



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:17 AM UTC

PDB ID : 3K71 / pdb_00003k71
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 types of validation reports are described at

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

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

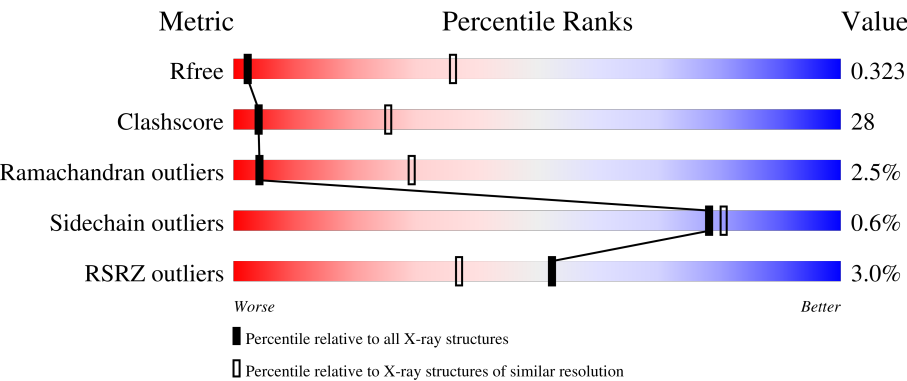
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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

Mol	Chain	Length	Quality of chain
1	A	1095	2% 41% 37% 20%
1	C	1095	3% 42% 36% 19%
1	E	1095	2% 41% 37% 19%
1	G	1095	2% 51% 44% ..
2	B	687	3% 63% 34% ..

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Mol	Chain	Length	Quality of chain
2	D	687	
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	MAN	Q	3	X	-	-	-
4	MAN	R	3	X	-	-	-
4	MAN	U	3	X	-	-	-
5	MAN	T	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	D	3479	-	-	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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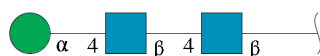
Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	expression tag	UNP P05107
B	682	GLU	-	expression tag	UNP P05107
B	684	LEU	-	expression tag	UNP P05107
B	685	TYR	-	expression tag	UNP P05107
B	686	PHE	-	expression tag	UNP P05107
B	687	GLN	-	expression tag	UNP P05107
D	678	ASP	-	expression tag	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.



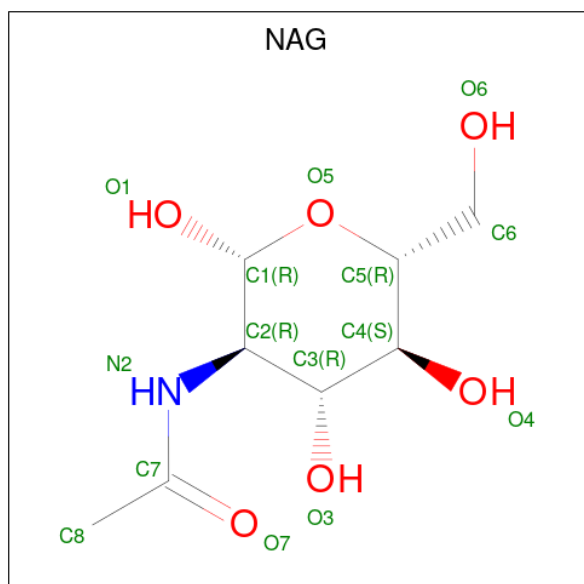
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	U	3	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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

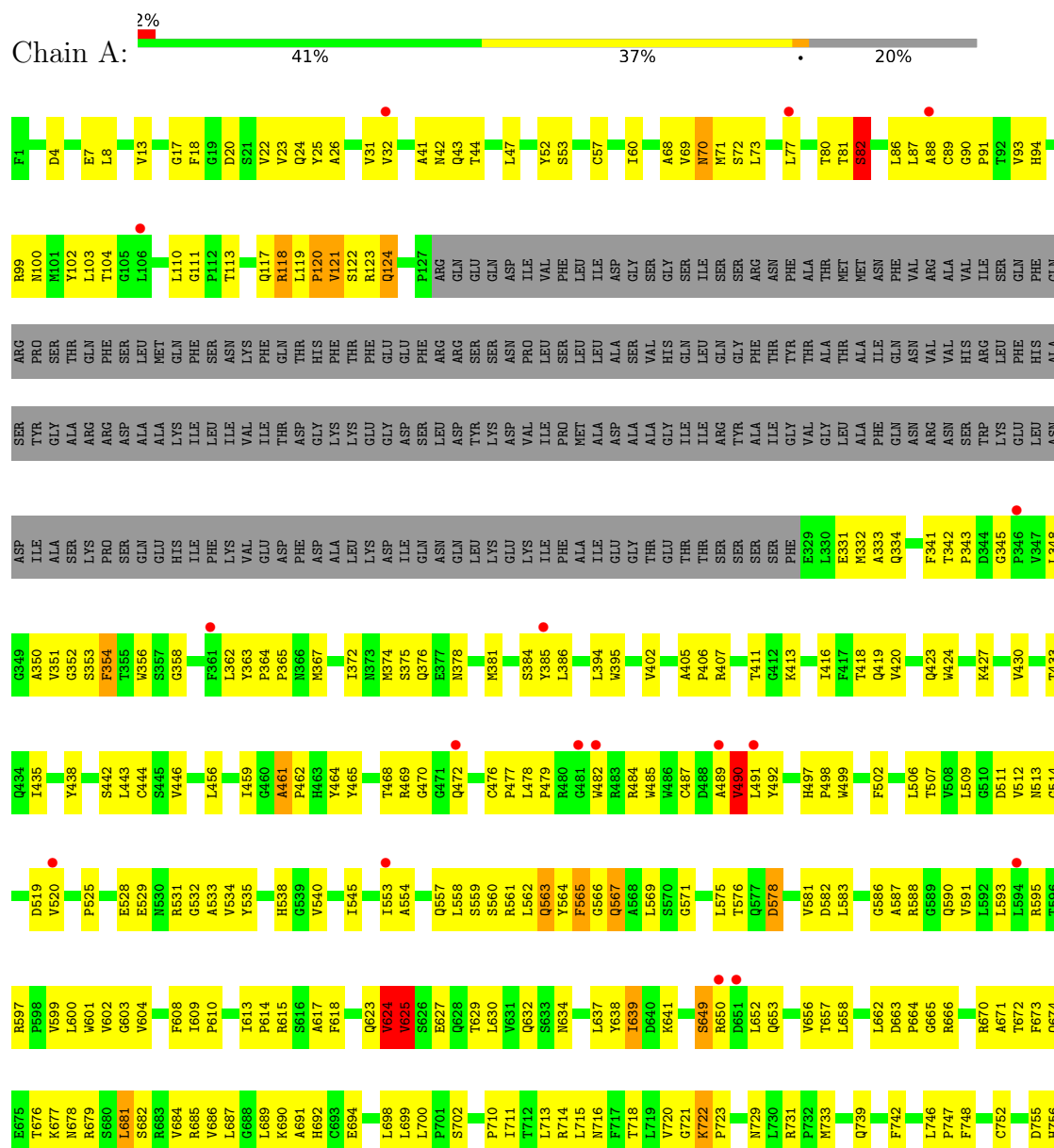
- Molecule 9 is water.

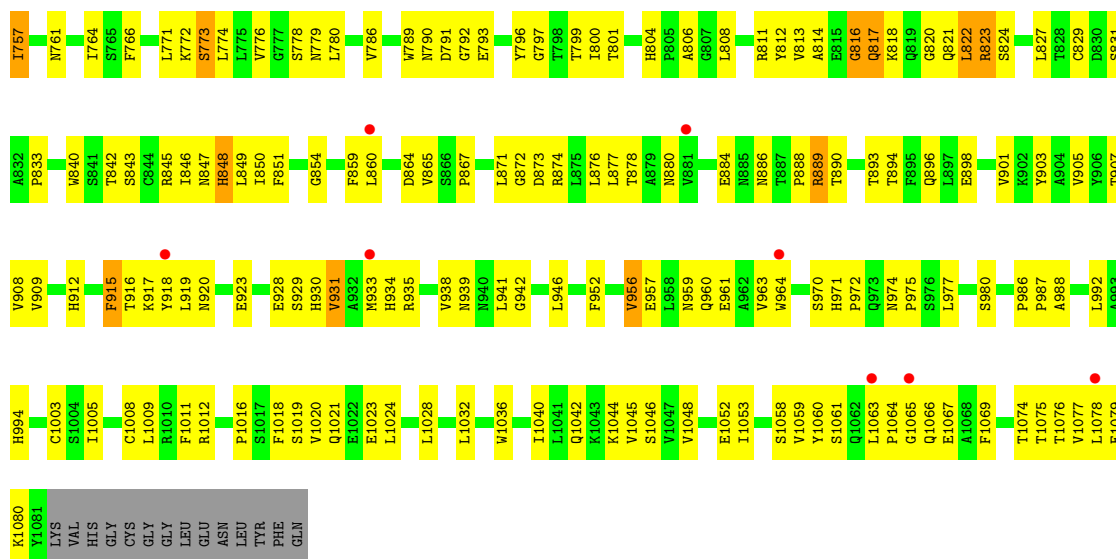
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	3	Total	O	0	0
			3	3		

3 Residue-property plots

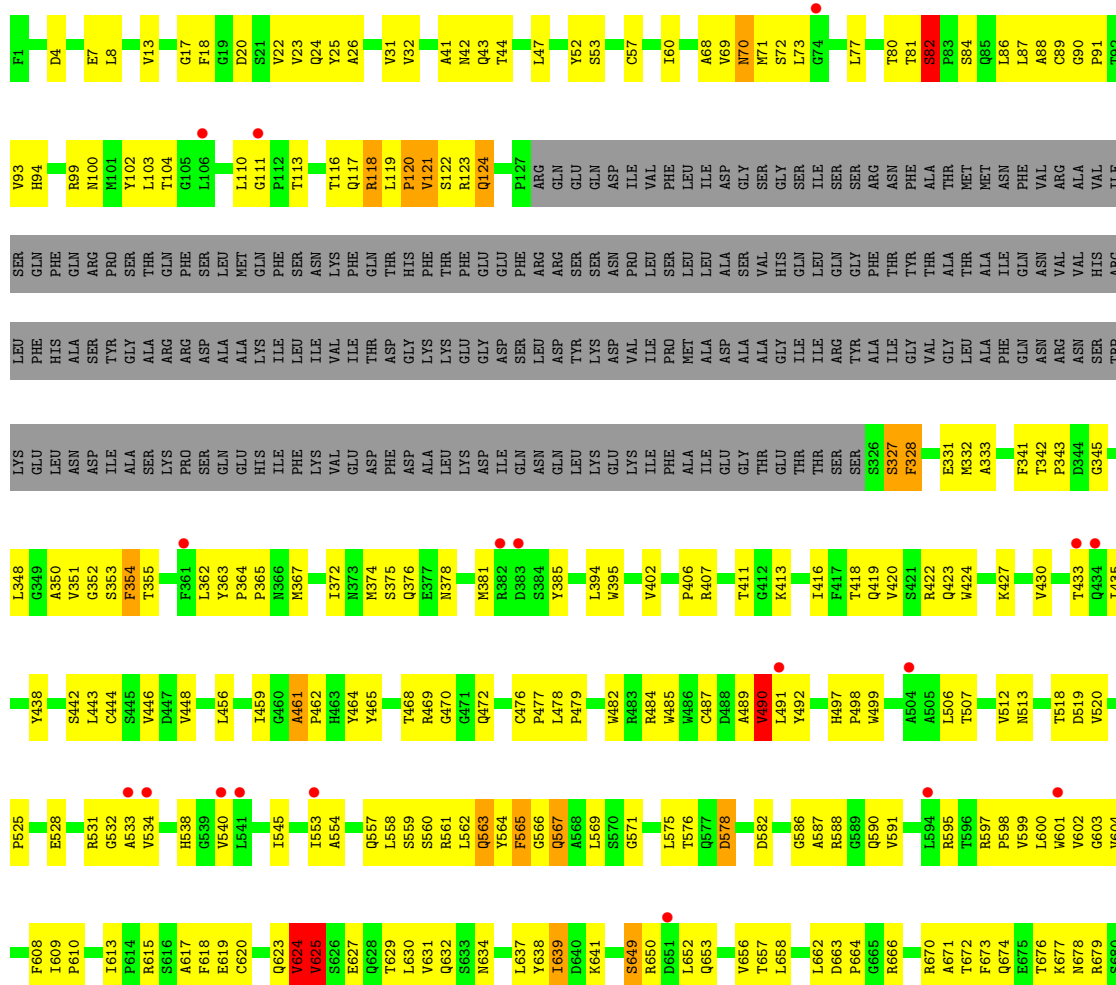
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

