



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:37 AM UTC

PDB ID : 2WIN / pdb_00002win
Title : C3 convertase (C3bBb) stabilized by SCIN
Authors : Wu, J.; Janssen, B.J.; Gros, P.
Deposited on : 2009-05-13
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

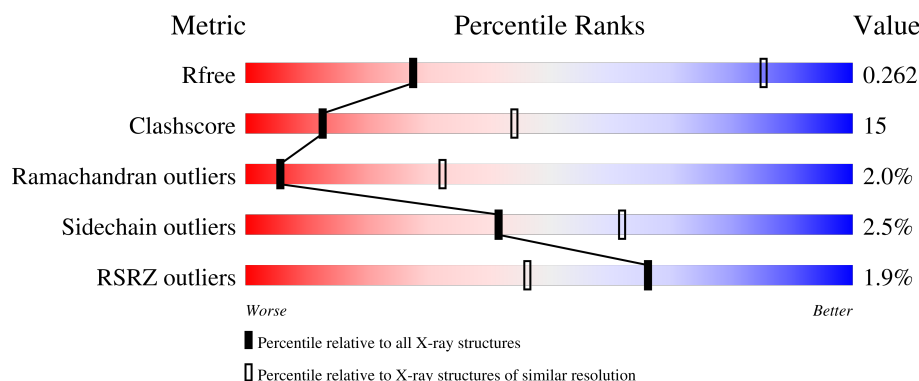
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	645	% 71% 27% ..
1	C	645	% 71% 27% ..
1	E	645	2% 70% 28% ..
1	G	645	4% 70% 29% ..
2	B	915	% 68% 27% ...

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Mol	Chain	Length	Quality of chain
2	D	915	
2	F	915	
2	H	915	
3	I	507	
3	J	507	
3	K	507	
3	L	507	
4	M	92	
4	N	92	
4	P	92	
4	Q	92	
5	O	4	
5	R	4	
5	T	4	
5	U	4	
6	S	5	
6	W	5	
7	V	6	
8	X	4	
9	Y	3	
9	a	3	
10	Z	2	
11	b	5	
12	c	3	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	Z	1	X	-	-	-
11	NAG	b	1	X	-	-	-
11	MAN	b	3	X	-	-	-
11	MAN	b	4	X	-	-	-
11	MAN	b	5	X	-	-	-
16	NAG	K	803	X	-	-	-
16	NAG	L	802	X	-	-	-
5	NAG	O	1	X	-	-	-
7	NAG	V	1	X	-	-	-
8	MAN	X	3	X	-	-	-
8	MAN	X	4	X	-	-	-
9	MAN	Y	3	X	-	-	-
9	MAN	a	3	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 67989 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	C	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	E	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	G	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7177	4545	1209	1386	37			
2	D	901	Total	C	N	O	S	0	0	0
			7166	4537	1208	1384	37			
2	F	900	Total	C	N	O	S	0	0	0
			7172	4545	1206	1384	37			
2	H	900	Total	C	N	O	S	2313	0	0
			7175	4547	1209	1382	37			

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	J	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	K	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	L	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			

- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

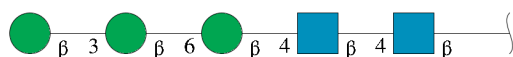
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	N	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	Q	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

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



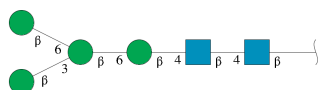
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



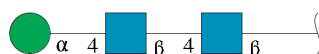
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	V	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 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
8	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 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.



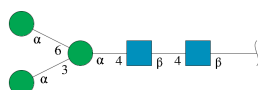
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	a	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



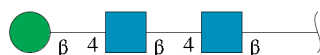
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



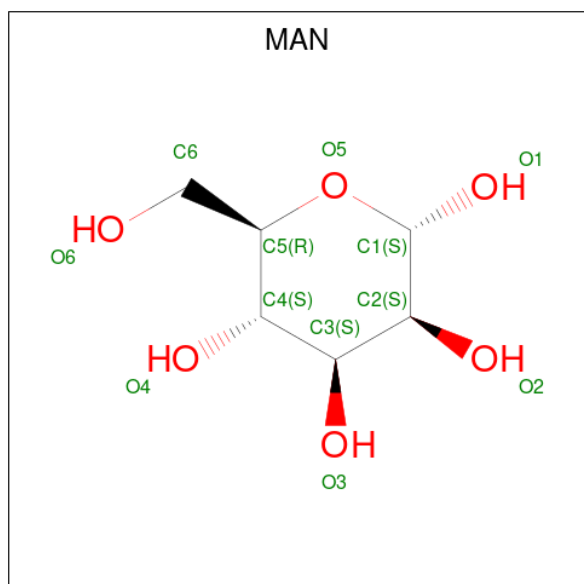
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	b	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



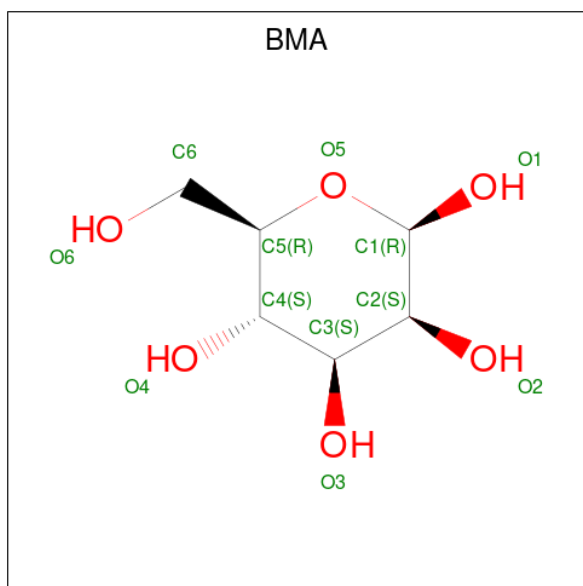
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	c	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 13 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 14 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	C	O	0	0
			11	6	5		
14	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total	Mg	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		
15	L	1	Total	Mg	0	0
			1	1		

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			14	8	1	5		
16	L	1	Total	C	N	O	0	0
			14	8	1	5		

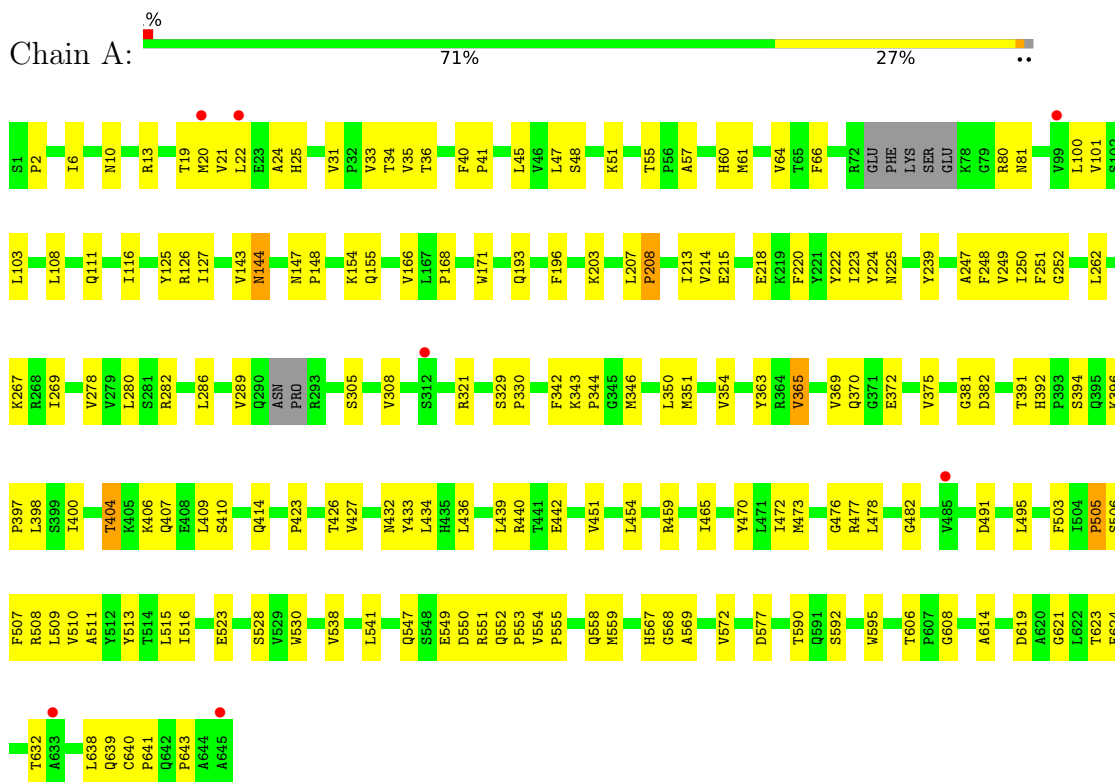
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	O	0	0
			1	1		
17	I	2	Total	O	0	0
			2	2		
17	J	2	Total	O	0	0
			2	2		
17	K	2	Total	O	0	0
			2	2		
17	L	1	Total	O	0	0
			1	1		

3 Residue-property plots

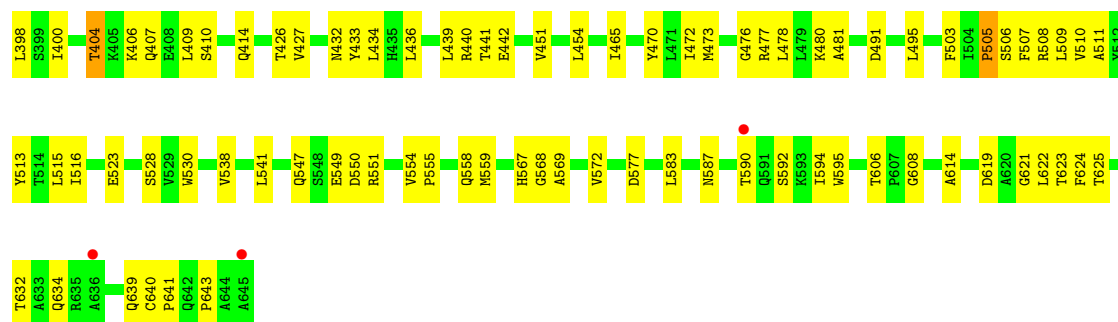
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: COMPLEMENT C3 BETA CHAIN

