	5.1
2	D	161	HIS	5.1
1	G	234	ILE	5.0
2	B	73	GLN	5.0
2	D	91	ALA	5.0
2	H	72	GLY	5.0
1	G	135	PHE	5.0
1	E	124	GLN	5.0
1	G	251	LYS	4.9
2	F	71	GLY	4.9
2	D	389	PHE	4.8
1	C	9	THR	4.8
1	A	95	HIS	4.8
1	A	1078	LEU	4.7
2	D	432	ARG	4.7
2	B	318	SER	4.7
2	F	386	PRO	4.7
1	G	266	ALA	4.6
2	B	415	VAL	4.6
2	D	160	THR	4.6
2	D	668	ASP	4.6
1	G	108	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	416	THR	4.5
2	H	180	PHE	4.5
1	G	267	ILE	4.5
2	H	470	GLU	4.5
2	F	72	GLY	4.5
1	G	483	ARG	4.4
2	B	32	PRO	4.4
2	F	664	LEU	4.4
1	A	594	LEU	4.3
2	D	37	SER	4.3
2	D	367	GLY	4.3
2	B	237	LEU	4.3
2	D	237	LEU	4.2
2	F	109	TYR	4.2
2	B	433	ASP	4.2
2	B	432	ARG	4.1
1	E	1044	LYS	4.1
2	F	144	ILE	4.1
2	D	236	LEU	4.1
1	C	623	GLN	4.1
2	F	160	THR	4.1
2	H	629	GLN	4.1
1	E	95	HIS	4.1
1	A	87	LEU	4.1
2	D	62	LEU	4.1
1	E	102	TYR	4.1
1	A	127	PRO	4.0
1	E	594	LEU	4.0
1	C	817	GLN	4.0
1	G	217	VAL	4.0
2	F	161	HIS	4.0
1	E	817	GLN	4.0
2	F	389	PHE	4.0
1	G	285	ILE	3.9
1	A	106	LEU	3.9
1	A	346	PRO	3.9
1	A	821	GLN	3.9
2	B	389	PHE	3.9
2	D	433	ASP	3.9
1	A	102	TYR	3.9
1	A	77	LEU	3.9
2	D	92	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	13	VAL	3.8
2	B	107	LEU	3.8
1	E	117	GLN	3.8
2	H	91	ALA	3.8
2	F	145	GLY	3.8
2	B	328	SER	3.8
1	A	88	ALA	3.8
2	B	236	LEU	3.7
2	B	664	LEU	3.7
2	D	431	SER	3.7
2	B	629	GLN	3.7
1	G	127	PRO	3.7
2	H	227	GLU	3.7
2	H	335	LYS	3.7
2	H	1	GLN	3.7
2	D	63	ALA	3.7
1	G	277	ASN	3.7
1	E	1078	LEU	3.7
2	F	81	VAL	3.7
2	F	106	ASP	3.7
1	G	216	VAL	3.7
2	F	433	ASP	3.6
1	G	821	GLN	3.6
2	D	443	LEU	3.6
2	B	330	VAL	3.6
2	F	416	THR	3.6
1	G	1045	VAL	3.6
1	G	320	THR	3.6
1	G	124	GLN	3.6
2	D	429	ASP	3.6
1	G	250	TYR	3.6
2	B	31	GLY	3.6
1	G	171	LEU	3.6
2	D	622	SER	3.6
2	B	186	LEU	3.6
1	A	817	GLN	3.6
2	H	133	ARG	3.6
2	F	414	ILE	3.6
2	B	463	THR	3.5
2	H	37	SER	3.5
1	G	236	ILE	3.5
2	H	393	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	236	LEU	3.5
2	D	206	GLY	3.5
2	D	393	VAL	3.5
2	F	266	LEU	3.5
2	B	663	TYR	3.5
2	B	391	VAL	3.5
2	B	430	GLN	3.5
1	G	88	ALA	3.5
2	B	202	GLN	3.5
1	G	106	LEU	3.5
2	H	389	PHE	3.5
1	G	332	MET	3.5
1	E	918	TYR	3.5
2	F	428	ARG	3.4
2	H	433	ASP	3.4
1	G	125	GLU	3.4
1	C	483	ARG	3.4
1	G	221	PHE	3.4
2	F	133	ARG	3.4
2	D	107	LEU	3.4
1	G	137	ILE	3.4
1	G	172	MET	3.4
2	F	92	ALA	3.4
1	E	1045	VAL	3.4
1	C	124	GLN	3.4
2	F	68	ASP	3.4
2	F	430	GLN	3.4
2	F	665	ILE	3.4
1	E	483	ARG	3.4
1	G	235	LEU	3.3
1	G	213	ILE	3.3
2	H	432	ARG	3.3
2	F	635	VAL	3.3
2	D	93	PHE	3.3
2	H	391	VAL	3.3
2	D	331	VAL	3.3
2	B	171	ASN	3.3
1	A	108	PHE	3.3
2	F	97	PHE	3.3
2	D	171	ASN	3.3
1	A	918	TYR	3.3
2	D	122	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1078	LEU	3.3
2	B	68	ASP	3.2
2	F	76	LEU	3.2
1	G	209	THR	3.2
2	F	1	GLN	3.2
2	D	634	PRO	3.2
1	G	87	LEU	3.2
2	D	669	GLU	3.2
1	C	821	GLN	3.2
2	F	29	PHE	3.2
1	G	1078	LEU	3.2
2	B	122	ARG	3.1
2	D	651	ALA	3.1
2	F	93	PHE	3.1
2	H	430	GLN	3.1
1	E	1065	GLY	3.1
2	H	650	VAL	3.1
2	B	72	GLY	3.1
2	H	161	HIS	3.1
2	B	1	GLN	3.1
2	F	622	SER	3.1
2	B	23	TRP	3.1
2	B	470	GLU	3.1
1	G	233	LYS	3.1
1	C	10	ALA	3.1
2	B	37	SER	3.1
2	F	371	ARG	3.1
2	H	71	GLY	3.1
1	A	347	VAL	3.0
2	H	107	LEU	3.0
1	G	237	VAL	3.0
1	G	138	ASP	3.0
2	F	387	ILE	3.0
2	B	366	ASN	3.0
2	D	133	ARG	3.0
2	H	331	VAL	3.0
2	F	318	SER	3.0
2	D	8	VAL	3.0
1	G	918	TYR	3.0
1	E	119	LEU	3.0
1	A	553	ILE	3.0
2	F	369	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	335	GLU	3.0
2	B	323	LEU	3.0
2	H	272	LYS	3.0
2	F	663	TYR	3.0
1	C	533	ALA	3.0
2	F	26	LYS	3.0
2	D	100	ALA	2.9
2	B	414	ILE	2.9
1	C	907	THR	2.9
2	H	334	ILE	2.9
1	E	9	THR	2.9
2	H	664	LEU	2.9
2	D	38	ILE	2.9
1	A	481	GLY	2.9
1	C	74	GLY	2.9
2	D	602	LYS	2.9
1	A	46	GLY	2.9
1	E	61	GLY	2.9
1	C	102	TYR	2.9
2	F	49	ARG	2.9
1	C	108	PHE	2.9
1	C	624	VAL	2.9
2	B	630	LEU	2.9
2	D	623	ALA	2.9
2	D	415	VAL	2.9
2	F	122	ARG	2.9
1	A	61	GLY	2.9
2	H	207	ASN	2.9
1	E	13	VAL	2.8
2	D	43	ARG	2.8
2	F	207	ASN	2.8
2	H	651	ALA	2.8
2	D	296	PRO	2.8
1	E	106	LEU	2.8
2	D	391	VAL	2.8
1	C	594	LEU	2.8
1	G	245	GLY	2.8
1	G	481	GLY	2.8
2	H	206	GLY	2.8
2	B	161	HIS	2.8
2	D	399	ILE	2.8
2	H	145	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	96	THR	2.8
2	B	67	GLU	2.8
2	H	610	LEU	2.8
1	A	529	GLU	2.8
2	B	654	LEU	2.8
1	A	425	ARG	2.8
2	D	629	GLN	2.8
2	F	202	GLN	2.7
2	F	206	GLY	2.7
2	D	395	ALA	2.7
2	B	93	PHE	2.7