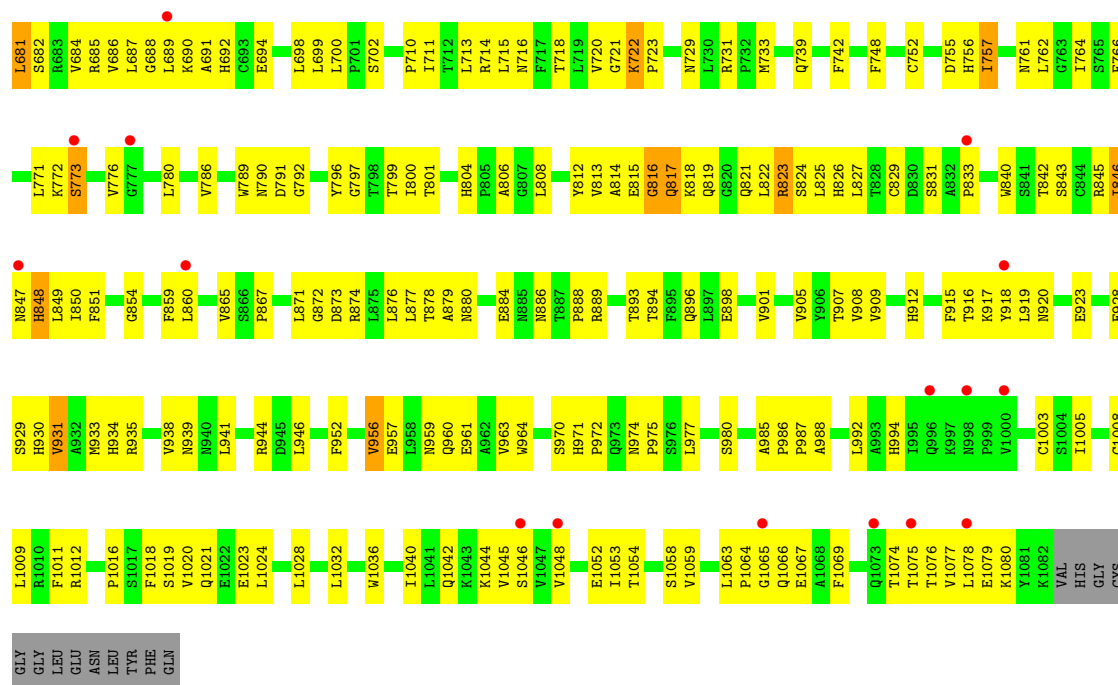
• Molecule 1: Integrin alpha-X



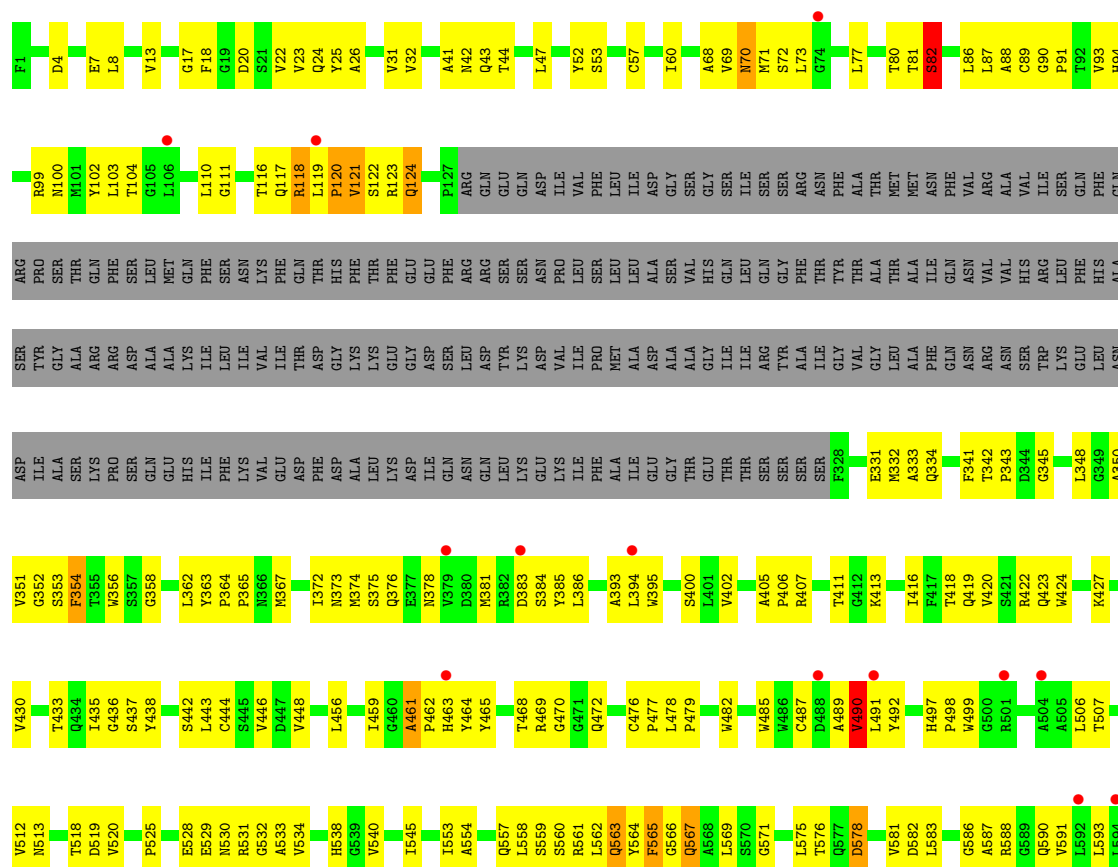


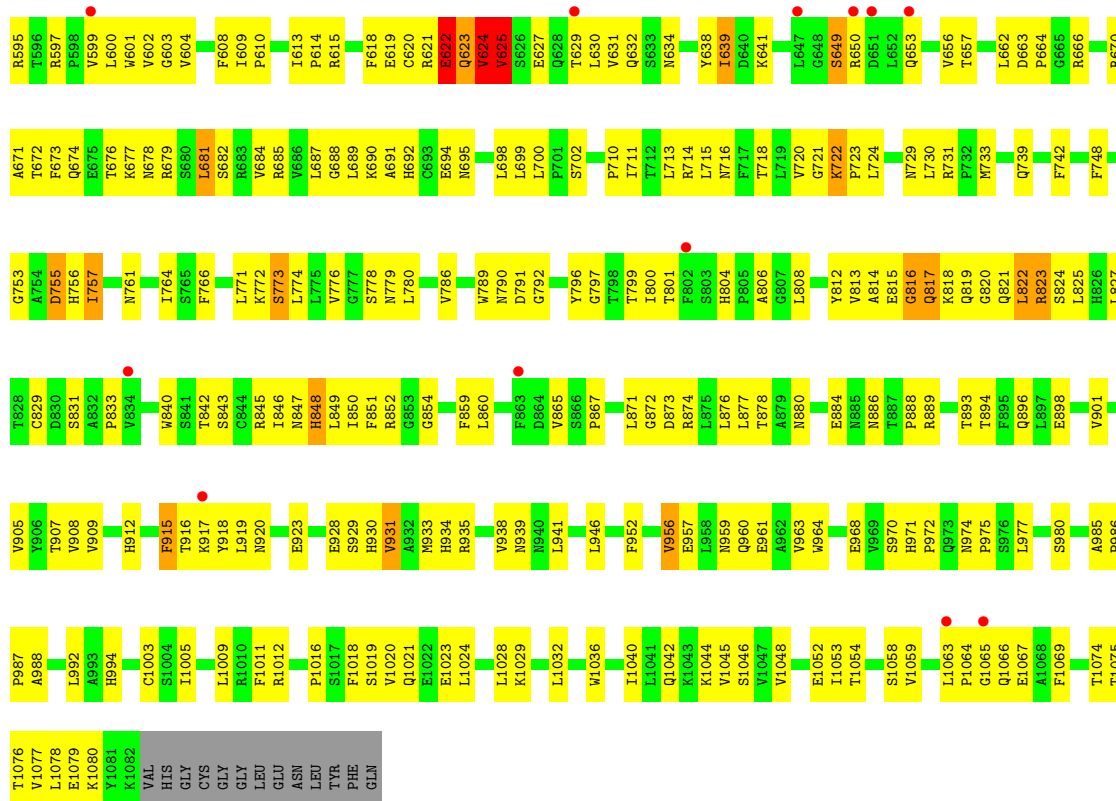
• Molecule 1: Integrin alpha-X



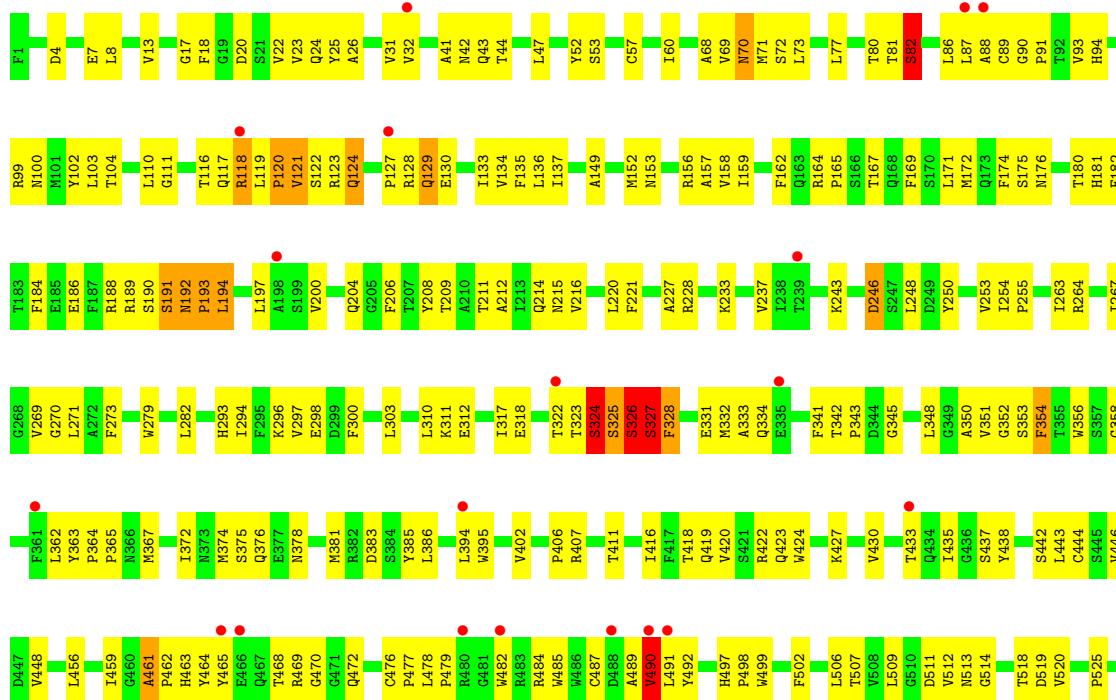


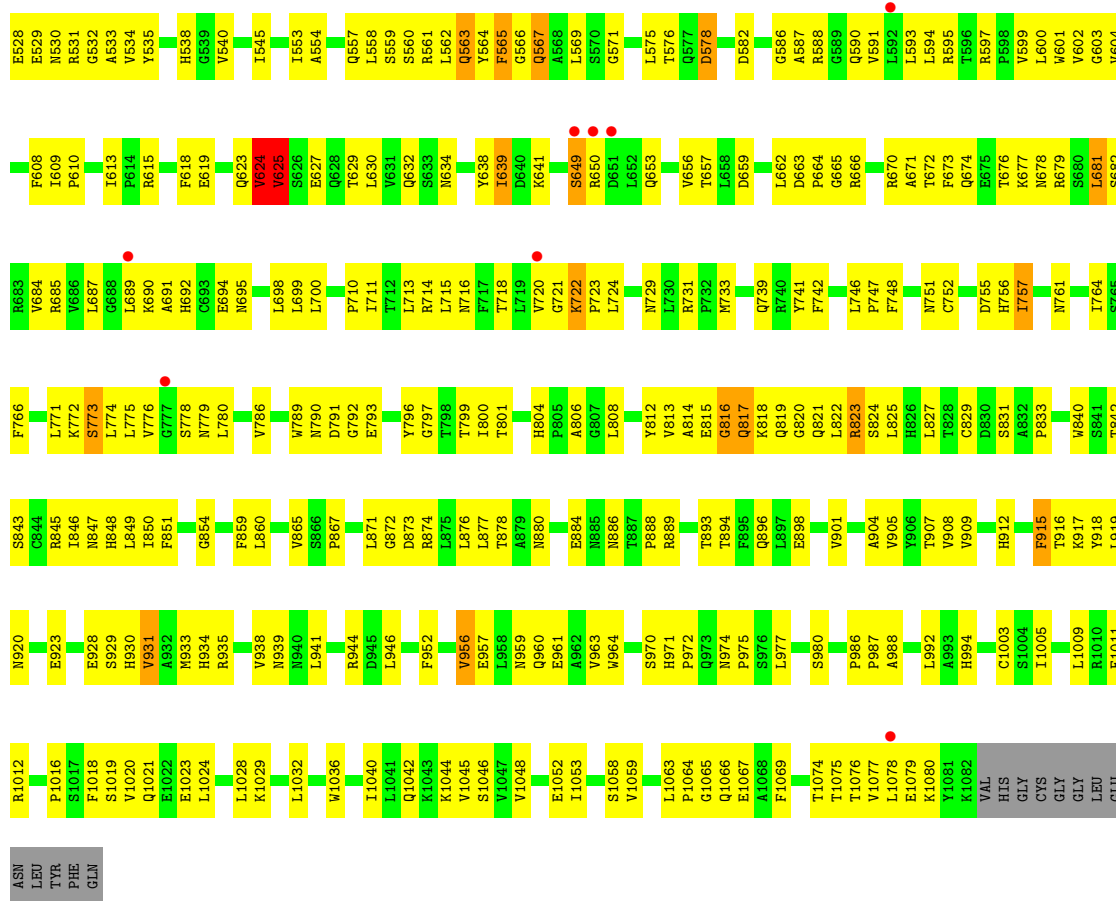
• Molecule 1: Integrin alpha-X



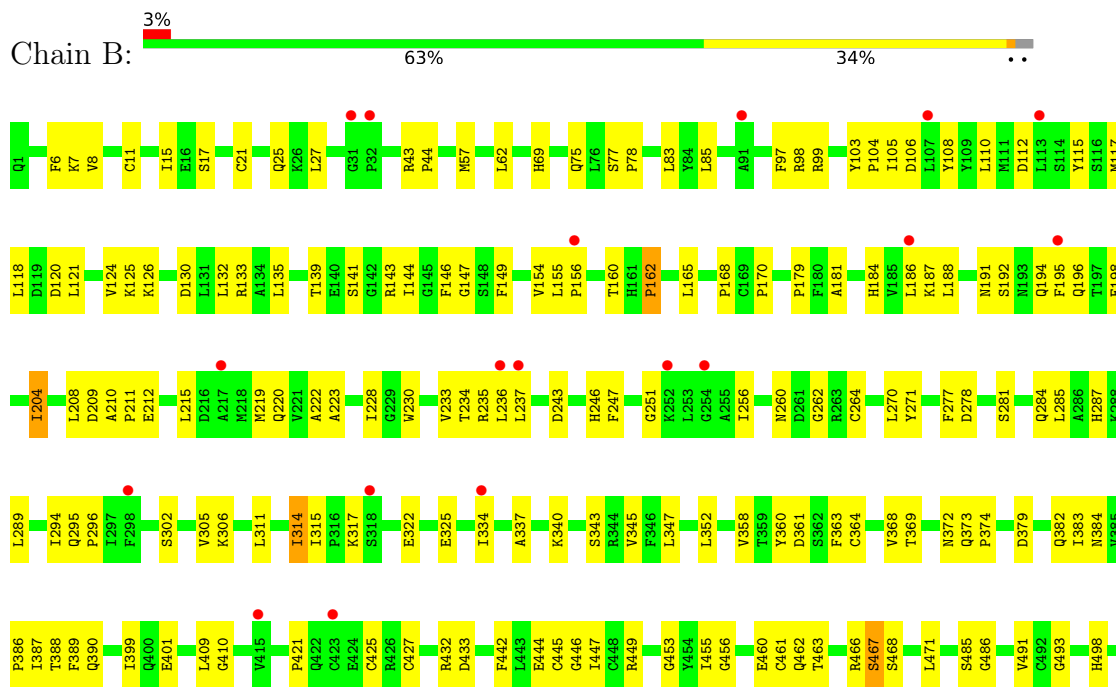


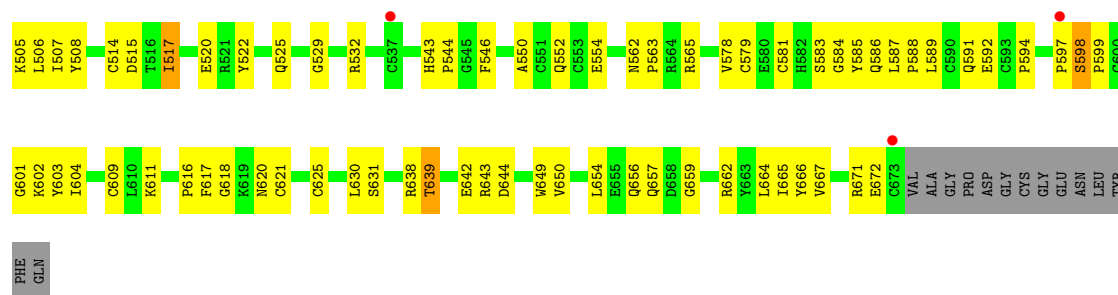
• Molecule 1: Integrin alpha-X



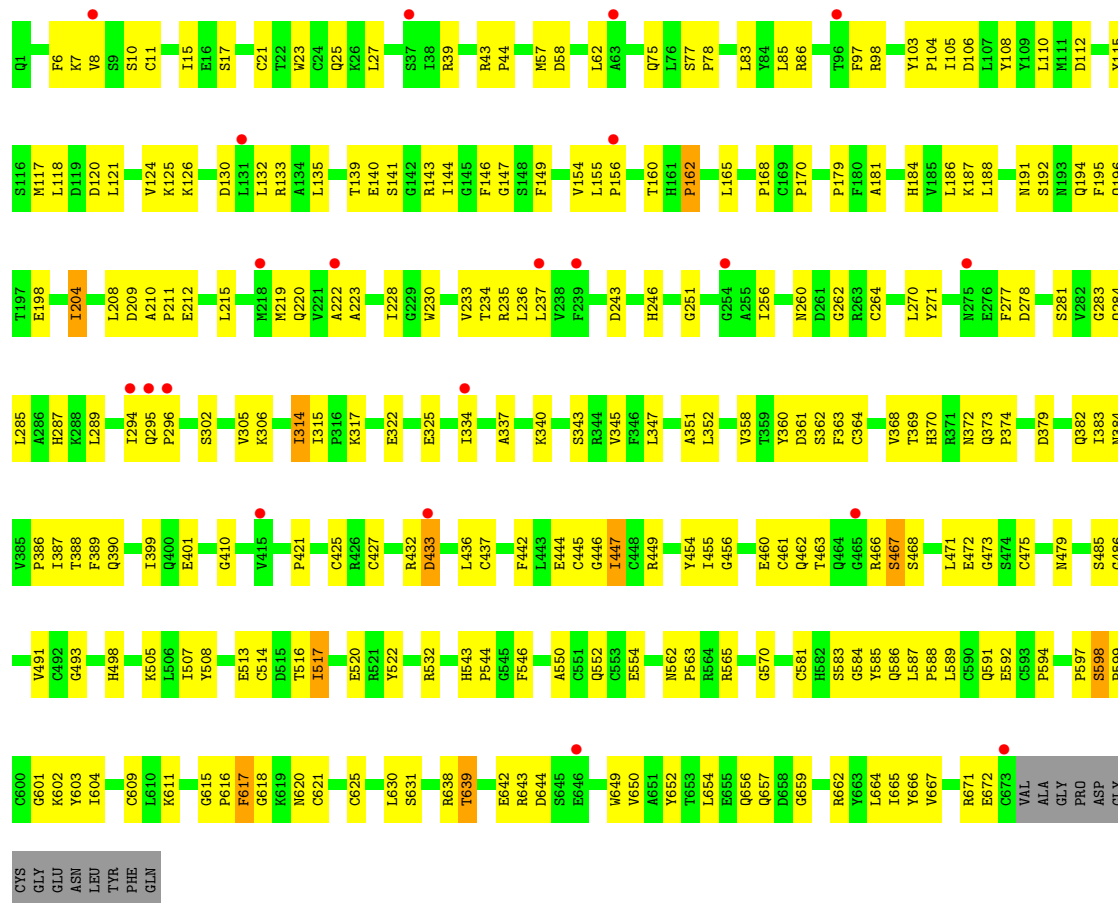


• Molecule 2: Integrin beta-2

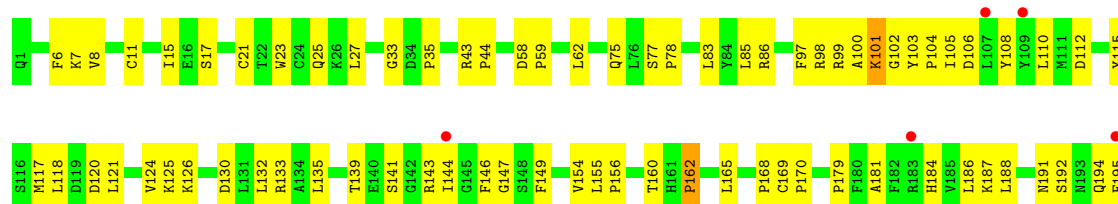


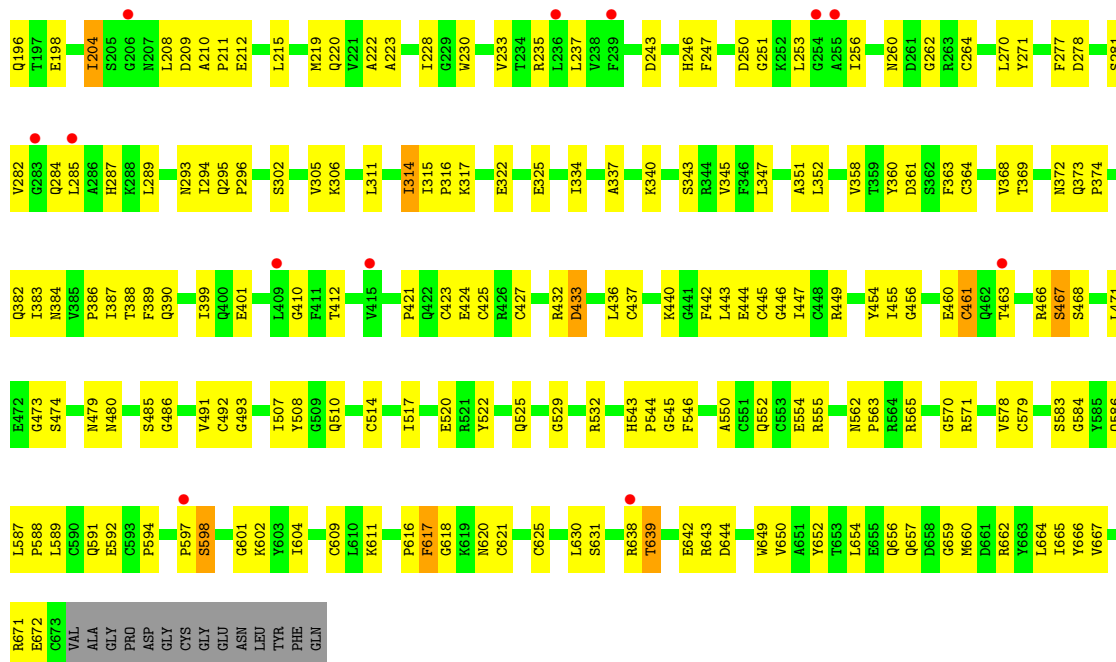


• Molecule 2: Integrin beta-2

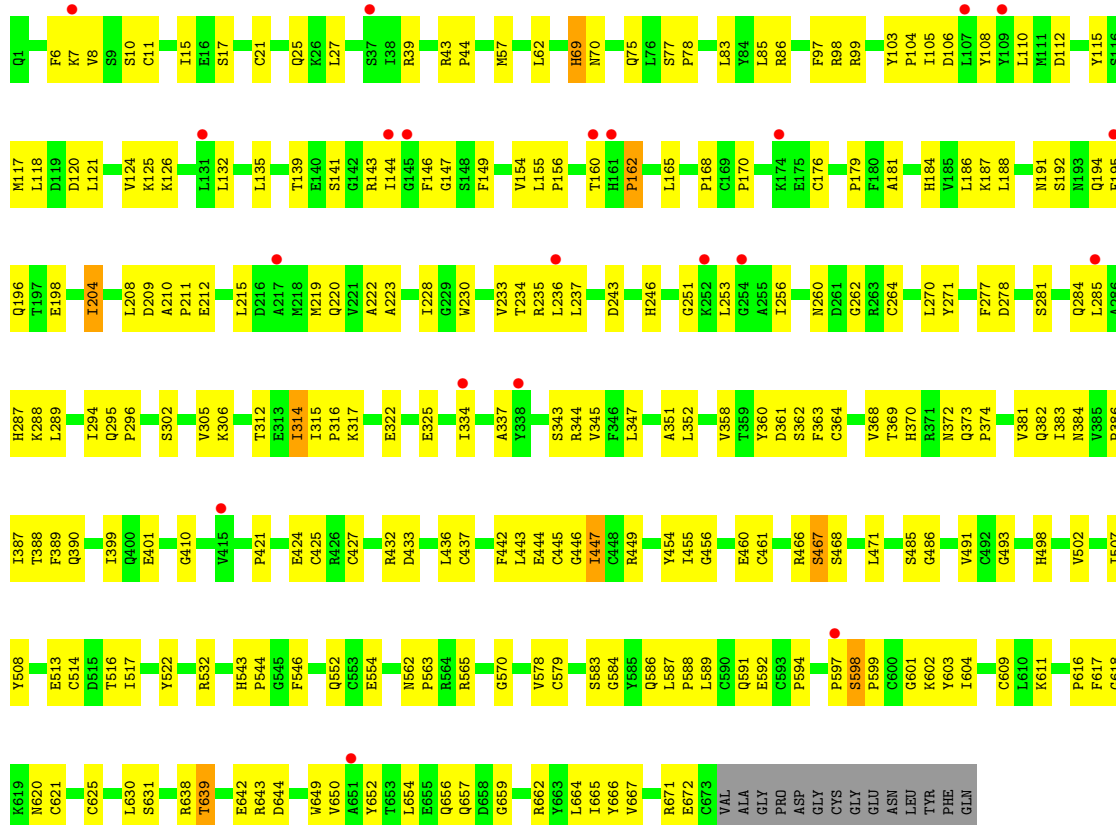


• Molecule 2: Integrin beta-2





• 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%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

- 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%

MAG1
MAG2
MAN3

- 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:  33% 67%

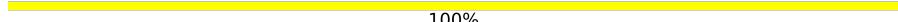
MAG1
MAG2
MAN3

- 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%



- 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%

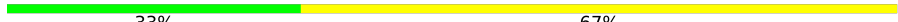


- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 67%



- 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:  33% 67%

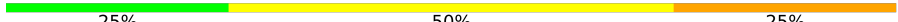


- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:  25% 50% 25%



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 0.309 , 0.323	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)	0.30 , 202.3	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	0.85	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: MAN, NAG, MG, CA

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	0.31	0/6936	0.76	10/9437 (0.1%)
1	C	0.31	0/6969	0.76	9/9480 (0.1%)
1	E	0.32	1/6957 (0.0%)	0.77	12/9464 (0.1%)
1	G	0.33	0/8579	0.77	12/11652 (0.1%)
2	B	0.29	0/5273	0.73	1/7119 (0.0%)
2	D	0.29	0/5273	0.73	3/7119 (0.0%)
2	F	0.30	0/5273	0.73	3/7119 (0.0%)
2	H	0.29	0/5273	0.73	1/7119 (0.0%)
All	All	0.31	1/50533 (0.0%)	0.75	51/68509 (0.1%)

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	-5.33	1.38	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	625	VAL	N-CA-C	7.25	119.52	109.45
1	C	625	VAL	N-CA-C	7.16	119.41	109.45
1	A	625	VAL	N-CA-C	7.15	119.39	109.45
1	E	625	VAL	N-CA-C	7.14	119.38	109.45
1	E	622	GLU	N-CA-C	6.52	118.11	110.41
2	F	423	CYS	N-CA-C	6.43	118.68	107.49
1	E	625	VAL	CB-CA-C	-6.43	102.62	111.49
1	C	625	VAL	CB-CA-C	-6.42	102.64	111.49
1	A	82	SER	CA-C-N	-6.36	111.66	120.25
1	A	82	SER	C-N-CA	-6.36	111.66	120.25
1	A	625	VAL	CB-CA-C	-6.25	102.86	111.49
1	E	82	SER	CA-C-N	-6.20	111.87	120.25
1	E	82	SER	C-N-CA	-6.20	111.87	120.25
1	G	625	VAL	CB-CA-C	-6.16	102.99	111.49
1	G	82	SER	CA-C-N	-6.12	111.99	120.25
1	G	82	SER	C-N-CA	-6.12	111.99	120.25
1	C	82	SER	CA-C-N	-6.11	112.00	120.25
1	C	82	SER	C-N-CA	-6.11	112.00	120.25
1	E	623	GLN	N-CA-C	-5.87	99.63	109.07
1	A	817	GLN	N-CA-C	5.59	117.59	110.61
2	H	583	SER	CB-CA-C	-5.55	109.19	115.79
1	G	461	ALA	CA-C-N	5.53	125.88	119.47
1	G	461	ALA	C-N-CA	5.53	125.88	119.47
1	C	461	ALA	CA-C-N	5.51	125.87	119.47
1	C	461	ALA	C-N-CA	5.51	125.87	119.47
1	A	461	ALA	CA-C-N	5.48	125.83	119.47
1	A	461	ALA	C-N-CA	5.48	125.83	119.47
1	E	817	GLN	N-CA-C	5.44	117.41	110.61
1	E	461	ALA	CA-C-N	5.42	125.75	119.47
1	E	461	ALA	C-N-CA	5.42	125.75	119.47
1	C	817	GLN	N-CA-C	5.36	117.73	110.06
2	D	58	ASP	CA-C-N	5.32	126.49	119.84
2	D	58	ASP	C-N-CA	5.32	126.49	119.84
2	D	583	SER	CB-CA-C	-5.25	109.55	115.79
2	F	583	SER	CB-CA-C	-5.22	109.58	115.79
1	G	817	GLN	N-CA-C	5.22	117.53	110.06
1	G	192	ASN	CA-C-N	5.21	126.35	119.84
1	G	192	ASN	C-N-CA	5.21	126.35	119.84
2	B	583	SER	CB-CA-C	-5.20	109.60	115.79
2	F	461	CYS	CB-CA-C	-5.16	105.06	113.37
1	G	578	ASP	N-CA-C	-5.09	102.75	110.28
1	E	578	ASP	N-CA-C	-5.08	102.76	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	326	SER	N-CA-C	5.08	121.62	110.80
1	E	822	LEU	N-CA-C	5.07	114.98	108.34
1	E	848	HIS	N-CA-C	5.07	115.69	108.54
1	A	848	HIS	N-CA-C	5.06	115.67	108.54
1	C	848	HIS	N-CA-C	5.06	115.67	108.54
1	A	578	ASP	N-CA-C	-5.05	102.81	110.28
1	C	578	ASP	N-CA-C	-5.04	102.82	110.28
1	A	822	LEU	N-CA-C	5.03	114.93	108.34
1	G	129	GLN	N-CA-C	5.02	116.50	108.41

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

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Mol	Chain	Res	Type	Group
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
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

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	455	0
1	C	6814	0	6672	444	0
1	E	6802	0	6662	460	2
1	G	8392	0	8229	530	2
2	B	5177	0	4966	217	0
2	D	5177	0	4966	249	0
2	F	5177	0	4966	251	0
2	H	5177	0	4966	240	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2721	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 28.