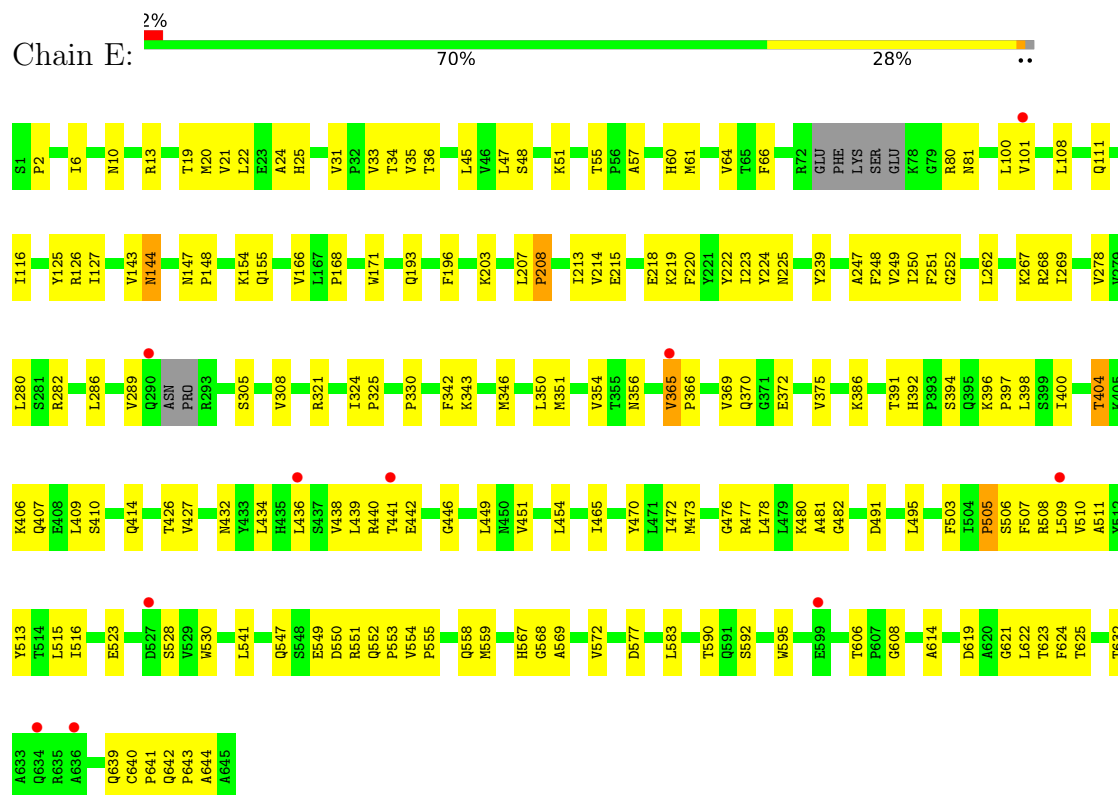


• Molecule 1: COMPLEMENT C3 BETA CHAIN

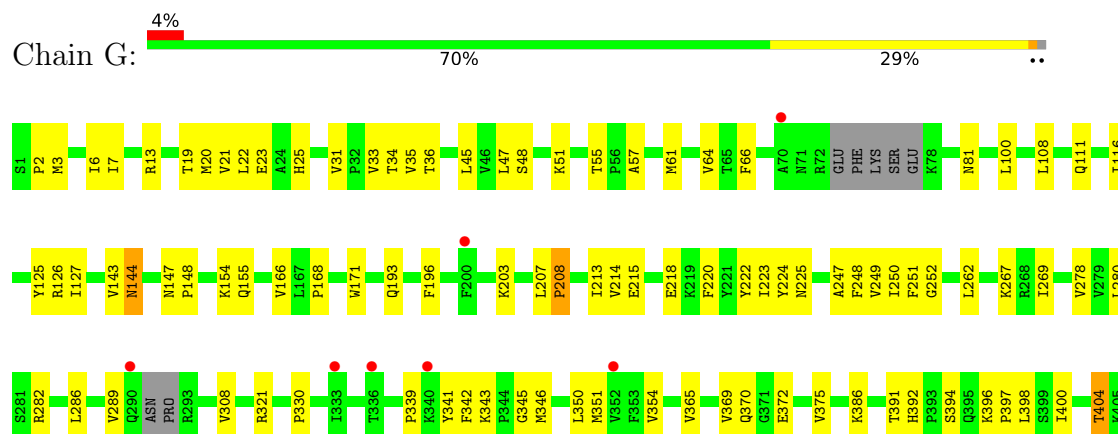


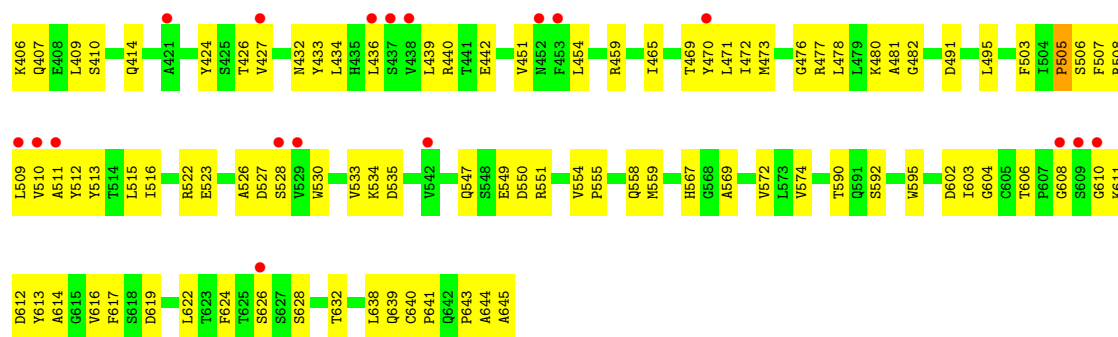


● Molecule 1: COMPLEMENT C3 BETA CHAIN

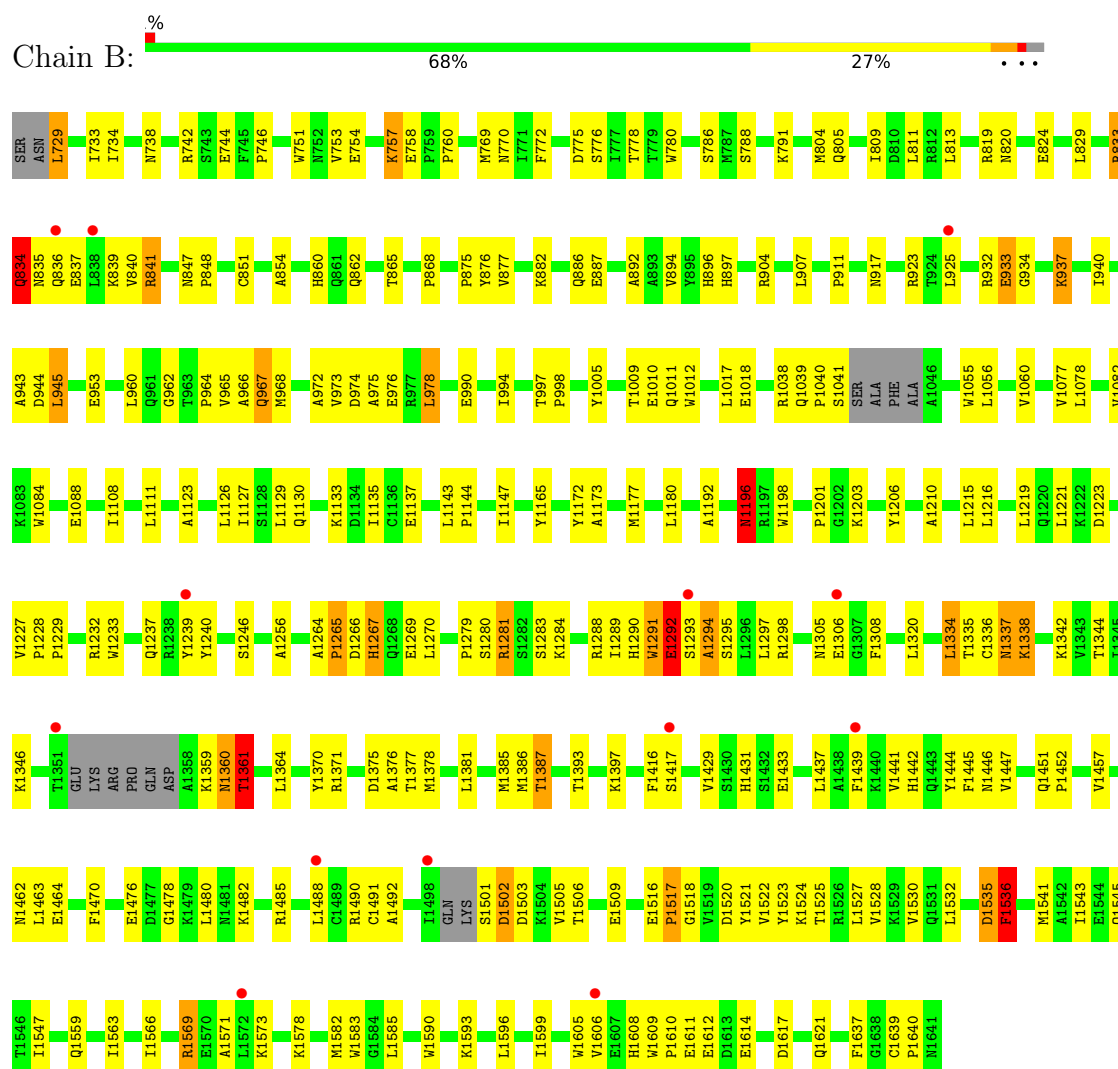


● Molecule 1: COMPLEMENT C3 BETA CHAIN

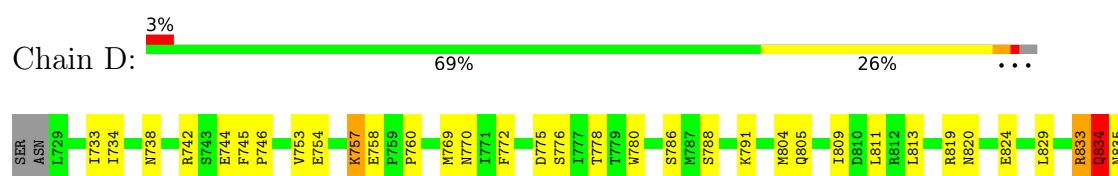


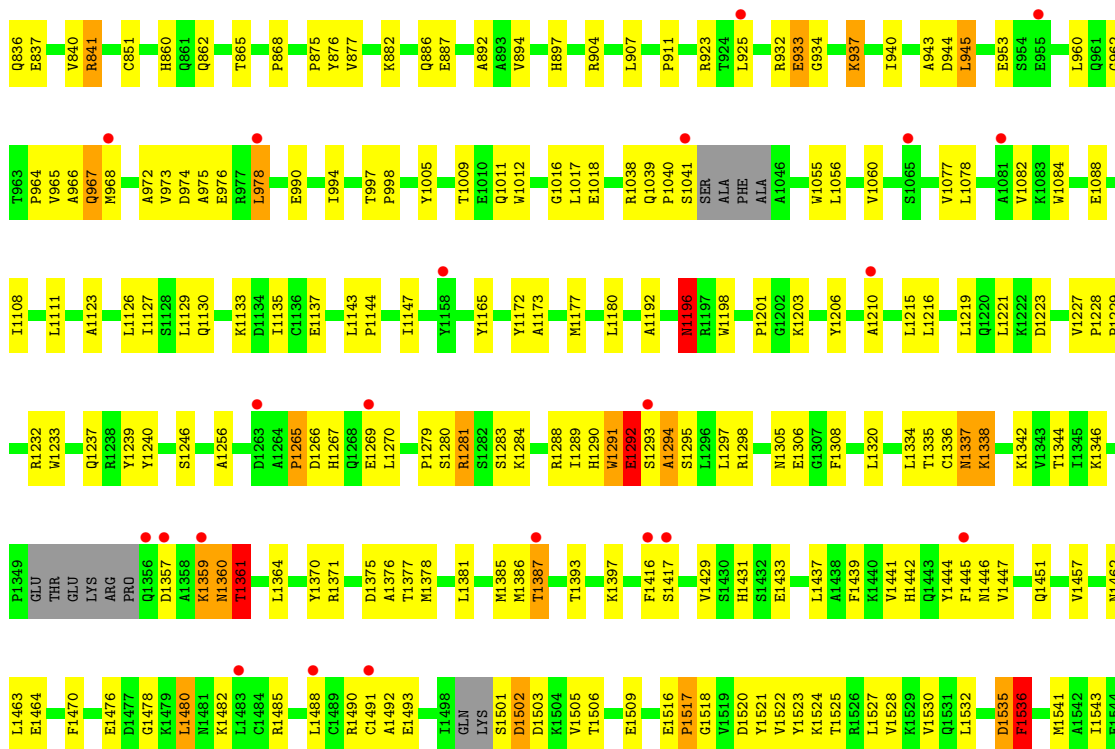


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

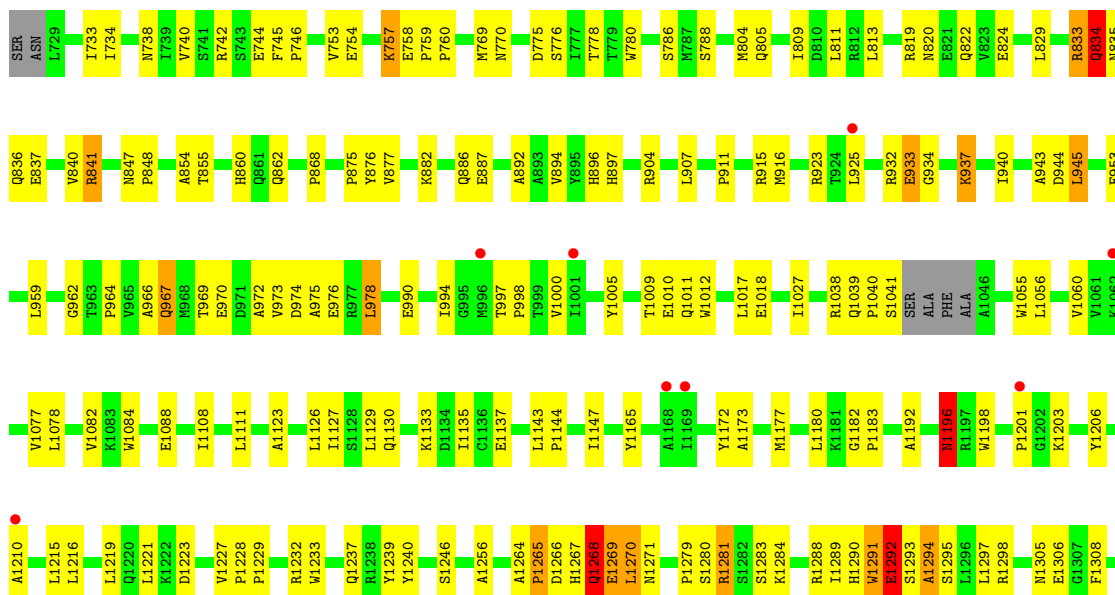


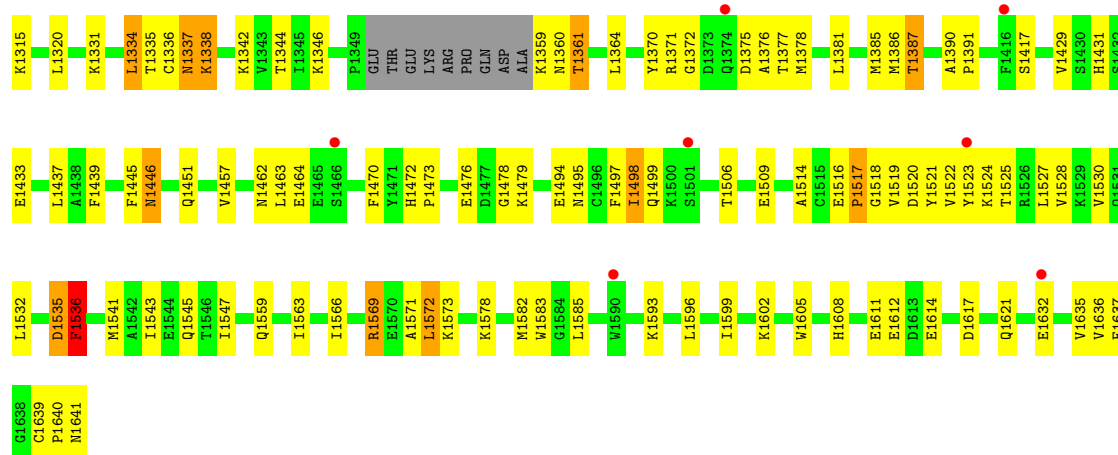
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



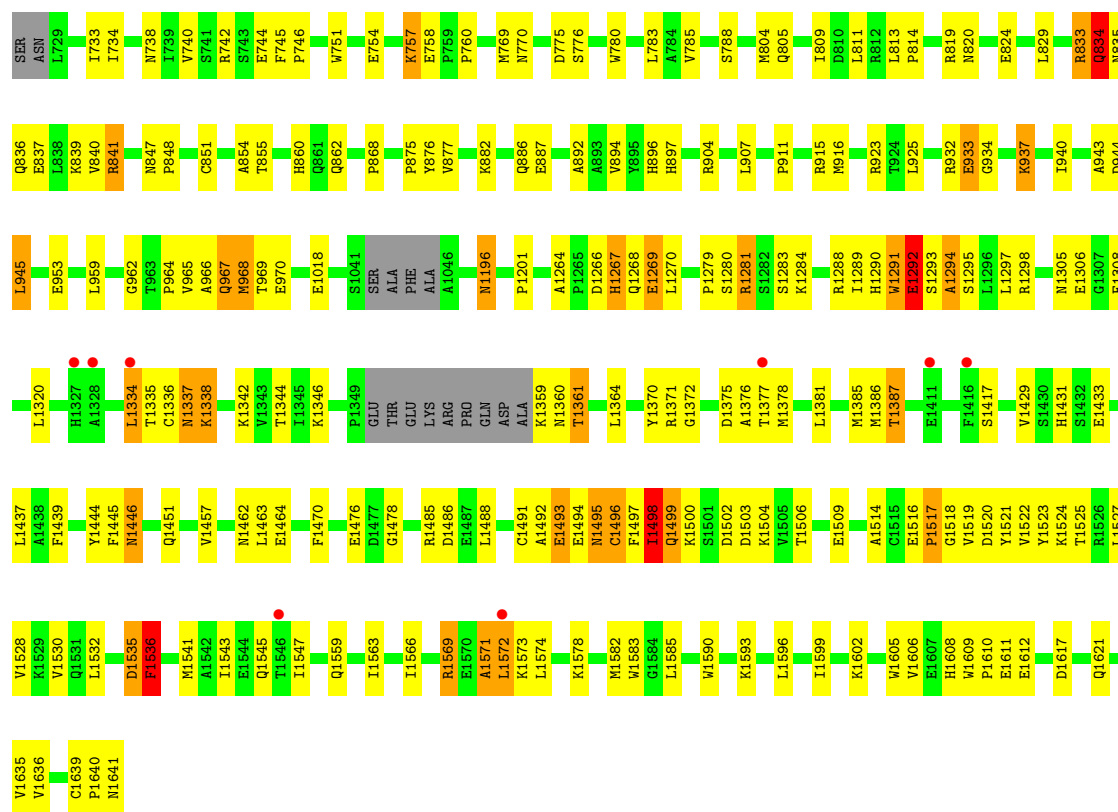
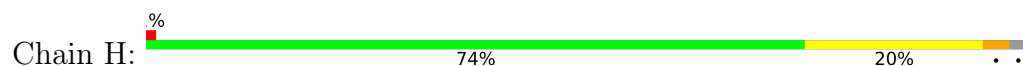


● Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



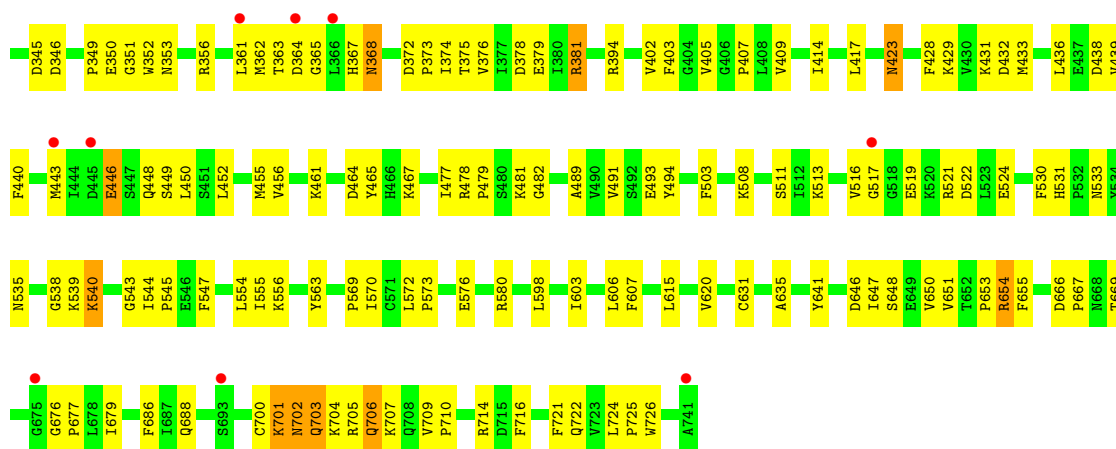


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

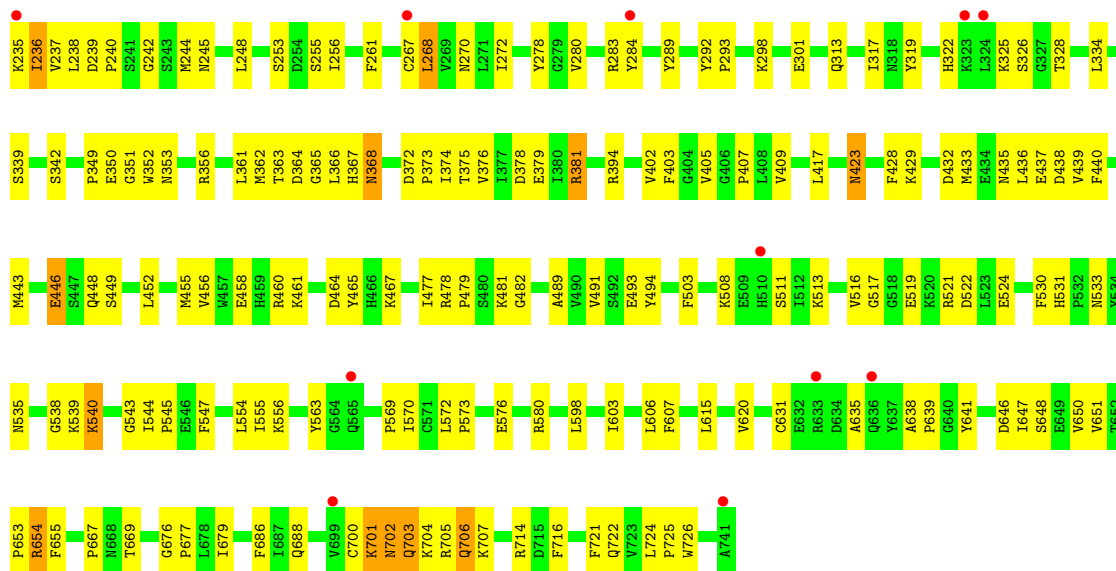


• Molecule 3: COMPLEMENT FACTOR B

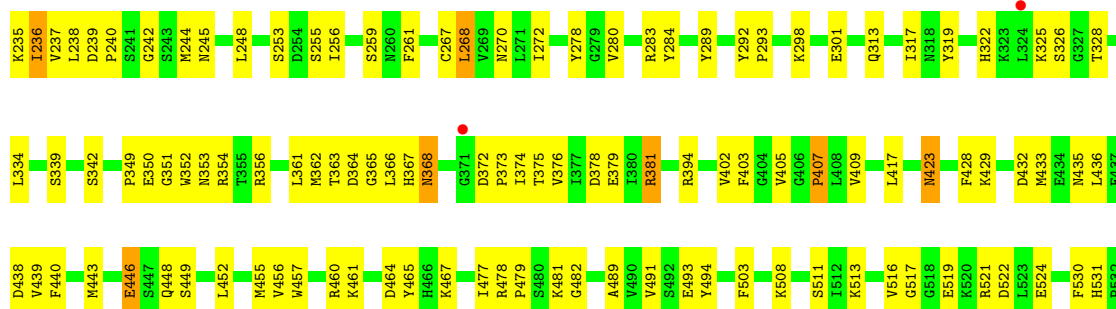


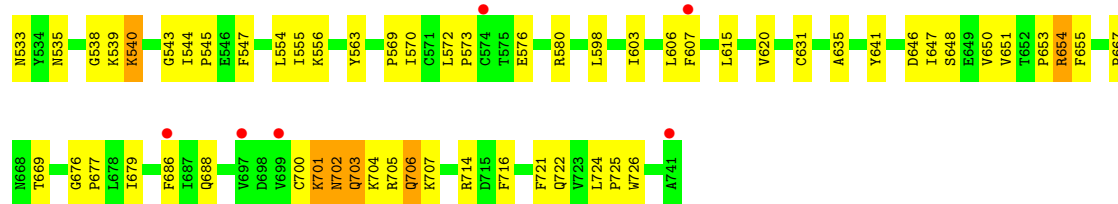


• Molecule 3: COMPLEMENT FACTOR B

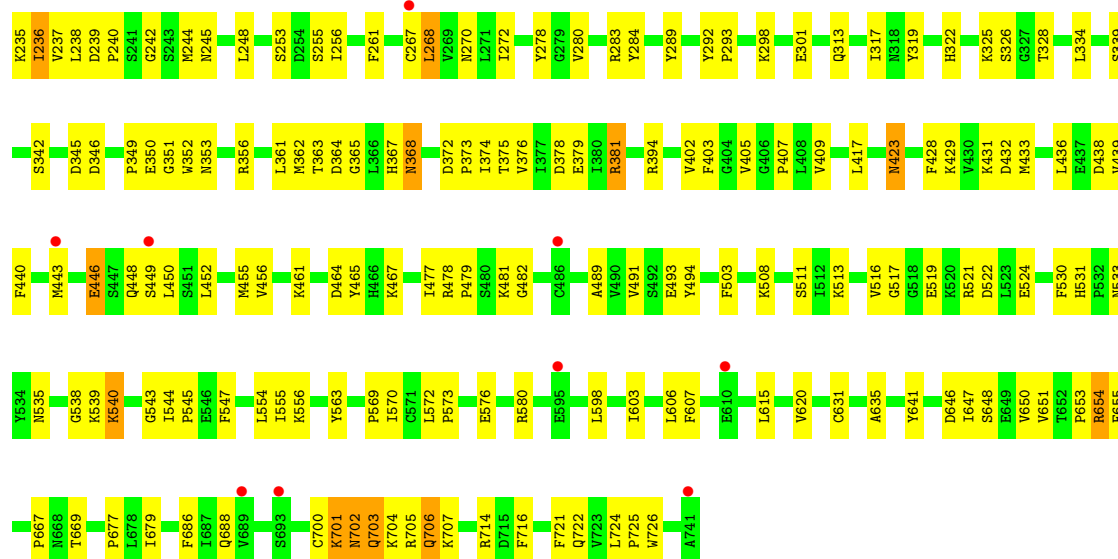


• Molecule 3: COMPLEMENT FACTOR B

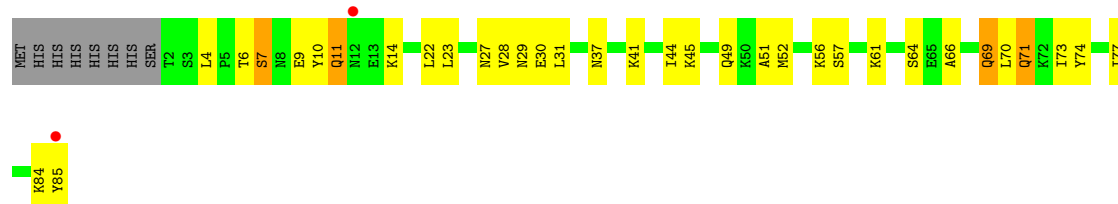




• Molecule 3: COMPLEMENT FACTOR B



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



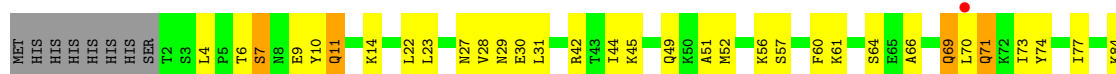
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



- Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



Y85

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



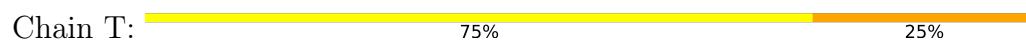
MAG1
MAG2
BMA3
BMA4

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



MAG1
MAG2
BMA3
BMA4

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



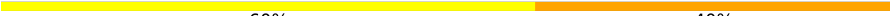
MAG1
MAG2
BMA3
BMA4

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



MAG1
MAG2
BMA3
BMA4

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

Chain S:  60% 40%



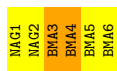
- Molecule 6: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  20% 80%



- Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  67% 33%



- Molecule 8: 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 X:  25% 25% 50%



- Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  33% 67%



- Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  33% 67%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