1	C	553	ILE	2.7
2	H	667	VAL	2.7
1	G	240	ASP	2.7
1	G	296	LYS	2.7
2	H	49	ARG	2.7
1	G	816	GLY	2.7
2	F	320	VAL	2.7
1	G	529	GLU	2.7
2	F	185	VAL	2.7
2	D	667	VAL	2.7
2	F	624	ALA	2.7
1	E	108	PHE	2.7
1	G	295	PHE	2.7
1	C	729	ASN	2.7
1	G	173	GLN	2.7
2	D	345	VAL	2.7
2	F	667	VAL	2.7
2	D	267	GLU	2.6
1	G	180	THR	2.6
2	H	35	PRO	2.6
2	H	628	LEU	2.6
1	E	591	VAL	2.6
1	C	724	LEU	2.6
1	E	593	LEU	2.6
2	F	95	VAL	2.6
2	F	345	VAL	2.6
1	E	12	ARG	2.6
2	B	176	CYS	2.6
2	D	95	VAL	2.6
1	G	480	ARG	2.6
2	B	39	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	387	ILE	2.6
2	D	185	VAL	2.6
1	G	118	ARG	2.6
2	D	96	THR	2.6
2	D	466	ARG	2.6
1	E	592	LEU	2.6
1	G	1044	LYS	2.6
1	E	721	GLY	2.6
1	E	907	THR	2.5
1	C	534	VAL	2.5
2	F	171	ASN	2.5
1	G	133	ILE	2.5
1	C	88	ALA	2.5
2	D	102	GLY	2.5
2	F	627	GLY	2.5
1	G	181	HIS	2.5
2	D	172	LYS	2.5
2	F	438	HIS	2.5
2	B	393	VAL	2.5
2	F	415	VAL	2.5
1	E	480	ARG	2.5
2	D	56	ILE	2.5
2	F	651	ALA	2.5
2	B	160	THR	2.5
2	B	347	LEU	2.5
2	F	623	ALA	2.5
2	F	602	LYS	2.5
1	E	484	ARG	2.5
2	F	407	ARG	2.5
2	F	85	LEU	2.5
2	D	79	GLN	2.5
2	B	404	PHE	2.5
2	D	664	LEU	2.5
2	H	474	SER	2.5
2	H	109	TYR	2.4
2	B	30	THR	2.4
2	B	443	LEU	2.4
2	D	226	GLU	2.4
2	D	416	THR	2.4
1	G	261	GLY	2.4
1	G	973	GLN	2.4
2	D	390	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	404	PHE	2.4
2	B	407	ARG	2.4
2	F	190	ASN	2.4
1	E	623	GLN	2.4
2	B	49	ARG	2.4
1	E	125	GLU	2.4
2	B	406	ILE	2.4
2	F	195	PHE	2.4
2	D	101	LYS	2.4
1	E	10	ALA	2.4
2	H	369	THR	2.4
2	D	123	ASN	2.4
2	F	466	ARG	2.4
1	G	215	ASN	2.3
2	F	339	ASN	2.3
1	G	324	SER	2.3
2	D	294	ILE	2.3
1	A	963	VAL	2.3
1	G	592	LEU	2.3
2	D	35	PRO	2.3
2	H	189	THR	2.3
1	C	95	HIS	2.3
2	B	375	ARG	2.3
1	A	101	MET	2.3
2	D	68	ASP	2.3
2	F	35	PRO	2.3
2	B	424	GLU	2.3
1	E	653	GLN	2.3
2	F	418	GLN	2.3
2	B	185	VAL	2.3
1	G	268	GLY	2.3
1	A	1079	GLU	2.3
1	A	848	HIS	2.3
2	B	102	GLY	2.3
1	C	326	SER	2.3
1	G	557	GLN	2.3
1	C	918	TYR	2.3
1	G	282	LEU	2.3
2	B	95	VAL	2.3
2	D	368	VAL	2.3
1	E	104	THR	2.3
2	B	623	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	407	ARG	2.3
1	C	653	GLN	2.3
2	F	105	ILE	2.3
1	G	594	LEU	2.3
2	B	622	SER	2.3
1	C	592	LEU	2.3
2	H	73	GLN	2.3
2	H	226	GLU	2.3
2	H	363	PHE	2.3
1	G	225	TYR	2.3
2	B	109	TYR	2.3
1	G	169	PHE	2.3
2	B	665	ILE	2.3
2	D	74	LYS	2.3
2	D	330	VAL	2.3
2	F	446	GLY	2.2
2	F	384	ASN	2.2
2	H	186	LEU	2.2
1	G	281	GLU	2.2
2	B	351	ALA	2.2
2	F	443	LEU	2.2
1	E	332	MET	2.2
1	E	485	TRP	2.2
2	H	663	TYR	2.2
2	H	70	ASN	2.2
2	H	136	ASN	2.2
2	F	669	GLU	2.2
1	E	973	GLN	2.2
2	F	331	VAL	2.2
2	B	431	SER	2.2
2	B	628	LEU	2.2
1	C	1047	VAL	2.2
2	B	8	VAL	2.2
2	B	345	VAL	2.2
2	D	454	TYR	2.2
2	H	179	PRO	2.2
1	C	46	GLY	2.2
1	E	599	VAL	2.2
1	G	394	LEU	2.2
1	G	422	ARG	2.2
2	B	35	PRO	2.2
1	E	725	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	392	LYS	2.2
1	A	394	LEU	2.2
1	C	87	LEU	2.2
2	B	203	LEU	2.2
2	B	390	GLN	2.2
2	H	345	VAL	2.2
2	B	29	PHE	2.2
2	F	189	THR	2.2
2	D	650	VAL	2.2
1	E	996	GLN	2.2
2	D	73	GLN	2.2
2	D	70	ASN	2.1
2	F	630	LEU	2.1
2	D	414	ILE	2.1
2	H	395	ALA	2.1
2	B	331	VAL	2.1
1	A	964	TRP	2.1
1	E	1043	LYS	2.1
1	C	8	LEU	2.1
1	E	87	LEU	2.1
1	E	347	VAL	2.1
2	F	84	TYR	2.1
2	B	101	LYS	2.1
2	H	113	LEU	2.1
1	A	1081	TYR	2.1
1	C	1044	LYS	2.1
1	E	62	LEU	2.1
2	H	618	GLY	2.1
2	H	390	GLN	2.1
2	H	406	ILE	2.1
2	F	5	LYS	2.1
1	C	1001	LEU	2.1
1	E	626	SER	2.1
2	B	423	CYS	2.1
2	D	611	LYS	2.1
1	C	12	ARG	2.1
1	E	481	GLY	2.1
2	F	226	GLU	2.1
2	F	27	LEU	2.1
2	B	66	GLN	2.1
1	E	651	ASP	2.1
2	D	118	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	186	LEU	2.1
1	A	78	ALA	2.1
2	D	235	ARG	2.1
2	F	32	PRO	2.1
2	F	432	ARG	2.1
1	A	340	VAL	2.1
1	G	139	GLY	2.1
1	A	523	GLY	2.1
1	G	253	VAL	2.1
1	C	57	CYS	2.1
1	G	252	ASP	2.1
2	H	665	ILE	2.1
1	G	95	HIS	2.1
1	G	848	HIS	2.1
2	B	363	PHE	2.1
1	G	653	GLN	2.1
2	B	180	PHE	2.1
2	B	57	MET	2.0
2	D	59	PRO	2.0
2	D	29	PHE	2.0
2	H	36	ASP	2.0
2	B	190	ASN	2.0
1	G	187	PHE	2.0
1	G	283	ASN	2.0
1	G	339	ALA	2.0
1	G	197	LEU	2.0
2	D	113	LEU	2.0
2	H	95	VAL	2.0
2	H	69	HIS	2.0
1	G	468	THR	2.0
2	B	429	ASP	2.0
2	D	369	THR	2.0
1	E	398	VAL	2.0
1	E	118	ARG	2.0
2	B	371	ARG	2.0
2	F	98	ARG	2.0
2	F	344	ARG	2.0
2	H	39	ARG	2.0
2	H	431	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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