All (2721) 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
2:F:35:PRO:HG2	2:F:510:GLN:CD	1.90	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:119:LEU:N	1:G:120:PRO:HA	1.83	0.90
2:H:532:ARG:HD3	2:H:554:GLU:CD	1.97	0.88
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
1:G:99:ARG:HH12	1:G:318:GLU:HG3	1.41	0.86
1:E:1064:PRO:HG3	1:E:1067:GLU:CD	2.01	0.85
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.01	0.85
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.01	0.85
2:D:532:ARG:HD3	2:D:554:GLU:CD	2.02	0.85
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
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.03	0.83
2:H:25:GLN:OE1	2:H:427:CYS:SG	2.36	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:1064:PRO:HG3	1:G:1067:GLU:CD	2.04	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:570:GLY:HA2	2:H:659:GLY:HA2	1.64	0.79
1:E:923:GLU:HB2	1:E:1080:LYS:HB3	1.63	0.79
1:E:1052:GLU:OE1	1:G:756:HIS:HA	1.83	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: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:623:GLN:O	1:G:624:VAL:HG22	1.84	0.78
1:E:789:TRP:CZ2	1:G:772:LYS:HA	2.20	0.77
1:G:99:ARG:NH1	1:G:318:GLU:CG	2.47	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:E:721:GLY:C	1:E:723:PRO:HD3	2.10	0.76
1:G:119:LEU:H	1:G:120:PRO:HA	1.50	0.76
1:A:721:GLY:C	1:A:723:PRO:HD3	2.11	0.76
1:G:721:GLY:C	1:G:723:PRO:HD3	2.10	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
1:C:721:GLY:C	1:C:723:PRO:HD3	2.11	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:15:ILE:HG23	2:F:86:ARG:CZ	2.17	0.74
2:F:461:CYS:HB3	2:F:466:ARG:HD2	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:662:LEU:HD11	1:E:673:PHE:CZ	2.24	0.71
1:E:1064:PRO:CG	1:E:1067:GLU:HG3	2.20	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
1:E:817:GLN:N	1:E:818:LYS:HA	2.05	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
2:F:35:PRO:CG	2:F:510:GLN:CD	2.63	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:A:731:ARG:HG3	1:A:731:ARG:O	1.92	0.70
1:C:731:ARG:HG3	1:C:731:ARG:O	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:491:LEU:HD11	1:C:545:ILE:HG12	1.75	0.69
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.75	0.68
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	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
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:HG3	1:G:731:ARG:O	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:A:519:ASP:CG	1:A:538:HIS:HD1	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:TYR:CE2	1:E:814:ALA:HB2	2.31	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:15:ILE:HG23	2:H:86:ARG:CZ	2.25	0.66
2:H:103:TYR:HB3	2:H:104:PRO:HD2	1.77	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
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:630:LEU:HD21	1:E:653:GLN:HB2	1.77	0.65
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.26	0.65
1:C:519:ASP:CG	1:C:538:HIS:HD1	2.05	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:27:LEU:HD21	2:F:443:LEU:HD11	1.78	0.65
2:F:103:TYR:HB3	2:F:104:PRO:HD2	1.77	0.65
1:E:609:ILE:HB	1:E:610:PRO:HD3	1.77	0.65
1:G:519:ASP:CG	1:G:538:HIS:HD1	2.03	0.65
1:C:103:LEU:CD1	2:D:155:LEU:HD13	2.26	0.64
1:E:519:ASP:CG	1:E:538:HIS:HD1	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:812:TYR:CD2	1:G:814:ALA:HB2	2.32	0.64
1:A:599:VAL:HG23	1:A:599:VAL:O	1.95	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:G:1064:PRO:HG2	1:G:1067:GLU:HG3	1.79	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
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
2:F:532:ARG:HD3	2:F:554:GLU:CD	2.22	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:O	1:G:121:VAL:HG12	1.98	0.63
2:H:104:PRO:HD2	2:H:233:VAL:HG11	1.78	0.63
1:G:721:GLY:C	1:G:723:PRO:CD	2.72	0.63
2:H:39:ARG:NE	2:H:447:ILE:HG23	2.13	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
2:B:597:PRO:O	2:B:598:SER:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:121:VAL:HG12	1.98	0.62
1:C:721:GLY:C	1:C:723:PRO:CD	2.72	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:E:721:GLY:C	1:E:723:PRO:CD	2.72	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
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:HG23	1:G:599:VAL:O	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:721:GLY:C	1:A:723:PRO:CD	2.72	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
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:C:630:LEU:HD21	1:G:653:GLN:HB2	1.82	0.61
1:E:871:LEU:HD11	1:E:901:VAL:HG21	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:971:HIS:CE1	1:E:974:ASN:HB2	2.35	0.61
1:E:1064:PRO:HG3	1:E:1067:GLU:CG	2.30	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: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
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	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
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:80:THR:HB	1:G:341:PHE:CG	2.36	0.60
1:G:1064:PRO:HG3	1:G:1067:GLU:CG	2.31	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:214:GLN:CD	1:G:253:VAL:HG12	2.27	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:A:876:LEU:C	1:A:876:LEU:HD12	2.27	0.60
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.83	0.60
1:E:876:LEU:C	1:E:876:LEU:HD12	2.26	0.60
1:E:928:GLU:HG3	1:E:929:SER:N	2.17	0.60
1:G:876:LEU:C	1:G:876:LEU:HD12	2.27	0.60
1:G:971:HIS:CE1	1:G:974:ASN:HB2	2.36	0.60
1:G:1064:PRO:HG3	1:G:1067:GLU:HG3	1.83	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:469:ARG:NH2	2:F:287:HIS:HB2	2.15	0.60
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
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.27	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
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.27	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:C:653:GLN:CB	1:G:630:LEU:HD21	2.32	0.59
1:C:876:LEU:HD12	1:C:876:LEU:C	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:615:ARG:HA	1:G:618:PHE:HB2	1.83	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:G:1065:GLY:C	1:G:1066:GLN:HG3	2.28	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:44:THR:HG22	1:G:71:MET:HG2	1.83	0.59
1:G:362:LEU:HD23	1:G:363:TYR:N	2.18	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: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
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
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: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
1:E:1065:GLY:C	1:E:1066:GLN:HG3	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:GLN:CD	2:B:317:LYS:HE2	2.28	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
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.28	0.58
2:F:295:GLN:CD	2:F:317:LYS:HE2	2.28	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:E:468:THR:HG23	1:E:498:PRO:HG3	1.84	0.58
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:490:VAL:HG12	1:G:491:LEU:N	2.18	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:H:295:GLN:CD	2:H:317:LYS:HE2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:446:VAL:HG21	1:G:520:VAL:CG1	2.34	0.57
1:E:436:GLY:C	2:F:282:VAL:HG11	2.30	0.57
1:A:575:LEU:HD12	1:A:576:THR:N	2.20	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
1:G:491:LEU:HD12	1:G:491:LEU:C	2.30	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
1:A:491:LEU:C	1:A:491:LEU:HD12	2.30	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
2:B:285:LEU:O	2:B:289:LEU:HB3	2.06	0.56
1:C:491:LEU:C	1:C:491:LEU:HD12	2.30	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
1:E:491:LEU:C	1:E:491:LEU:HD12	2.30	0.56
1:G:873:ASP:C	1:G:901:VAL:HG12	2.30	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
1:C:575:LEU:HD12	1:C:576:THR:N	2.21	0.56
2:D:460:GLU:HG2	2:D:461:CYS:SG	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:666:ARG:HB3	2:H:498:HIS:NE2	2.20	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:99:ARG:NH1	1:G:318:GLU:CD	2.63	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:E:852:ARG:HD2	2:F:480:ASN:CG	2.30	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:A:873:ASP:C	1:A:901:VAL:HG12	2.30	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
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
1:C:873:ASP:C	1:C:901:VAL:HG12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.88	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
2:F:508:TYR:CZ	2:F:514:CYS:HB3	2.41	0.55
2:H:460:GLU:HG2	2:H:461:CYS:SG	2.47	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
1:E:873:ASP:C	1:E:901:VAL:HG12	2.32	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
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:94:HIS:CD2	2:F:155:LEU:HD21	2.41	0.55
1:E:822:LEU:HG	1:E:823:ARG:H	1.72	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:N	1:C:941:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:418:THR:HG21	1:G:482:TRP:CZ2	2.41	0.55
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.88	0.55
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.89	0.55
1:A:681:LEU:C	1:A:681:LEU:HD12	2.32	0.55
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.89	0.55
2:D:77:SER:HA	2:D:78:PRO:C	2.32	0.55
1:E:435:ILE:HD13	2:F:311:LEU:HB2	1.87	0.55
2:F:77:SER:HA	2:F:78:PRO:C	2.32	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:47:LEU:HD11	1:C:88:ALA:CB	2.37	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: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: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
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:6:PHE:O	2:H:8:VAL:HG23	2.07	0.54
2:H:103:TYR:HB3	2:H:104:PRO:CD	2.37	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
1:G:4:ASP:CG	1:G:597:ARG:NH2	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:G:772:LYS:O	2.08	0.54
2:H:77:SER:HA	2:H:78:PRO:C	2.32	0.54
1:A:941:LEU:HD12	1:A:941:LEU:N	2.22	0.54
1:C:103:LEU:HD21	2:D:155:LEU:CD2	2.38	0.54
1:C:327:SER:O	1:C:328:PHE:O	2.26	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:665:GLY:HA3	2:H:498:HIS:HB3	1.88	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:A:362:LEU:HD23	1:A:362:LEU:C	2.33	0.54
1:A:652:LEU:HD21	1:E:609:ILE:HG22	1.89	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:772:LYS:HG3	1:E:772:LYS:O	2.07	0.54
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:93:VAL:O	1:E:103:LEU:HA	2.08	0.54
1:E:964:TRP:CB	1:E:1032:LEU:HA	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:LEU:HD23	1:C:362:LEU:C	2.33	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:58:ASP:N	2:F:59:PRO:HD3	2.23	0.54
2:F:471:LEU:O	2:F:493:GLY:HA2	2.08	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
1:C:681:LEU:C	1:C:681:LEU:HD12	2.33	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:6:PHE:O	2:F:8:VAL:HG23	2.07	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
1:G:184:PHE:CD2	1:G:227:ALA:HB2	2.43	0.53
1:G:600:LEU:HD12	1:G:600:LEU:O	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
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: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
1:G:681:LEU:HD12	1:G:681:LEU:C	2.32	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:94:HIS:CD2	2:B:155:LEU:HD21	2.43	0.53
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:LEU:CD1	2:D:156:PRO:HG3	2.39	0.53
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.38	0.53
1:E:362:LEU:HD23	1:E:362:LEU:C	2.34	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
2:B:77:SER:HA	2:B:78:PRO:C	2.32	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:362:LEU:HD23	1:G:362:LEU:C	2.33	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:93:VAL:O	1:A:103:LEU:HA	2.08	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
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:211:THR:HA	1:G:248:LEU:HD12	1.91	0.53
1:G:964:TRP:CB	1:G:1032:LEU:HA	2.38	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
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:4:ASP:CG	1:A:597:ARG:NH2	2.67	0.53
1:A:531:ARG:HA	1:A:563:GLN:O	2.09	0.53
1:A:692:HIS:ND1	1:E:694:GLU:HA	2.24	0.53
1:C:766:PHE:CZ	1:C:877:LEU:CD1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1063:LEU:HD12	1:C:1064:PRO:HA	1.90	0.53
2:D:57:MET:SD	2:D:427:CYS:SG	3.07	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:652:LEU:HD21	1:G:609:ILE:HG22	1.90	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:E:716:ASN:C	1:E:716:ASN:OD1	2.52	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: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
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:484:ARG:NH1	2:H:586:GLN:CG	2.73	0.52
1:G:671:ALA:O	1:G:672:THR:HG23	2.10	0.52
1:G:1063:LEU:HD12	1:G:1064:PRO:HA	1.90	0.52
2:H:135:LEU:HD11	2:H:139:THR:HB	1.90	0.52
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD12	1:A:492:TYR:N	2.24	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:18:PHE:CZ	1:A:32:VAL:HG21	2.45	0.52
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.39	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:600:LEU:O	1:A:600:LEU:HD12	2.09	0.52
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	1.90	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:25:GLN:HB2	2:D:445:CYS:CA	2.39	0.52
2:D:135:LEU:HD11	2:D:139:THR:HB	1.90	0.52
1:E:89:CYS:C	1:E:91:PRO:HD3	2.35	0.52
1:E:119:LEU:HD21	1:E:124:GLN:NE2	2.25	0.52
1:E:917:LYS:HE3	1:E:1077:VAL:CG2	2.39	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
2:D:155:LEU:H	2:D:160:THR:CG2	2.23	0.52
1:E:4:ASP:CG	1:E:597:ARG:NH2	2.68	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:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.91	0.52
2:B:27:LEU:CD2	2:B:446:GLY:HA2	2.39	0.52
2:B:155:LEU:H	2:B:160:THR:CG2	2.23	0.52
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.44	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
2:D:23:TRP:CH2	2:D:447:ILE:HD13	2.45	0.52
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.44	0.52
1:E:815:GLU:HB3	1:E:819:GLN:NE2	2.25	0.52
1:E:1063:LEU:HD12	1:E:1064:PRO:HA	1.90	0.52
2:F:83:LEU:HD13	2:F:85:LEU:HB2	1.92	0.52
2:F:155:LEU:C	2:F:155:LEU:HD12	2.35	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:89:CYS:C	1:C:91:PRO:HD3	2.35	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:333:ALA:HA	1:G:352:GLY:H	1.74	0.52
1:G:917:LYS:HE3	1:G:1077:VAL:CG2	2.39	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:155:LEU:C	2:B:155:LEU:HD12	2.35	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:71:MET:HG3	1:C:90:GLY:HA3	1.92	0.51
1:C:685:ARG:NH2	1:G:685:ARG:CZ	2.73	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
1:C:716:ASN:C	1:C:716:ASN:OD1	2.54	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:681:LEU:C	1:E:681:LEU:HD12	2.35	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
1:A:89:CYS:C	1:A:91:PRO:HD3	2.34	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
2:D:143:ARG:C	2:D:144:ILE:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:TYR:CD1	1:E:86:LEU:HB2	2.44	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:89:CYS:C	1:G:91:PRO:HD3	2.34	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:A:41:ALA:O	1:A:42:ASN:C	2.54	0.51
1:C:671:ALA:O	1:C:672:THR:HG23	2.11	0.51
1:C:714:ARG:HD2	1:C:714:ARG:C	2.36	0.51
1:E:18:PHE:CZ	1:E:32:VAL:HG21	2.45	0.51
1:E:117:GLN:CB	1:E:121:VAL:HG21	2.41	0.51
1:E:532:GLY:HA3	1:E:565:PHE:HD2	1.75	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:155:LEU:C	2:H:155:LEU:HD12	2.35	0.51
2:H:638:ARG:HB2	2:H:654:LEU:O	2.11	0.51
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.45	0.51
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.39	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:714:ARG:HD2	1:G:714:ARG:C	2.36	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
1:A:68:ALA:HB1	1:A:71:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.93	0.51
2:B:143:ARG:C	2:B:144:ILE:HD12	2.36	0.51
1:C:553:ILE:HG23	1:C:557:GLN:HG3	1.93	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:HD12	2:D:587:LEU:N	2.26	0.51
1:E:383:ASP:OD2	2:F:211:PRO:HD3	2.11	0.51
1:E:755:ASP:O	1:E:756:HIS:HB3	2.10	0.51
1:E:780:LEU:C	1:E:780:LEU:HD23	2.36	0.51
1:E:907:THR:HG21	1:E:1053:ILE:HD13	1.93	0.51
2:F:347:LEU:HD22	2:F:389:PHE:CG	2.46	0.51
1:G:41:ALA:O	1:G:42:ASN:C	2.54	0.51
1:G:77:LEU:HD23	1:G:88:ALA:HA	1.93	0.51
1:G:833:PRO:HA	1:G:840:TRP:CB	2.40	0.51
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.91	0.51
1:A:714:ARG:HD2	1:A:714:ARG:C	2.36	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:C:780:LEU:HD23	1:C:780:LEU:C	2.36	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:491:LEU:HD11	1:C:545:ILE:CG1	2.39	0.51
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:TYR:CE1	2:H:253:LEU:HD11	2.46	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:1044:LYS:HA	1:G:1079:GLU:HB2	1.93	0.51
2:H:143:ARG:C	2:H:144:ILE:HD12	2.36	0.51
1:A:833:PRO:HA	1:A:840:TRP:CB	2.40	0.50
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.93	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
1:G:716:ASN:C	1:G:716:ASN:OD1	2.53	0.50
2:H:212:GLU:HG2	2:H:243:ASP:CB	2.41	0.50
1:A:89:CYS:O	1:A:91:PRO:HD3	2.11	0.50
1:A:634:ASN:ND2	1:E:690:LYS:HG3	2.26	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:N	2:H:587:LEU:HD12	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:77:LEU:HD23	1:C:88:ALA:HA	1.93	0.50
1:C:692:HIS:ND1	1:G:694:GLU:HA	2.27	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:F:143:ARG:C	2:F:144:ILE:HD12	2.36	0.50
1:G:68:ALA:HB1	1:G:71:MET:HE2	1.93	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:O	1:E:848:HIS:ND1	2.45	0.50
1:G:674:GLN:HB2	1:G:699:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:595:ARG:HB2	1:E:597:ARG:HH12	1.77	0.50
1:G:987:PRO:O	1:G:988:ALA:HB3	2.11	0.50
1:A:716:ASN:C	1:A:716:ASN:OD1	2.54	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:89:CYS:O	1:C:91:PRO:HD3	2.12	0.50
1:C:698:LEU:N	1:C:698:LEU:HD12	2.25	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: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
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.12	0.50
2:B:462:GLN:HG2	2:B:463:THR:N	2.26	0.50
2:B:587:LEU:HD12	2:B:587:LEU:N	2.26	0.50
1:E:89:CYS:O	1:E:91:PRO:HD3	2.12	0.50
1:E:373:ASN:OD1	4:Q:1:NAG:C2	2.58	0.50
1:G:89:CYS:O	1:G:91:PRO:HD3	2.12	0.50
1:G:323:THR:O	1:G:324:SER:C	2.54	0.50
1:G:525:PRO:HA	1:G:532:GLY:HA2	1.92	0.50
1:A:597:ARG:HB3	1:A:731:ARG:O	2.12	0.50
1:A:656:VAL:HG21	1:A:687:LEU:HD11	1.94	0.50
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.42	0.50
1:C:68:ALA:HB1	1:C:71:MET:HE2	1.93	0.50
1:C:685:ARG:CZ	1:G:685:ARG:NH2	2.75	0.50
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.42	0.50
2:F:587:LEU:N	2:F:587:LEU:HD12	2.27	0.50
1:G:780:LEU:HD23	1:G:780:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:LEU:HD12	2:D:155:LEU:C	2.36	0.49
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.42	0.49
1:E:41:ALA:O	1:E:42:ASN:C	2.54	0.49
1:E:714:ARG:HD2	1:E:714:ARG:C	2.36	0.49
1:E:1044:LYS:HA	1:E:1079:GLU:HB2	1.93	0.49
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
1:A:461:ALA:N	1:A:462:PRO:HD3	2.27	0.49
1:A:713:LEU:HD23	1:A:713:LEU:C	2.38	0.49
1:A:886:ASN:O	1:A:888:PRO:HD3	2.12	0.49
1:C:41:ALA:O	1:C:42:ASN:C	2.55	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:70:ASN:HB3	1:G:94:HIS:ND1	2.27	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
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:CG	1:G:174:PHE:O	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:780:LEU:HD23	1:A:780:LEU:C	2.36	0.49
1:A:848:HIS:O	1:A:848:HIS:ND1	2.45	0.49
1:A:992:LEU:HD23	1:A:992:LEU:C	2.37	0.49
1:C:848:HIS:O	1:C:848:HIS:ND1	2.45	0.49
1:E:68:ALA:HB1	1:E:71:MET:HE2	1.93	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:666:ARG:HB3	2:B:498:HIS:NE2	2.28	0.49
1:A:698:LEU:HD12	1:A:698:LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG23	1:A:893:THR:O	2.12	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: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
1:C:4:ASP:CG	1:C:597:ARG:NH2	2.70	0.49
2:D:39:ARG:NE	2:D:447:ILE:HG23	2.28	0.49
2:D:135:LEU:CD1	2:D:139:THR:HB	2.43	0.49
1:E:886:ASN:O	1:E:888:PRO:HD3	2.12	0.49
1:E:1024:LEU:C	1:E:1024:LEU:HD23	2.38	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: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:C:1063:LEU:HG	1:C:1064:PRO:HD3	1.95	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:827:LEU:CD1	1:C:829:CYS:SG	3.00	0.49
1:C:1058:SER:O	1:C:1059:VAL:HB	2.13	0.49
1:E:827:LEU:CD1	1:E:829:CYS:SG	3.01	0.49
2:F:75:GLN:O	2:F:97:PHE:CD1	2.66	0.49
2:F:251:GLY:HA3	2:F:278:ASP:OD1	2.13	0.49
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.43	0.49
1:C:1024:LEU:HD23	1:C:1024:LEU:C	2.37	0.49
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.93	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:469:ARG:NH2	2:B:287:HIS:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ARG:HH11	2:B:594:PRO:HG2	1.77	0.49
1:A:771:LEU:O	1:C:789:TRP:CZ2	2.66	0.49
1:A:986:PRO:CB	1:A:987:PRO:CD	2.90	0.49
1:C:47:LEU:HB2	1:C:60:ILE:CG2	2.43	0.49
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.48	0.49
1:E:47:LEU:HB2	1:E:60:ILE:CG2	2.43	0.49
1:E:1058:SER:O	1:E:1059:VAL:HB	2.13	0.49
2:H:154:VAL:HG23	2:H:160:THR:HG21	1.94	0.49
2:H:285:LEU:C	2:H:287:HIS:N	2.71	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:110:LEU:HD11	2:B:237:LEU:HD23	1.95	0.48
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.47	0.48
1:C:992:LEU:HD23	1:C:992:LEU:C	2.38	0.48
1:E:31:VAL:HG21	1:E:86:LEU:HD13	1.94	0.48
1:E:70:ASN:HB3	1:E:94:HIS:ND1	2.28	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:70:ASN:HB3	1:A:94:HIS:ND1	2.28	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
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:385:TYR:CZ	2:F:253:LEU:HD11	2.48	0.48
1:E:780:LEU:O	1:E:865:VAL:HG12	2.14	0.48
1:G:780:LEU:O	1:G:865:VAL:HG12	2.13	0.48
1:G:907:THR:HG21	1:G:1053:ILE:HD13	1.93	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
1:C:73:LEU:C	1:C:73:LEU:HD12	2.38	0.48
1:C:689:LEU:C	1:C:689:LEU:HD12	2.39	0.48
1:C:986:PRO:HB3	1:C:987:PRO:HD2	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
1:E:1063:LEU:HG	1:E:1064:PRO:HD3	1.95	0.48
2:F:121:LEU:O	2:F:121:LEU:HD23	2.14	0.48
1:G:657:THR:HG23	1:G:720:VAL:HB	1.95	0.48
2:H:132:LEU:HA	2:H:135:LEU:HB3	1.95	0.48
2:H:135:LEU:CD1	2:H:139:THR:HB	2.43	0.48
1:A:576:THR:HG23	1:A:582:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:569:LEU:HD12	1:E:569:LEU:O	2.14	0.48
1:E:657:THR:HG23	1:E:720:VAL:HB	1.94	0.48
1:E:715:LEU:HD12	1:E:715:LEU:O	2.13	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:31:VAL:HG21	1:G:86:LEU:HD13	1.95	0.48
1:G:47:LEU:HB2	1:G:60:ILE:CG2	2.43	0.48
1:G:992:LEU:HD23	1:G:992:LEU:C	2.37	0.48
2:H:75:GLN:O	2:H:97:PHE:CD1	2.66	0.48
2:H:532:ARG:HD3	2:H:554:GLU:CG	2.43	0.48
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.28	0.48
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.14	0.48
2:D:656:GLN:HG2	2:D:657:GLN:N	2.28	0.48
1:E:470:GLY:HA2	1:E:497:HIS:O	2.13	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:679:ARG:C	1:C:679:ARG:HD3	2.39	0.48
1:C:797:GLY:HA3	1:C:884:GLU:HB2	1.95	0.48
1:E:656:VAL:HG21	1:E:687:LEU:HD11	1.95	0.48
1:E:1009:LEU:HD22	1:E:1011:PHE:CE1	2.49	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:73:LEU:C	1:A:73:LEU:HD12	2.38	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:25:TYR:CG	1:C:26:ALA:N	2.82	0.48
1:C:117:GLN:HB2	1:C:121:VAL:HG21	1.95	0.48
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.95	0.48
2:D:39:ARG:CD	2:D:447:ILE:HG23	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:938:VAL:HG12	1:E:1024:LEU:O	2.13	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
2:F:285:LEU:C	2:F:287:HIS:N	2.71	0.48
1:G:73:LEU:HD12	1:G:73:LEU:C	2.38	0.48
1:G:656:VAL:HG13	1:G:718:THR:O	2.14	0.48
1:G:752:CYS:HB2	1:G:793:GLU:CD	2.39	0.48
2:H:270:LEU:HD23	2:H:271:TYR:O	2.13	0.48
1:A:68:ALA:CB	1:A:71:MET:HE2	2.44	0.48
1:A:470:GLY:HA2	1:A:497:HIS:O	2.14	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:A:1063:LEU:HG	1:A:1064:PRO:HD3	1.96	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
1:G:713:LEU:HD23	1:G:713:LEU:C	2.38	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
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.96	0.48
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.44	0.48
1:C:569:LEU:HD12	1:C:569:LEU:O	2.14	0.48
1:C:715:LEU:HD12	1:C:715:LEU:O	2.13	0.48
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.49	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: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
1:A:608:PHE:O	1:A:609:ILE:C	2.57	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
1:C:930:HIS:O	1:C:931:VAL:C	2.57	0.48
2:D:222:ALA:HB2	2:D:294:ILE:CD1	2.44	0.48
1:G:575:LEU:HD12	1:G:576:THR:CG2	2.44	0.48
1:G:908:VAL:HG13	1:G:1069:PHE:HB3	1.96	0.48
1:G:986:PRO:CB	1:G:987:PRO:CD	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:N	1:A:110:LEU:HD12	2.29	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:C:713:LEU:HD23	1:C:713:LEU:C	2.39	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:71:MET:CG	1:G:90:GLY:HA3	2.44	0.47
1:G:121:VAL:O	1:G:121:VAL:CG1	2.62	0.47
1:G:478:LEU:HA	1:G:485:TRP:HE1	1.79	0.47
1:G:739:GLN:HB2	1:G:742:PHE:CE1	2.49	0.47
1:G:986:PRO:HG3	1:G:1003:CYS:O	2.13	0.47
1:A:4:ASP:HB2	1:A:597:ARG:CZ	2.44	0.47
1:A:73:LEU:HA	1:A:90:GLY:HA2	1.96	0.47
1:A:679:ARG:HD3	1:A:679:ARG:C	2.39	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:1024:LEU:HD23	1:A:1024:LEU:C	2.39	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:HG23	1:E:893:THR:O	2.13	0.47
2:F:110:LEU:HD11	2:F:237:LEU:HD23	1.95	0.47
2:F:222:ALA:HB2	2:F:294:ILE:CD1	2.45	0.47
2:F:270:LEU:HD23	2:F:271:TYR:O	2.14	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:689:LEU:C	1:G:689:LEU:HD12	2.39	0.47
1:G:741:TYR:CD2	2:H:502:VAL:HG22	2.49	0.47
1:G:961:GLU:HG2	1:G:1036:TRP:HA	1.96	0.47
1:G:1009:LEU:HD22	1:G:1011:PHE:CE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:LEU:C	1:E:73:LEU:HD12	2.39	0.47
1:E:73:LEU:HA	1:E:90:GLY:HA2	1.96	0.47
1:E:444:CYS:CB	1:E:506:LEU:CD1	2.93	0.47
1:E:689:LEU:C	1:E:689:LEU:HD12	2.39	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:273:PHE:CB	1:G:296:LYS:HD2	2.42	0.47
1:G:293:HIS:O	1:G:294:ILE:HG13	2.14	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:57:MET:HE2	2:H:57:MET:HA	1.96	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:789:TRP:CZ2	1:C:771:LEU:O	2.66	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:68:ALA:CB	1:C:71:MET:HE2	2.44	0.47
1:C:110:LEU:HD12	1:C:110:LEU:N	2.30	0.47
2:D:11:CYS:O	2:D:15:ILE:HG12	2.14	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
1:E:980:SER:HB3	1:E:1012:ARG:HB3	1.96	0.47
2:F:135:LEU:HD11	2:F:139:THR:HB	1.95	0.47
1:G:86:LEU:HD23	1:G:87:LEU:N	2.30	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
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:57:MET:HE2	2:B:57:MET:HA	1.96	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:353:SER:C	1:C:354:PHE:CG	2.92	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:C:961:GLU:HG2	1:C:1036:TRP:HA	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:609:ILE:CB	1:G:610:PRO:HD3	2.42	0.47
1:G:918:TYR:O	1:G:919:LEU:C	2.57	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
1:A:698:LEU:C	1:A:699:LEU:HD12	2.40	0.47
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.47
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.96	0.47
2:B:121:LEU:O	2:B:121:LEU:HD23	2.14	0.47
1:C:71:MET:CG	1:C:90:GLY:HA3	2.44	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:731:ARG:NH2	1:C:733:MET:SD	2.88	0.47
1:C:980:SER:HB3	1:C:1012:ARG:HB3	1.96	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:68:ALA:CB	1:G:71:MET:HE2	2.45	0.47
1:G:608:PHE:O	1:G:609:ILE:C	2.57	0.47
1:G:822:LEU:HG	1:G:823:ARG:N	2.30	0.47
1:G:893:THR:HG23	1:G:893:THR:O	2.15	0.47
1:G:1024:LEU:HD23	1:G:1024:LEU:C	2.39	0.47
1:G:1058:SER:O	1:G:1059:VAL:HB	2.13	0.47
2:H:39:ARG:CZ	2:H:447:ILE:HG23	2.43	0.47
1:A:13:VAL:HG21	1:A:57:CYS:HB2	1.96	0.47
1:A:117:GLN:HB2	1:A:121:VAL:HG21	1.95	0.47
1:A:121:VAL:O	1:A:121:VAL:CG1	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:930:HIS:O	1:A:931:VAL:C	2.57	0.47
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.14	0.47
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.96	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.97	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:D:659:GLY:O	2:D:662:ARG:HG2	2.15	0.47
1:E:68:ALA:CB	1:E:71:MET:HE2	2.44	0.47
1:E:831:SER:HB3	1:E:842:THR:HG22	1.96	0.47
2:F:43:ARG:N	2:F:44:PRO:CD	2.78	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
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:43:ARG:HB3	2:H:44:PRO:HD3	1.96	0.47
2:H:222:ALA:HB2	2:H:294:ILE:CD1	2.45	0.47
2:H:656:GLN:HG2	2:H:657:GLN:N	2.29	0.47
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.96	0.47
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.14	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: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:HB2	1:G:506:LEU:HD12	1.97	0.47
1:G:444:CYS:CB	1:G:506:LEU:CD1	2.92	0.47
1:G:657:THR:HG22	1:G:684:VAL:HG22	1.97	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
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
1:E:713:LEU:C	1:E:713:LEU:HD23	2.39	0.47
1:E:930:HIS:O	1:E:931:VAL:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:HIS:CE1	1:G:200:VAL:CG1	2.97	0.47
1:G:353:SER:C	1:G:354:PHE:CG	2.92	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
1:A:752:CYS:HB2	1:A:793:GLU:CD	2.40	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: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
1:G:156:ARG:HB3	1:G:197:LEU:HD13	1.97	0.47
1:G:679:ARG:C	1:G:679:ARG:HD3	2.40	0.47
1:G:1063:LEU:HG	1:G:1064:PRO:HD3	1.95	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:25:TYR:CG	1:A:26:ALA:N	2.82	0.46
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.45	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:71:MET:SD	1:C:90:GLY:HA3	2.55	0.46
2:D:149:PHE:HA	2:D:181:ALA:O	2.14	0.46
1:E:71:MET:SD	1:E:90:GLY:HA3	2.55	0.46
1:G:385:TYR:CZ	2:H:253:LEU:CD1	2.98	0.46
1:G:698:LEU:C	1:G:699:LEU:HD12	2.40	0.46
1:G:930:HIS:O	1:G:931:VAL:C	2.57	0.46
2:H:118:LEU:HD21	2:H:204:ILE:CD1	2.45	0.46
1:A:71:MET:CG	1:A:90:GLY:HA3	2.44	0.46
1:A:685:ARG:NH2	1:E:685:ARG:CZ	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:905:VAL:CG1	1:G:946:LEU:HD21	2.45	0.46
2:H:43:ARG:N	2:H:44:PRO:CD	2.78	0.46
2:H:149:PHE:HA	2:H:181:ALA:O	2.14	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:608:PHE:O	1:C:609:ILE:C	2.59	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:71:MET:CG	1:E:90:GLY:HA3	2.44	0.46
1:E:575:LEU:HD12	1:E:576:THR:CG2	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:71:MET:O	1:A:72:SER:C	2.58	0.46
1:A:93:VAL:HB	1:A:104:THR:CG2	2.45	0.46
1:A:103:LEU:HD13	2:B:156:PRO:HG3	1.97	0.46
1:A:689:LEU:C	1:A:689:LEU:HD12	2.40	0.46
1:C:698:LEU:C	1:C:699:LEU:HD12	2.41	0.46
1:E:608:PHE:O	1:E:609:ILE:C	2.58	0.46
1:E:679:ARG:C	1:E:679:ARG:HD3	2.40	0.46
1:E:753:GLY:C	1:E:755:ASP:H	2.22	0.46
1:G:93:VAL:HB	1:G:104:THR:CG2	2.45	0.46
2:H:277:PHE:CE1	2:H:278:ASP:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:277:PHE:CE1	2:D:278:ASP:O	2.68	0.46
1:E:93:VAL:HB	1:E:104:THR:CG2	2.44	0.46
1:E:353:SER:C	1:E:354:PHE:CG	2.92	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
2:F:363:PHE:HB2	2:F:388:THR:HB	1.96	0.46
1:G:71:MET:SD	1:G:90:GLY:HA3	2.55	0.46
1:G:73:LEU:HA	1:G:90:GLY:HA2	1.97	0.46
1:G:576:THR:HG23	1:G:582:ASP:OD2	2.14	0.46
1:G:731:ARG:NH2	1:G:733:MET:SD	2.88	0.46
2:H:27:LEU:HD21	2:H:446:GLY:C	2.40	0.46
1:A:559:SER:O	1:A:560:SER:C	2.59	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
1:E:918:TYR:O	1:E:919:LEU:C	2.58	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:71:MET:SD	1:A:90:GLY:HA3	2.55	0.46
1:A:406:PRO:HB3	1:A:438:TYR:CZ	2.51	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:285:LEU:C	2:D:287:HIS:N	2.71	0.46
2:D:340:LYS:HD2	2:D:379:ASP:CG	2.41	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:O	2:F:98:ARG:HG2	2.15	0.46
1:G:850:ILE:HG22	1:G:851:PHE:N	2.30	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
2:B:334:ILE:HA	2:B:337:ALA:CB	2.46	0.46
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:GLY:O	2:B:662:ARG:HG2	2.15	0.46
1:C:601:TRP:HZ2	1:C:641:LYS:HD3	1.81	0.46
2:D:75:GLN:CD	2:D:98:ARG:O	2.59	0.46
1:E:975:PRO:HG2	1:E:977:LEU:HD11	1.98	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:772:LYS:O	1:G:773:SER:HB3	2.16	0.46
1:G:980:SER:HB3	1:G:1012:ARG:HB3	1.97	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:659:GLY:O	2:B:662:ARG:CG	2.63	0.46
1:C:71:MET:O	1:C:72:SER:C	2.59	0.46
1:E:71:MET:O	1:E:72:SER:C	2.58	0.46
1:E:656:VAL:HG13	1:E:718:THR:O	2.16	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:823:ARG:NH1	1:E:825:LEU:O	2.49	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