NAG1
NAG2

- Molecule 11: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

100%

NAG1
NAG2
MAN3
MAN4
MAN5

- Molecule 12: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

33%

67%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	39.67 – 3.90 39.67 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.67-3.90) 97.5 (39.67-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.268 0.247 , 0.262	Depositor DCC
R_{free} test set	2089 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAG, MAN, MG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/5056	0.69	0/6870
1	C	0.24	0/5056	0.69	0/6870
1	E	0.24	0/5056	0.69	0/6870
1	G	0.26	0/5056	0.69	0/6870
2	B	0.25	0/7317	0.67	0/9907
2	D	0.25	0/7306	0.67	0/9894
2	F	0.25	0/7314	0.67	0/9905
2	H	0.26	0/7315	0.67	1/9902 (0.0%)
3	I	0.24	0/4092	0.69	0/5543
3	J	0.24	0/4092	0.69	0/5543
3	K	0.24	0/4092	0.69	0/5543
3	L	0.24	0/4092	0.70	0/5543
4	M	0.24	0/690	0.61	0/923
4	N	0.24	0/690	0.61	0/923
4	P	0.24	0/690	0.61	0/923
4	Q	0.24	0/690	0.61	0/923
All	All	0.25	0/68604	0.68	1/92952 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	970	GLU	CB-CA-C	-5.25	109.52	117.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4958	0	5017	136	0
1	C	4958	0	5017	136	0
1	E	4958	0	5017	141	0
1	G	4958	0	5016	156	0
2	B	7177	0	7085	216	0
2	D	7166	0	7062	210	0
2	F	7172	0	7080	239	0
2	H	7175	0	7087	211	0
3	I	4004	0	3966	131	0
3	J	4004	0	3967	133	0
3	K	4004	0	3965	132	0
3	L	4004	0	3966	132	0
4	M	682	0	697	36	0
4	N	682	0	697	39	0
4	P	682	0	697	34	0
4	Q	682	0	697	39	0
5	O	50	0	43	1	0
5	R	50	0	42	1	0
5	T	50	0	43	1	0
5	U	50	0	43	3	0
6	S	61	0	52	1	0
6	W	61	0	52	5	0
7	V	72	0	61	2	0
8	X	50	0	43	2	0
9	Y	39	0	34	2	0
9	a	39	0	34	2	0
10	Z	28	0	25	0	0
11	b	61	0	52	5	0
12	c	39	0	34	0	0
13	A	11	0	10	1	0
14	B	11	0	10	0	0
14	K	11	0	10	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
16	K	14	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	14	0	13	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	2	0	0	1	0
17	K	2	0	0	0	0
17	L	1	0	0	0	0
All	All	67989	0	67647	1986	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1986) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:THR:HG21	1:G:432:ASN:H	1.20	1.07
2:H:1494:GLU:HB3	2:H:1602:LYS:HB3	1.36	1.04
2:D:1569:ARG:HB2	2:D:1569:ARG:HH11	1.32	0.94
2:F:1569:ARG:HB2	2:F:1569:ARG:HH11	1.32	0.94
2:H:1569:ARG:HB2	2:H:1569:ARG:HH11	1.32	0.94
2:B:1569:ARG:HH11	2:B:1569:ARG:HB2	1.32	0.94
2:H:1268:GLN:HG3	2:H:1269:GLU:H	1.34	0.92
1:G:505:PRO:HG3	1:G:595:TRP:CE3	2.08	0.88
3:I:267:CYS:HB2	3:I:433:MET:HE1	1.54	0.88
3:K:267:CYS:HB2	3:K:433:MET:HE1	1.54	0.88
3:J:267:CYS:HB2	3:J:433:MET:HE1	1.54	0.87
2:F:1359:LYS:HD2	4:M:4:LEU:HD11	1.58	0.86
3:L:267:CYS:HB2	3:L:433:MET:HE1	1.54	0.85
1:A:549:GLU:HG2	1:A:550:ASP:H	1.44	0.83
1:G:477:ARG:HG2	1:G:477:ARG:HH11	1.44	0.83
1:C:549:GLU:HG2	1:C:550:ASP:H	1.44	0.82
1:E:477:ARG:HG2	1:E:477:ARG:HH11	1.44	0.82
2:H:1497:PHE:HE2	2:H:1571:ALA:HB1	1.43	0.82
1:E:547:GLN:HE22	1:E:559:MET:HA	1.44	0.82
1:G:549:GLU:HG2	1:G:550:ASP:H	1.44	0.82
3:J:381:ARG:HG2	3:J:381:ARG:HH21	1.45	0.82
1:E:549:GLU:HG2	1:E:550:ASP:H	1.44	0.82
4:Q:6:THR:H	4:Q:9:GLU:HB3	1.45	0.82
4:N:6:THR:H	4:N:9:GLU:HB3	1.45	0.81
4:P:6:THR:H	4:P:9:GLU:HB3	1.45	0.81
1:A:547:GLN:HE22	1:A:559:MET:HA	1.44	0.81
2:H:1485:ARG:HD3	2:H:1536:PHE:CZ	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:547:GLN:HE22	1:G:559:MET:HA	1.44	0.81
3:K:381:ARG:HH21	3:K:381:ARG:HG2	1.45	0.81
1:C:547:GLN:HE22	1:C:559:MET:HA	1.44	0.81
4:M:6:THR:H	4:M:9:GLU:HB3	1.45	0.81
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.44	0.80
1:C:477:ARG:HG2	1:C:477:ARG:HH11	1.44	0.80
2:H:1291:TRP:CD1	2:H:1292:GLU:H	1.99	0.80
1:G:508:ARG:CZ	1:G:604:GLY:HA3	2.12	0.80
3:L:381:ARG:HG2	3:L:381:ARG:HH21	1.45	0.80
2:B:819:ARG:HG2	2:B:819:ARG:HH11	1.46	0.80
2:D:819:ARG:HG2	2:D:819:ARG:HH11	1.46	0.80
3:I:381:ARG:HH21	3:I:381:ARG:HG2	1.45	0.80
1:C:45:LEU:HD11	1:C:48:SER:HB3	1.64	0.79
2:F:1291:TRP:CD1	2:F:1292:GLU:H	1.99	0.79
2:H:833:ARG:HH11	2:H:833:ARG:HG2	1.48	0.79
2:D:833:ARG:HG2	2:D:833:ARG:HH11	1.48	0.79
2:H:1488:LEU:HG	2:H:1590:TRP:HH2	1.47	0.79
2:F:819:ARG:HG2	2:F:819:ARG:HH11	1.46	0.79
2:H:819:ARG:HG2	2:H:819:ARG:HH11	1.46	0.79
2:D:1532:LEU:HD11	2:D:1569:ARG:HD3	1.65	0.78
3:I:244:MET:HG3	3:I:356:ARG:HB2	1.65	0.78
1:G:45:LEU:HD11	1:G:48:SER:HB3	1.64	0.78
2:H:1532:LEU:HD11	2:H:1569:ARG:HD3	1.65	0.78
2:F:1532:LEU:HD11	2:F:1569:ARG:HD3	1.65	0.78
1:E:45:LEU:HD11	1:E:48:SER:HB3	1.64	0.78
1:A:45:LEU:HD11	1:A:48:SER:HB3	1.64	0.78
2:B:1532:LEU:HD11	2:B:1569:ARG:HD3	1.65	0.78
2:F:738:ASN:HD22	4:P:45:LYS:HE2	1.47	0.78
2:F:833:ARG:HG2	2:F:833:ARG:HH11	1.48	0.78
2:H:966:ALA:O	2:H:967:GLN:HB2	1.83	0.78
2:B:833:ARG:HG2	2:B:833:ARG:HH11	1.48	0.77
2:F:932:ARG:NH1	3:L:339:SER:HB2	1.99	0.77
2:H:738:ASN:HD22	4:Q:45:LYS:HE2	1.49	0.77
2:F:841:ARG:HG2	2:F:841:ARG:HH11	1.50	0.77
3:J:244:MET:HG3	3:J:356:ARG:HB2	1.65	0.77
3:K:244:MET:HG3	3:K:356:ARG:HB2	1.65	0.77
3:L:244:MET:HG3	3:L:356:ARG:HB2	1.65	0.77
2:F:742:ARG:HB3	2:F:775:ASP:HB3	1.67	0.77
1:G:506:SER:HB2	1:G:530:TRP:HE1	1.50	0.77
2:B:841:ARG:HH11	2:B:841:ARG:HG2	1.50	0.76
2:F:740:VAL:HB	4:P:42:ARG:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.50	0.76
1:E:506:SER:HB2	1:E:530:TRP:HE1	1.50	0.76
3:I:705:ARG:O	3:I:706:GLN:HB2	1.86	0.75
3:L:705:ARG:O	3:L:706:GLN:HB2	1.86	0.75
3:K:354:ARG:HB2	16:K:803:NAG:H81	1.67	0.75
2:D:841:ARG:HG2	2:D:841:ARG:HH11	1.50	0.75
2:H:1498:ILE:HD12	2:H:1605:TRP:HA	1.65	0.75
3:J:705:ARG:O	3:J:706:GLN:HB2	1.86	0.75
2:F:1569:ARG:HH11	2:F:1569:ARG:CB	2.00	0.75
2:H:841:ARG:HG2	2:H:841:ARG:HH11	1.50	0.75
1:C:440:ARG:HG3	1:C:440:ARG:O	1.85	0.75
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.50	0.75
3:L:446:GLU:O	3:L:450:LEU:HG	1.86	0.74
2:B:1569:ARG:HH11	2:B:1569:ARG:CB	2.00	0.74
2:D:1291:TRP:CD1	2:D:1292:GLU:H	2.05	0.74
1:C:404:THR:HG23	1:C:414:GLN:HE21	1.53	0.74
3:L:489:ALA:HB2	3:L:677:PRO:HG3	1.70	0.74
1:E:440:ARG:O	1:E:440:ARG:HG3	1.85	0.74
3:K:705:ARG:O	3:K:706:GLN:HB2	1.86	0.74
2:H:1569:ARG:HH11	2:H:1569:ARG:CB	2.00	0.74
3:I:464:ASP:HB3	3:I:615:LEU:HB2	1.70	0.74
1:A:440:ARG:HG3	1:A:440:ARG:O	1.86	0.74
1:G:440:ARG:HG3	1:G:440:ARG:O	1.85	0.74
2:H:877:VAL:HG22	2:H:1451:GLN:HE21	1.53	0.74
3:K:464:ASP:HB3	3:K:615:LEU:HB2	1.70	0.74
1:A:404:THR:HG23	1:A:414:GLN:HE21	1.53	0.74
1:E:223:ILE:H	1:E:223:ILE:HD12	1.53	0.74
2:B:1291:TRP:CD1	2:B:1292:GLU:H	2.05	0.74
2:H:740:VAL:HB	4:Q:42:ARG:HB2	1.69	0.74
2:F:834:GLN:NE2	2:F:835:ASN:H	1.86	0.73
2:D:1569:ARG:HH11	2:D:1569:ARG:CB	2.00	0.73
1:G:223:ILE:H	1:G:223:ILE:HD12	1.53	0.73
3:I:248:LEU:HD22	3:I:268:LEU:HD22	1.71	0.73
2:B:834:GLN:NE2	2:B:835:ASN:H	1.86	0.73
1:E:404:THR:HG23	1:E:414:GLN:HE21	1.53	0.73
2:H:742:ARG:HB3	2:H:775:ASP:HB3	1.71	0.73
1:C:223:ILE:HD12	1:C:223:ILE:H	1.53	0.73
1:G:404:THR:HG23	1:G:414:GLN:HE21	1.52	0.73
1:A:223:ILE:H	1:A:223:ILE:HD12	1.53	0.73
3:L:248:LEU:HD22	3:L:268:LEU:HD22	1.71	0.73
2:B:966:ALA:O	2:B:967:GLN:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:489:ALA:HB2	3:I:677:PRO:HG3	1.70	0.73
2:D:834:GLN:NE2	2:D:835:ASN:H	1.86	0.73
2:F:966:ALA:O	2:F:967:GLN:HB2	1.89	0.73
2:D:966:ALA:O	2:D:967:GLN:HB2	1.88	0.73
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.71	0.72
3:L:464:ASP:HB3	3:L:615:LEU:HB2	1.70	0.72
1:G:424:TYR:O	1:G:433:TYR:HE1	1.73	0.72
2:F:1269:GLU:HG3	2:F:1315:LYS:HB3	1.70	0.72
2:F:937:LYS:HG2	3:L:345:ASP:OD1	1.88	0.72
2:H:1497:PHE:CE2	2:H:1571:ALA:HB1	2.24	0.72
3:K:489:ALA:HB2	3:K:677:PRO:HG3	1.70	0.72
3:J:489:ALA:HB2	3:J:677:PRO:HG3	1.70	0.72
1:G:426:THR:HG21	1:G:432:ASN:N	2.02	0.72
3:K:635:ALA:HB3	3:K:647:ILE:HD11	1.71	0.72
3:J:248:LEU:HD22	3:J:268:LEU:HD22	1.70	0.72
3:J:464:ASP:HB3	3:J:615:LEU:HB2	1.70	0.72
3:J:653:PRO:HD2	3:J:654:ARG:HH12	1.55	0.72
2:H:834:GLN:NE2	2:H:835:ASN:H	1.86	0.72
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.72	0.71
1:G:6:ILE:HD13	1:G:22:LEU:HD23	1.72	0.71
3:L:461:LYS:HE2	3:L:461:LYS:HA	1.73	0.71
3:J:539:LYS:HG2	3:J:544:ILE:HD12	1.73	0.71
3:J:576:GLU:HB3	3:J:580:ARG:HH22	1.55	0.71
3:K:539:LYS:HG2	3:K:544:ILE:HD12	1.73	0.71
1:C:13:ARG:HH22	1:C:476:GLY:HA3	1.54	0.71
3:J:635:ALA:HB3	3:J:647:ILE:HD11	1.71	0.71
3:K:461:LYS:HA	3:K:461:LYS:HE2	1.73	0.71
3:I:461:LYS:HE2	3:I:461:LYS:HA	1.73	0.71
3:I:653:PRO:HD2	3:I:654:ARG:HH12	1.55	0.71
3:J:461:LYS:HE2	3:J:461:LYS:HA	1.73	0.71
3:K:576:GLU:HB3	3:K:580:ARG:HH22	1.55	0.71
1:C:439:LEU:HG	1:E:439:LEU:HG	1.71	0.71
3:I:635:ALA:HB3	3:I:647:ILE:HD11	1.71	0.71
3:K:248:LEU:HD22	3:K:268:LEU:HD22	1.70	0.71
3:L:635:ALA:HB3	3:L:647:ILE:HD11	1.71	0.70
1:E:6:ILE:HD13	1:E:22:LEU:HD23	1.72	0.70
1:C:98:VAL:HG11	2:D:1017:LEU:HD13	1.73	0.70
3:K:653:PRO:HD2	3:K:654:ARG:HH12	1.55	0.70
1:A:239:TYR:HB2	2:B:804:MET:HE2	1.73	0.70
4:Q:71:GLN:HA	4:Q:71:GLN:HE21	1.57	0.70
3:I:539:LYS:HG2	3:I:544:ILE:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:576:GLU:HB3	3:L:580:ARG:HH22	1.55	0.70
2:H:1446:ASN:HB2	4:N:4:LEU:HD13	1.74	0.70
4:P:71:GLN:HE21	4:P:71:GLN:HA	1.57	0.70
1:C:239:TYR:HB2	2:D:804:MET:HE2	1.74	0.70
3:I:576:GLU:HB3	3:I:580:ARG:HH22	1.55	0.70
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.74	0.70
3:L:539:LYS:HG2	3:L:544:ILE:HD12	1.73	0.69
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.72	0.69
2:D:1416:PHE:HZ	2:D:1442:HIS:HB2	1.57	0.69
3:I:381:ARG:HH21	3:I:381:ARG:CG	2.05	0.69
3:J:238:LEU:HD11	3:J:278:TYR:HB3	1.74	0.69
3:L:373:PRO:HB2	3:L:417:LEU:HD21	1.75	0.69
3:I:238:LEU:HD11	3:I:278:TYR:HB3	1.74	0.69
3:K:381:ARG:HH21	3:K:381:ARG:CG	2.06	0.69
3:L:653:PRO:HD2	3:L:654:ARG:HH12	1.55	0.69
2:H:962:GLY:O	2:H:964:PRO:HD3	1.92	0.69
1:E:426:THR:HG21	1:E:432:ASN:H	1.57	0.69
2:F:1387:THR:HG22	2:F:1451:GLN:H	1.58	0.69
2:H:1446:ASN:HB2	4:N:4:LEU:CD1	2.21	0.69
3:L:238:LEU:HD11	3:L:278:TYR:HB3	1.74	0.69
1:G:505:PRO:HG3	1:G:595:TRP:HE3	1.55	0.69
2:H:855:THR:HB	2:H:1602:LYS:HZ3	1.56	0.69
4:N:71:GLN:HA	4:N:71:GLN:HE21	1.56	0.69
2:H:1387:THR:HG22	2:H:1451:GLN:H	1.58	0.69
3:J:381:ARG:HH21	3:J:381:ARG:CG	2.05	0.69
2:D:962:GLY:O	2:D:964:PRO:HD3	1.93	0.69
3:L:381:ARG:HH21	3:L:381:ARG:CG	2.05	0.69
2:B:1416:PHE:HZ	2:B:1442:HIS:HB2	1.57	0.68
3:J:705:ARG:O	3:J:705:ARG:HG3	1.93	0.68
2:B:841:ARG:HG2	2:B:841:ARG:NH1	2.08	0.68
2:B:1488:LEU:HG	2:B:1590:TRP:CZ2	2.27	0.68
2:F:841:ARG:HG2	2:F:841:ARG:NH1	2.08	0.68
2:D:1488:LEU:HG	2:D:1590:TRP:CZ2	2.27	0.68
4:M:71:GLN:HA	4:M:71:GLN:HE21	1.56	0.68
1:E:248:PHE:HD1	2:F:1378:MET:HE3	1.58	0.68
2:F:733:ILE:HG12	2:F:734:ILE:H	1.58	0.68
3:I:373:PRO:HB2	3:I:417:LEU:HD21	1.75	0.68
3:J:373:PRO:HB2	3:J:417:LEU:HD21	1.75	0.68
3:K:373:PRO:HB2	3:K:417:LEU:HD21	1.75	0.68
3:J:435:ASN:ND2	3:J:460:ARG:HH21	1.90	0.68
1:G:100:LEU:HD21	1:G:638:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:567:HIS:ND1	2:H:760:PRO:HG3	2.09	0.68
1:C:606:THR:HG22	1:C:608:GLY:H	1.59	0.68
2:D:1445:PHE:CZ	4:P:7:SER:HA	2.28	0.68
2:H:733:ILE:HG12	2:H:734:ILE:H	1.58	0.68
3:J:432:ASP:HA	4:Q:27:ASN:HD21	1.57	0.67
1:C:372:GLU:O	1:C:375:VAL:HG12	1.95	0.67
3:K:446:GLU:HB3	3:K:449:SER:HB2	1.77	0.67
2:D:733:ILE:HG12	2:D:734:ILE:H	1.58	0.67
2:D:1518:GLY:HA3	2:D:1585:LEU:HD22	1.77	0.67
3:K:705:ARG:O	3:K:705:ARG:HG3	1.93	0.67
2:H:841:ARG:HG2	2:H:841:ARG:NH1	2.08	0.67
3:K:238:LEU:HD11	3:K:278:TYR:HB3	1.74	0.67
2:B:733:ILE:HG12	2:B:734:ILE:H	1.58	0.67
3:I:705:ARG:O	3:I:705:ARG:HG3	1.94	0.67
2:B:1518:GLY:HA3	2:B:1585:LEU:HD22	1.77	0.67
1:G:351:MET:SD	1:G:440:ARG:HD2	2.35	0.67