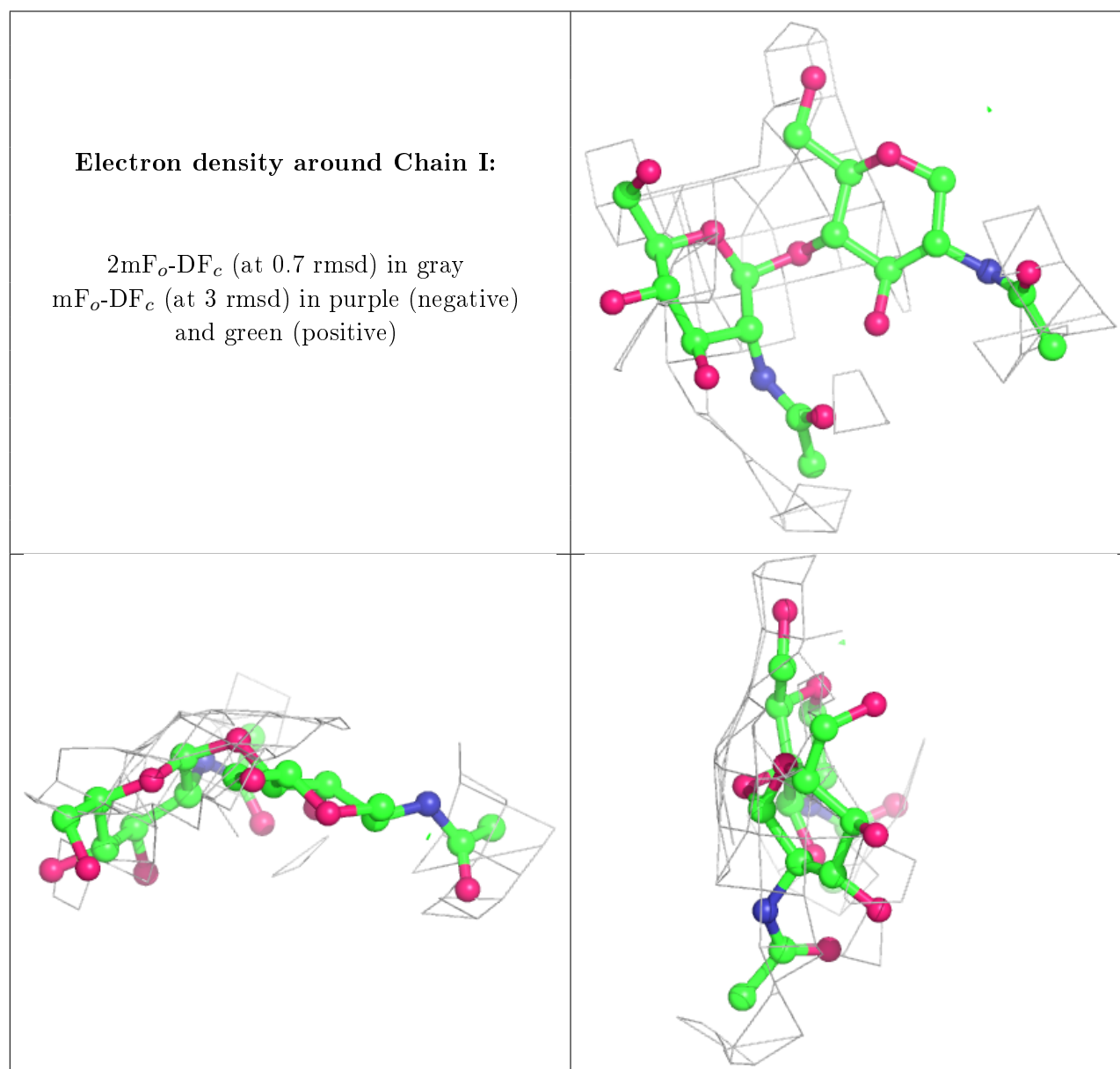
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	T	3	11/12	0.47	0.29	286,318,328,335	0
4	MAN	R	3	11/12	0.48	0.25	156,276,306,313	0
4	NAG	Q	2	14/15	0.53	0.52	286,310,336,351	0
4	MAN	K	3	11/12	0.54	0.25	271,295,318,322	0
4	NAG	Q	1	14/15	0.57	0.32	290,333,360,390	0
4	MAN	O	3	11/12	0.59	0.25	267,322,330,331	0
4	MAN	Q	3	11/12	0.65	0.41	242,273,308,315	0
4	NAG	J	2	14/15	0.65	0.30	260,301,316,331	0
5	MAN	T	4	11/12	0.65	0.36	270,291,333,336	0
3	NAG	I	2	14/15	0.66	0.33	190,302,317,324	0
4	MAN	U	3	11/12	0.68	0.24	266,274,284,288	0
4	MAN	J	3	11/12	0.68	0.18	229,283,307,312	0
3	NAG	P	1	14/15	0.72	0.29	182,235,257,271	0
3	NAG	M	2	14/15	0.73	0.27	204,296,319,331	0
5	NAG	T	2	14/15	0.77	0.38	263,314,342,363	0
4	NAG	L	1	14/15	0.77	0.32	140,205,251,290	0
3	NAG	M	1	14/15	0.77	0.35	224,274,288,298	0
3	NAG	N	1	14/15	0.78	0.22	186,260,283,292	0
3	NAG	S	2	14/15	0.79	0.30	189,282,303,305	0
3	NAG	I	1	14/15	0.81	0.18	216,243,262,294	0
5	NAG	T	1	14/15	0.81	0.30	257,281,310,318	0
3	NAG	N	2	14/15	0.81	0.25	154,257,273,298	0
4	MAN	L	3	11/12	0.81	0.39	187,257,308,323	0
4	NAG	J	1	14/15	0.82	0.27	237,325,347,352	0
3	NAG	S	1	14/15	0.83	0.24	184,229,251,262	0
4	NAG	L	2	14/15	0.83	0.24	222,253,284,303	0
3	NAG	P	2	14/15	0.86	0.14	209,276,288,291	0
4	NAG	K	2	14/15	0.86	0.27	231,265,291,318	0
4	NAG	U	2	14/15	0.87	0.26	229,249,267,274	0
4	NAG	R	2	14/15	0.88	0.14	161,245,265,293	0
4	NAG	O	1	14/15	0.90	0.19	125,169,213,220	0
4	NAG	O	2	14/15	0.91	0.13	227,256,296,312	0