1:A:25:TYR:O	1:A:26:ALA:C	2.59	0.46
1:A:353:SER:C	1:A:354:PHE:CG	2.92	0.46
1:A:656:VAL:HG13	1:A:718:THR:O	2.15	0.46
2:B:6:PHE:CG	2:B:7:LYS:N	2.83	0.46
2:B:135:LEU:CD1	2:B:139:THR:HB	2.45	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:559:SER:O	1:E:560:SER:C	2.59	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:99:ARG:HG3	1:G:100:ASN:OD1	2.16	0.46
1:G:939:ASN:HB3	1:G:1023:GLU:HA	1.98	0.46
2:H:6:PHE:CG	2:H:7:LYS:N	2.83	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:878:THR:HG22	1:A:896:GLN:HB3	1.99	0.45
1:A:939:ASN:HB3	1:A:1023:GLU:HA	1.98	0.45
1:C:575:LEU:HD12	1:C:576:THR:HG23	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
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
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
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.98	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:98:ARG:HG2	2:H:98:ARG:O	2.15	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:710:PRO:HG3	1:A:884:GLU:OE2	2.17	0.45
1:A:850:ILE:HG22	1:A:851:PHE:N	2.32	0.45
2:B:75:GLN:CD	2:B:98:ARG:O	2.59	0.45
2:B:305:VAL:HG13	2:B:306:LYS:N	2.32	0.45
1:C:25:TYR:O	1:C:26:ALA:C	2.59	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
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.45
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.52	0.45
1:E:4:ASP:HB2	1:E:597:ARG:CZ	2.46	0.45
1:E:446:VAL:CG1	1:E:456:LEU:HD11	2.47	0.45
1:E:698:LEU:C	1:E:699:LEU:HD12	2.41	0.45
1:E:790:ASN:HB2	1:E:851:PHE:CE1	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:559:SER:O	1:G:560:SER:C	2.59	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
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
1:A:685:ARG:CZ	1:E:685:ARG:NH2	2.79	0.45
2:B:98:ARG:O	2:B:98:ARG:HG2	2.15	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
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
2:F:652:TYR:HB3	2:F:667:VAL:HA	1.99	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:44:THR:CG2	1:A:71:MET:HE3	2.47	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:559:SER:O	1:C:560:SER:C	2.59	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:98:ARG:O	2:D:98:ARG:HG2	2.15	0.45
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.52	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:663:ASP:N	1:G:664:PRO:HD3	2.32	0.45
1:G:916:THR:O	1:G:1076:THR:HG23	2.17	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:75:GLN:CD	2:H:98:ARG:O	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:HIS:O	1:A:849:LEU:CB	2.65	0.45
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:919:LEU:HD11	2:D:643:ARG:NH1	2.32	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:E:121:VAL:O	1:E:121:VAL:CG1	2.62	0.45
1:E:623:GLN:C	1:E:624:VAL:HG22	2.39	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:71:MET:O	1:G:72:SER:C	2.58	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:446:VAL:CG1	1:A:456:LEU:HD11	2.47	0.45
1:A:662:LEU:HD21	1:A:698:LEU:HD23	1.99	0.45
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.46	0.45
1:A:686:VAL:CG1	1:E:695:ASN:O	2.64	0.45
1:A:804:HIS:CE1	1:A:840:TRP:NE1	2.85	0.45
1:A:1003:CYS:HB3	1:A:1008:CYS:HB2	1.85	0.45
2:B:665:ILE:N	2:B:665:ILE:HD12	2.32	0.45
1:C:22:VAL:HG22	1:C:23:VAL:N	2.32	0.45
1:C:23:VAL:HG22	1:C:24:GLN:N	2.31	0.45
1:C:1064:PRO:HG3	1:C:1067:GLU:OE2	2.16	0.45
2:D:345:VAL:HG11	2:D:387:ILE:HD11	1.98	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:E:724:LEU:HD12	1:E:729:ASN:ND2	2.32	0.45
1:E:964:TRP:HB3	1:E:1032:LEU:HA	1.99	0.45
2:F:99:ARG:O	2:F:383:ILE:O	2.35	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
1:G:243:LYS:HD2	1:G:246:ASP:OD2	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:52:TYR:O	1:A:53:SER:C	2.60	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: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
1:A:1023:GLU:O	1:A:1024:LEU:C	2.60	0.45
2:B:83:LEU:HD12	2:B:83:LEU:O	2.16	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
1:C:99:ARG:HG3	1:C:100:ASN:OD1	2.17	0.45
1:C:599:VAL:HG12	1:C:733:MET:HG3	1.99	0.45
1:C:676:THR:O	1:C:677:LYS:CB	2.65	0.45
1:C:766:PHE:HZ	1:C:877:LEU:HD12	1.82	0.45
1:C:804:HIS:CE1	1:C:840:TRP:NE1	2.85	0.45
1:C:831:SER:HA	1:C:842:THR:HG22	1.98	0.45
1:E:435:ILE:O	2:F:282:VAL:HG21	2.16	0.45
1:G:152:MET:HE1	1:G:171:LEU:HD21	1.98	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:285:LEU:C	2:B:287:HIS:N	2.71	0.45
2:B:383:ILE:HG22	2:B:384:ASN:N	2.32	0.45
1:C:69:VAL:HG12	1:C:70:ASN:N	2.32	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:44:THR:CG2	1:E:71:MET:HE3	2.47	0.45
1:E:416:ILE:HG22	1:E:427:LYS:HD3	1.99	0.45
1:E:599:VAL:HG12	1:E:733:MET:HG3	1.98	0.45
1:E:649:SER:O	1:E:650:ARG:HB3	2.16	0.45
1:G:69:VAL:HG12	1:G:70:ASN:N	2.32	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:848:HIS:O	1:G:849:LEU:CB	2.65	0.45
1:A:694:GLU:HA	1:E:692:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ASP:O	2:B:124:VAL:HB	2.17	0.45
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
1:C:8:LEU:C	1:C:8:LEU:HD12	2.42	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
1:E:8:LEU:C	1:E:8:LEU:HD12	2.42	0.45
1:E:348:LEU:N	1:E:348:LEU:HD12	2.32	0.45
1:E:525:PRO:HB3	1:E:564:TYR:HB2	1.99	0.45
1:E:772:LYS:O	1:E:773:SER:HB3	2.17	0.45
1:E:1064:PRO:HG3	1:E:1067:GLU:OE2	2.16	0.45
2:F:75:GLN:CD	2:F:98:ARG:O	2.59	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
1:G:665:GLY:C	2:H:498:HIS:HB3	2.42	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:25:TYR:OH	1:A:111:GLY:HA2	2.17	0.44
1:A:435:ILE:HD13	2:B:311:LEU:HB2	1.98	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:1045:VAL:HG22	1:A:1046:SER:N	2.32	0.44
1:C:4:ASP:HB2	1:C:597:ARG:CZ	2.46	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: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:57:MET:HE2	2:D:57:MET: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.99	0.44
1:C:419:GLN:HA	1:C:424:TRP:HA	1.99	0.44
1:C:761:ASN:O	1:C:762:LEU:HD23	2.17	0.44
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.99	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
1:G:8:LEU:C	1:G:8:LEU:HD12	2.42	0.44
2:H:108:TYR:CE2	2:H:147:GLY:HA3	2.52	0.44
1:A:8:LEU:C	1:A:8:LEU:HD12	2.42	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
2:B:671:ARG:C	2:B:672:GLU:HG3	2.42	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
1:C:1003:CYS:HB3	1:C:1008:CYS:HB2	1.85	0.44
2:D:215:LEU:HD12	2:D:246:HIS:O	2.17	0.44
2:D:219:MET:CE	2:D:262:GLY:HA2	2.47	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:113:THR:HG22	1:G:1029:LYS:CE	2.48	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: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:916:THR:O	1:C:1076:THR:HG23	2.17	0.44
1:C:971:HIS:CE1	1:C:974:ASN:CB	3.01	0.44
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.98	0.44
2:D:120:ASP:O	2:D:124:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:ALA:HB2	2:D:294:ILE:HD12	2.00	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:HA	2:D:565:ARG:HD3	1.83	0.44
2:D:665:ILE:HG22	2:D:666:TYR:N	2.32	0.44
1:E:662:LEU:HD21	1:E:698:LEU:HD23	1.98	0.44
1:E:880:ASN:OD1	1:E:894:THR:HG22	2.17	0.44
1:E:992:LEU:C	1:E:992:LEU:HD23	2.42	0.44
2:F:98:ARG:HB2	2:F:386:PRO:HG3	1.98	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
1:G:25:TYR:OH	1:G:111:GLY:HA2	2.17	0.44
1:G:52:TYR:O	1:G:53:SER:C	2.60	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:444:CYS:HB2	1:C:506:LEU:HD12	1.97	0.44
1:C:476:CYS:HB3	1:C:487:CYS:HA	1.98	0.44
1:C:507:THR:HG21	1:C:571:GLY:N	2.33	0.44
1:C:662:LEU:O	1:C:663:ASP:C	2.61	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:317:ILE:O	1:G:317:ILE:HG23	2.17	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: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
1:A:1028:LEU:HD12	1:A:1028:LEU:O	2.17	0.44
2:B:237:LEU:HD13	2:B:294:ILE:HG23	1.99	0.44
2:B:432:ARG:O	2:B:433:ASP:HB2	2.16	0.44
2:B:507:ILE:HG22	2:B:508:TYR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:987:PRO:O	1:E:988:ALA:HB3	2.16	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
1:G:860:LEU:HD23	1:G:860:LEU:C	2.43	0.44
1:G:934:HIS:ND1	1:G:1074:THR:CG2	2.80	0.44
1:G:1020:VAL:HG12	1:G:1021:GLN:HG3	1.98	0.44
2:H:120:ASP:O	2:H:124:VAL:HB	2.17	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:25:TYR:OH	1:C:111:GLY:HA2	2.18	0.44
1:C:103:LEU:HD21	2:D:155:LEU:HD22	1.99	0.44
1:C:365:PRO:C	1:C:367:MET:H	2.26	0.44
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.98	0.44
1:C:565:PHE:CD2	1:C:565:PHE:C	2.96	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:HD12	2:F:83:LEU:O	2.17	0.44
1:G:122:SER:O	1:G:123:ARG:C	2.60	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
1:G:964:TRP:HB3	1:G:1032:LEU:HA	1.99	0.44
2:H:120:ASP:OD1	2:H:325:GLU:O	2.36	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
1:A:102:TYR:CG	1:A:331:GLU:HB3	2.52	0.44
1:A:477:PRO:C	1:A:479:PRO:HD3	2.43	0.44
1:A:565:PHE:CD2	1:A:565:PHE:C	2.95	0.44
1:A:916:THR:O	1:A:1076:THR:HG23	2.17	0.44
1:C:52:TYR:O	1:C:53:SER:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:VAL:HG12	1:E:70:ASN:N	2.32	0.44
1:E:676:THR:O	1:E:677:LYS:CB	2.65	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:44:THR:CG2	1:G:71:MET:HE3	2.48	0.44
1:G:172:MET:HE1	1:G:215:ASN:O	2.18	0.44
1:G:477:PRO:C	1:G:479:PRO:HD3	2.43	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
1:G:1020:VAL:O	1:G:1021:GLN:HB2	2.17	0.44
1:G:1028:LEU:HD12	1:G:1028:LEU:O	2.18	0.44
2:H:83:LEU:HD12	2:H:83:LEU:O	2.17	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
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.99	0.44
1:A:964:TRP:HB2	1:A:1032:LEU:HA	2.00	0.44
2:B:219:MET:CE	2:B:262:GLY:HA2	2.48	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
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.32	0.44
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.85	0.44
1:E:52:TYR:O	1:E:53:SER:C	2.60	0.44
1:E:419:GLN:HA	1:E:424:TRP:HA	1.99	0.44
1:E:874:ARG:NH2	1:G:894:THR:O	2.51	0.44
1:E:916:THR:O	1:E:1076:THR:HG23	2.18	0.44
1:G:158:VAL:O	1:G:158:VAL:HG12	2.17	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:G:1048:VAL:HG22	1:G:1075:THR:HB	2.00	0.44
1:A:122:SER:O	1:A:123:ARG:C	2.61	0.43
1:A:860:LEU:HD23	1:A:860:LEU:C	2.43	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:456:LEU:HA	1:E:477:PRO:HA	1.99	0.43
1:E:678:ASN:ND2	6:E:3678:NAG:C7	2.78	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
2:F:671:ARG:C	2:F:672:GLU:HG3	2.43	0.43
1:G:22:VAL:HG22	1:G:23:VAL:N	2.31	0.43
1:G:136:LEU:HD23	1:G:237:VAL:HG22	1.99	0.43
1:G:383:ASP:OD2	2:H:211:PRO:HD3	2.18	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:964:TRP:HB2	1:G:1032:LEU:HA	2.00	0.43
1:G:1023:GLU:O	1:G:1024:LEU:C	2.61	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
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:25:TYR:O	1:E:26:ALA:C	2.59	0.43
1:E:939:ASN:HB3	1:E:1023:GLU:HA	1.99	0.43
1:E:1020:VAL:O	1:E:1021:GLN:HB2	2.18	0.43
1:G:23:VAL:HG22	1:G:24:GLN:N	2.31	0.43
2:H:671:ARG:C	2:H:672:GLU:HG3	2.42	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
1:A:1048:VAL:HG22	1:A:1075:THR:HB	2.00	0.43
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.53	0.43
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.53	0.43
1:C:1028:LEU:HD12	1:C:1028:LEU:O	2.19	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:804:HIS:CE1	1:E:840:TRP:NE1	2.86	0.43
1:E:1018:PHE:O	1:E:1019:SER:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1048:VAL:HG22	1:E:1075:THR:HB	2.00	0.43
2:F:126:LYS:HG2	2:F:196:GLN:O	2.18	0.43
1:G:94:HIS:CD2	2:H:155:LEU:HD21	2.53	0.43
1:G:365:PRO:C	1:G:367:MET:H	2.26	0.43
1:G:601:TRP:HZ2	1:G:641:LYS:HD3	1.82	0.43
1:G:959:ASN:O	1:G:960:GLN:HB3	2.18	0.43
1:G:1018:PHE:O	1:G:1019:SER:C	2.61	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:69:VAL:HG12	1:A:70:ASN:N	2.32	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
1:A:970:SER:C	1:A:972:PRO:HD3	2.43	0.43
2:B:644:ASP:HB3	2:B:650:VAL:CG2	2.47	0.43
1:C:44:THR:CG2	1:C:71:MET:HE3	2.47	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:860:LEU:C	1:C:860:LEU:HD23	2.44	0.43
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.99	0.43
1:C:964:TRP:HB2	1:C:1032:LEU:HA	2.00	0.43
1:C:971:HIS:NE2	1:C:974:ASN:CB	2.82	0.43
2:D:383:ILE:HG22	2:D:384:ASN:N	2.32	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:565:PHE:CD2	1:E:565:PHE:C	2.95	0.43
1:E:919:LEU:C	1:E:919:LEU:HD12	2.44	0.43
1:E:964:TRP:HB3	1:E:1032:LEU:HG	2.00	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
2:F:237:LEU:HD13	2:F:294:ILE:HG23	1.99	0.43
1:G:351:VAL:HG23	1:G:352:GLY:N	2.33	0.43
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
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:81:THR:O	1:A:82:SER:C	2.62	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:686:VAL:HG11	1:E:695:ASN:O	2.18	0.43
1:A:964:TRP:HB3	1:A:1032:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:GLY:O	1:A:1066:GLN:HG3	2.19	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:465:TYR:CD1	1:C:469:ARG:HG2	2.54	0.43
1:C:477:PRO:C	1:C:479:PRO:HD3	2.43	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
1:C:964:TRP:HB3	1:C:1032:LEU:HG	2.01	0.43
1:C:1018:PHE:O	1:C:1019:SER:C	2.61	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:E:560:SER:C	1:E:561:ARG:CG	2.92	0.43
2:F:611:LYS:CB	2:F:667:VAL:HB	2.49	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
1:G:970:SER:C	1:G:972:PRO:HD3	2.44	0.43
2:H:6:PHE:CD2	2:H:7:LYS:N	2.85	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
1:A:348:LEU:HD12	1:A:348:LEU:N	2.33	0.43
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.99	0.43
1:A:909:VAL:HG12	1:A:1069:PHE:O	2.19	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:351:VAL:HG23	1:E:352:GLY:N	2.33	0.43
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
1:E:860:LEU:HD23	1:E:860:LEU:C	2.44	0.43
1:E:1045:VAL:HG22	1:E:1046:SER:N	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1020:VAL:O	1:G:1021:GLN:CB	2.67	0.43
2:H:25:GLN:HB2	2:H:445:CYS:CB	2.49	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:663:ASP:N	1:A:664:PRO:HD3	2.32	0.43
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.82	0.43
1:C:472:GLN:NE2	1:C:492:TYR:HB2	2.33	0.43
1:C:560:SER:C	1:C:561:ARG:CG	2.92	0.43
1:C:970:SER:C	1:C:972:PRO:HD3	2.44	0.43
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.19	0.43
2:D:6:PHE:CD2	2:D:7:LYS:N	2.87	0.43
2:D:237:LEU:HD13	2:D:294:ILE:HG23	1.99	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
1:E:1028:LEU:HD12	1:E:1028:LEU:O	2.19	0.43
2:F:6:PHE:CD2	2:F:7:LYS:N	2.86	0.43
2:F:144:ILE:HG22	2:F:195:PHE:CZ	2.54	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:566:GLY:O	1:G:567:GLN:C	2.62	0.43
1:A:365:PRO:C	1:A:367:MET:H	2.26	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
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.19	0.43
2:B:256:ILE:O	2:B:256:ILE:HG13	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
2:D:671:ARG:C	2:D:672:GLU:HG3	2.44	0.43
1:E:477:PRO:C	1:E:479:PRO:HD3	2.43	0.43
1:E:613:ILE:HD12	1:E:748:PHE:CD2	2.54	0.43
1:E:761:ASN:HB3	1:E:792:GLY:HA3	2.01	0.43
1:E:771:LEU:O	1:G:789:TRP:CZ2	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:25:TYR:O	1:G:26:ALA:C	2.59	0.43
1:G:172:MET:SD	1:G:216:VAL:CG2	3.07	0.43
1:G:662:LEU:O	1:G:663:ASP:C	2.62	0.43
1:G:796:TYR:CE2	1:G:850:ILE:HD13	2.54	0.43
2:H:99:ARG:O	2:H:383:ILE:O	2.37	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
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:1018:PHE:O	1:A:1019:SER:C	2.61	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: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
1:A:44:THR:HG21	1:A:71:MET:HE3	2.01	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
2:B:617:PHE:O	2:B:618:GLY:C	2.62	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:909:VAL:HG12	1:C:1069:PHE:O	2.19	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:99:ARG:HG3	1:E:100:ASN:OD1	2.18	0.43
1:E:374:MET:HE2	1:E:381:MET:HE1	2.01	0.43
1:E:766:PHE:CE1	1:E:877:LEU:HD11	2.54	0.43
1:E:799:THR:HA	1:E:845:ARG:HA	2.01	0.43
1:E:971:HIS:CE1	1:E:974:ASN:CB	3.00	0.43
2:F:617:PHE:O	2:F:618:GLY:C	2.62	0.43
1:G:81:THR:O	1:G:82:SER:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:874:ARG:NH2	1:C:894:THR:O	2.52	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
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:D:617:PHE:O	2:D:618:GLY:C	2.62	0.42
1:E:365:PRO:C	1:E:367:MET:H	2.26	0.42
1:E:970:SER:C	1:E:972:PRO:HD3	2.44	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:778:SER:O	1:G:779:ASN:C	2.62	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:84:SER:OG	1:E:968:GLU:OE1	2.32	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
2:F:401:GLU:HA	2:F:421:PRO:HD3	2.00	0.42
1:G:509:LEU:HB3	1:G:519:ASP:O	2.19	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:778:SER:O	1:A:779:ASN:C	2.62	0.42
1:C:919:LEU:C	1:C:919:LEU:HD12	2.44	0.42
2:D:584:GLY:O	2:D:586:GLN:HG2	2.20	0.42
2:D:639:THR:HG23	2:D:639:THR:O	2.19	0.42
1:E:44:THR:HG21	1:E:71:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:778:SER:O	1:E:779:ASN:C	2.63	0.42
1:E:920:ASN:O	1:E:1080:LYS:HG2	2.19	0.42
1:E:1054:THR:HG21	1:G:757:ILE:HG21	2.01	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:919:LEU:C	1:G:919:LEU:HD12	2.45	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:O	2:H:639:THR:HG23	2.19	0.42
1:A:7:GLU:O	1:A:595:ARG:NH2	2.53	0.42
1:A:374:MET:HE2	1:A:381:MET:HE1	2.01	0.42
1:A:433:THR:HG23	1:A:464:TYR:CE1	2.54	0.42
1:A:442:SER:O	1:A:459:ILE:HA	2.20	0.42
1:A:919:LEU:C	1:A:919:LEU:HD12	2.44	0.42
1:C:686:VAL:HG11	1:G:695:ASN:O	2.19	0.42
1:C:690:LYS:HG3	1:G:634:ASN:ND2	2.35	0.42
1:C:796:TYR:CE2	1:C:850:ILE:HD13	2.55	0.42
1:C:1065:GLY:O	1:C:1066:GLN:HG3	2.18	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:565:PHE:CD2	1:G:565:PHE:C	2.95	0.42
1:G:939:ASN:HA	1:G:1018:PHE:HZ	1.84	0.42
1:A:560:SER:C	1:A:561:ARG:HG3	2.45	0.42
1:A:761:ASN:HB3	1:A:792:GLY:HA3	2.00	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:374:MET:HE2	1:C:381:MET:HE1	2.01	0.42
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.84	0.42
1:E:620:CYS:HB3	1:E:702:SER:O	2.19	0.42
1:E:676:THR:O	1:E:677:LYS:HB3	2.19	0.42
1:E:748:PHE:N	1:E:748:PHE:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:263:ILE:HD12	1:G:317:ILE:CD1	2.49	0.42
1:G:560:SER:C	1:G:561:ARG:CG	2.92	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:529:GLU:C	1:A:531:ARG:H	2.28	0.42
1:A:560:SER:C	1:A:561:ARG:CG	2.92	0.42
1:A:566:GLY:O	1:A:567:GLN:C	2.62	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: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:C:1040:ILE:CD1	1:C:1042:GLN:HB2	2.49	0.42
1:E:430:VAL:HG23	1:E:430:VAL:O	2.20	0.42
1:E:586:GLY:HA2	1:E:591:VAL:HG23	2.00	0.42
1:E:934:HIS:ND1	1:E:1074:THR:CG2	2.82	0.42
1:E:1040:ILE:CD1	1:E:1042:GLN:HB2	2.49	0.42
1:G:374:MET:HE2	1:G:381:MET:HE1	2.01	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:G:1045:VAL:HG22	1:G:1046:SER:N	2.33	0.42
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.55	0.42
1:A:1040:ILE:CD1	1:A:1042:GLN:HB2	2.50	0.42
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.49	0.42
1:C:73:LEU:HA	1:C:89:CYS:O	2.20	0.42
1:C:87:LEU:HD21	1:C:348:LEU:HD11	2.00	0.42
1:C:122:SER:O	1:C:123:ARG:C	2.61	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:1065:GLY:O	1:C:1066:GLN:CG	2.68	0.42
2:D:281:SER:OG	2:D:284:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LEU:HA	1:E:89:CYS:O	2.20	0.42
1:E:122:SER:O	1:E:123:ARG:C	2.61	0.42
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.02	0.42
1:E:407:ARG:HD2	2:F:250:ASP:OD2	2.20	0.42
1:E:529:GLU:C	1:E:531:ARG:H	2.27	0.42
1:E:871:LEU:CD1	1:E:901:VAL:HG11	2.50	0.42
1:E:1023:GLU:O	1:E:1024:LEU:C	2.62	0.42
2:F:455:ILE:HG22	2:F:456:GLY:N	2.35	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
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
2:B:99:ARG:O	2:B:383:ILE:O	2.37	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
1:C:44:THR:HG21	1:C:71:MET:HE3	2.02	0.42
1:C:81:THR:O	1:C:82:SER:C	2.63	0.42
1:C:748:PHE:N	1:C:748:PHE:CD1	2.88	0.42
1:C:766:PHE:CE1	1:C:877:LEU:HD11	2.55	0.42
1:C:826:HIS:HB3	1:C:848:HIS:NE2	2.35	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:7:GLU:O	1:E:595:ARG:NH2	2.53	0.42
1:E:81:THR:O	1:E:82:SER:C	2.63	0.42
1:E:629:THR:CG2	1:E:630:LEU:N	2.83	0.42
1:E:909:VAL:HG12	1:E:1069:PHE:O	2.19	0.42
1:E:959:ASN:C	1:E:961:GLU:H	2.28	0.42
1:E:1020:VAL:O	1:E:1021:GLN:CB	2.68	0.42
2:F:120:ASP:OD1	2:F:325:GLU:O	2.36	0.42
2:F:315:ILE:HA	2:F:316:PRO:HD3	1.87	0.42
1:G:676:THR:O	1:G:677:LYS:HB3	2.19	0.42
1:G:774:LEU:O	1:G:774:LEU:HG	2.20	0.42
1:G:1065:GLY:O	1:G:1066:GLN:HG3	2.19	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
1:A:918:TYR:CD1	1:A:918:TYR:C	2.98	0.42
2:B:162:PRO:O	2:B:165:LEU:CB	2.67	0.42
1:C:7:GLU:O	1:C:595:ARG:NH2	2.53	0.42
1:C:560:SER:C	1:C:561:ARG:HG3	2.45	0.42
1:C:678:ASN:ND2	6:C:3678:NAG:C7	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG23	2:F:639:THR:O	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:17:SER:HB2	2:H:21:CYS:SG	2.60	0.42
2:H:132:LEU:HD22	2:H:192:SER:HB3	2.01	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: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
1:C:1048:VAL:HG22	1:C:1075:THR:HB	2.00	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: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: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:1040:ILE:CD1	1:G:1042:GLN:HB2	2.49	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
1:C:694:GLU:HA	1:G:692:HIS:ND1	2.35	0.41
1:E:663:ASP:HB3	1:E:666:ARG:HD3	2.01	0.41
1:E:666:ARG:CZ	1:E:670:ARG:HH21	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:ARG:CD	2:H:447:ILE:HG23	2.49	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
1:A:469:ARG:C	1:A:498:PRO:HA	2.45	0.41
1:A:511:ASP:OD1	1:A:514:GLY:HA2	2.21	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
2:B:361:ASP:HB2	2:B:390:GLN:HB3	2.02	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:566:GLY:O	1:C:567:GLN:C	2.62	0.41
1:C:602:VAL:HG23	1:C:638:TYR:C	2.45	0.41
1:C:919:LEU:CB	1:C:1079:GLU:HB3	2.47	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:333:ALA:O	1:E:334:GLN:C	2.63	0.41
1:E:662:LEU:O	1:E:663:ASP:C	2.63	0.41
2:F:187:LYS:HG2	2:F:188:LEU:N	2.35	0.41
1:G:73:LEU:HA	1:G:89:CYS:O	2.20	0.41
1:G:191:SER:C	1:G:192:ASN:OD1	2.63	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
2:H:187:LYS:HG2	2:H:188:LEU:N	2.35	0.41
1:A:73:LEU:HA	1:A:89:CYS:O	2.20	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:766:PHE:HB3	1:A:786:VAL:HG23	2.02	0.41
1:A:848:HIS:HB2	2:B:485:SER:HB3	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
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:671:ALA:HB2	1:C:700:LEU:HD23	2.01	0.41
1:C:959:ASN:C	1:C:961:GLU:H	2.28	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:560:SER:C	1:E:561:ARG:HG3	2.45	0.41
1:E:602:VAL:HG23	1:E:638:TYR:C	2.46	0.41
1:E:985:ALA:HA	1:E:986:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:132:LEU:HD22	2:F:192:SER:HB3	2.01	0.41
2:F:162:PRO:O	2:F:165:LEU:CB	2.67	0.41
1:G:44:THR:HG21	1:G:71:MET:HE3	2.02	0.41
1:G:372:ILE:HG13	1:G:372:ILE:O	2.20	0.41
1:G:385:TYR:CE1	2:H:253:LEU:CD1	3.04	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:1065:GLY:O	1:G:1066:GLN:CG	2.68	0.41
2:H:302:SER:HB3	2:H:322:GLU:CG	2.50	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:A:1060:TYR:O	1:A:1061:SER:HB3	2.21	0.41
1:C:871:LEU:CD1	1:C:901:VAL:HG11	2.50	0.41
1:C:918:TYR:CD1	1:C:918:TYR:C	2.98	0.41
2:D:188:LEU:CD1	2:D:230:TRP:HA	2.51	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:671:ALA:O	1:E:672:THR:CG2	2.68	0.41
1:E:1065:GLY:O	1:E:1066:GLN:CG	2.68	0.41
2:F:584:GLY:O	2:F:586:GLN:HG2	2.20	0.41
1:G:117:GLN:HB3	1:G:121:VAL:CG2	2.50	0.41
1:G:560:SER:C	1:G:561:ARG:HG3	2.45	0.41
1:G:564:TYR:CZ	1:G:588:ARG:HD2	2.55	0.41
1:G:602:VAL:HG23	1:G:638:TYR:C	2.45	0.41
1:G:915:PHE:CD1	1:G:1074:THR:CG2	3.03	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:H:617:PHE:O	2:H:618:GLY:C	2.62	0.41
1:A:959:ASN:C	1:A:961:GLU:H	2.28	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: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
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:ILE:HG22	2:D:315:ILE:N	2.35	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:522:TYR:CE1	2:F:552:GLN:HA	2.54	0.41
2:F:545:GLY:O	2:F:555:ARG:HA	2.19	0.41
1:G:529:GLU:C	1:G:531:ARG:H	2.28	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
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:HG	1:A:774:LEU:O	2.21	0.41
1:A:789:TRP:NE1	1:C:772:LYS:HB3	2.35	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: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
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:58:ASP:N	2:F:59:PRO:CD	2.84	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
1:G:206:PHE:HB2	1:G:208:TYR:HE2	1.85	0.41
1:G:271:LEU:C	1:G:273:PHE:N	2.77	0.41
1:G:469:ARG:C	1:G:498:PRO:HA	2.46	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: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
1:A:1065:GLY:O	1:A:1066:GLN:CG	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:E:372:ILE:HG13	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:376:GLN:C	1:G:378:ASN:N	2.79	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
1:G:848:HIS:HB2	2:H:485:SER:HB3	2.02	0.41
2:H:98:ARG:HD3	2:H:386:PRO:HG3	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
5:T:2:NAG:C3	5:T:3:MAN:H2	2.50	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:106:ASP:OD2	2:B:188:LEU:HD13	2.21	0.41
2:B:130:ASP:HA	2:B:133:ARG:HB3	2.02	0.41
2:B:317:LYS:HZ1	2:B:409:LEU:HB3	1.85	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: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
1:G:665:GLY:CA	2:H:498:HIS:HB3	2.50	0.41
1:G:746:LEU:HD23	1:G:746:LEU:C	2.46	0.41
1:G:918:TYR:CD1	1:G:918:TYR:C	2.98	0.41
2:H:436:LEU:O	2:H:437:CYS:HB2	2.21	0.41
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:HB3	1:A:519:ASP:O	2.21	0.41
1:A:662:LEU:O	1:A:663:ASP:C	2.64	0.41
1:A:746:LEU:C	1:A:746:LEU:HD23	2.46	0.41
1:A:797:GLY:N	1:A:884:GLU:HB2	2.35	0.41
1:A:840:TRP:N	1:A:840:TRP:CD1	2.89	0.41
1:A:871:LEU:HD12	1:A:903:TYR:OH	2.20	0.41
1:A:871:LEU:CD1	1:A:901:VAL:HG11	2.50	0.41
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.51	0.41
2:B:317:LYS:NZ	2:B:409:LEU:HB3	2.36	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:422:ARG:HA	1:C:424:TRP:HZ3	1.86	0.41
1:C:507:THR:HG22	1:C:569:LEU:CD1	2.51	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
1:C:919:LEU:CD1	2:D:643:ARG:NH1	2.84	0.41
2:D:219:MET:SD	2:D:285:LEU:HD23	2.60	0.41
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.51	0.41
2:D:271:TYR:O	2:D:271:TYR:CG	2.74	0.41
2:D:442:PHE:CE1	2:D:449:ARG:HD3	2.55	0.41
2:D:532:ARG:HD3	2:D:554:GLU:CG	2.49	0.41
2:D:581:CYS:HB3	2:D:585:TYR:HB2	2.03	0.41
1:E:358:GLY:HA3	1:E:386:LEU:HB3	2.03	0.41
1:E:422:ARG:HA	1:E:424:TRP:HZ3	1.86	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
1:E:819:GLN:HA	1:E:820:GLY:HA2	1.80	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:956:VAL:O	1:E:963:VAL:HG23	2.21	0.41
2:F:154:VAL:HA	2:F:160:THR:CG2	2.49	0.41
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:HD3	2:F:565:ARG:HA	1.83	0.41
1:G:149:ALA:O	1:G:153:ASN:CG	2.64	0.41
1:G:352:GLY:HA2	1:G:356:TRP:HA	2.03	0.41
1:G:562:LEU:HD23	1:G:562:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:671:ALA:O	1:G:672:THR:CG2	2.69	0.41
1:G:908:VAL:HG12	1:G:909:VAL:N	2.35	0.41
1:G:959:ASN:C	1:G:961:GLU:H	2.28	0.41
2:H:69:HIS:HB2	2:H:70:ASN:H	1.73	0.41
2:H:352:LEU:HD22	2:H:358:VAL:HG23	2.03	0.41
2:H:565:ARG:HA	2:H:565:ARG:HD3	1.83	0.41
1:A:602:VAL:HB	1:A:639:ILE:CG2	2.51	0.41
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.68	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:469:ARG:HD3	2:D:283:GLY:HA3	2.03	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
1:C:1065:GLY:C	1:C:1066:GLN:CG	2.93	0.41
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.51	0.41
2:D:106:ASP:OD2	2:D:188:LEU:HD13	2.21	0.41
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:N	1:E:840:TRP:CD1	2.88	0.41
1:E:918:TYR:CD1	1:E:918:TYR:C	2.99	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
2:F:471:LEU:C	2:F:473:GLY:H	2.30	0.41
1:G:333:ALA:O	1:G:334:GLN:C	2.64	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: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:83:LEU:HD12	2:H:83:LEU:C	2.47	0.41
2:H:424:GLU:OE1	2:H:424:GLU:HA	2.21	0.41
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.56	0.40
1:A:484:ARG:HH12	2:B:586:GLN:HG3	1.80	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
1:A:1064:PRO:HG3	1:A:1067:GLU:OE2	2.18	0.40
2:B:345:VAL:HG11	2:B:387:ILE:HD11	2.03	0.40
1:C:430:VAL:O	1:C:430:VAL:HG23	2.20	0.40
1:C:1023:GLU:O	1:C:1024:LEU:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:601:GLY:C	2:H:603:TYR:H	2.29	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:915:PHE:CD1	1:A:1074:THR:CG2	3.04	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
2:B:599:PRO:O	2:B:603:TYR:CD2	2.75	0.40
1:C:43:GLN:O	1:C:70:ASN:HA	2.22	0.40
1:C:599:VAL:CG2	1:C:599:VAL:O	2.68	0.40
1:C:637:LEU:HD11	1:C:658:LEU:HD21	2.03	0.40
1:C:764:ILE:HD12	1:C:800:ILE:HD13	2.03	0.40
1:C:772:LYS:O	1:C:773:SER:CB	2.68	0.40
2:D:317:LYS:HE2	2:D:317:LYS:HB2	1.93	0.40
2:D:471:LEU:C	2:D:473:GLY:H	2.30	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:279:TRP:CD1	1:G:279:TRP:C	3.00	0.40
1:G:310:LEU:O	1:G:311:LYS:C	2.64	0.40
1:G:618:PHE:CE2	1:G:619:GLU:HG3	2.56	0.40
2:H:260:ASN:C	2:H:260:ASN:OD1	2.64	0.40
2:H:611:LYS:HG2	2:H:667:VAL:HB	2.03	0.40
1:A:332:MET:SD	2:B:208:LEU:HD13	2.61	0.40
1:A:614:PRO:O	1:A:615:ARG:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:LYS:HE3	1:A:1077:VAL:HG21	2.03	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:376:GLN:C	1:C:378:ASN:N	2.79	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:566:GLY:O	1:E:567:GLN:C	2.63	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:593:LEU:C	1:G:594:LEU:HD12	2.46	0.40
1:G:775:LEU:CD1	1:G:904:ALA:HB2	2.51	0.40
1:G:827:LEU:O	1:G:827:LEU:HD12	2.21	0.40
2:H:543:HIS:HB3	2:H:544:PRO:HD2	2.02	0.40
1:A:333:ALA:O	1:A:334:GLN:C	2.64	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
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:764:ILE:HD13	1:C:879:ALA:HB1	2.03	0.40
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.03	0.40
2:D:83:LEU:HD12	2:D:83:LEU:C	2.47	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: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:HD23	1:E:562:LEU:HA	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:402:VAL:CG1	1:G:443:LEU:HD22	2.51	0.40
1:G:422:ARG:HA	1:G:424:TRP:HZ3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:G:840:TRP:CD1	2.89	0.40
2:H:176:CYS:HB2	2:H:204:ILE:O	2.22	0.40
2:H:188:LEU:CD1	2:H:230:TRP:HA	2.51	0.40
2:H:234:THR:HG22	2:H:235:ARG:N	2.36	0.40
2:H:522:TYR:CD2	2:H:522:TYR:C	2.99	0.40
1:A:68:ALA:HA	1:A:93:VAL:HG13	2.04	0.40
1:A:358:GLY:HA3	1:A:386:LEU:HB3	2.03	0.40
1:A:376:GLN:C	1:A:378:ASN:N	2.79	0.40
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.51	0.40
1:A:419:GLN:CD	1:A:424:TRP:CD1	3.00	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:617:ALA:HB1	1:A:702:SER:HA	2.03	0.40
1:A:679:ARG:HD3	1:A:679:ARG:O	2.22	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
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:376:GLN:C	1:E:378:ASN:N	2.79	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.03	0.40
1:E:469:ARG:C	1:E:498:PRO:HA	2.46	0.40
1:E:609:ILE:HB	1:E:610:PRO:CD	2.47	0.40
1:E:1065:GLY:C	1:E:1066:GLN:CG	2.94	0.40
2:F:130:ASP:HA	2:F:133:ARG:HB3	2.02	0.40
2:F:271:TYR:O	2:F:271:TYR:CG	2.74	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:CD1	1:G:748:PHE:N	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
1:G:1058:SER:O	1:G:1059:VAL:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:118:LEU:HD23	2:H:204:ILE:HG21	2.04	0.40
2:H:219:MET:HE1	2:H:288:LYS:HG2	2.03	0.40
2:H:219:MET:O	2:H:223:ALA:HB2	2.21	0.40
2:H:305:VAL:HG13	2:H:306:LYS:HG3	2.03	0.40
2:H:312:THR:CG2	2:H:344:ARG:HH22	2.34	0.40
2:H:315:ILE:HA	2:H:316:PRO:HD3	1.87	0.40
2:H:513:GLU:HG2	2:H:514:CYS:N	2.36	0.40
2:H:578:VAL:HG12	2:H:579:CYS:N	2.35	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	876/1095 (80%)	660 (75%)	190 (22%)	26 (3%)	3	26
1	C	880/1095 (80%)	662 (75%)	193 (22%)	25 (3%)	4	27
1	E	878/1095 (80%)	659 (75%)	192 (22%)	27 (3%)	3	25
1	G	1080/1095 (99%)	834 (77%)	214 (20%)	32 (3%)	3	26
2	B	671/687 (98%)	511 (76%)	149 (22%)	11 (2%)	7	37
2	D	671/687 (98%)	514 (77%)	144 (22%)	13 (2%)	6	33
2	F	671/687 (98%)	512 (76%)	145 (22%)	14 (2%)	5	32
2	H	671/687 (98%)	512 (76%)	147 (22%)	12 (2%)	6	34
All	All	6398/7128 (90%)	4864 (76%)	1374 (22%)	160 (2%)	4	29