2:H:1268:GLN:CG	2:H:1269:GLU:H	2.00	0.67
2:H:1359:LYS:HD2	4:N:4:LEU:HD11	1.75	0.67
3:L:705:ARG:O	3:L:705:ARG:HG3	1.94	0.67
2:D:876:TYR:HA	2:D:1451:GLN:HE22	1.60	0.66
2:F:962:GLY:O	2:F:964:PRO:HD3	1.95	0.66
2:H:1518:GLY:HA3	2:H:1585:LEU:HD22	1.77	0.66
2:H:1499:GLN:HG2	2:H:1500:LYS:HG3	1.77	0.66
2:D:1337:ASN:O	2:D:1338:LYS:HB2	1.95	0.66
1:G:606:THR:HG22	1:G:608:GLY:H	1.59	0.66
1:G:55:THR:HG22	1:G:57:ALA:H	1.61	0.66
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.78	0.66
1:A:606:THR:HG22	1:A:608:GLY:H	1.59	0.66
2:B:877:VAL:HG22	2:B:1451:GLN:HE21	1.59	0.66
2:D:841:ARG:HG2	2:D:841:ARG:NH1	2.08	0.66
1:G:473:MET:HE2	1:G:603:ILE:HD11	1.77	0.66
2:H:1498:ILE:HG12	2:H:1499:GLN:H	1.60	0.66
2:B:1041:SER:HG	2:B:1084:TRP:CD1	2.14	0.66
2:D:1041:SER:HG	2:D:1084:TRP:CD1	2.14	0.66
1:E:606:THR:HG22	1:E:608:GLY:H	1.59	0.66
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.60	0.66
3:J:446:GLU:HB3	3:J:449:SER:HB2	1.77	0.66
1:G:510:VAL:HG21	1:G:622:LEU:CD1	2.26	0.65
2:H:896:HIS:HB3	4:N:61:LYS:HD3	1.78	0.65
2:B:962:GLY:O	2:B:964:PRO:HD3	1.96	0.65
1:E:473:MET:HB2	1:E:508:ARG:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.65
2:B:1417:SER:HB2	4:Q:14:LYS:NZ	2.11	0.65
3:I:446:GLU:HB3	3:I:449:SER:HB2	1.79	0.65
3:I:478:ARG:HG3	3:I:479:PRO:HD2	1.79	0.65
2:F:1518:GLY:HA3	2:F:1585:LEU:HD22	1.77	0.65
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.78	0.65
2:F:829:LEU:HD23	2:F:840:VAL:HG11	1.78	0.65
2:F:1126:LEU:HG	2:F:1130:GLN:HE21	1.61	0.65
2:B:829:LEU:HD23	2:B:840:VAL:HG11	1.78	0.65
2:H:829:LEU:HD23	2:H:840:VAL:HG11	1.78	0.65
1:G:549:GLU:HG2	1:G:550:ASP:N	2.12	0.65
2:B:1337:ASN:O	2:B:1338:LYS:HB2	1.94	0.65
1:C:10:ASN:HB2	1:C:621:GLY:C	2.21	0.64
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.61	0.64
2:D:829:LEU:HD23	2:D:840:VAL:HG11	1.78	0.64
1:C:55:THR:HG22	1:C:57:ALA:H	1.61	0.64
2:F:1265:PRO:O	2:F:1266:ASP:HB2	1.96	0.64
3:I:446:GLU:O	3:I:450:LEU:HG	1.97	0.64
2:B:1265:PRO:O	2:B:1266:ASP:HB2	1.97	0.64
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.60	0.64
1:E:55:THR:HG22	1:E:57:ALA:H	1.61	0.64
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.61	0.64
1:G:473:MET:HB2	1:G:508:ARG:HB2	1.78	0.64
3:J:478:ARG:HG3	3:J:479:PRO:HD2	1.79	0.64
2:F:1268:GLN:O	2:F:1269:GLU:HG2	1.97	0.64
3:K:478:ARG:HG3	3:K:479:PRO:HD2	1.79	0.64
3:L:446:GLU:HB3	3:L:449:SER:HB2	1.79	0.64
2:B:837:GLU:HG2	4:Q:64:SER:OG	1.97	0.64
2:D:1265:PRO:O	2:D:1266:ASP:HB2	1.98	0.64
2:F:1337:ASN:O	2:F:1338:LYS:HB2	1.97	0.64
2:H:1338:LYS:HA	2:H:1371:ARG:HB2	1.80	0.64
1:C:549:GLU:HG2	1:C:550:ASP:N	2.12	0.63
2:D:1527:LEU:HD13	2:D:1541:MET:HG2	1.80	0.63
1:A:551:ARG:HD2	1:A:551:ARG:N	2.13	0.63
2:D:1416:PHE:CZ	2:D:1442:HIS:HB2	2.34	0.63
2:H:837:GLU:HG2	4:N:64:SER:OG	1.98	0.63
3:K:460:ARG:HE	4:P:28:VAL:HG21	1.63	0.63
3:K:513:LYS:HB3	3:K:522:ASP:HB3	1.81	0.63
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.81	0.63
1:G:3:MET:HE2	1:G:626:SER:CB	2.29	0.63
1:C:551:ARG:HD2	1:C:551:ARG:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1498:ILE:HG22	2:F:1499:GLN:N	2.13	0.63
3:L:478:ARG:HG3	3:L:479:PRO:HD2	1.79	0.63
2:D:962:GLY:C	2:D:964:PRO:HD3	2.24	0.63
1:E:551:ARG:N	1:E:551:ARG:HD2	2.13	0.63
1:E:567:HIS:ND1	2:F:760:PRO:HG3	2.13	0.63
1:G:551:ARG:N	1:G:551:ARG:HD2	2.13	0.63
2:H:876:TYR:HA	2:H:1451:GLN:HE22	1.64	0.63
2:H:1337:ASN:O	2:H:1338:LYS:HB2	1.97	0.63
6:S:1:NAG:H61	6:S:2:NAG:C7	2.29	0.63
2:B:1527:LEU:HD13	2:B:1541:MET:HG2	1.80	0.63
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.80	0.63
1:C:634:GLN:HE22	2:D:1016:GLY:HA2	1.64	0.63
1:A:351:MET:SD	1:A:440:ARG:HD2	2.39	0.63
2:B:1416:PHE:CZ	2:B:1442:HIS:HB2	2.34	0.63
3:J:460:ARG:HE	4:Q:28:VAL:HG21	1.64	0.62
1:E:147:ASN:HB2	1:E:148:PRO:HD2	1.81	0.62
1:G:512:TYR:CZ	1:G:624:PHE:HE1	2.16	0.62
2:H:1527:LEU:HD13	2:H:1541:MET:HG2	1.80	0.62
3:K:432:ASP:HA	4:P:27:ASN:HD21	1.63	0.62
3:L:513:LYS:HB3	3:L:522:ASP:HB3	1.81	0.62
2:B:1295:SER:O	2:B:1297:LEU:HD12	2.00	0.62
2:D:1295:SER:O	2:D:1297:LEU:HD12	2.00	0.62
2:B:876:TYR:HA	2:B:1451:GLN:HE22	1.63	0.62
3:I:513:LYS:HB3	3:I:522:ASP:HB3	1.81	0.62
1:G:147:ASN:HB2	1:G:148:PRO:HD2	1.81	0.62
2:F:877:VAL:HG22	2:F:1451:GLN:HE21	1.65	0.62
2:B:1446:ASN:HB2	4:Q:4:LEU:HB2	1.81	0.62
2:H:1498:ILE:HG13	2:H:1605:TRP:CE3	2.34	0.62
1:A:549:GLU:HG2	1:A:550:ASP:N	2.12	0.62
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.81	0.62
2:H:834:GLN:HE21	2:H:835:ASN:H	1.47	0.62
2:H:855:THR:HB	2:H:1602:LYS:NZ	2.14	0.62
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.35	0.62
2:F:1527:LEU:HD13	2:F:1541:MET:HG2	1.80	0.62
3:J:513:LYS:HB3	3:J:522:ASP:HB3	1.81	0.62
1:A:248:PHE:HD1	2:B:1378:MET:HE3	1.63	0.61
1:G:248:PHE:HD1	2:H:1378:MET:HE3	1.65	0.61
3:I:423:ASN:HD22	3:I:423:ASN:N	1.98	0.61
1:G:19:THR:HB	1:G:478:LEU:HB2	1.81	0.61
2:B:834:GLN:HE21	2:B:835:ASN:H	1.47	0.61
1:E:222:TYR:CE2	1:E:224:TYR:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1295:SER:O	2:F:1297:LEU:HD12	2.00	0.61
2:H:1611:GLU:HG3	2:H:1612:GLU:H	1.66	0.61
3:I:650:VAL:HG23	3:I:651:VAL:HG23	1.83	0.61
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.15	0.61
2:H:1497:PHE:HB2	2:H:1498:ILE:HD13	1.82	0.61
3:K:423:ASN:HD22	3:K:423:ASN:N	1.98	0.61
3:L:461:LYS:HG2	4:N:28:VAL:HG12	1.81	0.61
2:B:1490:ARG:HB3	2:B:1590:TRP:CH2	2.36	0.61
1:E:372:GLU:O	1:E:375:VAL:HG12	1.99	0.61
1:G:372:GLU:O	1:G:375:VAL:HG12	2.01	0.61
2:F:1385:MET:HE2	2:F:1385:MET:HA	1.83	0.61
1:G:222:TYR:CE2	1:G:224:TYR:HB2	2.35	0.61
3:I:461:LYS:HG2	4:M:28:VAL:HG12	1.82	0.61
3:K:478:ARG:HE	3:K:481:LYS:HD2	1.65	0.61
2:H:1498:ILE:HG12	2:H:1499:GLN:N	2.13	0.61
3:L:650:VAL:HG23	3:L:651:VAL:HG23	1.83	0.61
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.83	0.61
2:D:1490:ARG:HB3	2:D:1590:TRP:CH2	2.36	0.61
2:H:1385:MET:HA	2:H:1385:MET:HE2	1.83	0.61
2:H:1498:ILE:CG1	2:H:1499:GLN:H	2.12	0.61
3:J:423:ASN:HD22	3:J:423:ASN:N	1.98	0.61
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.35	0.61
2:H:923:ARG:HH22	2:H:940:ILE:HG12	1.66	0.61
2:F:834:GLN:HE21	2:F:835:ASN:H	1.47	0.61
2:F:1338:LYS:HA	2:F:1371:ARG:HB2	1.81	0.61
2:F:1527:LEU:HD21	2:F:1530:VAL:HG22	1.83	0.61
3:K:650:VAL:HG23	3:K:651:VAL:HG23	1.83	0.61
1:A:10:ASN:HB2	1:A:621:GLY:C	2.25	0.60
2:B:1527:LEU:HD21	2:B:1530:VAL:HG22	1.83	0.60
2:D:1291:TRP:CG	2:D:1292:GLU:H	2.19	0.60
2:F:1611:GLU:HG3	2:F:1612:GLU:H	1.66	0.60
3:I:478:ARG:HE	3:I:481:LYS:HD2	1.65	0.60
1:A:372:GLU:O	1:A:375:VAL:HG12	2.01	0.60
1:C:248:PHE:HD1	2:D:1378:MET:HE3	1.66	0.60
2:D:1291:TRP:O	2:D:1292:GLU:C	2.45	0.60
2:D:1611:GLU:HG3	2:D:1612:GLU:H	1.66	0.60
2:F:923:ARG:HH22	2:F:940:ILE:HG12	1.66	0.60
3:J:478:ARG:HE	3:J:481:LYS:HD2	1.65	0.60
2:F:837:GLU:HG2	4:M:64:SER:OG	2.00	0.60
1:G:20:MET:HB3	1:G:64:VAL:HG23	1.83	0.60
1:C:426:THR:HG21	1:C:432:ASN:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1295:SER:O	2:H:1297:LEU:HD12	2.00	0.60
3:L:449:SER:HA	3:L:452:LEU:HD13	1.84	0.60
3:L:478:ARG:HE	3:L:481:LYS:HD2	1.65	0.60
4:P:84:LYS:O	4:P:85:TYR:HB2	2.02	0.60
2:B:973:VAL:HG11	2:B:978:LEU:HD12	1.83	0.60
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.82	0.60
2:D:772:PHE:HD1	4:M:37:ASN:ND2	1.99	0.60
2:D:973:VAL:HG11	2:D:978:LEU:HD12	1.83	0.60
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.83	0.60
1:G:143:VAL:C	1:G:144:ASN:HD22	2.10	0.60
3:K:407:PRO:HD3	11:b:1:NAG:H82	1.83	0.60
2:B:1385:MET:HE2	2:B:1385:MET:HA	1.83	0.60
2:B:1532:LEU:HD11	2:B:1569:ARG:CD	2.32	0.60
2:D:1385:MET:HE2	2:D:1385:MET:HA	1.83	0.60
4:M:84:LYS:O	4:M:85:TYR:HB2	2.02	0.60
1:A:143:VAL:C	1:A:144:ASN:HD22	2.09	0.60
2:B:1039:GLN:HB3	2:B:1040:PRO:HD2	1.83	0.60
1:E:143:VAL:C	1:E:144:ASN:HD22	2.10	0.60
3:J:650:VAL:HG23	3:J:651:VAL:HG23	1.83	0.60
3:L:374:ILE:HD13	3:L:417:LEU:HD23	1.84	0.60
2:B:1291:TRP:CG	2:B:1292:GLU:N	2.69	0.60
2:D:834:GLN:HE21	2:D:835:ASN:H	1.47	0.60
1:E:20:MET:HB3	1:E:64:VAL:HG23	1.83	0.60
2:F:1041:SER:HG	2:F:1084:TRP:CD1	2.20	0.60
2:F:1291:TRP:CD1	2:F:1292:GLU:N	2.70	0.60
2:F:1446:ASN:HB2	4:M:4:LEU:CD1	2.32	0.60
3:J:460:ARG:NE	4:Q:28:VAL:HG21	2.16	0.60
2:D:1532:LEU:HD11	2:D:1569:ARG:CD	2.32	0.59
1:E:220:PHE:CZ	1:E:330:PRO:HB3	2.37	0.59
2:F:876:TYR:HA	2:F:1451:GLN:HE22	1.67	0.59
2:F:1039:GLN:HB3	2:F:1040:PRO:HD2	1.83	0.59
2:D:877:VAL:HG22	2:D:1451:GLN:HE21	1.67	0.59
2:D:1039:GLN:HB3	2:D:1040:PRO:HD2	1.83	0.59
3:J:570:ILE:HD13	3:J:688:GLN:HB2	1.84	0.59
3:K:436:LEU:HB3	3:K:440:PHE:CE2	2.37	0.59
3:L:423:ASN:HD22	3:L:423:ASN:N	1.98	0.59
2:B:1611:GLU:HG3	2:B:1612:GLU:H	1.66	0.59
2:F:1291:TRP:O	2:F:1292:GLU:C	2.44	0.59
2:D:1527:LEU:HD21	2:D:1530:VAL:HG22	1.83	0.59
1:E:549:GLU:HG2	1:E:550:ASP:N	2.12	0.59
2:F:1291:TRP:CG	2:F:1292:GLU:H	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ARG:NH2	1:G:476:GLY:HA3	2.18	0.59
2:H:833:ARG:HH11	2:H:833:ARG:CG	2.15	0.59
3:I:563:TYR:CE2	3:I:569:PRO:HG3	2.38	0.59
3:I:570:ILE:HD13	3:I:688:GLN:HB2	1.84	0.59
1:G:555:PRO:HB3	2:H:775:ASP:HA	1.83	0.59
2:B:1291:TRP:CG	2:B:1292:GLU:H	2.19	0.59
2:D:1337:ASN:O	2:D:1338:LYS:CB	2.51	0.59
2:H:744:GLU:C	2:H:746:PRO:HD3	2.28	0.59
2:H:1291:TRP:CG	2:H:1292:GLU:H	2.19	0.59
2:H:1527:LEU:HD21	2:H:1530:VAL:HG22	1.83	0.59
3:L:570:ILE:HD13	3:L:688:GLN:HB2	1.84	0.59
4:N:84:LYS:O	4:N:85:TYR:HB2	2.02	0.59
2:H:1291:TRP:O	2:H:1292:GLU:C	2.45	0.59
2:B:1291:TRP:O	2:B:1292:GLU:C	2.45	0.59
1:C:143:VAL:C	1:C:144:ASN:HD22	2.10	0.59
1:G:61:MET:HE1	1:G:482:GLY:HA2	1.83	0.59
3:K:563:TYR:CE2	3:K:569:PRO:HG3	2.38	0.59
1:C:558:GLN:HB3	2:D:770:ASN:HD21	1.68	0.59
1:G:350:LEU:HD21	1:G:400:ILE:HG21	1.83	0.59
3:J:436:LEU:HB3	3:J:440:PHE:CE2	2.37	0.59
3:J:563:TYR:CE2	3:J:569:PRO:HG3	2.38	0.59
3:L:508:LYS:HE2	3:L:508:LYS:HA	1.85	0.59
4:N:22:LEU:HB3	4:N:74:TYR:HE2	1.68	0.59
4:Q:84:LYS:O	4:Q:85:TYR:HB2	2.02	0.59
3:L:563:TYR:CE2	3:L:569:PRO:HG3	2.38	0.59
2:F:973:VAL:HG11	2:F:978:LEU:HD12	1.84	0.58
3:I:374:ILE:HD13	3:I:417:LEU:HD23	1.84	0.58
2:D:833:ARG:HH11	2:D:833:ARG:CG	2.15	0.58
1:E:477:ARG:HH11	1:E:477:ARG:CG	2.16	0.58
2:F:1215:LEU:HD23	2:F:1256:ALA:HB1	1.85	0.58
3:L:436:LEU:HB3	3:L:440:PHE:CE2	2.37	0.58
3:I:436:LEU:HB3	3:I:440:PHE:CE2	2.37	0.58
3:K:374:ILE:HD13	3:K:417:LEU:HD23	1.84	0.58
1:C:40:PHE:CE2	2:D:1017:LEU:HD22	2.38	0.58
2:F:1291:TRP:CG	2:F:1292:GLU:N	2.70	0.58
2:F:1532:LEU:HD11	2:F:1569:ARG:CD	2.34	0.58
3:J:374:ILE:HD13	3:J:417:LEU:HD23	1.84	0.58
4:P:22:LEU:HB3	4:P:74:TYR:HE2	1.68	0.58
2:H:1535:ASP:O	2:H:1536:PHE:HB3	2.04	0.58
4:M:22:LEU:HB3	4:M:74:TYR:HE2	1.68	0.58
3:I:508:LYS:HE2	3:I:508:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:508:LYS:HE2	3:J:508:LYS:HA	1.85	0.58
2:D:1291:TRP:CG	2:D:1292:GLU:N	2.69	0.58
2:F:744:GLU:C	2:F:746:PRO:HD3	2.29	0.58
3:K:570:ILE:HD13	3:K:688:GLN:HB2	1.84	0.58
2:H:877:VAL:H	2:H:1451:GLN:NE2	2.01	0.58
3:L:477:ILE:O	3:L:511:SER:HB2	2.04	0.58
2:B:833:ARG:HH11	2:B:833:ARG:CG	2.15	0.58
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	1.85	0.58
2:F:1359:LYS:HD2	4:M:4:LEU:CD1	2.32	0.58
2:H:1532:LEU:HD11	2:H:1569:ARG:CD	2.34	0.58
3:J:477:ILE:O	3:J:511:SER:HB2	2.04	0.58
2:D:1470:PHE:HB2	2:D:1478:GLY:HA3	1.86	0.57
1:G:527:ASP:N	1:G:616:VAL:HG11	2.19	0.57
4:Q:6:THR:H	4:Q:9:GLU:CB	2.16	0.57
1:E:350:LEU:HD21	1:E:400:ILE:HG21	1.86	0.57
1:G:510:VAL:HG11	1:G:622:LEU:HD12	1.86	0.57
2:H:1291:TRP:CD1	2:H:1292:GLU:N	2.70	0.57
2:H:1497:PHE:CZ	2:H:1572:LEU:HD23	2.39	0.57
3:I:477:ILE:O	3:I:511:SER:HB2	2.04	0.57
3:K:477:ILE:O	3:K:511:SER:HB2	2.04	0.57
2:B:1445:PHE:CZ	4:Q:7:SER:HA	2.40	0.57
2:F:1133:LYS:O	2:F:1137:GLU:HG3	2.04	0.57