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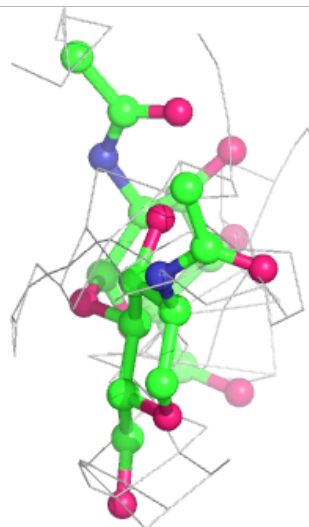
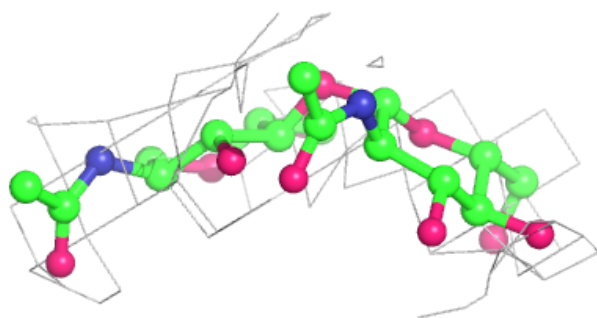
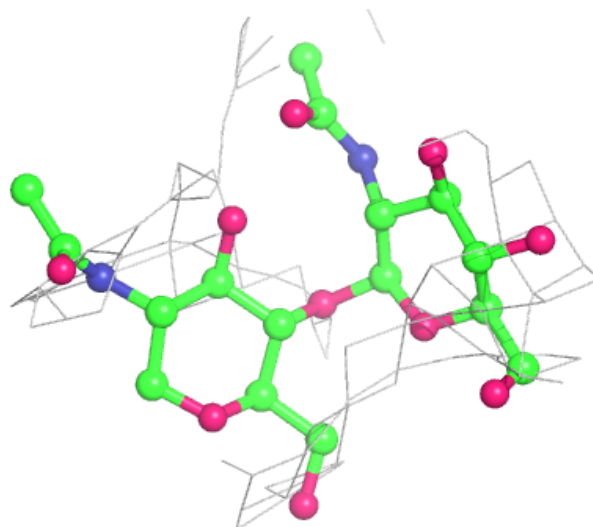
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	K	1	14/15	0.91	0.21	116,183,224,247	0
4	NAG	U	1	14/15	0.93	0.15	133,181,218,231	0
4	NAG	R	1	14/15	0.94	0.16	108,165,197,198	0