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	742 (99%)	7 (1%)	70	76
1	C	753/934 (81%)	746 (99%)	7 (1%)	70	76
1	E	751/934 (80%)	744 (99%)	7 (1%)	70	76
1	G	924/934 (99%)	914 (99%)	10 (1%)	65	74
2	B	582/592 (98%)	581 (100%)	1 (0%)	87	87
2	D	582/592 (98%)	581 (100%)	1 (0%)	87	87
2	F	582/592 (98%)	581 (100%)	1 (0%)	87	87
2	H	582/592 (98%)	581 (100%)	1 (0%)	87	87
All	All	5505/6104 (90%)	5470 (99%)	35 (1%)	78	81

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	PHE
1	A	567	GLN
1	A	639	ILE
1	A	681	LEU
1	A	823	ARG
1	A	915	PHE
1	A	933	MET
2	B	62	LEU
1	C	565	PHE
1	C	567	GLN
1	C	639	ILE
1	C	681	LEU
1	C	823	ARG
1	C	915	PHE
1	C	933	MET
2	D	62	LEU
1	E	565	PHE
1	E	567	GLN
1	E	639	ILE
1	E	681	LEU
1	E	823	ARG
1	E	915	PHE
1	E	933	MET
2	F	62	LEU
1	G	128	ARG
1	G	129	GLN
1	G	191	SER

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Mol	Chain	Res	Type
1	G	565	PHE
1	G	567	GLN
1	G	639	ILE
1	G	681	LEU
1	G	823	ARG
1	G	915	PHE
1	G	933	MET
2	H	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	366	ASN
1	A	463	HIS
1	A	472	GLN
1	A	495	GLN
1	A	623	GLN
1	A	692	HIS
1	A	1039	GLN
2	B	123	ASN
2	B	246	HIS
2	B	350	ASN
2	B	418	GLN
2	B	422	GLN
1	C	334	GLN
1	C	366	ASN
1	C	463	HIS
1	C	472	GLN
1	C	495	GLN
1	C	692	HIS
1	C	819	GLN
1	C	1039	GLN
2	D	123	ASN
2	D	194	GLN
2	D	246	HIS
2	D	293	ASN
2	D	350	ASN
2	D	418	GLN
2	D	422	GLN
2	D	479	ASN
2	D	510	GLN

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Mol	Chain	Res	Type
1	E	334	GLN
1	E	366	ASN
1	E	463	HIS
1	E	472	GLN
1	E	495	GLN
1	E	692	HIS
1	E	819	GLN
1	E	826	HIS
1	E	1039	GLN
2	F	123	ASN
2	F	194	GLN
2	F	246	HIS
2	F	265	HIS
2	F	350	ASN
2	F	418	GLN
2	F	422	GLN
2	F	479	ASN
1	G	168	GLN
1	G	179	GLN
1	G	334	GLN
1	G	366	ASN
1	G	463	HIS
1	G	495	GLN
1	G	692	HIS
1	G	697	ASN
1	G	819	GLN
1	G	1039	GLN
2	H	123	ASN
2	H	194	GLN
2	H	246	HIS
2	H	350	ASN
2	H	418	GLN
2	H	629	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	3,1	14,14,15	0.57	0	17,19,21	0.58	0
3	NAG	I	2	3	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.52	0	17,19,21	0.99	1 (5%)
4	NAG	J	2	4	14,14,15	0.53	0	17,19,21	2.17	2 (11%)
4	MAN	J	3	4	11,11,12	0.54	0	15,15,17	0.95	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.74	0	17,19,21	1.16	2 (11%)
4	NAG	K	2	4	14,14,15	0.65	0	17,19,21	0.82	0
4	MAN	K	3	4	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
4	NAG	L	1	4,1	14,14,15	0.71	0	17,19,21	2.16	5 (29%)
4	NAG	L	2	4	14,14,15	0.57	0	17,19,21	0.82	0
4	MAN	L	3	4	11,11,12	0.63	0	15,15,17	1.47	2 (13%)
3	NAG	M	1	3,1	14,14,15	0.48	0	17,19,21	0.74	0
3	NAG	M	2	3	14,14,15	0.64	0	17,19,21	1.17	1 (5%)
3	NAG	N	1	3,1	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
3	NAG	N	2	3	14,14,15	0.65	0	17,19,21	2.02	2 (11%)
4	NAG	O	1	4,1	14,14,15	0.61	0	17,19,21	1.34	1 (5%)
4	NAG	O	2	4	14,14,15	0.61	0	17,19,21	0.95	1 (5%)
4	MAN	O	3	4	11,11,12	0.66	0	15,15,17	1.34	2 (13%)
3	NAG	P	1	3,1	14,14,15	0.50	0	17,19,21	0.83	0
3	NAG	P	2	3	14,14,15	0.66	0	17,19,21	1.14	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.36	0	17,19,21	1.03	1 (5%)
4	NAG	Q	2	4	14,14,15	0.75	0	17,19,21	1.71	3 (17%)
4	MAN	Q	3	4	11,11,12	0.63	0	15,15,17	1.12	1 (6%)
4	NAG	R	1	4,1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
4	NAG	R	2	4	14,14,15	0.61	0	17,19,21	0.93	0
4	MAN	R	3	4	11,11,12	0.67	0	15,15,17	1.40	2 (13%)
3	NAG	S	1	3,1	14,14,15	0.57	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	S	2	3	14,14,15	0.63	0	17,19,21	1.08	1 (5%)
5	NAG	T	1	5,1	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
5	NAG	T	2	5	14,14,15	0.59	0	17,19,21	2.11	2 (11%)
5	MAN	T	3	5	11,11,12	0.54	0	15,15,17	0.73	0
5	MAN	T	4	5	11,11,12	0.62	0	15,15,17	0.49	0
4	NAG	U	1	4,1	14,14,15	0.65	0	17,19,21	1.82	3 (17%)
4	NAG	U	2	4	14,14,15	0.64	0	17,19,21	0.86	1 (5%)
4	MAN	U	3	4	11,11,12	0.66	0	15,15,17	1.27	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	3,1	-	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	4,1	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	4,1	-	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	4,1	-	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	3,1	-	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	3,1	-	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	4,1	-	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
3	NAG	P	1	3,1	-	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	4,1	-	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	Q	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	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	3,1	-	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	5,1	-	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	4,1	-	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 (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-O5-C5	7.64	122.42	112.19
5	T	2	NAG	C1-O5-C5	7.49	122.23	112.19
3	N	2	NAG	C1-O5-C5	7.14	121.76	112.19
4	U	1	NAG	C1-O5-C5	6.06	120.31	112.19
4	L	1	NAG	C1-O5-C5	5.45	119.49	112.19
4	O	1	NAG	C1-O5-C5	4.53	118.25	112.19
4	Q	2	NAG	C1-O5-C5	4.50	118.22	112.19
4	Q	2	NAG	C4-C3-C2	4.14	117.08	111.02
4	L	3	MAN	C1-O5-C5	4.10	117.68	112.19
4	R	3	MAN	C1-O5-C5	3.80	117.28	112.19
3	M	2	NAG	C1-O5-C5	3.53	116.92	112.19
4	L	1	NAG	C3-C4-C5	3.40	116.39	110.23
4	U	3	MAN	C1-O5-C5	3.26	116.55	112.19
4	K	3	MAN	C1-O5-C5	3.25	116.55	112.19
4	R	3	MAN	C1-C2-C3	3.23	114.35	109.64
4	O	3	MAN	C1-O5-C5	3.21	116.49	112.19
4	O	3	MAN	C1-C2-C3	3.20	114.31	109.64
4	J	2	NAG	O5-C1-C2	3.18	116.21	111.29
3	P	2	NAG	C1-O5-C5	3.18	116.45	112.19
3	N	2	NAG	O5-C1-C2	3.18	116.21	111.29
4	K	1	NAG	C4-C3-C2	3.17	115.66	111.02
4	L	3	MAN	C1-C2-C3	3.13	114.21	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1	NAG	O5-C5-C4	3.06	118.27	110.83
3	N	1	NAG	C1-O5-C5	3.03	116.25	112.19
3	I	2	NAG	C1-O5-C5	3.01	116.21	112.19
5	T	2	NAG	O5-C1-C2	2.95	115.85	111.29
4	U	3	MAN	C1-C2-C3	2.88	113.84	109.64
4	K	3	MAN	C1-C2-C3	2.86	113.80	109.64
4	R	1	NAG	C4-C3-C2	2.82	115.16	111.02
3	S	2	NAG	C1-O5-C5	2.82	115.96	112.19
4	J	1	NAG	C1-O5-C5	2.74	115.86	112.19
4	L	1	NAG	C4-C3-C2	2.74	115.04	111.02
4	K	1	NAG	C1-O5-C5	2.61	115.68	112.19
4	U	1	NAG	O5-C1-C2	2.59	115.30	111.29
4	Q	1	NAG	O5-C1-C2	2.58	115.28	111.29
4	L	1	NAG	O5-C1-C2	2.54	115.21	111.29
4	U	1	NAG	C4-C3-C2	2.41	114.55	111.02
4	Q	3	MAN	C1-O5-C5	-2.32	109.08	112.19
4	O	2	NAG	O4-C4-C3	2.27	115.72	110.38
4	Q	2	NAG	C3-C4-C5	2.21	114.25	110.23
5	T	1	NAG	C1-O5-C5	2.21	115.14	112.19
4	U	2	NAG	O4-C4-C3	2.19	115.54	110.38
4	J	3	MAN	C2-C3-C4	-2.15	107.08	110.86
4	J	3	MAN	O5-C5-C6	2.14	111.83	107.66

All (9) chirality outliers are listed below:

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

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C3-C2-N2-C7

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

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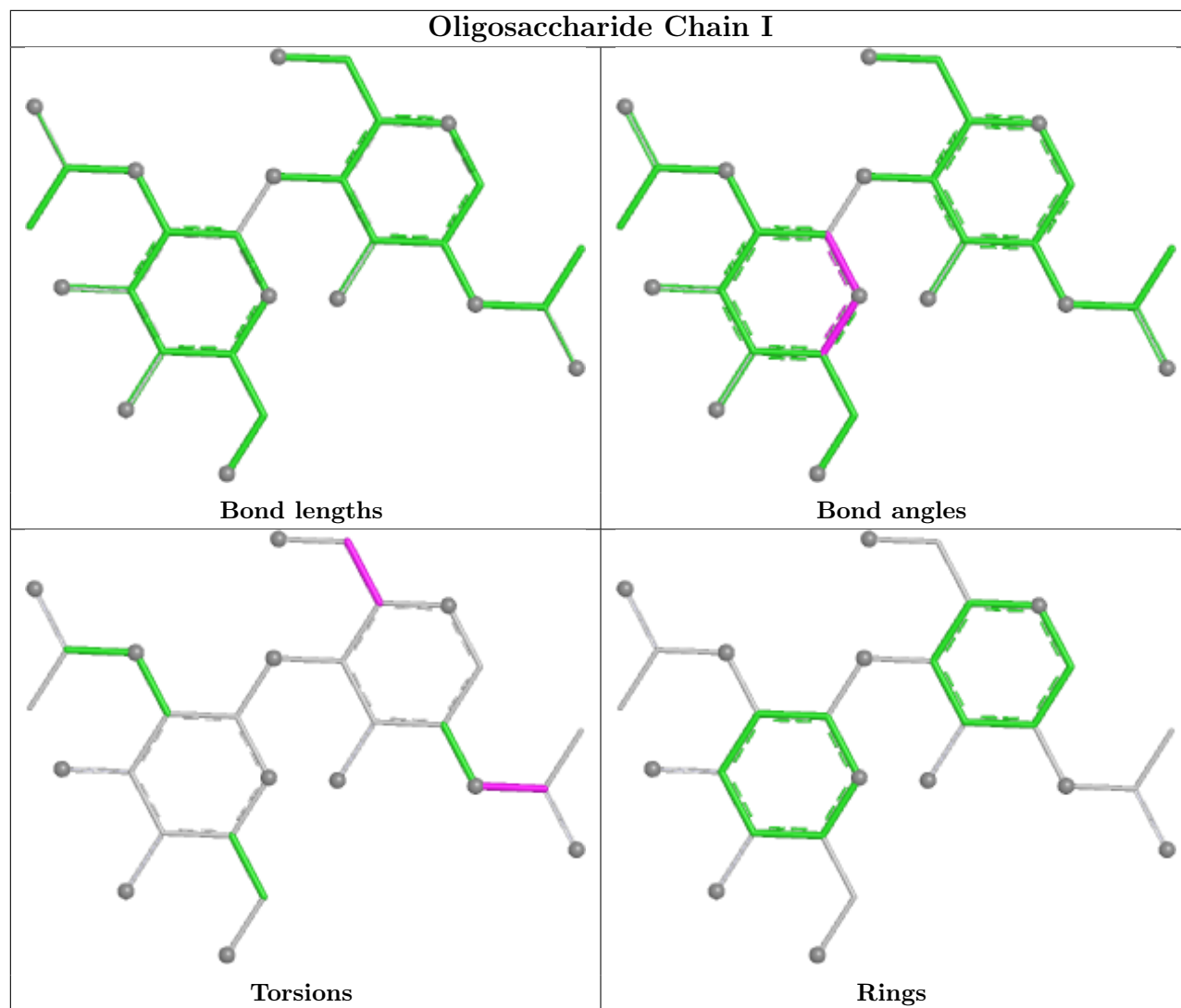
Mol	Chain	Res	Type	Atoms
5	T	1	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	M	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6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

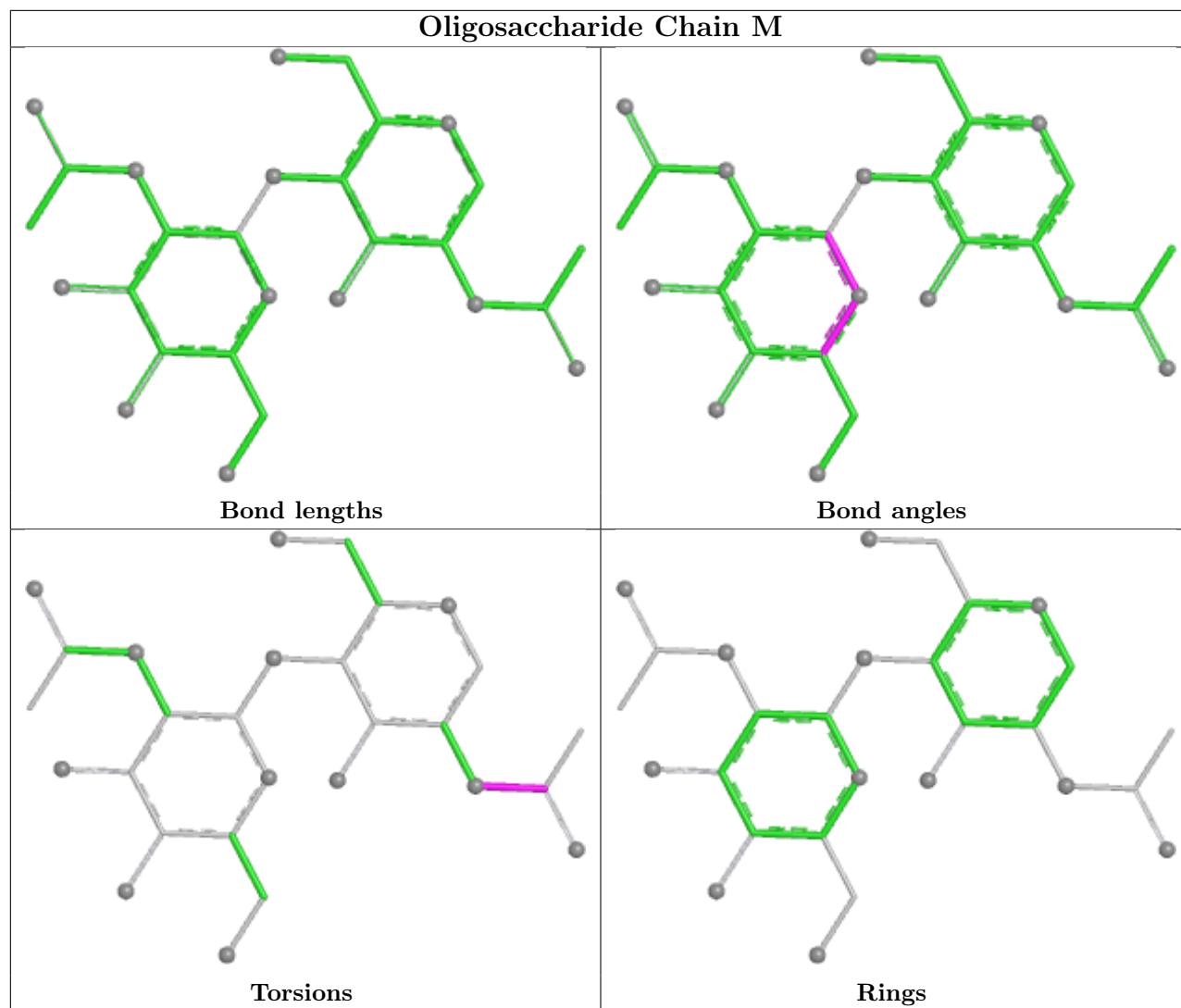
There are no ring outliers.