2:H:1291:TRP:CG	2:H:1292:GLU:N	2.70	0.57
1:A:614:ALA:HB1	1:A:632:THR:HA	1.86	0.57
2:D:809:ILE:HD11	2:D:892:ALA:HB3	1.87	0.57
2:D:1215:LEU:HD23	2:D:1256:ALA:HB1	1.85	0.57
1:G:13:ARG:HH22	1:G:476:GLY:HA3	1.69	0.57
4:Q:22:LEU:HB3	4:Q:74:TYR:HE2	1.68	0.57
2:B:962:GLY:C	2:B:964:PRO:HD3	2.29	0.57
2:B:1133:LYS:O	2:B:1137:GLU:HG3	2.04	0.57
2:B:1337:ASN:O	2:B:1338:LYS:CB	2.51	0.57
2:F:1535:ASP:O	2:F:1536:PHE:HB3	2.03	0.57
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.87	0.57
2:F:1269:GLU:HG3	2:F:1315:LYS:CB	2.35	0.57
2:F:1446:ASN:HB2	4:M:4:LEU:HD13	1.85	0.57
1:C:567:HIS:ND1	2:D:760:PRO:HG3	2.19	0.57
3:K:460:ARG:NE	4:P:28:VAL:HG21	2.19	0.57
3:K:508:LYS:HE2	3:K:508:LYS:HA	1.85	0.57
2:B:836:GLN:HG2	2:B:897:HIS:HE1	1.70	0.57
2:D:1360:ASN:O	2:D:1361:THR:C	2.48	0.57
1:E:614:ALA:HB1	1:E:632:THR:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1470:PHE:HB2	2:B:1478:GLY:HA3	1.86	0.57
2:D:1462:ASN:HD22	2:D:1463:LEU:N	2.03	0.57
2:H:923:ARG:NH2	2:H:940:ILE:HG12	2.19	0.57
2:H:1582:MET:HA	2:H:1605:TRP:O	2.05	0.57
2:F:1055:TRP:CZ2	2:F:1108:ILE:HA	2.40	0.57
2:H:819:ARG:HG2	2:H:819:ARG:NH1	2.19	0.57
2:H:1462:ASN:HD22	2:H:1463:LEU:N	2.03	0.57
2:B:965:VAL:O	2:B:1267:HIS:HD2	1.88	0.56
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.86	0.56
1:C:268:ARG:HD3	2:D:1378:MET:SD	2.44	0.56
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.40	0.56
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.86	0.56
3:L:253:SER:HB2	3:L:326:SER:O	2.05	0.56
2:F:809:ILE:HD11	2:F:892:ALA:HB3	1.87	0.56
2:F:833:ARG:HH11	2:F:833:ARG:CG	2.15	0.56
2:F:1582:MET:HA	2:F:1605:TRP:O	2.05	0.56
1:G:614:ALA:HB1	1:G:632:THR:HA	1.86	0.56
2:H:1494:GLU:HG2	2:H:1602:LYS:HD3	1.87	0.56
3:L:461:LYS:HD2	4:N:29:ASN:OD1	2.05	0.56
9:a:1:NAG:H61	9:a:2:NAG:C7	2.35	0.56
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.70	0.56
2:B:923:ARG:HH22	2:B:940:ILE:HG12	1.70	0.56
2:B:925:LEU:HD11	2:B:1320:LEU:HD22	1.87	0.56
2:B:1462:ASN:HD22	2:B:1463:LEU:N	2.03	0.56
2:B:1516:GLU:HB3	2:B:1517:PRO:HD2	1.88	0.56
1:C:614:ALA:HB1	1:C:632:THR:HA	1.86	0.56
2:D:925:LEU:HD11	2:D:1320:LEU:HD22	1.86	0.56
2:D:1133:LYS:O	2:D:1137:GLU:HG3	2.05	0.56
1:E:572:VAL:HG12	2:F:753:VAL:HG22	1.87	0.56
2:F:1462:ASN:HD22	2:F:1463:LEU:N	2.03	0.56
2:H:1337:ASN:O	2:H:1338:LYS:CB	2.53	0.56
2:H:1566:ILE:O	2:H:1569:ARG:HG3	2.06	0.56
3:K:364:ASP:O	3:K:409:VAL:HG23	2.06	0.56
2:D:1535:ASP:O	2:D:1536:PHE:HB3	2.05	0.56
2:F:836:GLN:HG2	2:F:897:HIS:HE1	1.70	0.56
2:H:925:LEU:HD11	2:H:1320:LEU:HD22	1.88	0.56
3:I:353:ASN:HB2	3:I:394:ARG:NH1	2.20	0.56
3:K:253:SER:HB2	3:K:326:SER:O	2.05	0.56
3:L:364:ASP:O	3:L:409:VAL:HG23	2.06	0.56
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.40	0.56
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:923:ARG:NH2	2:F:940:ILE:HG12	2.19	0.56
2:B:1360:ASN:O	2:B:1361:THR:C	2.48	0.56
2:B:1535:ASP:O	2:B:1536:PHE:HB3	2.05	0.56
1:C:441:THR:HG21	1:E:441:THR:HG21	1.88	0.56
1:E:116:ILE:HD11	1:E:203:LYS:HB3	1.88	0.56
1:G:477:ARG:HH11	1:G:477:ARG:CG	2.16	0.56
2:H:836:GLN:HG2	2:H:897:HIS:HE1	1.70	0.56
3:I:253:SER:HB2	3:I:326:SER:O	2.05	0.56
2:D:1180:LEU:HD23	2:D:1221:LEU:HD11	1.88	0.56
3:J:253:SER:HB2	3:J:326:SER:O	2.06	0.56
3:J:438:ASP:OD2	4:Q:28:VAL:HG13	2.05	0.56
2:D:923:ARG:HH22	2:D:940:ILE:HG12	1.70	0.56
2:D:1279:PRO:HG2	2:D:1306:GLU:HB3	1.88	0.56
2:F:1337:ASN:O	2:F:1338:LYS:CB	2.53	0.56
3:I:364:ASP:O	3:I:409:VAL:HG23	2.06	0.56
3:L:381:ARG:CG	3:L:381:ARG:NH2	2.68	0.56
2:F:1143:LEU:HB3	2:F:1144:PRO:HD3	1.86	0.56
2:H:809:ILE:HD11	2:H:892:ALA:HB3	1.87	0.56
2:H:964:PRO:HG3	2:H:1270:LEU:HD11	1.88	0.56
3:J:364:ASP:O	3:J:409:VAL:HG23	2.06	0.56
3:L:353:ASN:HB2	3:L:394:ARG:NH1	2.20	0.56
3:L:513:LYS:HZ2	3:L:524:GLU:HG2	1.71	0.56
4:N:6:THR:H	4:N:9:GLU:CB	2.16	0.56
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.16	0.56
2:F:1012:TRP:HB3	2:F:1017:LEU:HD23	1.88	0.56
3:K:513:LYS:HZ2	3:K:524:GLU:HG2	1.70	0.56
4:P:6:THR:H	4:P:9:GLU:CB	2.16	0.56
2:B:966:ALA:O	2:B:967:GLN:CB	2.54	0.55
2:F:1566:ILE:O	2:F:1569:ARG:HG3	2.06	0.55
3:I:461:LYS:HG2	4:M:28:VAL:CG1	2.36	0.55
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.88	0.55
2:D:1291:TRP:CD1	2:D:1292:GLU:N	2.75	0.55
2:D:1516:GLU:HB3	2:D:1517:PRO:HD2	1.88	0.55
2:F:804:MET:HG2	2:F:805:GLN:H	1.72	0.55
2:F:925:LEU:HD11	2:F:1320:LEU:HD22	1.88	0.55
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.88	0.55
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.88	0.55
2:B:1563:ILE:HB	2:B:1599:ILE:HD13	1.88	0.55
2:F:1516:GLU:HB3	2:F:1517:PRO:HD2	1.88	0.55
2:H:839:LYS:HE2	4:N:60:PHE:CD1	2.41	0.55
2:B:804:MET:HG2	2:B:805:GLN:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ILE:HD11	1:C:515:LEU:HD22	1.89	0.55
1:C:477:ARG:HH11	1:C:477:ARG:CG	2.16	0.55
2:F:738:ASN:ND2	4:P:45:LYS:HE2	2.19	0.55
1:G:116:ILE:HD11	1:G:203:LYS:HB3	1.88	0.55
2:H:1525:THR:HG22	2:H:1543:ILE:HA	1.88	0.55
2:H:1563:ILE:HB	2:H:1599:ILE:HD13	1.89	0.55
2:B:1566:ILE:O	2:B:1569:ARG:HG3	2.07	0.55
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.88	0.55
2:D:836:GLN:HG2	2:D:897:HIS:HE1	1.70	0.55
1:E:13:ARG:HH22	1:E:476:GLY:HA3	1.71	0.55
2:F:740:VAL:O	4:P:42:ARG:HD3	2.06	0.55
2:F:1498:ILE:HD12	2:F:1498:ILE:N	2.21	0.55
2:H:1338:LYS:CA	2:H:1371:ARG:HB2	2.36	0.55
3:K:353:ASN:HB2	3:K:394:ARG:NH1	2.21	0.55
2:B:1291:TRP:CD1	2:B:1292:GLU:N	2.75	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.89	0.55
2:D:1012:TRP:HB3	2:D:1017:LEU:HD23	1.88	0.55
2:F:776:SER:HB2	2:F:780:TRP:CZ2	2.42	0.55
2:F:1525:THR:HG22	2:F:1543:ILE:HA	1.88	0.55
2:B:877:VAL:H	2:B:1451:GLN:NE2	2.03	0.55
2:B:1012:TRP:HB3	2:B:1017:LEU:HD23	1.88	0.55
2:F:896:HIS:HB3	4:M:61:LYS:HD3	1.88	0.55
2:F:1640:PRO:O	2:F:1641:ASN:HB2	2.07	0.55
1:G:252:GLY:HA2	1:G:262:LEU:HG	1.89	0.55
2:H:1498:ILE:CD1	2:H:1605:TRP:HA	2.35	0.55
2:B:1417:SER:HB2	4:Q:14:LYS:HZ3	1.71	0.55
1:G:386:LYS:HD3	1:G:440:ARG:HG2	1.87	0.55
1:G:465:ILE:HD11	1:G:515:LEU:HD22	1.89	0.55
1:G:473:MET:CE	1:G:603:ILE:HD11	2.37	0.55
2:H:1516:GLU:HB3	2:H:1517:PRO:HD2	1.88	0.55
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.88	0.55
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.89	0.55
2:F:1084:TRP:CD1	2:F:1088:GLU:HG3	2.42	0.55
2:F:1268:GLN:O	2:F:1269:GLU:CG	2.55	0.55
1:C:116:ILE:HD11	1:C:203:LYS:HB3	1.88	0.55
2:F:1338:LYS:CA	2:F:1371:ARG:HB2	2.37	0.55
2:H:1641:ASN:HD21	3:J:366:LEU:HB3	1.72	0.55
3:J:353:ASN:HB2	3:J:394:ARG:NH1	2.21	0.55
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.42	0.54
1:E:10:ASN:HA	1:E:623:THR:HG23	1.89	0.54
2:F:1180:LEU:HD23	2:F:1221:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1279:PRO:HG2	2:F:1306:GLU:HB3	1.88	0.54
1:G:508:ARG:NH1	1:G:604:GLY:HA3	2.22	0.54
2:H:962:GLY:C	2:H:964:PRO:HD3	2.31	0.54
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.89	0.54
2:H:1279:PRO:HG2	2:H:1306:GLU:HB3	1.88	0.54
3:L:461:LYS:HG2	4:N:28:VAL:CG1	2.37	0.54
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.42	0.54
2:H:1445:PHE:CE2	4:N:7:SER:HA	2.43	0.54
1:E:478:LEU:HD21	1:E:622:LEU:HD21	1.88	0.54
2:H:1289:ILE:HD13	2:H:1298:ARG:HE	1.73	0.54
1:A:465:ILE:HD11	1:A:515:LEU:HD22	1.89	0.54
1:E:252:GLY:HA2	1:E:262:LEU:HG	1.89	0.54
3:I:535:ASN:O	3:I:547:PHE:HB3	2.07	0.54
3:L:452:LEU:HD23	3:L:455:MET:HE1	1.90	0.54
3:L:535:ASN:O	3:L:547:PHE:HB3	2.07	0.54
2:B:1041:SER:HG	2:B:1084:TRP:CG	2.26	0.54
2:D:804:MET:HG2	2:D:805:GLN:H	1.71	0.54
2:H:804:MET:HG2	2:H:805:GLN:H	1.72	0.54
3:K:535:ASN:O	3:K:547:PHE:HB3	2.07	0.54
2:B:1084:TRP:CD1	2:B:1088:GLU:HG3	2.42	0.54
2:D:966:ALA:O	2:D:967:GLN:CB	2.54	0.54
2:D:1566:ILE:O	2:D:1569:ARG:HG3	2.07	0.54
1:E:396:LYS:HG3	1:E:397:PRO:HD2	1.90	0.54
1:E:555:PRO:HB3	2:F:775:ASP:HA	1.90	0.54
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.90	0.54
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.54
2:D:837:GLU:HG2	4:P:64:SER:OG	2.07	0.54
2:D:1563:ILE:HB	2:D:1599:ILE:HD13	1.88	0.54
2:F:1289:ILE:HD13	2:F:1298:ARG:HE	1.73	0.54
1:G:534:LYS:HD2	1:G:535:ASP:H	1.72	0.54
3:J:631:CYS:SG	3:J:714:ARG:HD2	2.48	0.54
3:K:631:CYS:SG	3:K:714:ARG:HD2	2.48	0.54
3:L:478:ARG:NE	3:L:481:LYS:HD2	2.23	0.54
2:D:1041:SER:HG	2:D:1084:TRP:CG	2.26	0.54
2:F:1563:ILE:HB	2:F:1599:ILE:HD13	1.89	0.54
1:G:396:LYS:HG3	1:G:397:PRO:HD2	1.90	0.54
3:J:452:LEU:HD23	3:J:455:MET:HE1	1.90	0.54
3:K:478:ARG:NE	3:K:481:LYS:HD2	2.23	0.54
2:B:819:ARG:HG2	2:B:819:ARG:NH1	2.19	0.53
2:B:1582:MET:HA	2:B:1605:TRP:O	2.08	0.53
2:D:1084:TRP:CD1	2:D:1088:GLU:HG3	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:MET:HE1	1:E:482:GLY:HA2	1.89	0.53
3:I:452:LEU:HD23	3:I:455:MET:HE1	1.90	0.53
3:K:381:ARG:CG	3:K:381:ARG:NH2	2.68	0.53
3:L:436:LEU:HB3	3:L:440:PHE:HE2	1.73	0.53
1:A:13:ARG:HH22	1:A:476:GLY:HA3	1.73	0.53
2:B:923:ARG:NH2	2:B:940:ILE:HG12	2.23	0.53
2:B:1279:PRO:HG2	2:B:1306:GLU:HB3	1.88	0.53
1:C:436:LEU:HD11	1:C:511:ALA:HB3	1.90	0.53
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.42	0.53
2:D:997:THR:N	2:D:998:PRO:HD2	2.24	0.53
1:E:568:GLY:HA2	2:F:757:LYS:HE2	1.89	0.53
2:F:804:MET:HG2	2:F:805:GLN:N	2.23	0.53
1:G:451:VAL:HB	1:G:495:LEU:HB3	1.91	0.53
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.90	0.53
2:D:804:MET:HG2	2:D:805:GLN:N	2.23	0.53
3:J:535:ASN:O	3:J:547:PHE:HB3	2.07	0.53
3:K:435:ASN:ND2	3:K:460:ARG:HH21	2.06	0.53
3:L:631:CYS:SG	3:L:714:ARG:HD2	2.48	0.53
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.89	0.53
1:A:436:LEU:HD11	1:A:511:ALA:HB3	1.90	0.53
1:E:465:ILE:HD11	1:E:515:LEU:HD22	1.89	0.53
2:F:940:ILE:HD12	2:F:1308:PHE:CE1	2.44	0.53
2:D:1289:ILE:HD13	2:D:1298:ARG:HE	1.74	0.53
2:D:1582:MET:HA	2:D:1605:TRP:O	2.08	0.53
1:E:219:LYS:NZ	1:E:356:ASN:HD22	2.07	0.53
1:G:269:ILE:HD13	1:G:278:VAL:HB	1.90	0.53
2:H:1485:ARG:HH21	2:H:1590:TRP:CD1	2.27	0.53
3:I:513:LYS:HZ2	3:I:524:GLU:HG2	1.74	0.53
3:J:478:ARG:NE	3:J:481:LYS:HD2	2.23	0.53
1:A:451:VAL:HB	1:A:495:LEU:HB3	1.91	0.53
2:B:997:THR:N	2:B:998:PRO:HD2	2.24	0.53
1:C:269:ILE:HD13	1:C:278:VAL:HB	1.90	0.53
2:D:923:ARG:NH2	2:D:940:ILE:HG12	2.23	0.53
2:D:967:GLN:O	2:D:968:MET:HB2	2.08	0.53
2:H:940:ILE:HD12	2:H:1308:PHE:CE1	2.43	0.53
2:B:804:MET:HG2	2:B:805:GLN:N	2.23	0.53
1:E:477:ARG:HG2	1:E:477:ARG:NH1	2.21	0.53
2:F:1541:MET:HE1	2:F:1582:MET:SD	2.49	0.53
2:H:1521:TYR:HB2	2:H:1523:TYR:CE2	2.44	0.53
3:I:478:ARG:NE	3:I:481:LYS:HD2	2.23	0.53
3:K:452:LEU:HD23	3:K:455:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:456:VAL:HG13	3:K:467:LYS:HA	1.91	0.53
1:A:506:SER:CB	1:A:530:TRP:HE1	2.21	0.53
2:F:937:LYS:HD2	2:F:937:LYS:O	2.09	0.53
2:H:776:SER:HB2	2:H:780:TRP:CZ2	2.42	0.53
3:I:456:VAL:HG13	3:I:467:LYS:HA	1.91	0.53
3:J:456:VAL:HG13	3:J:467:LYS:HA	1.91	0.53
3:L:438:ASP:OD2	4:N:28:VAL:HG13	2.09	0.53
4:M:6:THR:H	4:M:9:GLU:CB	2.16	0.53
2:D:865:THR:OG1	4:P:11:GLN:HG2	2.08	0.53
2:D:877:VAL:H	2:D:1451:GLN:NE2	2.07	0.53
2:D:1470:PHE:CB	2:D:1478:GLY:HA3	2.39	0.53
1:E:505:PRO:HG3	1:E:595:TRP:CE3	2.44	0.53
2:F:822:GLN:OE1	2:F:1479:LYS:HA	2.09	0.53
2:F:973:VAL:HG12	2:F:975:ALA:H	1.73	0.53
2:F:997:THR:N	2:F:998:PRO:HD2	2.24	0.53
2:F:1387:THR:CG2	2:F:1451:GLN:H	2.21	0.53
3:I:631:CYS:SG	3:I:714:ARG:HD2	2.48	0.53
3:J:436:LEU:HB3	3:J:440:PHE:HE2	1.73	0.53
3:K:436:LEU:HB3	3:K:440:PHE:HE2	1.73	0.53
2:B:1289:ILE:HD13	2:B:1298:ARG:HE	1.73	0.52
1:C:439:LEU:H	1:C:439:LEU:HD12	1.74	0.52
1:E:590:THR:HG22	1:E:592:SER:H	1.75	0.52
1:G:569:ALA:HB2	2:H:788:SER:HB2	1.90	0.52
2:H:740:VAL:O	4:Q:42:ARG:HD3	2.09	0.52
2:D:1196:ASN:HD22	2:D:1196:ASN:N	2.07	0.52
2:F:978:LEU:HG	2:F:1240:TYR:HB3	1.91	0.52