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



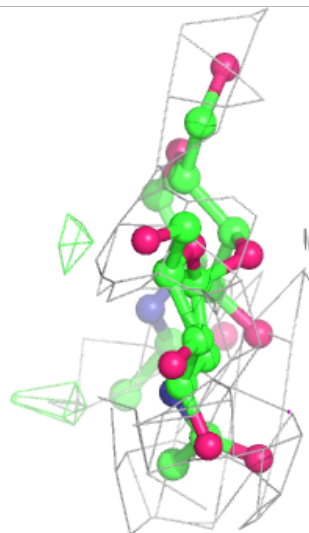
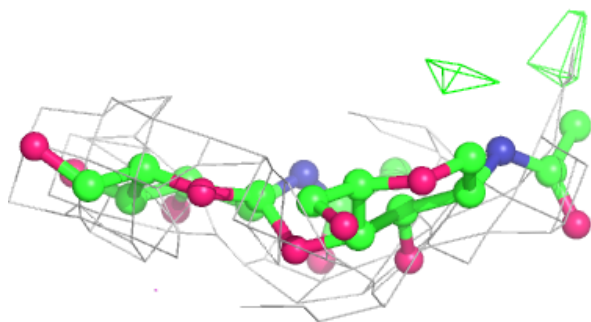
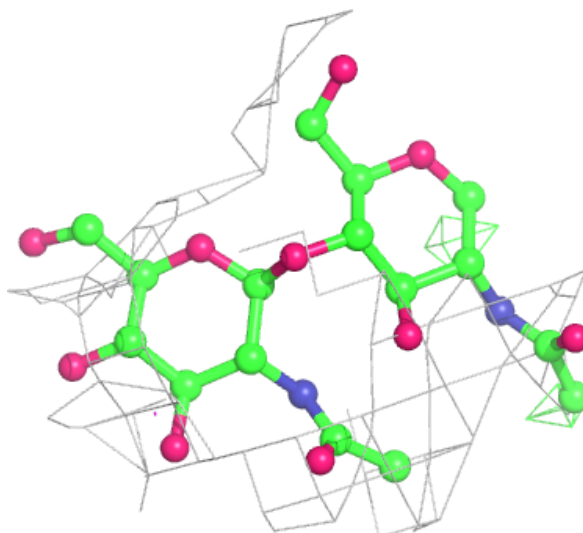
Electron density around Chain M:

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



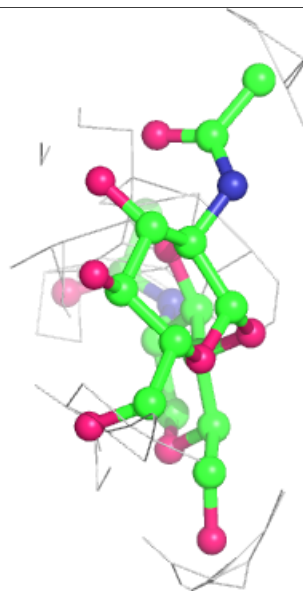
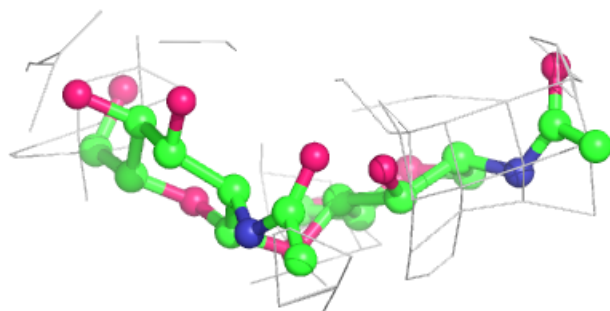
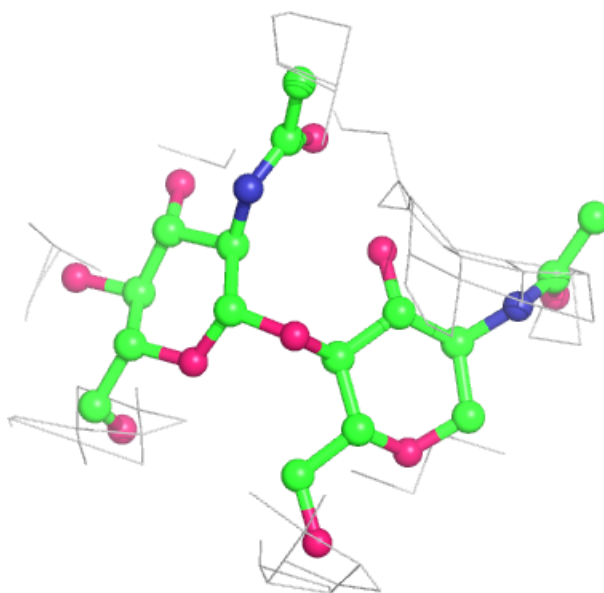
Electron density around Chain N:

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



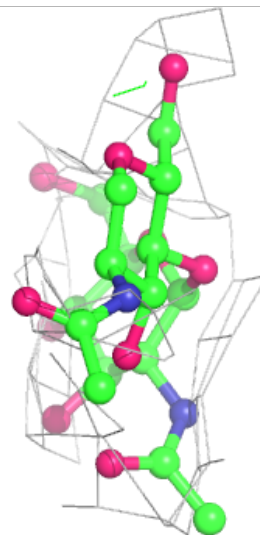
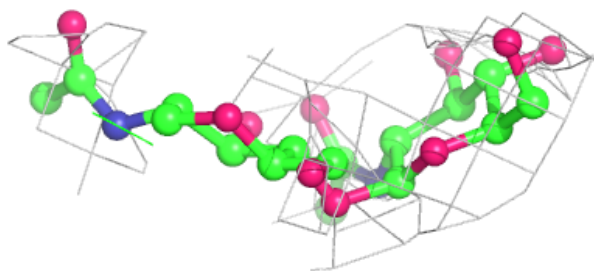
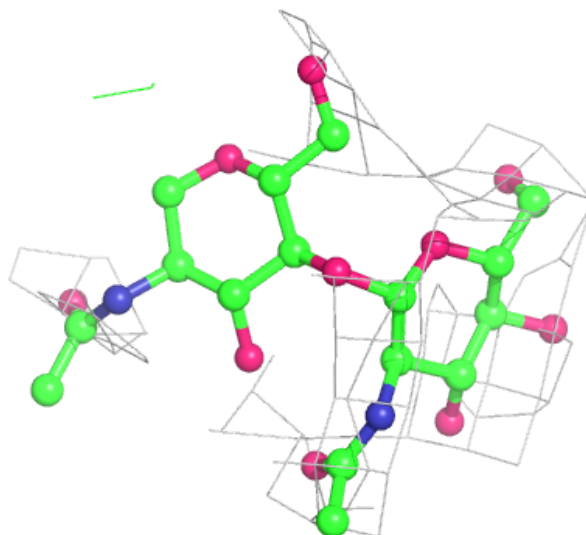
Electron density around Chain P:

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



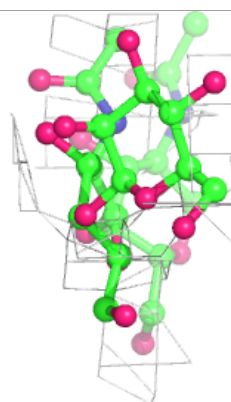
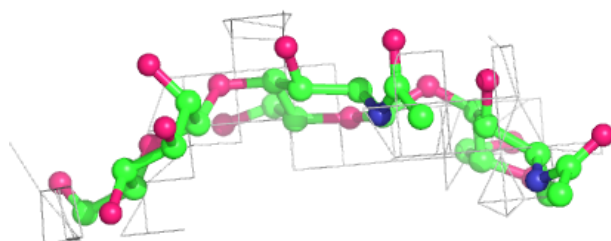
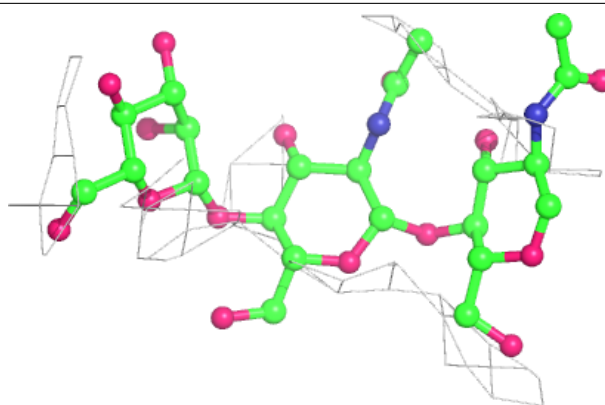
Electron density around Chain S:

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

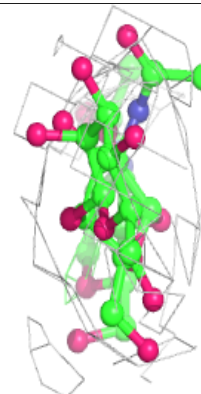
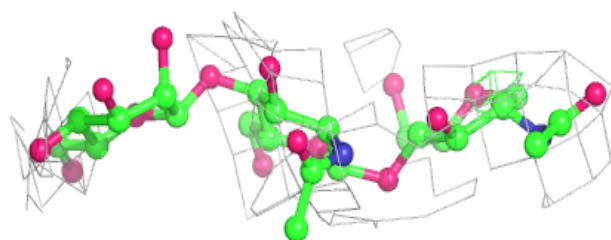
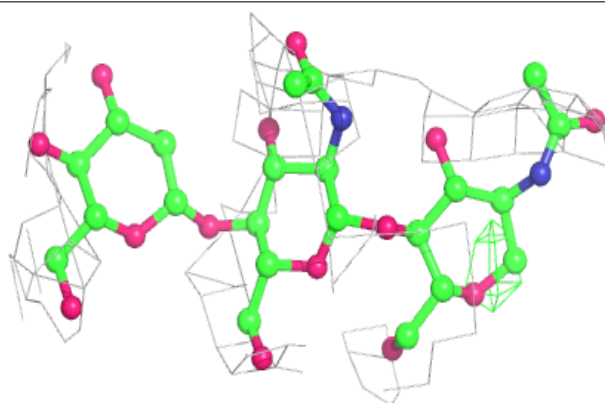


Electron density around Chain J:

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

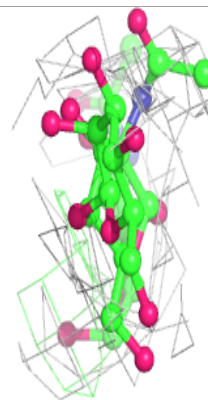
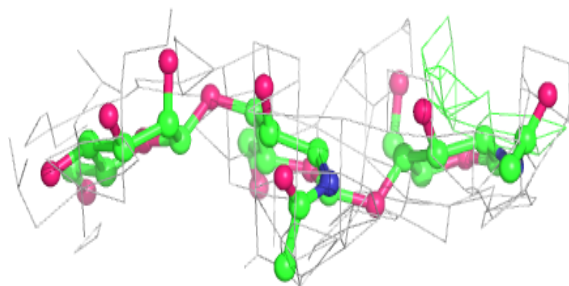
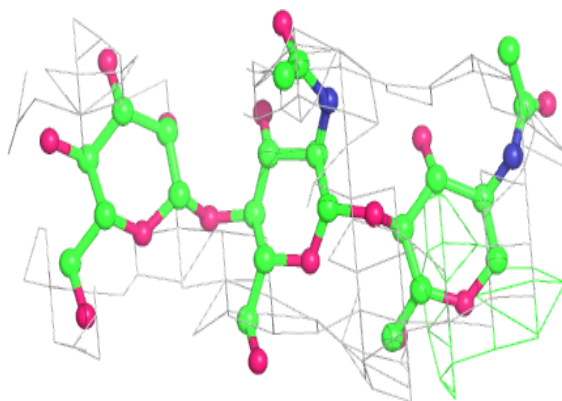
**Electron density around Chain K:**

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

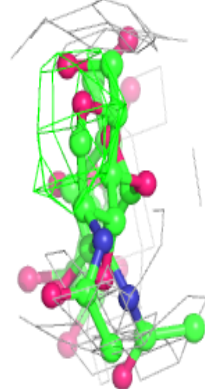
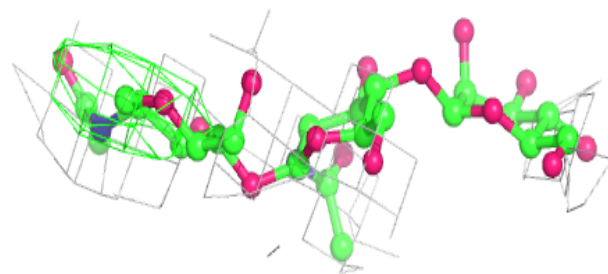
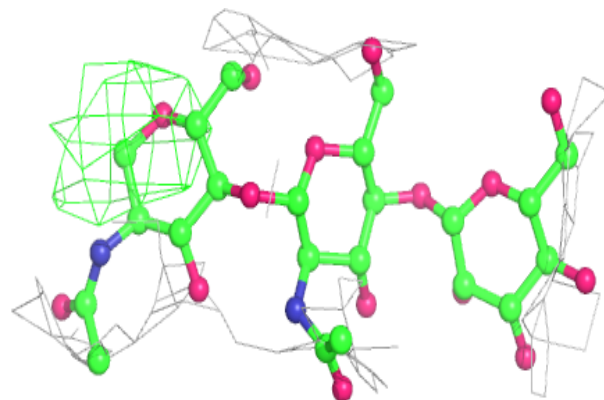


Electron density around Chain L:

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

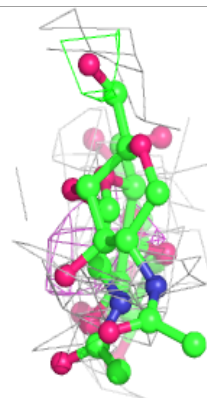
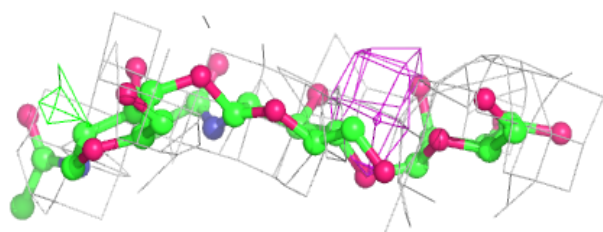
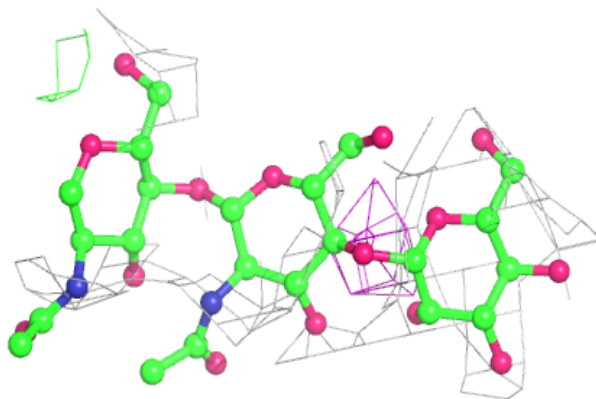
**Electron density around Chain O:**

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

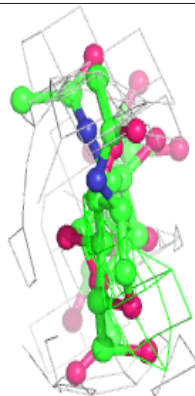
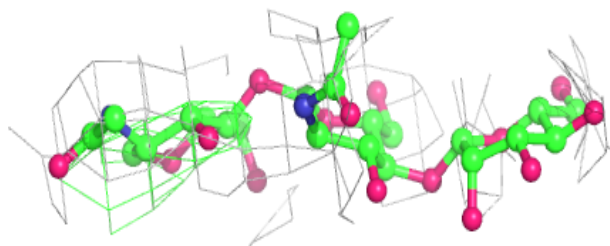
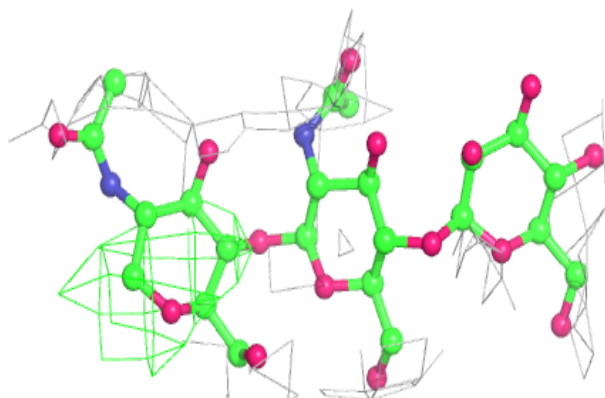