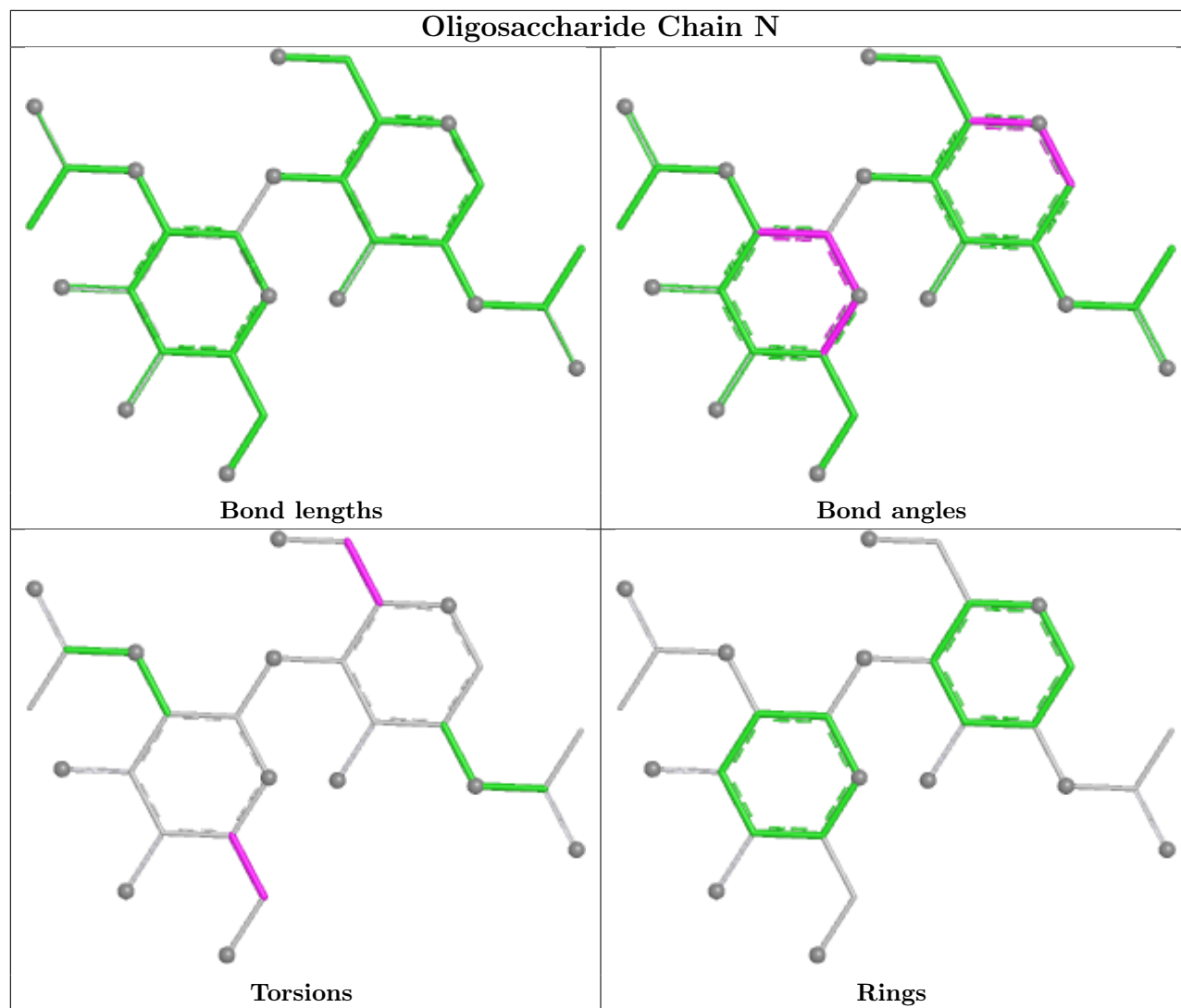
8 monomers are involved in 14 short contacts:

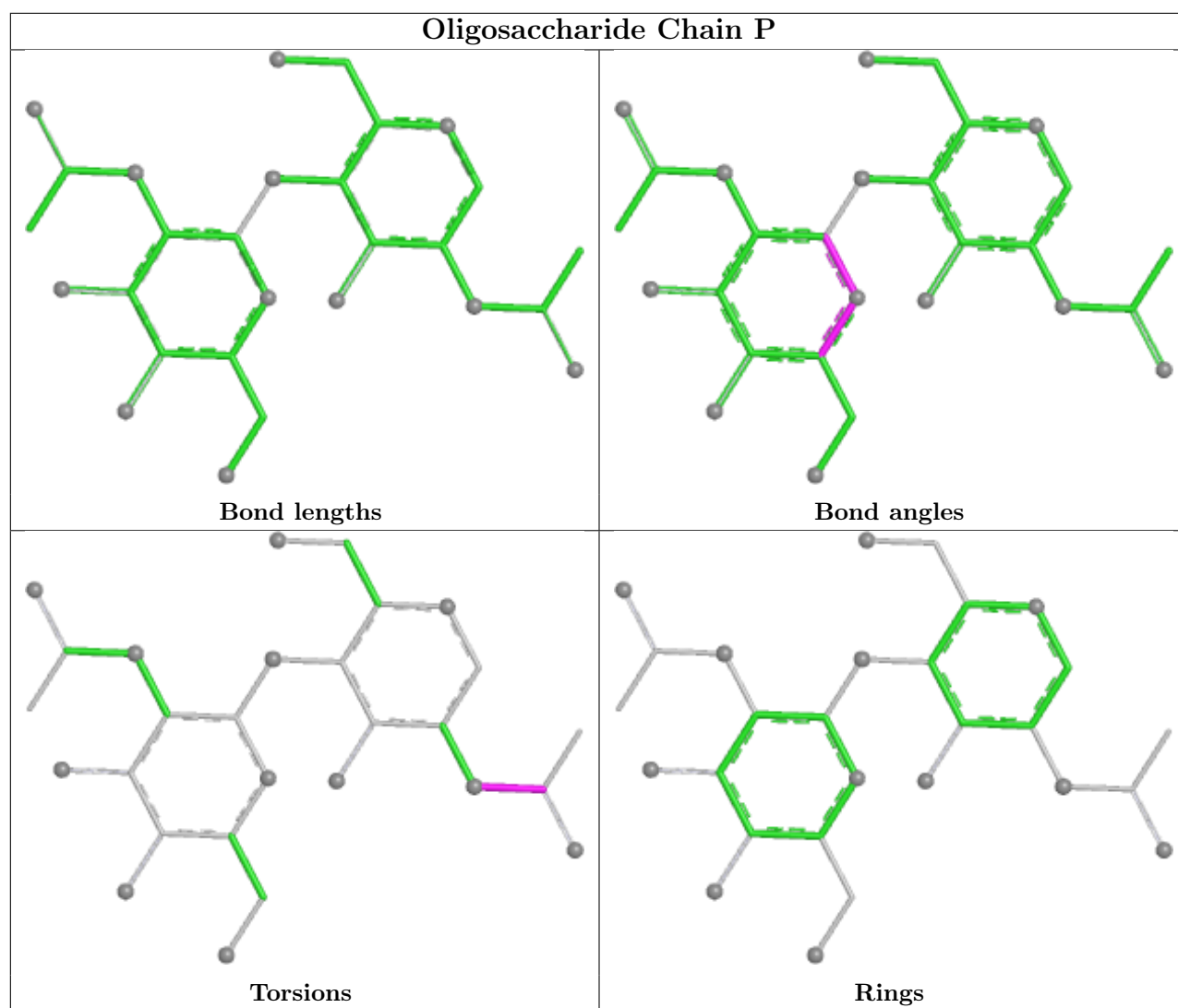
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	1	NAG	1	0
4	J	2	NAG	2	0
4	Q	2	NAG	5	0
4	J	3	MAN	2	0
5	T	3	MAN	2	0
4	J	1	NAG	1	0
4	Q	1	NAG	8	0
5	T	2	NAG	2	0

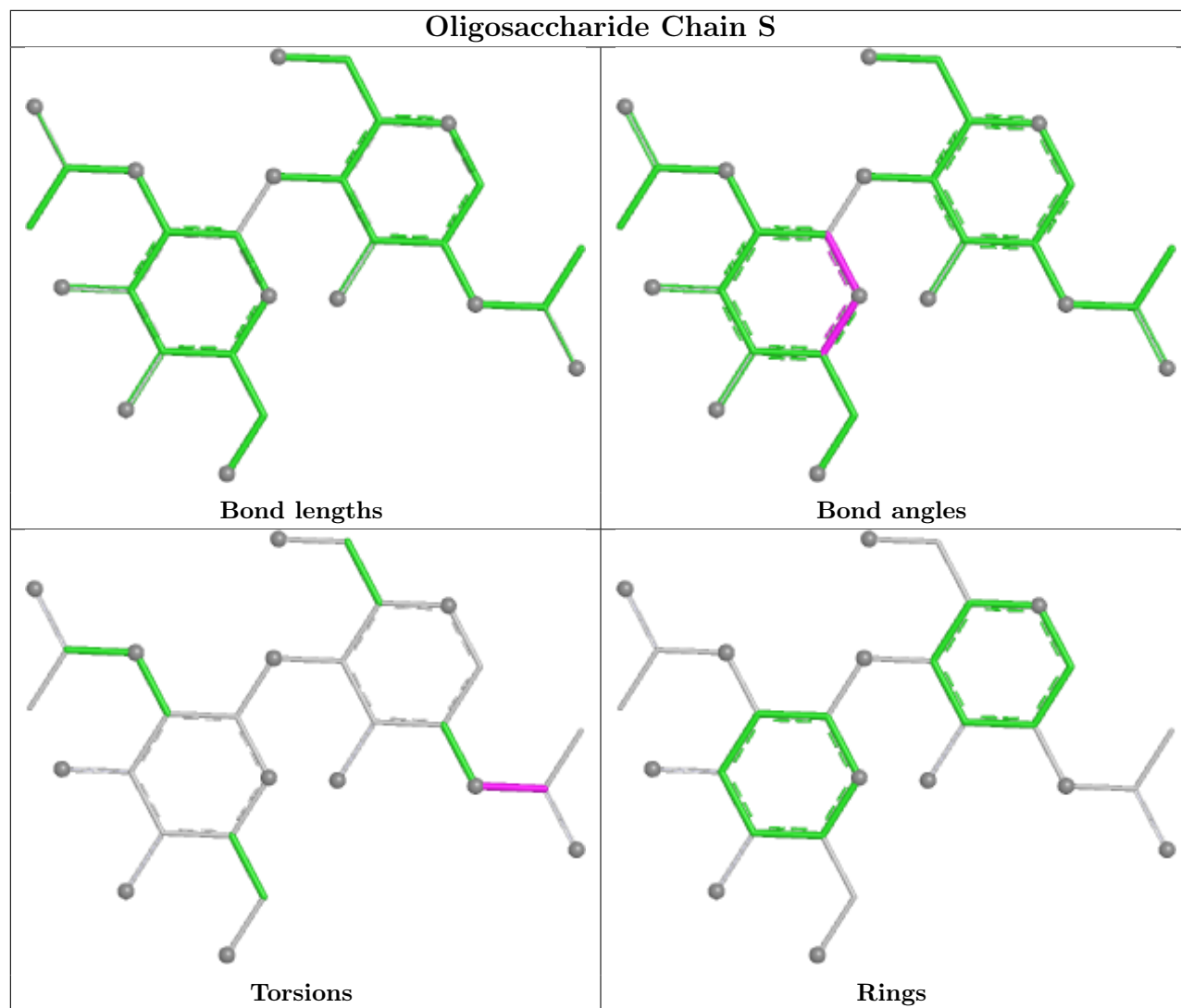
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

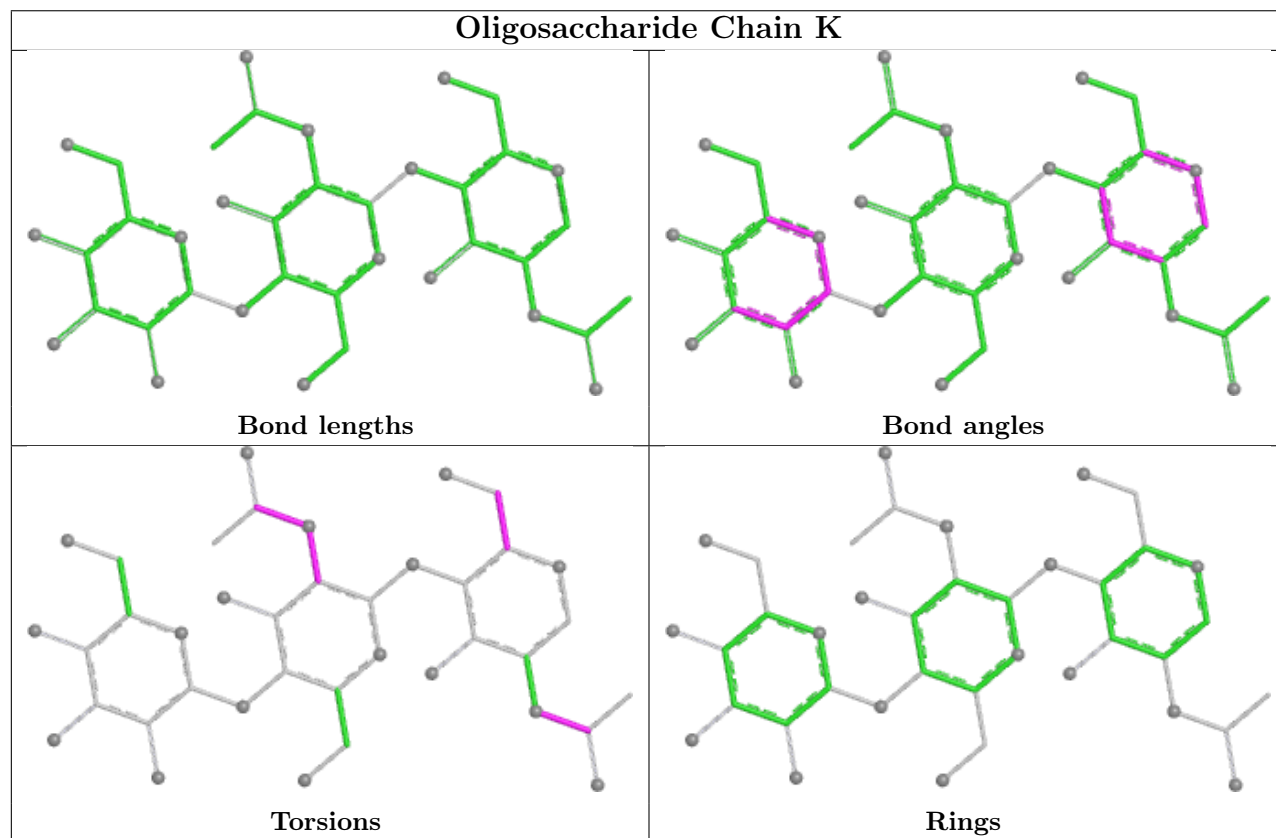
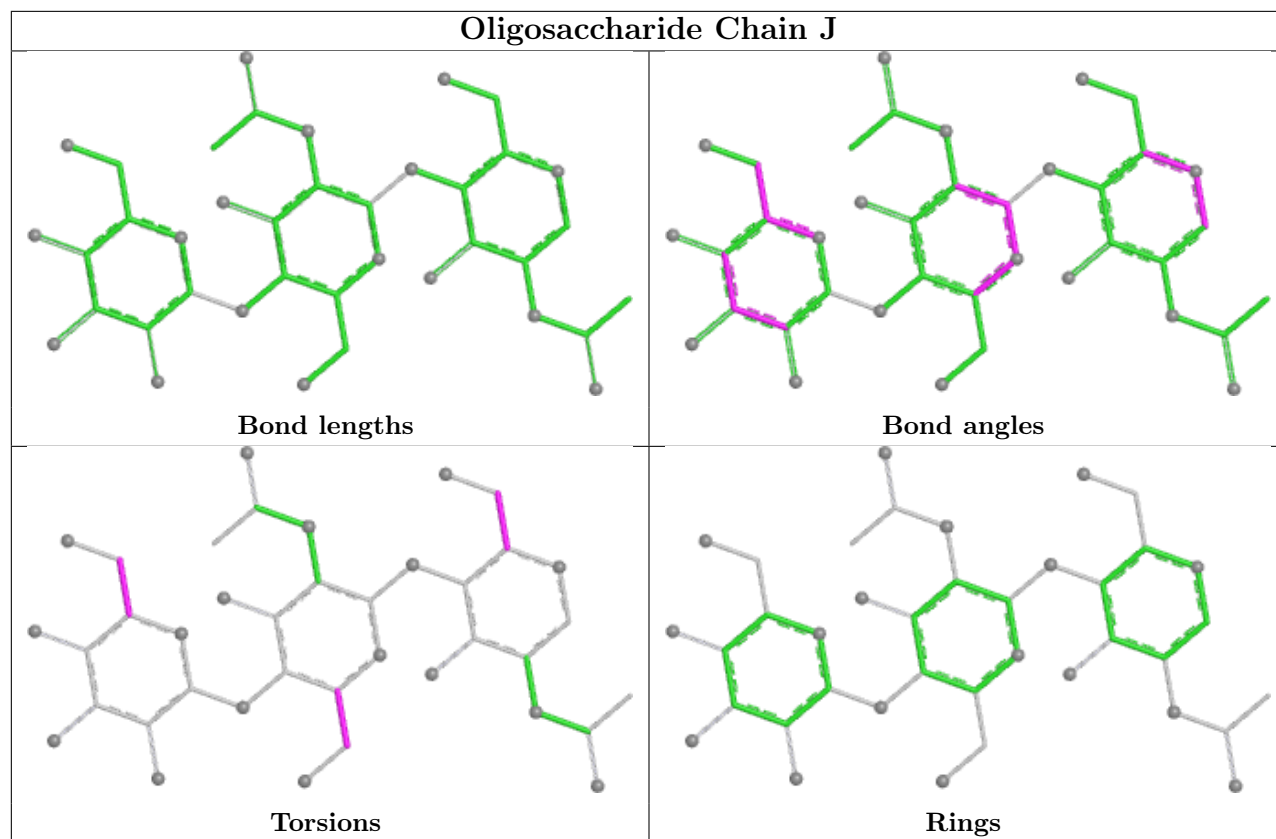


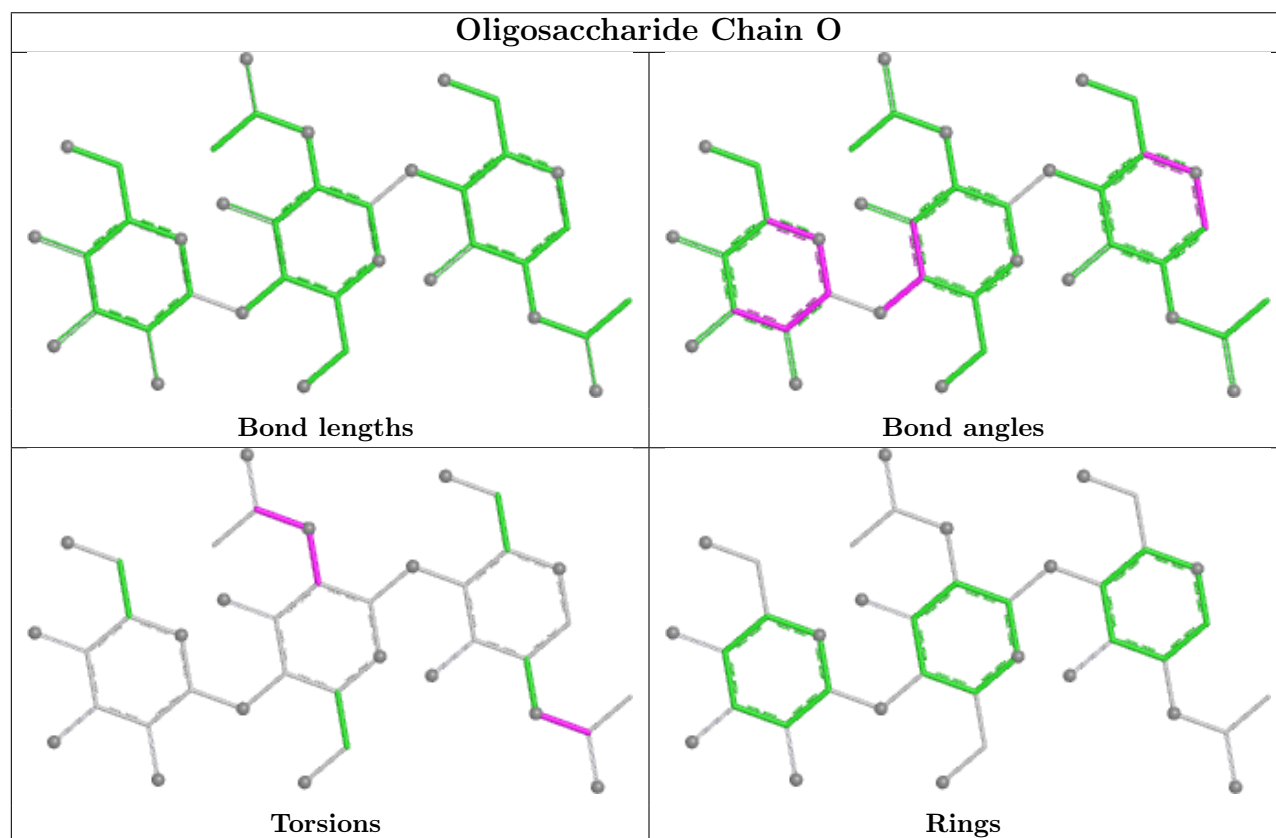
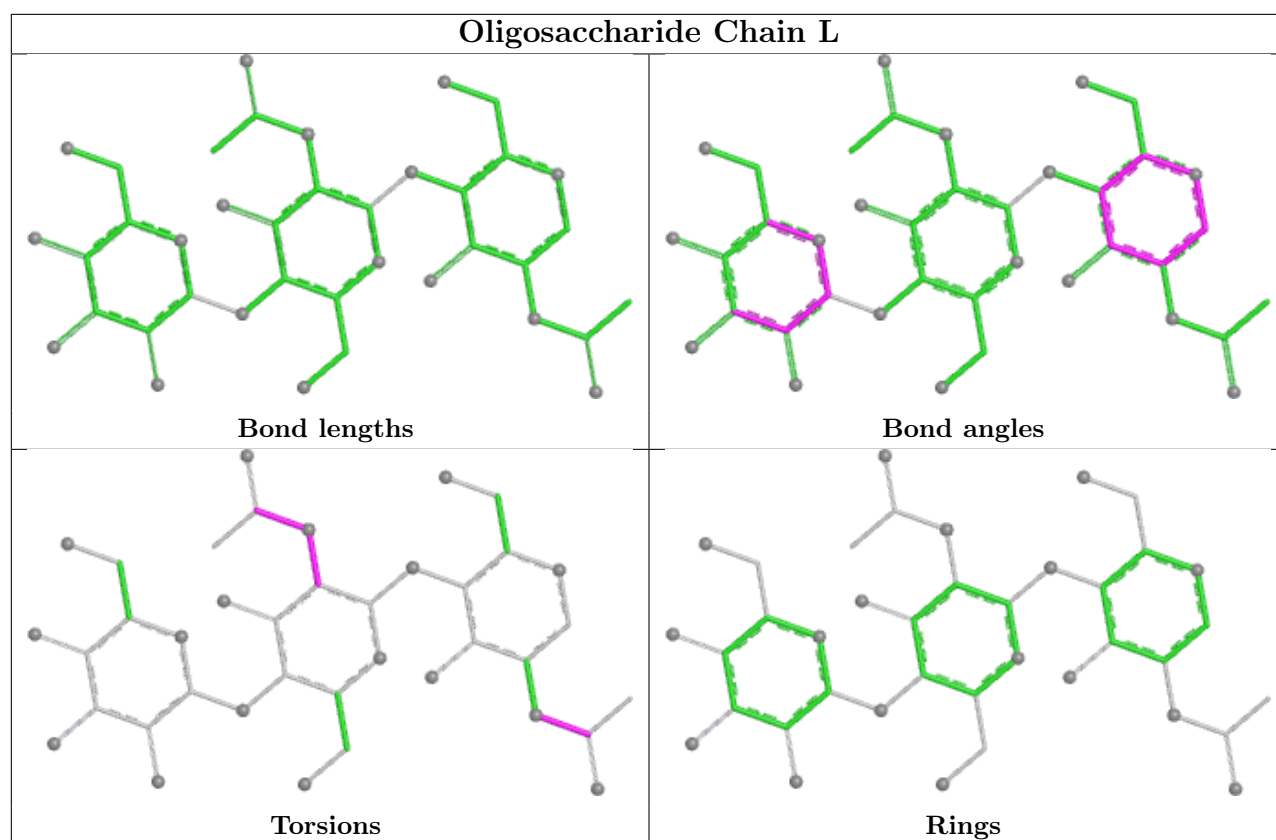