1:G:342:PHE:CE1	1:G:391:THR:HG21	2.45	0.52
1:G:472:ILE:HD13	1:G:509:LEU:HD23	1.90	0.52
3:K:438:ASP:OD2	4:P:28:VAL:HG13	2.09	0.52
3:K:654:ARG:HA	3:K:722:GLN:HG3	1.91	0.52
3:L:368:ASN:ND2	3:L:368:ASN:H	2.08	0.52
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.22	0.52
2:B:1446:ASN:CB	4:Q:4:LEU:HB2	2.40	0.52
2:B:1470:PHE:CB	2:B:1478:GLY:HA3	2.39	0.52
1:C:19:THR:HB	1:C:478:LEU:HB2	1.91	0.52
1:C:396:LYS:HG3	1:C:397:PRO:HD2	1.90	0.52
1:C:569:ALA:HB2	2:D:788:SER:HB2	1.89	0.52
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.22	0.52
1:E:439:LEU:H	1:E:439:LEU:HD12	1.74	0.52
1:G:527:ASP:CA	1:G:616:VAL:HG11	2.40	0.52
2:H:804:MET:HG2	2:H:805:GLN:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:461:LYS:HD2	4:P:29:ASN:OD1	2.10	0.52
3:K:598:LEU:HA	3:K:603:ILE:HD13	1.91	0.52
2:B:973:VAL:HG12	2:B:975:ALA:H	1.73	0.52
2:B:978:LEU:HG	2:B:1240:TYR:HB3	1.91	0.52
1:E:451:VAL:HB	1:E:495:LEU:HB3	1.91	0.52
3:J:654:ARG:HA	3:J:722:GLN:HG3	1.91	0.52
2:B:1344:THR:HG21	2:B:1346:LYS:HE2	1.92	0.52
2:D:744:GLU:C	2:D:746:PRO:HD3	2.34	0.52
2:D:973:VAL:HG12	2:D:975:ALA:H	1.73	0.52
2:F:932:ARG:HH11	3:L:339:SER:HB2	1.73	0.52
3:I:461:LYS:HD2	4:M:29:ASN:OD1	2.09	0.52
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.44	0.52
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.75	0.52
1:C:451:VAL:HB	1:C:495:LEU:HB3	1.91	0.52
2:D:1521:TYR:HB2	2:D:1523:TYR:CE2	2.44	0.52
1:E:434:LEU:HB2	1:E:513:TYR:HE2	1.75	0.52
1:G:339:PRO:HB3	1:G:608:GLY:O	2.09	0.52
1:G:436:LEU:HD11	1:G:511:ALA:HB3	1.90	0.52
2:H:1541:MET:HE1	2:H:1582:MET:SD	2.49	0.52
2:H:1578:LYS:HD3	2:H:1608:HIS:HE1	1.74	0.52
3:J:598:LEU:HA	3:J:603:ILE:HD13	1.91	0.52
3:K:531:HIS:CD2	3:K:533:ASN:H	2.27	0.52
8:X:2:NAG:H82	8:X:2:NAG:O3	2.10	0.52
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.75	0.52
1:E:472:ILE:HD13	1:E:509:LEU:HD23	1.90	0.52
2:F:1196:ASN:HD22	2:F:1196:ASN:N	2.07	0.52
2:F:1521:TYR:HB2	2:F:1523:TYR:CE2	2.44	0.52
2:H:1470:PHE:HB2	2:H:1478:GLY:HA3	1.92	0.52
3:I:313:GLN:O	3:I:317:ILE:HG13	2.10	0.52
3:I:531:HIS:CD2	3:I:533:ASN:H	2.27	0.52
3:I:538:GLY:C	3:I:539:LYS:HD2	2.35	0.52
3:L:256:ILE:HD12	3:L:405:VAL:HG23	1.92	0.52
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.92	0.52
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.90	0.52
2:D:1541:MET:HE1	2:D:1582:MET:SD	2.50	0.52
3:I:292:TYR:HD1	3:I:325:LYS:HD3	1.74	0.52
3:I:368:ASN:ND2	3:I:368:ASN:H	2.08	0.52
3:I:654:ARG:HA	3:I:722:GLN:HG3	1.91	0.52
3:J:531:HIS:CD2	3:J:533:ASN:H	2.27	0.52
3:L:292:TYR:HD1	3:L:325:LYS:HD3	1.74	0.52
2:B:1521:TYR:HB2	2:B:1523:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1541:MET:HE1	2:B:1582:MET:SD	2.50	0.52
2:D:978:LEU:HG	2:D:1240:TYR:HB3	1.91	0.52
2:F:1470:PHE:HB2	2:F:1478:GLY:HA3	1.92	0.52
1:G:214:VAL:HG23	1:G:321:ARG:HB2	1.92	0.52
1:G:506:SER:CB	1:G:530:TRP:HE1	2.21	0.52
2:H:1359:LYS:HD2	4:N:4:LEU:CD1	2.40	0.52
2:H:1387:THR:CG2	2:H:1451:GLN:H	2.21	0.52
2:H:1641:ASN:O	3:J:368:ASN:ND2	2.43	0.52
3:J:239:ASP:HB3	3:J:448:GLN:HB2	1.92	0.52
3:J:256:ILE:HD12	3:J:405:VAL:HG23	1.92	0.52
3:J:381:ARG:CG	3:J:381:ARG:NH2	2.68	0.52
3:L:598:LEU:HA	3:L:603:ILE:HD13	1.91	0.52
1:A:396:LYS:HG3	1:A:397:PRO:HD2	1.90	0.52
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.92	0.52
1:E:269:ILE:HD13	1:E:278:VAL:HB	1.90	0.52
1:E:436:LEU:HD11	1:E:511:ALA:HB3	1.90	0.52
1:G:424:TYR:O	1:G:433:TYR:CE1	2.59	0.52
3:I:436:LEU:HB3	3:I:440:PHE:HE2	1.73	0.52
3:J:368:ASN:ND2	3:J:368:ASN:H	2.06	0.52
3:L:654:ARG:HA	3:L:722:GLN:HG3	1.91	0.52
4:P:30:GLU:HA	4:P:44:ILE:HD13	1.92	0.52
2:B:1196:ASN:HD22	2:B:1196:ASN:N	2.07	0.51
2:F:1228:PRO:HB2	2:F:1229:PRO:HD3	1.92	0.51
3:K:538:GLY:C	3:K:539:LYS:HD2	2.35	0.51
3:L:239:ASP:HB3	3:L:448:GLN:HB2	1.92	0.51
1:A:439:LEU:H	1:A:439:LEU:HD12	1.74	0.51
2:H:860:HIS:CE1	2:H:862:GLN:HE22	2.29	0.51
3:K:313:GLN:O	3:K:317:ILE:HG13	2.10	0.51
3:K:368:ASN:ND2	3:K:368:ASN:H	2.07	0.51
3:L:531:HIS:CD2	3:L:533:ASN:H	2.27	0.51
4:N:30:GLU:HA	4:N:44:ILE:HD13	1.92	0.51
1:C:126:ARG:HG2	1:C:168:PRO:HA	1.93	0.51
1:E:214:VAL:HG23	1:E:321:ARG:HB2	1.92	0.51
1:A:590:THR:HG22	1:A:592:SER:H	1.75	0.51
2:D:972:ALA:HB1	2:D:1005:TYR:OH	2.10	0.51
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.92	0.51
2:D:1344:THR:HG21	2:D:1346:LYS:HE2	1.92	0.51
1:E:410:SER:O	1:E:414:GLN:HG2	2.11	0.51
2:F:754:GLU:HG3	2:F:769:MET:SD	2.51	0.51
3:I:598:LEU:HA	3:I:603:ILE:HD13	1.91	0.51
3:J:292:TYR:HD1	3:J:325:LYS:HD3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:313:GLN:O	3:L:317:ILE:HG13	2.10	0.51
1:C:568:GLY:HA2	2:D:757:LYS:HE2	1.93	0.51
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.92	0.51
2:F:972:ALA:HB1	2:F:1005:TYR:OH	2.09	0.51
2:F:1578:LYS:HD3	2:F:1608:HIS:HE1	1.74	0.51
3:I:700:CYS:O	3:I:701:LYS:C	2.53	0.51
3:K:256:ILE:HD12	3:K:405:VAL:HG23	1.92	0.51
4:M:70:LEU:HG	4:M:74:TYR:CE2	2.46	0.51
2:B:972:ALA:HB1	2:B:1005:TYR:OH	2.10	0.51
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.91	0.51
2:D:754:GLU:HG3	2:D:769:MET:SD	2.51	0.51
3:J:461:LYS:HD2	4:Q:29:ASN:OD1	2.10	0.51
3:J:538:GLY:C	3:J:539:LYS:HD2	2.35	0.51
3:K:292:TYR:HD1	3:K:325:LYS:HD3	1.74	0.51
3:K:700:CYS:O	3:K:701:LYS:C	2.53	0.51
3:L:538:GLY:C	3:L:539:LYS:HD2	2.35	0.51
3:L:700:CYS:O	3:L:701:LYS:C	2.53	0.51
1:A:640:CYS:HB3	1:A:641:PRO:HD2	1.93	0.51
2:B:754:GLU:HG3	2:B:769:MET:SD	2.51	0.51
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.93	0.51
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.92	0.51
2:D:1233:TRP:O	2:D:1237:GLN:HG2	2.11	0.51
1:E:19:THR:HB	1:E:478:LEU:HB2	1.93	0.51
1:E:506:SER:CB	1:E:530:TRP:HE1	2.21	0.51
2:F:1041:SER:HG	2:F:1084:TRP:CG	2.28	0.51
1:G:36:THR:HG23	1:G:48:SER:HA	1.93	0.51
1:G:439:LEU:HD12	1:G:439:LEU:H	1.74	0.51
1:G:590:THR:HG22	1:G:592:SER:H	1.74	0.51
2:H:937:LYS:O	2:H:937:LYS:HD2	2.10	0.51
3:L:235:LYS:O	3:L:236:ILE:HB	2.11	0.51
3:L:456:VAL:HG13	3:L:467:LYS:HA	1.91	0.51
1:A:36:THR:HG23	1:A:48:SER:HA	1.93	0.51
1:A:410:SER:O	1:A:414:GLN:HG2	2.11	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.51
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.93	0.51
2:D:1126:LEU:HD23	2:D:1173:ALA:HB1	1.93	0.51
2:D:1480:LEU:HB3	2:D:1493:GLU:OE2	2.10	0.51
1:G:404:THR:HG23	1:G:414:GLN:HB3	1.92	0.51
1:G:640:CYS:HB3	1:G:641:PRO:HD2	1.93	0.51
3:J:700:CYS:O	3:J:701:LYS:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:LYS:HE2	4:Q:60:PHE:CD1	2.46	0.51
1:C:590:THR:HG22	1:C:592:SER:H	1.75	0.51
2:D:819:ARG:HG2	2:D:819:ARG:NH1	2.19	0.51
1:G:126:ARG:HG2	1:G:168:PRO:HA	1.93	0.51
4:Q:30:GLU:HA	4:Q:44:ILE:HD13	1.92	0.51
4:Q:70:LEU:HG	4:Q:74:TYR:CE2	2.46	0.51
2:B:1578:LYS:HD3	2:B:1608:HIS:HE1	1.75	0.51
1:C:640:CYS:HB3	1:C:641:PRO:HD2	1.93	0.51
2:D:772:PHE:CD1	4:M:37:ASN:ND2	2.78	0.51
2:F:860:HIS:CE1	2:F:862:GLN:HE22	2.29	0.51
2:F:966:ALA:O	2:F:967:GLN:CB	2.57	0.51
2:F:1126:LEU:HD23	2:F:1173:ALA:HB1	1.93	0.51
2:F:1233:TRP:O	2:F:1237:GLN:HG2	2.11	0.51
1:G:434:LEU:HB2	1:G:513:TYR:HE2	1.75	0.51
2:H:738:ASN:ND2	4:Q:45:LYS:HE2	2.22	0.51
2:H:754:GLU:HG3	2:H:769:MET:SD	2.51	0.51
3:I:334:LEU:HB3	3:I:376:VAL:HG11	1.93	0.51
3:I:381:ARG:CG	3:I:381:ARG:NH2	2.68	0.51
3:L:339:SER:HA	3:L:342:SER:HB3	1.93	0.51
3:L:724:LEU:HB3	3:L:725:PRO:HD3	1.92	0.51
1:E:36:THR:HG23	1:E:48:SER:HA	1.93	0.50
1:E:248:PHE:CD1	2:F:1378:MET:HE3	2.44	0.50
3:I:256:ILE:HD12	3:I:405:VAL:HG23	1.92	0.50
3:J:513:LYS:HZ2	3:J:524:GLU:HG2	1.75	0.50
3:J:563:TYR:CZ	3:J:569:PRO:HG3	2.47	0.50
3:K:724:LEU:HB3	3:K:725:PRO:HD3	1.92	0.50
4:P:70:LEU:HG	4:P:74:TYR:CE2	2.46	0.50
1:C:36:THR:HG23	1:C:48:SER:HA	1.93	0.50
2:D:1593:LYS:HG2	2:D:1596:LEU:HD11	1.94	0.50
1:E:404:THR:HG23	1:E:414:GLN:HB3	1.92	0.50
1:E:640:CYS:HB3	1:E:641:PRO:HD2	1.93	0.50
2:F:882:LYS:HG3	2:F:886:GLN:NE2	2.27	0.50
2:H:1381:LEU:HD23	2:H:1457:VAL:HG12	1.93	0.50
3:I:724:LEU:HB3	3:I:725:PRO:HD3	1.92	0.50
3:L:334:LEU:HB3	3:L:376:VAL:HG11	1.93	0.50
2:B:744:GLU:C	2:B:746:PRO:HD3	2.35	0.50
2:B:772:PHE:HD1	4:N:37:ASN:ND2	2.10	0.50
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.11	0.50
1:C:410:SER:O	1:C:414:GLN:HG2	2.11	0.50
1:E:10:ASN:HB2	1:E:621:GLY:C	2.36	0.50
2:F:1344:THR:HG21	2:F:1346:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:313:GLN:O	3:J:317:ILE:HG13	2.10	0.50
3:K:239:ASP:HB3	3:K:448:GLN:HB2	1.92	0.50
3:L:439:VAL:HG22	4:N:31:LEU:HD21	1.91	0.50
1:G:554:VAL:HG13	1:G:555:PRO:HD2	1.94	0.50
3:I:239:ASP:HB3	3:I:448:GLN:HB2	1.92	0.50
3:J:334:LEU:HB3	3:J:376:VAL:HG11	1.93	0.50
3:L:465:TYR:CD1	3:L:517:GLY:HA2	2.46	0.50
3:L:641:TYR:HE2	3:L:650:VAL:HB	1.77	0.50
2:B:940:ILE:HD12	2:B:1308:PHE:CE1	2.47	0.50
2:B:964:PRO:HG3	2:B:1270:LEU:HD11	1.92	0.50
2:B:1569:ARG:HH11	2:B:1569:ARG:CG	2.25	0.50
1:C:404:THR:HG23	1:C:414:GLN:HB3	1.92	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.29	0.50
2:D:1578:LYS:HD3	2:D:1608:HIS:HE1	1.75	0.50
2:F:819:ARG:HH11	2:F:819:ARG:CG	2.22	0.50
1:G:369:VAL:HG12	1:G:370:GLN:H	1.77	0.50
1:G:410:SER:O	1:G:414:GLN:HG2	2.11	0.50
2:H:882:LYS:HG3	2:H:886:GLN:NE2	2.27	0.50
3:I:563:TYR:CZ	3:I:569:PRO:HG3	2.46	0.50
3:I:641:TYR:HE2	3:I:650:VAL:HB	1.77	0.50
3:J:235:LYS:O	3:J:236:ILE:HB	2.11	0.50
3:J:724:LEU:HB3	3:J:725:PRO:HD3	1.92	0.50
2:B:882:LYS:HG3	2:B:886:GLN:NE2	2.27	0.50
2:B:1593:LYS:HG2	2:B:1596:LEU:HD11	1.94	0.50
3:J:339:SER:HA	3:J:342:SER:HB3	1.93	0.50
3:J:465:TYR:CD1	3:J:517:GLY:HA2	2.46	0.50
3:K:641:TYR:HE2	3:K:650:VAL:HB	1.77	0.50
3:L:513:LYS:NZ	3:L:524:GLU:HG2	2.27	0.50
4:M:30:GLU:HA	4:M:44:ILE:HD13	1.92	0.50
1:A:126:ARG:HG2	1:A:168:PRO:HA	1.93	0.50
1:E:126:ARG:HG2	1:E:168:PRO:HA	1.93	0.50
1:E:268:ARG:HD3	2:F:1378:MET:SD	2.51	0.50
2:F:962:GLY:C	2:F:964:PRO:HD3	2.37	0.50
2:F:964:PRO:HG3	2:F:1270:LEU:HD11	1.93	0.50
2:H:1617:ASP:O	2:H:1621:GLN:HG3	2.12	0.50
3:K:339:SER:HA	3:K:342:SER:HB3	1.93	0.50
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.94	0.50
2:D:907:LEU:HD23	2:D:907:LEU:H	1.77	0.50
2:D:1280:SER:O	2:D:1281:ARG:C	2.55	0.50
2:F:855:THR:HB	2:F:1602:LYS:HZ3	1.76	0.50
2:F:1617:ASP:O	2:F:1621:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:839:LYS:HE2	4:N:60:PHE:CE1	2.47	0.50
2:H:907:LEU:H	2:H:907:LEU:HD23	1.77	0.50
3:I:339:SER:HA	3:I:342:SER:HB3	1.93	0.50
3:J:478:ARG:CG	3:J:479:PRO:HD2	2.42	0.50
1:C:10:ASN:HA	1:C:623:THR:HG23	1.93	0.50
1:C:222:TYR:HB3	1:C:225:ASN:HB2	1.94	0.50
1:E:222:TYR:HB3	1:E:225:ASN:HB2	1.94	0.50
2:F:1268:GLN:O	2:F:1269:GLU:CB	2.59	0.50
2:H:1495:ASN:O	2:H:1496:CYS:C	2.54	0.50
3:K:334:LEU:HB3	3:K:376:VAL:HG11	1.93	0.50
3:K:563:TYR:CZ	3:K:569:PRO:HG3	2.47	0.50
3:L:431:LYS:HG3	4:N:27:ASN:ND2	2.27	0.50
1:A:103:LEU:HB3	1:A:193:GLN:HE21	1.77	0.49
1:A:568:GLY:HA2	2:B:757:LYS:HE2	1.94	0.49
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.12	0.49
2:H:1488:LEU:HG	2:H:1590:TRP:CH2	2.35	0.49
3:J:641:TYR:HE2	3:J:650:VAL:HB	1.77	0.49
1:A:426:THR:HG21	1:A:432:ASN:H	1.77	0.49
2:B:1280:SER:O	2:B:1281:ARG:C	2.55	0.49
2:D:733:ILE:HG12	2:D:734:ILE:N	2.26	0.49
2:F:1593:LYS:HG2	2:F:1596:LEU:HD11	1.94	0.49
3:I:465:TYR:CD1	3:I:517:GLY:HA2	2.46	0.49
3:K:465:TYR:CD1	3:K:517:GLY:HA2	2.46	0.49
1:C:351:MET:SD	1:C:440:ARG:HD2	2.53	0.49
2:D:841:ARG:HH11	2:D:841:ARG:CG	2.23	0.49
2:D:882:LYS:HG3	2:D:886:GLN:NE2	2.27	0.49
2:D:940:ILE:HD12	2:D:1308:PHE:CE1	2.47	0.49
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.12	0.49
1:G:572:VAL:CG2	2:H:785:VAL:HB	2.42	0.49
2:H:1497:PHE:C	2:H:1498:ILE:HD13	2.37	0.49
3:I:438:ASP:OD2	4:M:28:VAL:HG13	2.12	0.49
3:J:435:ASN:HD21	3:J:460:ARG:HH21	1.57	0.49