Electron density around Chain Q:

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

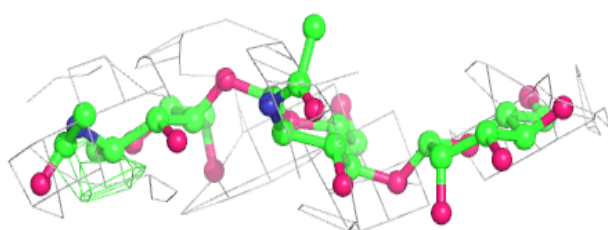
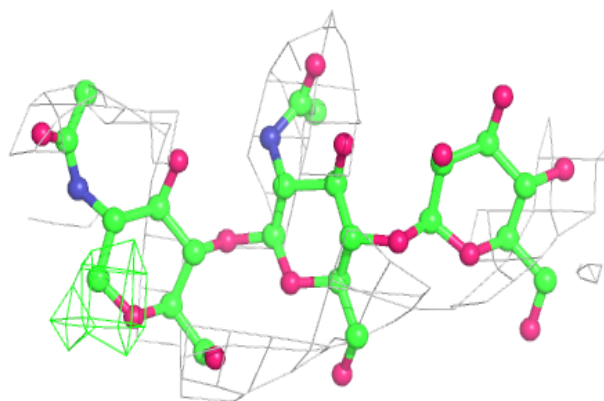
**Electron density around Chain R:**

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

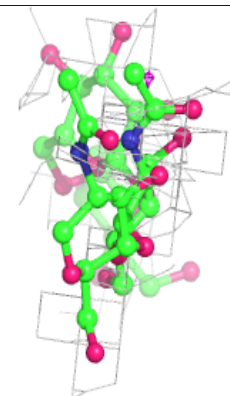
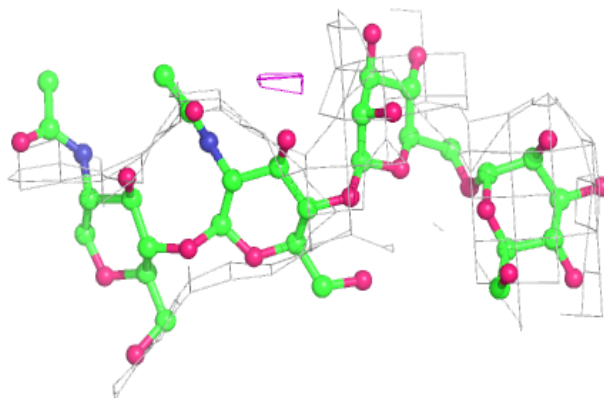


Electron density around Chain U:

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

**Electron density around Chain T:**

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



6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	CA	D	2002	1/1	0.40	0.12	533,533,533,533	0
7	CA	C	2005	1/1	0.42	0.13	235,235,235,235	0
6	NAG	F	3094	14/15	0.57	0.54	232,263,289,301	0
7	CA	G	2005	1/1	0.57	0.19	228,228,228,228	0
7	CA	E	2005	1/1	0.64	0.14	235,235,235,235	0
7	CA	A	2006	1/1	0.68	0.16	182,182,182,182	0
6	NAG	E	3678	14/15	0.69	0.29	172,234,258,258	0
7	CA	F	2002	1/1	0.71	0.10	534,534,534,534	0
7	CA	B	2002	1/1	0.71	0.15	533,533,533,533	0
6	NAG	F	3479	14/15	0.71	0.31	199,256,273,273	0
6	NAG	D	3479	14/15	0.72	0.32	192,213,248,259	0
7	CA	A	2007	1/1	0.72	0.14	279,279,279,279	0
7	CA	A	2005	1/1	0.74	0.23	235,235,235,235	0
7	CA	H	2002	1/1	0.74	0.12	532,532,532,532	0
6	NAG	H	3479	14/15	0.75	0.32	217,264,289,289	0
7	CA	E	2007	1/1	0.75	0.20	279,279,279,279	0
6	NAG	B	3479	14/15	0.76	0.26	232,258,304,321	0
8	MG	G	2009	1/1	0.79	0.47	414,414,414,414	0
6	NAG	C	3678	14/15	0.80	0.27	212,245,268,292	0
6	NAG	G	3678	14/15	0.80	0.33	129,233,286,308	0
7	CA	G	2007	1/1	0.81	0.16	284,284,284,284	0
6	NAG	E	3880	14/15	0.81	0.35	117,189,224,243	0
6	NAG	D	3094	14/15	0.82	0.26	212,265,297,302	0
6	NAG	A	3678	14/15	0.82	0.24	164,238,297,317	0
6	NAG	B	3094	14/15	0.82	0.30	236,271,288,298	0
6	NAG	G	3880	14/15	0.83	0.32	158,180,199,201	0
6	NAG	H	3094	14/15	0.83	0.33	209,244,295,296	0
6	NAG	C	3880	14/15	0.86	0.22	141,180,222,236	0
7	CA	C	2007	1/1	0.86	0.14	284,284,284,284	0
7	CA	C	2006	1/1	0.87	0.17	201,201,201,201	0
7	CA	G	2006	1/1	0.90	0.25	197,197,197,197	0
7	CA	E	2006	1/1	0.91	0.20	200,200,200,200	0

6.5 Other polymers ⓘ

There are no such residues in this entry.