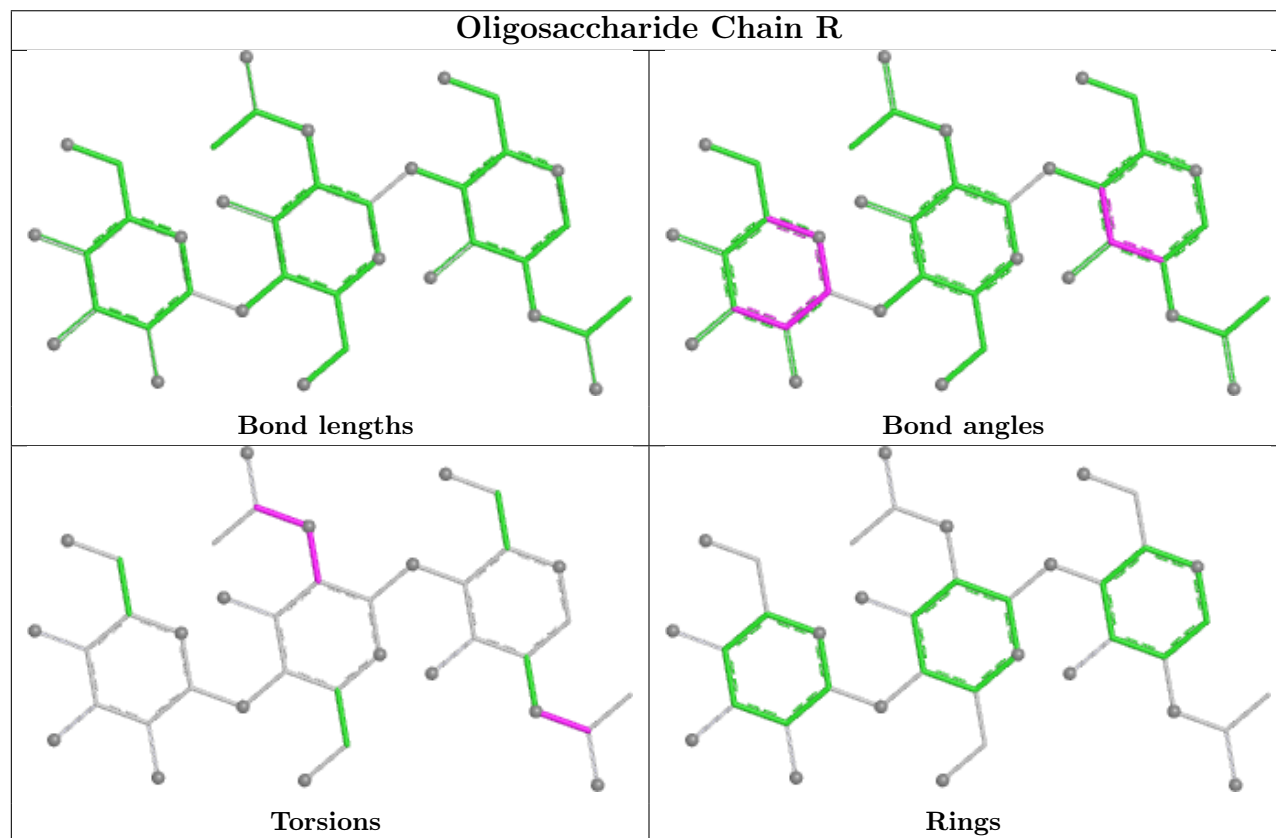
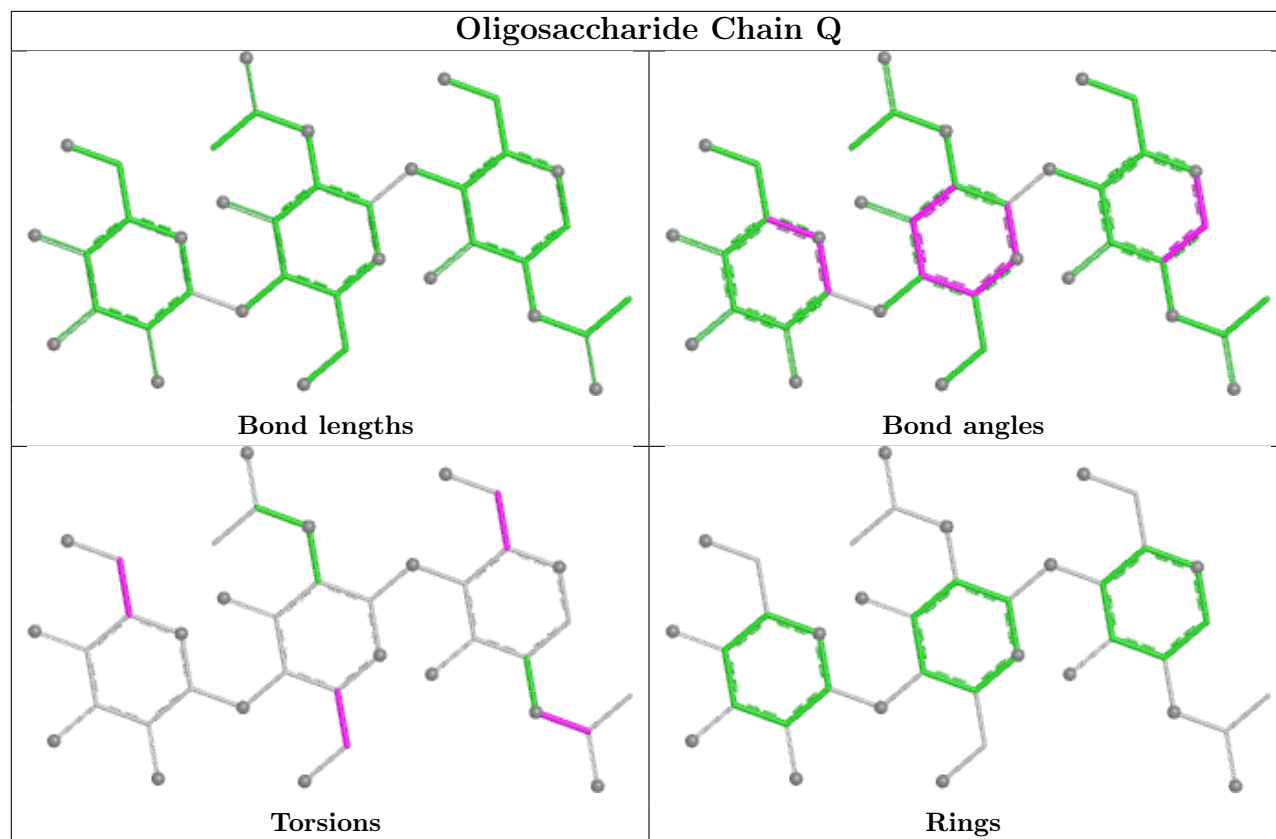


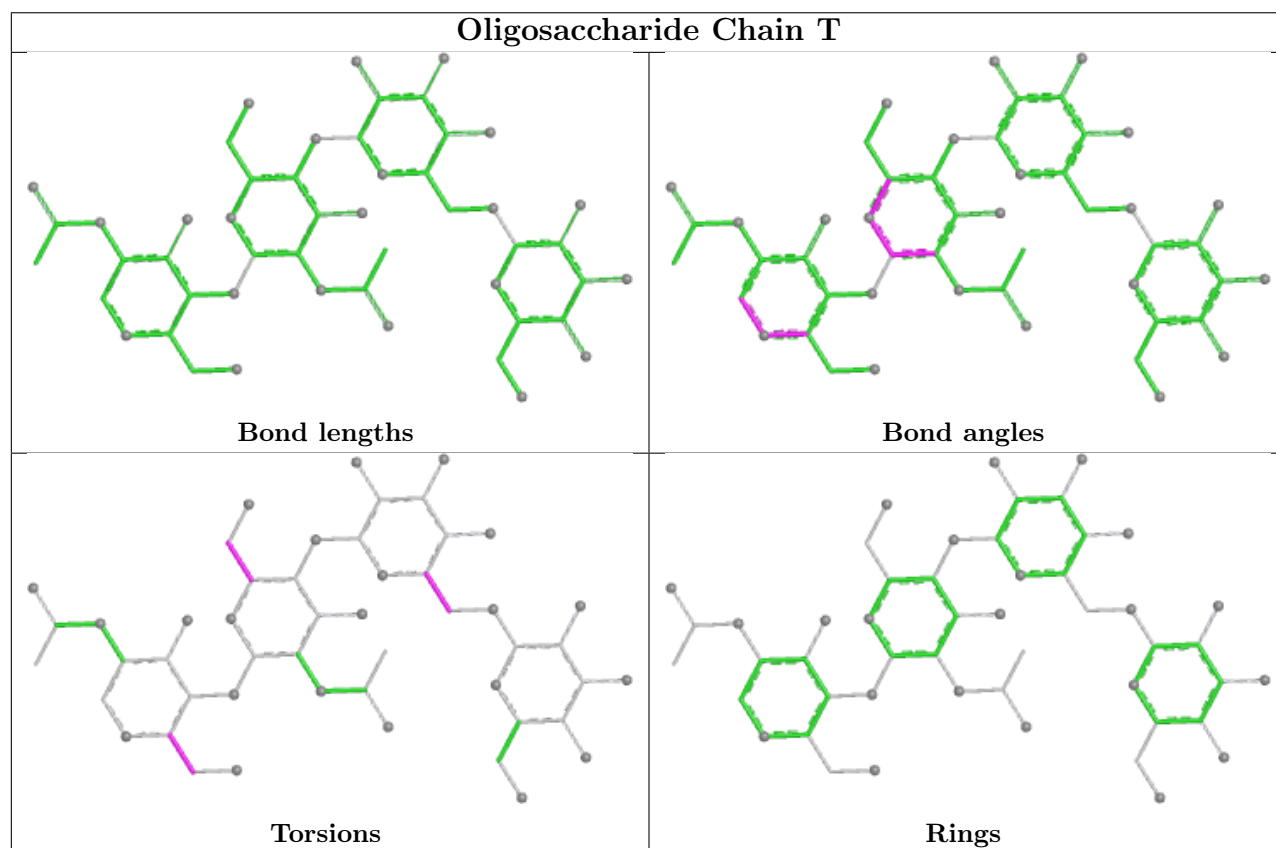
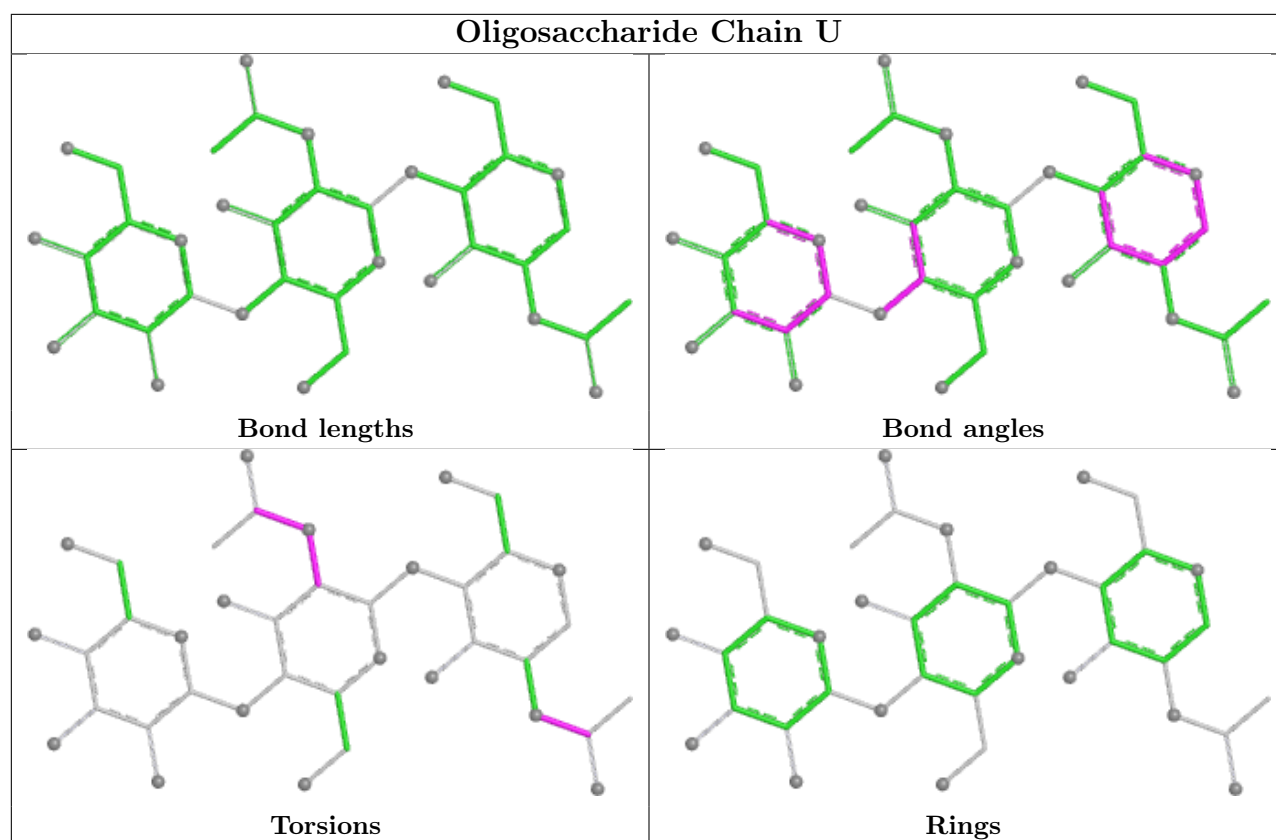












5.6 Ligand geometry

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	G	3678	1	14,14,15	0.50	0	17,19,21	0.93	2 (11%)
6	NAG	E	3880	1	14,14,15	0.45	0	17,19,21	1.71	1 (5%)
6	NAG	H	3479	-	14,14,15	0.48	0	17,19,21	0.92	0
6	NAG	C	3678	1	14,14,15	0.51	0	17,19,21	0.72	0
6	NAG	C	3880	1	14,14,15	0.47	0	17,19,21	1.51	1 (5%)
6	NAG	E	3678	1	14,14,15	0.51	0	17,19,21	0.97	2 (11%)
6	NAG	G	3880	1	14,14,15	0.48	0	17,19,21	1.58	1 (5%)
6	NAG	F	3479	-	14,14,15	0.54	0	17,19,21	0.87	1 (5%)
6	NAG	A	3678	1	14,14,15	0.50	0	17,19,21	0.90	2 (11%)
6	NAG	D	3094	2	14,14,15	0.45	0	17,19,21	0.78	0
6	NAG	B	3094	2	14,14,15	0.46	0	17,19,21	0.90	1 (5%)
6	NAG	D	3479	-	14,14,15	0.45	0	17,19,21	0.94	0
6	NAG	H	3094	2	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
6	NAG	B	3479	-	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
6	NAG	F	3094	2	14,14,15	0.49	0	17,19,21	0.90	1 (5%)

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	G	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	E	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	H	3479	-	-	0/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	2/6/23/26	0/1/1/1
6	NAG	C	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	E	3678	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	3880	NAG	C1-O5-C5	5.94	120.14	112.19
6	G	3880	NAG	C1-O5-C5	5.61	119.70	112.19
6	C	3880	NAG	C1-O5-C5	5.12	119.05	112.19
6	H	3094	NAG	C1-O5-C5	2.53	115.58	112.19
6	B	3094	NAG	C1-O5-C5	2.51	115.55	112.19
6	F	3094	NAG	C1-O5-C5	2.46	115.49	112.19
6	F	3479	NAG	C1-O5-C5	2.37	115.36	112.19
6	G	3678	NAG	O5-C1-C2	2.32	114.88	111.29
6	E	3678	NAG	O5-C1-C2	2.27	114.81	111.29
6	B	3479	NAG	C2-N2-C7	-2.26	119.88	122.90
6	G	3678	NAG	C1-O5-C5	2.25	115.20	112.19
6	E	3678	NAG	C1-O5-C5	2.18	115.11	112.19
6	A	3678	NAG	C1-O5-C5	2.14	115.05	112.19
6	A	3678	NAG	O5-C1-C2	2.03	114.44	111.29

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
6	G	3880	NAG	O7-C7-N2-C2
6	G	3880	NAG	O5-C5-C6-O6
6	C	3880	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
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	C	3678	NAG	1	0
6	E	3678	NAG	1	0
6	F	3479	NAG	3	0
6	D	3479	NAG	8	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%)	0.35	25 (2%)	55	39	101, 199, 283, 359	0
1	C	884/1095 (80%)	0.43	34 (3%)	44	32	97, 199, 280, 348	0
1	E	882/1095 (80%)	0.38	25 (2%)	55	39	96, 199, 283, 352	0
1	G	1082/1095 (98%)	0.40	27 (2%)	58	41	99, 211, 324, 419	0
2	B	673/687 (97%)	0.19	21 (3%)	51	36	70, 249, 313, 389	2 (0%)
2	D	673/687 (97%)	0.23	21 (3%)	51	36	70, 249, 312, 366	2 (0%)
2	F	673/687 (97%)	0.22	17 (2%)	58	41	71, 250, 314, 382	2 (0%)
2	H	673/687 (97%)	0.26	21 (3%)	51	36	70, 249, 313, 371	2 (0%)
All	All	6420/7128 (90%)	0.32	191 (2%)	52	37	70, 225, 307, 419	8 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	107	LEU	5.6
1	E	651	ASP	5.3
2	D	254	GLY	5.1
2	D	237	LEU	4.7
2	H	334	ILE	4.7
2	F	236	LEU	4.6
2	F	109	TYR	4.3
1	A	88	ALA	4.1
1	A	594	LEU	4.1
1	E	1065	GLY	4.1
2	H	254	GLY	4.0
1	C	433	THR	3.9
1	G	651	ASP	3.8
1	C	651	ASP	3.7
2	D	296	PRO	3.7
1	E	491	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	996	GLN	3.5
1	A	1078	LEU	3.5
1	E	599	VAL	3.4
2	B	597	PRO	3.4
1	A	385	TYR	3.4
2	B	32	PRO	3.3
1	C	541	LEU	3.2
1	A	77	LEU	3.2
1	C	491	LEU	3.2
2	D	37	SER	3.1
2	H	195	PHE	3.1
2	B	254	GLY	3.1
2	H	107	LEU	3.1
2	H	236	LEU	3.1
1	E	917	LYS	3.1
2	H	217	ALA	3.1
2	H	285	LEU	3.1
2	F	254	GLY	3.0
1	C	534	VAL	3.0
1	G	433	THR	3.0
1	E	74	GLY	3.0
1	C	382	ARG	3.0
2	B	236	LEU	2.9
1	A	553	ILE	2.9
1	C	74	GLY	2.9
1	A	918	TYR	2.9
1	E	106	LEU	2.9
1	E	594	LEU	2.9
1	G	465	TYR	2.9
2	H	161	HIS	2.8
1	G	394	LEU	2.8
1	G	466	GLU	2.8
1	A	1065	GLY	2.8
2	F	255	ALA	2.8
2	D	646	GLU	2.8
2	B	298	PHE	2.8
1	E	647	LEU	2.7
1	A	651	ASP	2.7
2	B	423	CYS	2.7
1	G	490	VAL	2.7
1	C	1048	VAL	2.7
1	G	777	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	239	THR	2.7
1	A	933	MET	2.7
1	G	88	ALA	2.6
2	H	651	ALA	2.6
1	E	383	ASP	2.6
1	A	106	LEU	2.6
1	E	394	LEU	2.6
2	D	294	ILE	2.6
2	F	283	GLY	2.6
1	C	1078	LEU	2.6
1	G	480	ARG	2.6
1	C	540	VAL	2.5
1	E	463	HIS	2.5
1	C	1000	VAL	2.5
1	A	346	PRO	2.5
1	C	553	ILE	2.5
1	C	777	GLY	2.5
1	C	504	ALA	2.5
2	F	597	PRO	2.5
2	F	638	ARG	2.5
1	E	379	VAL	2.5
1	A	964	TRP	2.5
1	G	127	PRO	2.5
2	B	537	CYS	2.5
2	D	239	PHE	2.4
2	H	7	LYS	2.4
2	H	144	ILE	2.4
1	G	118	ARG	2.4
2	F	463	THR	2.4
1	C	918	TYR	2.4
1	G	491	LEU	2.4
1	A	481	GLY	2.4
2	D	218	MET	2.4
2	D	96	THR	2.4
2	F	239	PHE	2.4
2	B	107	LEU	2.4
2	H	252	LYS	2.4
2	D	275	ASN	2.4
2	H	597	PRO	2.4
1	A	881	VAL	2.4
1	C	1075	THR	2.4
1	E	1063	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	87	LEU	2.4
2	F	409	LEU	2.4
1	C	533	ALA	2.4
1	G	198	ALA	2.4
1	C	106	LEU	2.4
2	D	295	GLN	2.3
1	E	629	THR	2.3
2	H	415	VAL	2.3
1	E	504	ALA	2.3
1	G	649	SER	2.3
1	G	689	LEU	2.3
1	A	32	VAL	2.3
1	C	434	GLN	2.3
2	D	131	LEU	2.3
1	C	1046	SER	2.3
2	B	156	PRO	2.3
1	A	482	TRP	2.3
2	H	131	LEU	2.3
2	D	433	ASP	2.3
1	G	32	VAL	2.3
2	B	415	VAL	2.3
1	C	383	ASP	2.3
1	A	1063	LEU	2.2
1	C	860	LEU	2.2
2	F	144	ILE	2.2
1	E	653	GLN	2.2
1	E	501	ARG	2.2
2	D	465	GLY	2.2
2	F	183	ARG	2.2
1	C	594	LEU	2.2
1	C	361	PHE	2.2
2	D	222	ALA	2.2
2	B	318	SER	2.2
2	D	156	PRO	2.2
2	D	63	ALA	2.2
1	E	802	PHE	2.2
1	C	601	TRP	2.2
1	A	472	GLN	2.2
1	E	592	LEU	2.2
2	H	174	LYS	2.2
1	C	847	ASN	2.2
2	B	217	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	237	LEU	2.2
1	E	834	VAL	2.2
2	D	415	VAL	2.2
2	B	334	ILE	2.2
2	F	195	PHE	2.2
1	A	491	LEU	2.2
1	E	119	LEU	2.2
1	E	650	ARG	2.1
2	H	37	SER	2.1
2	H	109	TYR	2.1
1	A	860	LEU	2.1
1	C	998	ASN	2.1
1	G	650	ARG	2.1
1	G	361	PHE	2.1
2	B	113	LEU	2.1
1	A	361	PHE	2.1
1	C	1065	GLY	2.1
2	B	31	GLY	2.1
2	D	673	CYS	2.1
2	H	145	GLY	2.1
1	C	773	SER	2.1
2	B	195	PHE	2.1
1	G	482	TRP	2.1
1	C	833	PRO	2.1
1	A	520	VAL	2.1
2	F	415	VAL	2.1
2	F	206	GLY	2.1
2	H	338	TYR	2.1
2	B	252	LYS	2.1
1	A	489	ALA	2.1
1	E	863	PHE	2.1
1	G	720	VAL	2.1
1	C	111	GLY	2.0
1	A	650	ARG	2.0
1	G	335	GLU	2.0
2	D	334	ILE	2.0
2	B	91	ALA	2.0
1	C	689	LEU	2.0
1	G	592	LEU	2.0
2	B	673	CYS	2.0
2	D	8	VAL	2.0
1	G	322	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	488	ASP	2.0
1	G	1078	LEU	2.0
1	C	1073	GLN	2.0
2	H	160	THR	2.0
1	E	488	ASP	2.0
2	B	186	LEU	2.0
2	F	285	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	I	2	14/15	-0.03	0.13	190,302,317,324	0
4	MAN	Q	3	11/12	-0.03	0.13	242,273,308,315	0
5	MAN	T	4	11/12	0.05	0.11	270,291,333,336	0
3	NAG	S	2	14/15	0.07	0.12	189,282,303,305	0
3	NAG	P	2	14/15	0.24	0.11	209,276,288,291	0
4	MAN	O	3	11/12	0.26	0.11	267,322,330,331	0
3	NAG	M	2	14/15	0.27	0.10	204,296,319,331	0
3	NAG	N	2	14/15	0.28	0.11	154,257,273,298	0
4	NAG	Q	2	14/15	0.29	0.12	286,310,336,351	0
5	MAN	T	3	11/12	0.31	0.12	286,318,328,335	0
4	MAN	L	3	11/12	0.33	0.12	187,257,308,323	0
4	NAG	Q	1	14/15	0.36	0.15	290,333,360,390	0
4	MAN	J	3	11/12	0.44	0.09	229,283,307,312	0
4	MAN	K	3	11/12	0.52	0.10	271,295,318,322	0
3	NAG	N	1	14/15	0.52	0.12	186,260,283,292	0
4	NAG	J	2	14/15	0.55	0.11	260,301,316,331	0
4	MAN	U	3	11/12	0.56	0.10	266,274,284,288	0
3	NAG	I	1	14/15	0.57	0.10	216,243,262,294	0
5	NAG	T	1	14/15	0.62	0.12	257,281,310,318	0
4	NAG	L	2	14/15	0.63	0.13	222,253,284,303	0
4	NAG	K	2	14/15	0.64	0.09	231,265,291,318	0

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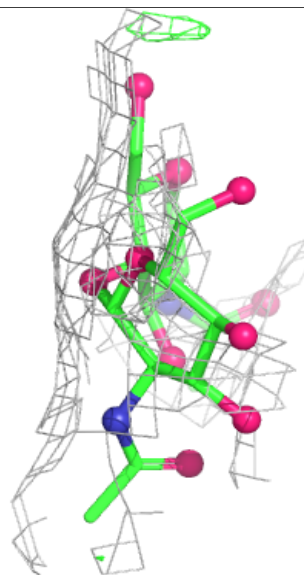
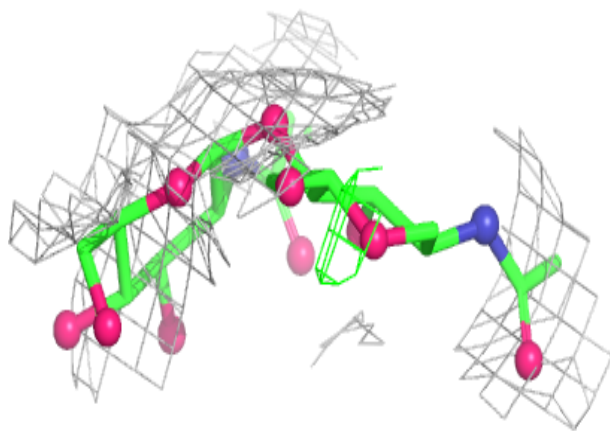
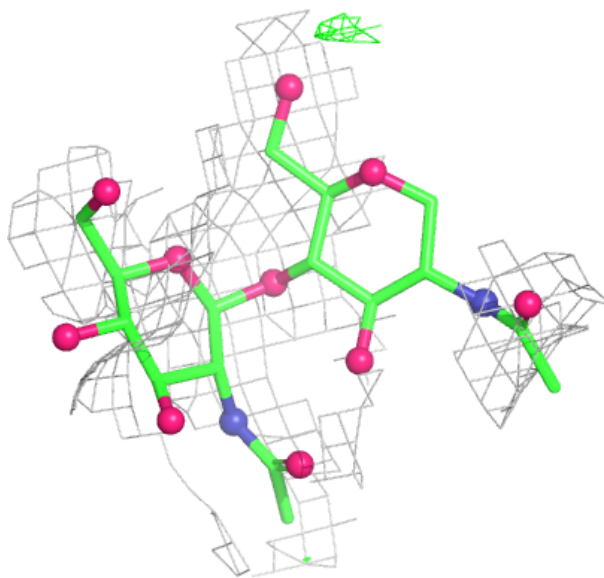
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	U	2	14/15	0.66	0.10	229,249,267,274	0
5	NAG	T	2	14/15	0.70	0.10	263,314,342,363	0
4	NAG	R	2	14/15	0.71	0.10	161,245,265,293	0
4	NAG	O	2	14/15	0.72	0.11	227,256,296,312	0
4	MAN	R	3	11/12	0.72	0.12	156,276,306,313	0
3	NAG	P	1	14/15	0.80	0.10	182,235,257,271	0
3	NAG	S	1	14/15	0.80	0.08	184,229,251,262	0
4	NAG	L	1	14/15	0.83	0.16	140,205,251,290	0
3	NAG	M	1	14/15	0.84	0.09	224,274,288,298	0
4	NAG	J	1	14/15	0.86	0.10	237,325,347,352	0
4	NAG	O	1	14/15	0.89	0.12	125,169,213,220	0
4	NAG	R	1	14/15	0.89	0.09	108,165,197,198	0
4	NAG	K	1	14/15	0.94	0.08	116,183,224,247	0
4	NAG	U	1	14/15	0.94	0.08	133,181,218,231	0

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

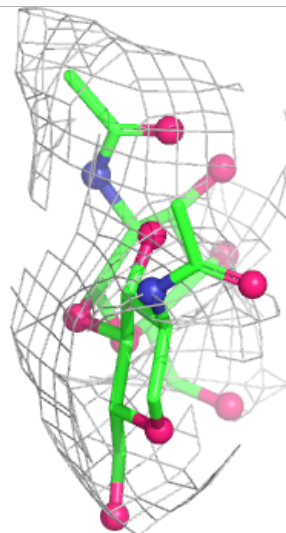
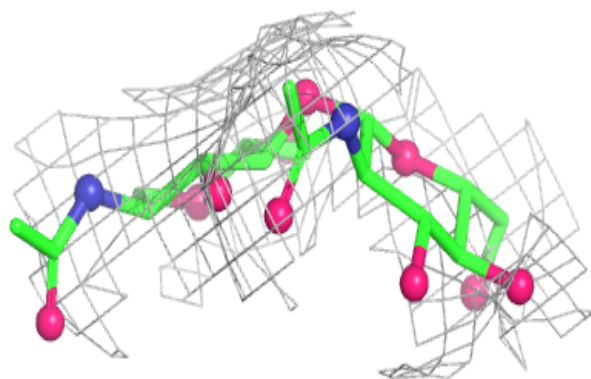
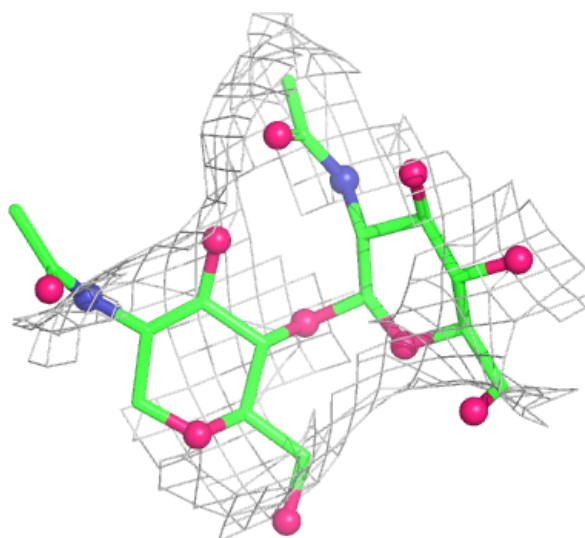
Electron density around Chain I:

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



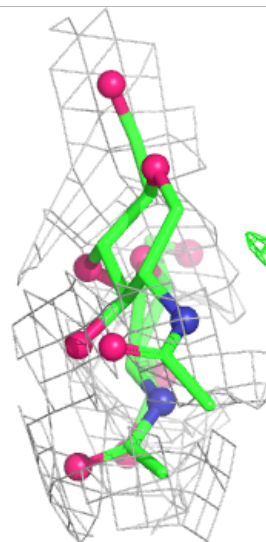
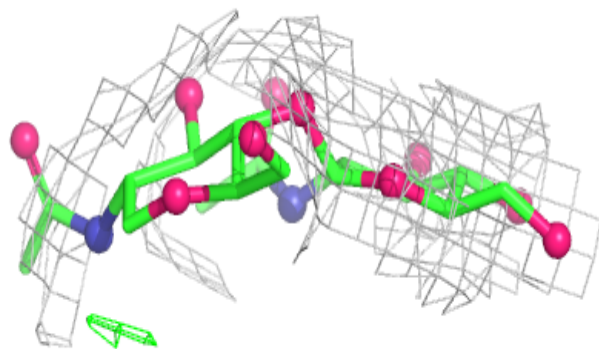
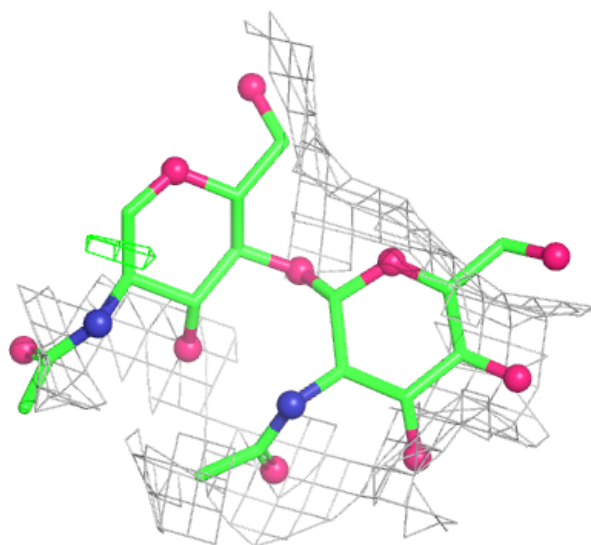
Electron density around Chain M:

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



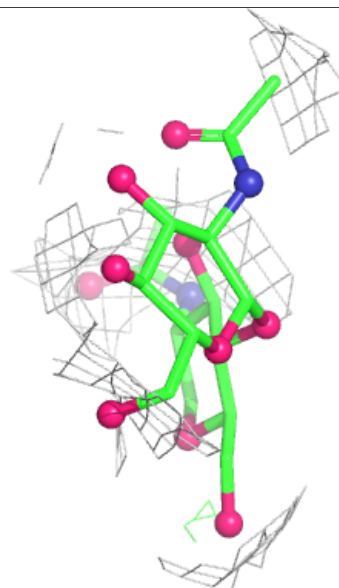
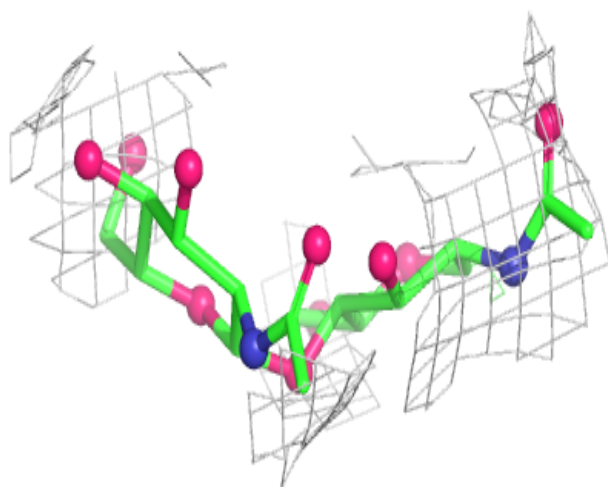
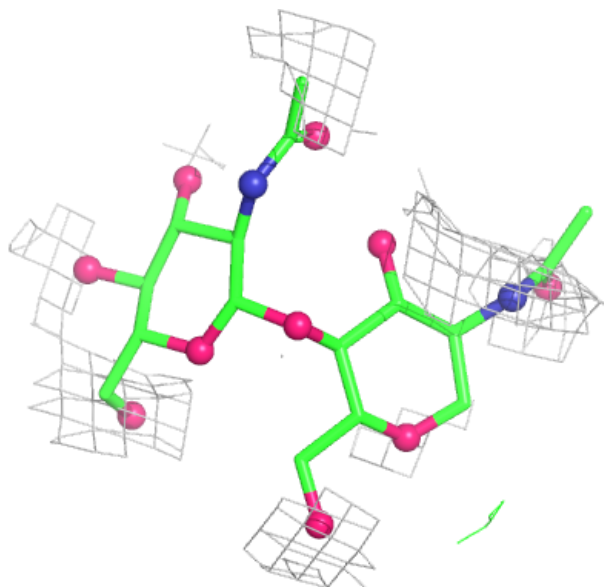
Electron density around Chain N:

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



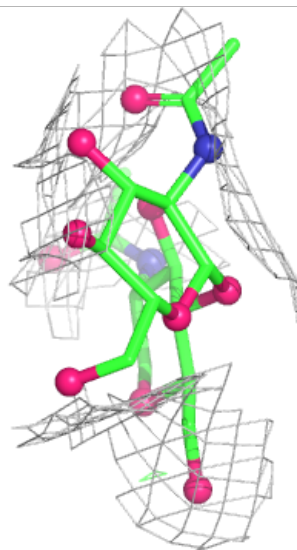
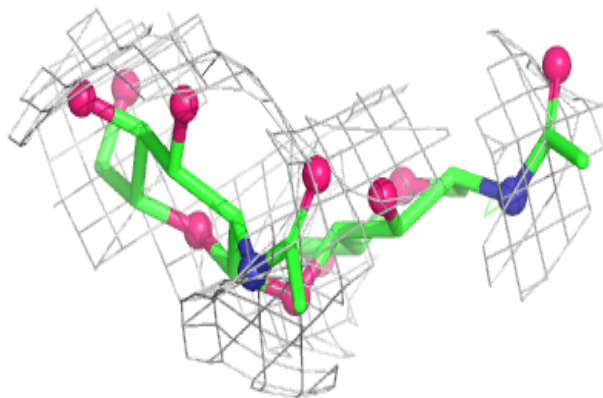
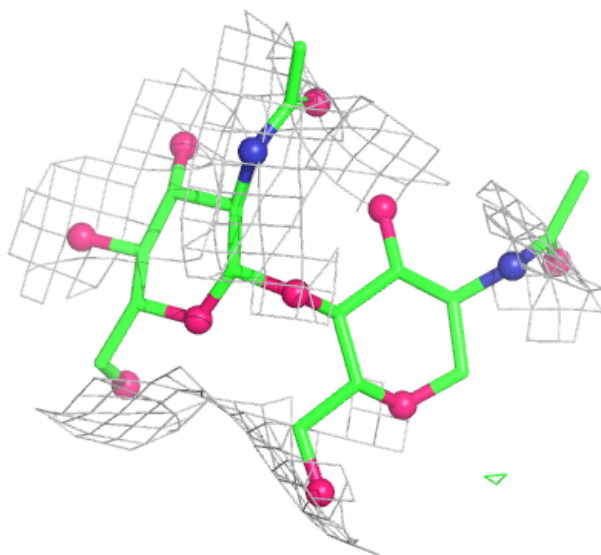
Electron density around Chain P:

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



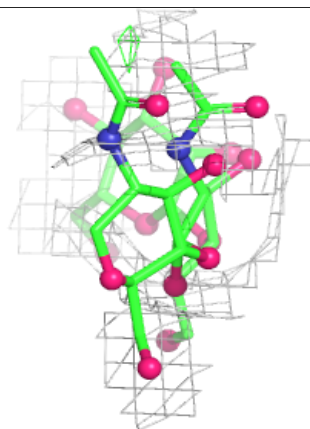
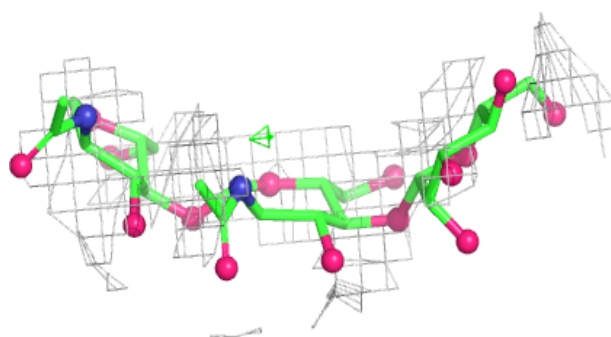
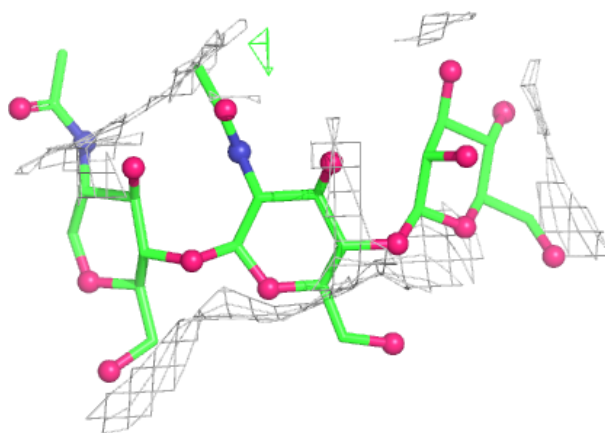
Electron density around Chain S:

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

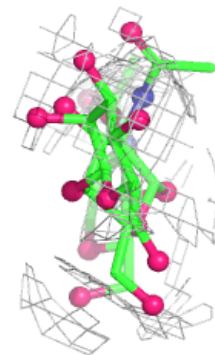
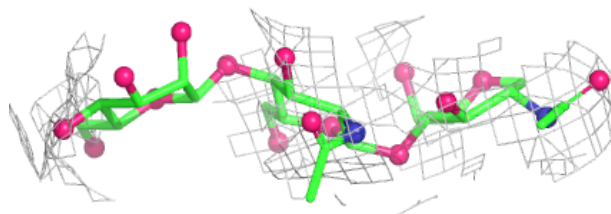
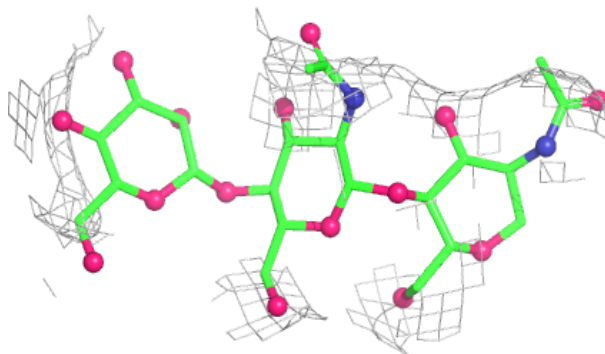


Electron density around Chain J:

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

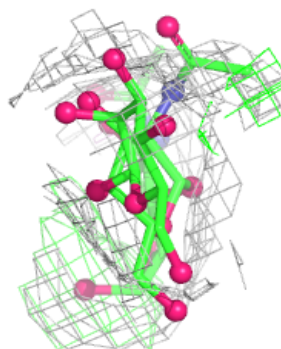
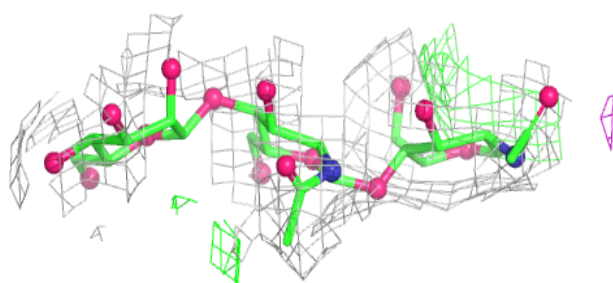
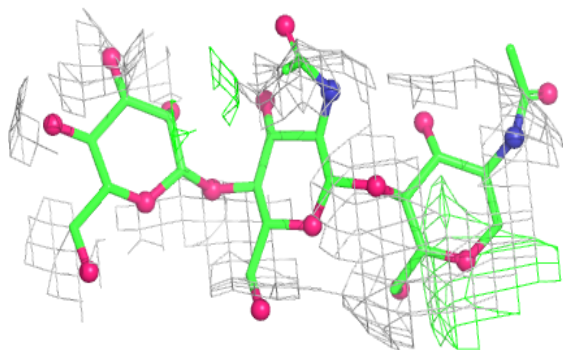
**Electron density around Chain K:**

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

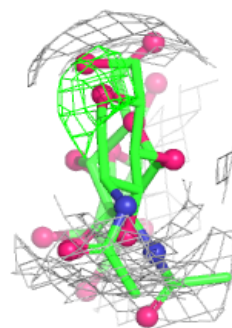
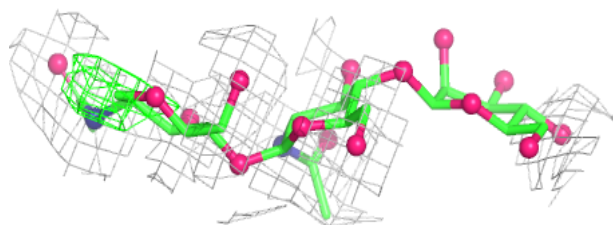
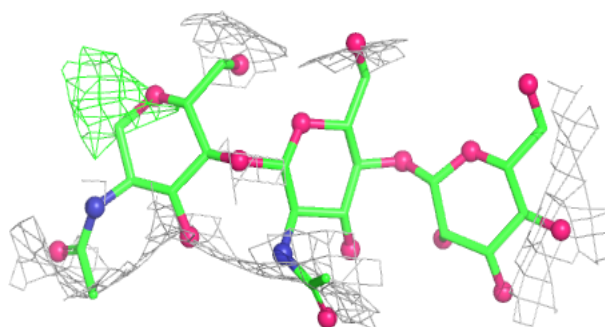


Electron density around Chain L:

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

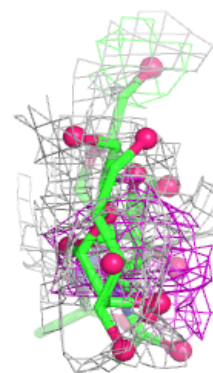
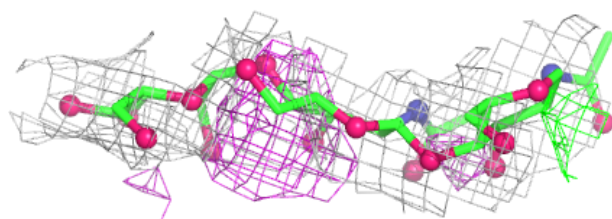
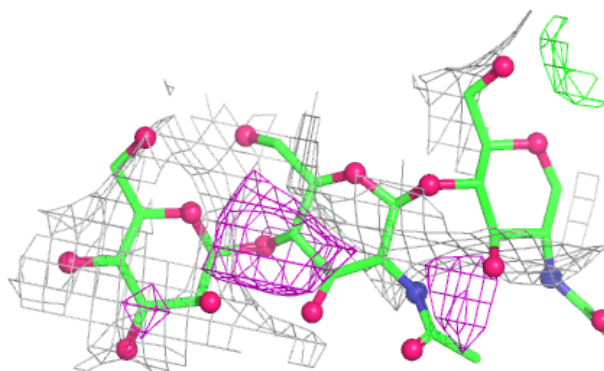
**Electron density around Chain O:**

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

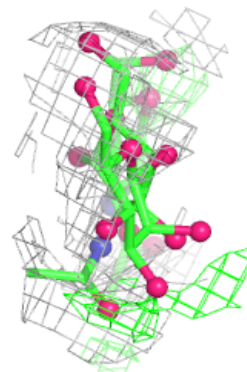
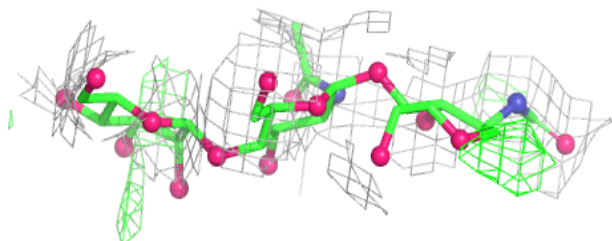
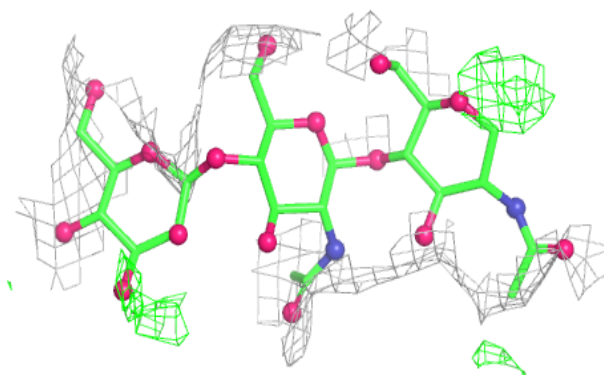


Electron density around Chain Q:

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

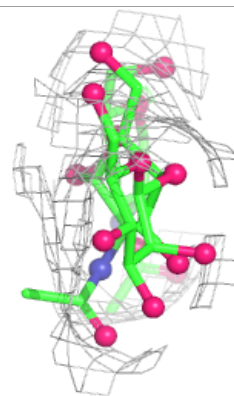
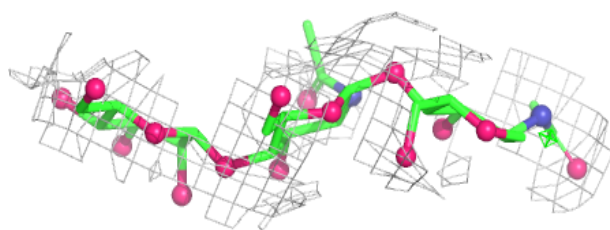
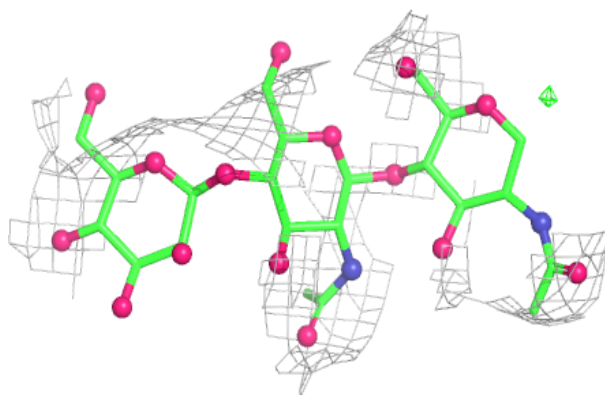
**Electron density around Chain R:**

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

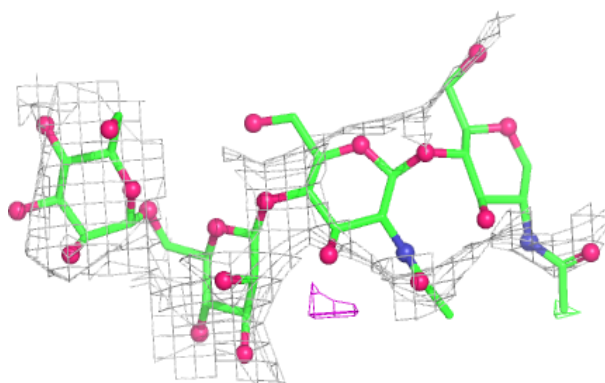


Electron density around Chain U:

$2mF_o - DF_c$ (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
6	NAG	F	3094	14/15	0.12	0.15	232,263,289,301	0
6	NAG	A	3678	14/15	0.30	0.15	164,238,297,317	0
6	NAG	F	3479	14/15	0.36	0.11	199,256,273,273	0
6	NAG	D	3479	14/15	0.41	0.10	192,213,248,259	0
6	NAG	H	3094	14/15	0.43	0.14	209,244,295,296	0
6	NAG	G	3678	14/15	0.44	0.14	129,233,286,308	0
6	NAG	E	3678	14/15	0.44	0.16	172,234,258,258	0
6	NAG	H	3479	14/15	0.44	0.11	217,264,289,289	0
6	NAG	C	3678	14/15	0.58	0.13	212,245,268,292	0
6	NAG	D	3094	14/15	0.71	0.09	212,265,297,302	0
6	NAG	B	3479	14/15	0.71	0.10	232,258,304,321	0
6	NAG	B	3094	14/15	0.76	0.09	236,271,288,298	0
7	CA	F	2002	1/1	0.78	0.07	534,534,534,534	0
6	NAG	G	3880	14/15	0.84	0.12	158,180,199,201	0
7	CA	H	2002	1/1	0.84	0.07	532,532,532,532	0
6	NAG	E	3880	14/15	0.86	0.11	117,189,224,243	0
8	MG	G	2009	1/1	0.87	0.07	414,414,414,414	0
7	CA	B	2002	1/1	0.88	0.08	533,533,533,533	0
7	CA	D	2002	1/1	0.90	0.06	533,533,533,533	0
7	CA	G	2007	1/1	0.90	0.06	284,284,284,284	0
6	NAG	C	3880	14/15	0.91	0.08	141,180,222,236	0
7	CA	E	2005	1/1	0.91	0.07	235,235,235,235	0
7	CA	C	2007	1/1	0.94	0.06	284,284,284,284	0
7	CA	A	2007	1/1	0.95	0.05	279,279,279,279	0
7	CA	C	2005	1/1	0.96	0.05	235,235,235,235	0
7	CA	C	2006	1/1	0.96	0.04	201,201,201,201	0
7	CA	G	2006	1/1	0.96	0.04	197,197,197,197	0
7	CA	E	2006	1/1	0.97	0.04	200,200,200,200	0
7	CA	A	2006	1/1	0.97	0.04	182,182,182,182	0
7	CA	A	2005	1/1	0.97	0.06	235,235,235,235	0
7	CA	E	2007	1/1	0.98	0.05	279,279,279,279	0
7	CA	G	2005	1/1	0.98	0.06	228,228,228,228	0

6.5 Other polymers

There are no such residues in this entry.