2:B:1505:VAL:HG23	2:B:1505:VAL:O	2.12	0.49
1:E:554:VAL:HG13	1:E:555:PRO:HD2	1.94	0.49
2:F:1495:ASN:O	2:F:1602:LYS:HA	2.13	0.49
3:I:328:THR:HB	3:I:367:HIS:HA	1.94	0.49
3:K:235:LYS:O	3:K:236:ILE:HB	2.11	0.49
3:L:478:ARG:CG	3:L:479:PRO:HD2	2.42	0.49
4:N:70:LEU:HG	4:N:74:TYR:CE2	2.46	0.49
2:B:1239:TYR:OH	2:B:1246:SER:HB2	2.13	0.49
2:F:841:ARG:HH11	2:F:841:ARG:CG	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1569:ARG:HH11	2:F:1569:ARG:CG	2.26	0.49
1:G:439:LEU:HD12	1:G:439:LEU:N	2.28	0.49
2:H:733:ILE:HG12	2:H:734:ILE:N	2.26	0.49
2:H:1593:LYS:HG2	2:H:1596:LEU:HD11	1.94	0.49
3:J:513:LYS:NZ	3:J:524:GLU:HG2	2.27	0.49
3:L:328:THR:HB	3:L:367:HIS:HA	1.94	0.49
2:H:1344:THR:HG21	2:H:1346:LYS:HE2	1.93	0.49
2:H:1635:VAL:HG23	2:H:1636:VAL:H	1.78	0.49
2:D:1485:ARG:HD3	2:D:1536:PHE:HZ	1.78	0.49
1:E:108:LEU:HB2	1:E:196:PHE:CD1	2.48	0.49
2:F:1381:LEU:HD23	2:F:1457:VAL:HG12	1.93	0.49
3:I:573:PRO:HB3	3:I:721:PHE:CZ	2.48	0.49
3:K:328:THR:HB	3:K:367:HIS:HA	1.95	0.49
3:L:563:TYR:CZ	3:L:569:PRO:HG3	2.47	0.49
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.48	0.49
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.94	0.49
2:D:1569:ARG:HH11	2:D:1569:ARG:CG	2.24	0.49
2:F:907:LEU:HD23	2:F:907:LEU:H	1.77	0.49
1:G:369:VAL:HG12	1:G:370:GLN:N	2.28	0.49
3:L:268:LEU:O	3:L:272:ILE:HG13	2.13	0.49
1:A:222:TYR:HB3	1:A:225:ASN:HB2	1.94	0.49
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.48	0.49
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.27	0.49
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.95	0.49
2:H:1280:SER:O	2:H:1281:ARG:C	2.55	0.49
2:H:1485:ARG:HH21	2:H:1590:TRP:NE1	2.11	0.49
3:I:235:LYS:O	3:I:236:ILE:HB	2.11	0.49
2:B:738:ASN:HD22	4:N:45:LYS:HE2	1.78	0.49
2:H:1462:ASN:HD22	2:H:1462:ASN:C	2.21	0.49
1:A:477:ARG:CG	1:A:477:ARG:NH1	2.76	0.48
2:B:907:LEU:HD23	2:B:907:LEU:H	1.77	0.48
2:D:813:LEU:HD23	2:D:907:LEU:HB3	1.95	0.48
2:D:833:ARG:CG	2:D:833:ARG:NH1	2.76	0.48
2:D:1239:TYR:OH	2:D:1246:SER:HB2	2.13	0.48
2:D:1417:SER:HB2	4:P:14:LYS:NZ	2.27	0.48
1:G:454:LEU:HA	1:G:491:ASP:O	2.13	0.48
1:G:477:ARG:CG	1:G:477:ARG:NH1	2.76	0.48
2:H:813:LEU:HD23	2:H:907:LEU:HB3	1.95	0.48
2:H:1497:PHE:O	2:H:1498:ILE:C	2.56	0.48
3:J:268:LEU:O	3:J:272:ILE:HG13	2.13	0.48
3:J:573:PRO:HB3	3:J:721:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:372:ASP:O	3:L:375:THR:HG22	2.13	0.48
3:L:573:PRO:HB3	3:L:721:PHE:CZ	2.48	0.48
1:C:477:ARG:CG	1:C:477:ARG:NH1	2.76	0.48
2:H:1446:ASN:HB2	4:N:4:LEU:HB2	1.94	0.48
2:H:1492:ALA:O	2:H:1494:GLU:N	2.46	0.48
2:H:1492:ALA:O	2:H:1493:GLU:C	2.55	0.48
3:I:620:VAL:HG12	3:I:667:PRO:HD2	1.95	0.48
3:K:372:ASP:O	3:K:375:THR:HG22	2.13	0.48
3:K:513:LYS:NZ	3:K:524:GLU:HG2	2.27	0.48
3:L:620:VAL:HG12	3:L:667:PRO:HD2	1.95	0.48
1:A:407:GLN:C	1:A:409:LEU:H	2.21	0.48
2:B:1462:ASN:HD22	2:B:1462:ASN:C	2.21	0.48
2:F:1635:VAL:HG23	2:F:1636:VAL:H	1.78	0.48
1:G:407:GLN:C	1:G:409:LEU:H	2.21	0.48
2:H:1338:LYS:H	2:H:1371:ARG:HD2	1.78	0.48
3:I:372:ASP:O	3:I:375:THR:HG22	2.13	0.48
3:I:513:LYS:NZ	3:I:524:GLU:HG2	2.27	0.48
3:J:328:THR:HB	3:J:367:HIS:HA	1.95	0.48
3:J:372:ASP:O	3:J:375:THR:HG22	2.13	0.48
3:K:268:LEU:O	3:K:272:ILE:HG13	2.13	0.48
3:K:478:ARG:CG	3:K:479:PRO:HD2	2.42	0.48
1:A:439:LEU:HD12	1:A:439:LEU:N	2.28	0.48
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.48	0.48
2:D:1505:VAL:O	2:D:1505:VAL:HG23	2.12	0.48
1:E:407:GLN:C	1:E:409:LEU:H	2.21	0.48
3:I:268:LEU:O	3:I:272:ILE:HG13	2.13	0.48
3:I:270:ASN:HD22	3:I:270:ASN:N	2.12	0.48
3:J:493:GLU:HG3	3:J:563:TYR:OH	2.14	0.48
3:J:620:VAL:HG12	3:J:667:PRO:HD2	1.95	0.48
5:U:1:NAG:H61	5:U:2:NAG:H83	1.94	0.48
2:F:1239:TYR:OH	2:F:1246:SER:HB2	2.13	0.48
2:F:1445:PHE:CE2	4:M:7:SER:HA	2.48	0.48
1:G:108:LEU:HB2	1:G:196:PHE:CD1	2.48	0.48
2:H:1569:ARG:HH11	2:H:1569:ARG:CG	2.26	0.48
3:I:478:ARG:CG	3:I:479:PRO:HD2	2.42	0.48
2:B:1485:ARG:HD3	2:B:1536:PHE:HZ	1.78	0.48
3:J:270:ASN:HD22	3:J:270:ASN:N	2.11	0.48
3:K:362:MET:HG2	3:K:403:PHE:HB2	1.95	0.48
4:N:11:GLN:NE2	4:N:11:GLN:H	2.11	0.48
2:D:738:ASN:HD22	4:M:45:LYS:HE2	1.77	0.48
3:L:493:GLU:HG3	3:L:563:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:11:GLN:NE2	4:P:11:GLN:H	2.11	0.48
4:Q:11:GLN:NE2	4:Q:11:GLN:H	2.11	0.48
1:C:407:GLN:C	1:C:409:LEU:H	2.21	0.48
1:C:506:SER:CB	1:C:530:TRP:HE1	2.21	0.48
1:E:369:VAL:HG12	1:E:370:GLN:H	1.78	0.48
2:F:1280:SER:O	2:F:1281:ARG:C	2.55	0.48
2:F:1462:ASN:HD22	2:F:1462:ASN:C	2.21	0.48
1:G:222:TYR:HB3	1:G:225:ASN:HB2	1.94	0.48
1:G:351:MET:HE1	1:G:386:LYS:HD2	1.95	0.48
3:I:439:VAL:HG22	4:M:31:LEU:HD21	1.95	0.48
3:I:465:TYR:CE1	3:I:517:GLY:HA2	2.49	0.48
3:I:493:GLU:HG3	3:I:563:TYR:OH	2.14	0.48
3:K:378:ASP:HA	3:K:381:ARG:HB2	1.96	0.48
3:K:573:PRO:HB3	3:K:721:PHE:CZ	2.48	0.48
2:D:944:ASP:O	2:D:945:LEU:C	2.57	0.48
2:D:1291:TRP:O	2:D:1294:ALA:N	2.47	0.48
2:D:1361:THR:HA	2:D:1441:VAL:O	2.14	0.48
2:F:1147:ILE:HG23	2:F:1177:MET:HE2	1.96	0.48
1:G:624:PHE:HB3	1:G:632:THR:HG23	1.96	0.48
2:H:1499:GLN:HG2	2:H:1500:LYS:N	2.27	0.48
3:J:465:TYR:CE1	3:J:517:GLY:HA2	2.49	0.48
3:K:465:TYR:CE1	3:K:517:GLY:HA2	2.49	0.48
3:L:328:THR:O	3:L:367:HIS:HB2	2.14	0.48
3:L:544:ILE:HD13	3:L:650:VAL:HG12	1.96	0.48
4:M:11:GLN:NE2	4:M:11:GLN:H	2.11	0.48
1:A:624:PHE:HB3	1:A:632:THR:HG23	1.96	0.48
2:B:865:THR:OG1	4:Q:11:GLN:HG2	2.14	0.48
2:B:944:ASP:O	2:B:945:LEU:C	2.57	0.48
1:C:439:LEU:HD12	1:C:439:LEU:N	2.28	0.48
2:D:1462:ASN:HD22	2:D:1462:ASN:C	2.21	0.48
1:E:606:THR:HB	1:E:619:ASP:HB3	1.96	0.48
2:F:819:ARG:HG2	2:F:819:ARG:NH1	2.19	0.48
1:G:528:SER:N	1:G:616:VAL:HG13	2.29	0.48
2:H:932:ARG:O	2:H:934:GLY:N	2.47	0.48
3:K:493:GLU:HG3	3:K:563:TYR:OH	2.14	0.48
1:A:351:MET:HE2	1:A:351:MET:HA	1.96	0.47
1:A:470:TYR:HA	1:A:510:VAL:O	2.14	0.47
2:B:1361:THR:HA	2:B:1441:VAL:O	2.14	0.47
2:D:964:PRO:HB3	2:D:1270:LEU:HD11	1.95	0.47
1:E:439:LEU:HD12	1:E:439:LEU:N	2.28	0.47
2:F:733:ILE:HG12	2:F:734:ILE:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:VAL:HG21	1:G:64:VAL:HG21	1.96	0.47
3:J:539:LYS:HD2	3:J:539:LYS:N	2.30	0.47
3:K:328:THR:O	3:K:367:HIS:HB2	2.14	0.47
3:L:361:LEU:O	3:L:402:VAL:HA	2.14	0.47
3:L:465:TYR:CE1	3:L:517:GLY:HA2	2.49	0.47
1:A:382:ASP:OD2	1:A:440:ARG:NH2	2.47	0.47
1:C:35:VAL:HG21	1:C:64:VAL:HG21	1.96	0.47
1:C:351:MET:HE2	1:C:351:MET:HA	1.96	0.47
2:F:877:VAL:H	2:F:1451:GLN:NE2	2.12	0.47
2:F:1338:LYS:H	2:F:1371:ARG:HD2	1.79	0.47
1:G:470:TYR:HA	1:G:510:VAL:O	2.14	0.47
1:G:510:VAL:HG21	1:G:622:LEU:HD12	1.96	0.47
5:O:1:NAG:H4	5:O:2:NAG:H2	1.61	0.47
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.47
2:B:1386:MET:O	2:B:1387:THR:C	2.57	0.47
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.50	0.47
1:G:345:GLY:HA2	1:G:391:THR:O	2.14	0.47
3:I:544:ILE:HD13	3:I:650:VAL:HG12	1.96	0.47
3:K:620:VAL:HG12	3:K:667:PRO:HD2	1.95	0.47
1:A:577:ASP:CG	2:B:778:THR:HG21	2.40	0.47
2:B:1291:TRP:O	2:B:1294:ALA:N	2.47	0.47
1:C:555:PRO:HB3	2:D:775:ASP:HA	1.96	0.47
2:D:965:VAL:O	2:D:1267:HIS:HD2	1.97	0.47
2:F:813:LEU:HD23	2:F:907:LEU:HB3	1.95	0.47
3:J:362:MET:HG2	3:J:403:PHE:HB2	1.95	0.47
3:J:378:ASP:HA	3:J:381:ARG:HB2	1.96	0.47
3:L:334:LEU:HD12	3:L:373:PRO:HB3	1.97	0.47
4:N:10:TYR:HE2	4:N:14:LYS:HE3	1.80	0.47
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.50	0.47
1:C:624:PHE:HB3	1:C:632:THR:HG23	1.96	0.47
1:E:13:ARG:NH2	1:E:476:GLY:HA3	2.28	0.47
1:E:351:MET:HE2	1:E:351:MET:HA	1.96	0.47
1:E:369:VAL:HG12	1:E:370:GLN:N	2.29	0.47
1:E:624:PHE:HB3	1:E:632:THR:HG23	1.96	0.47
2:H:1270:LEU:O	2:H:1290:HIS:HA	2.15	0.47
3:I:378:ASP:HA	3:I:381:ARG:HB2	1.96	0.47
3:K:334:LEU:HD12	3:K:373:PRO:HB3	1.97	0.47
4:M:10:TYR:HE2	4:M:14:LYS:HE3	1.79	0.47
2:B:932:ARG:O	2:B:933:GLU:C	2.57	0.47
1:C:166:VAL:O	1:C:168:PRO:HD3	2.15	0.47
1:E:35:VAL:HG21	1:E:64:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:932:ARG:O	2:F:934:GLY:N	2.47	0.47
1:G:606:THR:HB	1:G:619:ASP:HB3	1.96	0.47
3:I:334:LEU:HD12	3:I:373:PRO:HB3	1.97	0.47
3:I:349:PRO:O	3:I:352:TRP:HD1	1.98	0.47
3:I:361:LEU:O	3:I:402:VAL:HA	2.14	0.47
3:I:362:MET:HG2	3:I:403:PHE:HB2	1.95	0.47
3:J:349:PRO:O	3:J:352:TRP:HD1	1.98	0.47
3:J:437:GLU:CD	3:J:458:GLU:HB2	2.40	0.47
3:L:352:TRP:H	3:L:352:TRP:CD1	2.33	0.47
1:A:35:VAL:HG21	1:A:64:VAL:HG21	1.96	0.47
1:A:218:GLU:C	1:A:220:PHE:H	2.23	0.47
1:C:10:ASN:HB2	1:C:621:GLY:HA2	1.95	0.47
1:C:470:TYR:HA	1:C:510:VAL:O	2.14	0.47
2:D:932:ARG:O	2:D:933:GLU:C	2.57	0.47
2:D:1147:ILE:HG23	2:D:1177:MET:HE2	1.96	0.47
2:F:969:THR:O	2:F:970:GLU:C	2.57	0.47
2:F:1269:GLU:HG3	2:F:1269:GLU:O	2.15	0.47
2:F:1270:LEU:O	2:F:1290:HIS:HA	2.15	0.47
1:G:351:MET:HE2	1:G:351:MET:HA	1.96	0.47
2:H:1359:LYS:HD2	4:N:4:LEU:CG	2.45	0.47
2:H:1521:TYR:HB2	2:H:1523:TYR:CZ	2.49	0.47
3:J:236:ILE:HG21	3:J:443:MET:O	2.15	0.47
3:K:544:ILE:HD13	3:K:650:VAL:HG12	1.96	0.47
3:L:362:MET:HG2	3:L:403:PHE:HB2	1.95	0.47
3:L:539:LYS:HD2	3:L:539:LYS:N	2.30	0.47
1:A:248:PHE:CD1	2:B:1378:MET:HE3	2.47	0.47
1:A:606:THR:HB	1:A:619:ASP:HB3	1.96	0.47
2:B:967:GLN:O	2:B:968:MET:HB2	2.13	0.47
2:H:1446:ASN:CB	4:N:4:LEU:HB2	2.44	0.47
3:I:236:ILE:HG23	3:I:236:ILE:O	2.15	0.47
3:I:352:TRP:CD1	3:I:352:TRP:H	2.32	0.47
3:J:328:THR:O	3:J:367:HIS:HB2	2.15	0.47
3:J:544:ILE:HD13	3:J:650:VAL:HG12	1.96	0.47
3:K:363:THR:HG23	3:K:365:GLY:H	1.80	0.47
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.97	0.47
1:C:218:GLU:C	1:C:220:PHE:H	2.23	0.47
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.97	0.47
1:E:6:ILE:HG22	1:E:625:THR:O	2.14	0.47
1:E:219:LYS:HZ2	1:E:356:ASN:HD22	1.63	0.47
2:F:1521:TYR:HB2	2:F:1523:TYR:CZ	2.49	0.47
1:G:522:ARG:HG2	1:G:628:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1291:TRP:O	2:H:1294:ALA:N	2.48	0.47
2:H:1498:ILE:HG13	2:H:1605:TRP:CZ3	2.50	0.47
3:K:236:ILE:HG21	3:K:443:MET:O	2.15	0.47
1:C:325:PRO:HG2	1:C:357:PRO:HB2	1.97	0.47
1:E:470:TYR:HA	1:E:510:VAL:O	2.14	0.47
2:H:944:ASP:O	2:H:945:LEU:C	2.57	0.47
3:K:270:ASN:N	3:K:270:ASN:HD22	2.12	0.47
3:K:539:LYS:HD2	3:K:539:LYS:N	2.30	0.47
3:L:236:ILE:O	3:L:236:ILE:HG23	2.15	0.47
2:B:733:ILE:HD13	2:B:841:ARG:HD3	1.98	0.46
2:B:1640:PRO:HA	3:L:326:SER:OG	2.14	0.46
1:C:378:LEU:HD13	1:E:446:GLY:O	2.16	0.46
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.96	0.46
2:D:1386:MET:O	2:D:1387:THR:C	2.58	0.46
2:D:1524:LYS:HB3	2:D:1545:GLN:HG2	1.97	0.46
1:E:34:THR:HG22	1:E:51:LYS:HE3	1.97	0.46
2:F:1269:GLU:CG	2:F:1315:LYS:HB3	2.40	0.46
2:F:1524:LYS:HB3	2:F:1545:GLN:HG2	1.97	0.46
2:H:1386:MET:O	2:H:1387:THR:C	2.58	0.46
3:L:236:ILE:HG21	3:L:443:MET:O	2.15	0.46
1:A:166:VAL:O	1:A:168:PRO:HD3	2.15	0.46
1:A:213:ILE:HG22	1:A:215:GLU:HG3	1.97	0.46
2:B:1524:LYS:HB3	2:B:1545:GLN:HG2	1.97	0.46
1:C:6:ILE:HD12	1:C:21:VAL:O	2.14	0.46
1:C:369:VAL:HG12	1:C:370:GLN:N	2.31	0.46
2:D:990:GLU:O	2:D:994:ILE:HG13	2.16	0.46
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.46
2:F:733:ILE:HD13	2:F:841:ARG:HD3	1.97	0.46
2:F:1265:PRO:O	2:F:1266:ASP:CB	2.64	0.46
3:I:328:THR:O	3:I:367:HIS:HB2	2.14	0.46
3:L:270:ASN:HD22	3:L:270:ASN:N	2.11	0.46
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.51	0.46
1:E:6:ILE:HD12	1:E:21:VAL:O	2.14	0.46
1:E:207:LEU:HA	1:E:208:PRO:HD2	1.82	0.46
2:F:944:ASP:O	2:F:945:LEU:C	2.57	0.46
2:F:990:GLU:O	2:F:994:ILE:HG13	2.16	0.46
2:F:1291:TRP:O	2:F:1294:ALA:N	2.48	0.46
2:F:1336:CYS:O	2:F:1337:ASN:C	2.59	0.46
1:G:34:THR:HG22	1:G:51:LYS:HE3	1.97	0.46
1:G:477:ARG:HG2	1:G:477:ARG:NH1	2.21	0.46
2:H:1444:TYR:HB2	4:N:10:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:361:LEU:O	3:J:402:VAL:HA	2.14	0.46
3:L:679:ILE:HG21	3:L:686:PHE:HB3	1.97	0.46
11:b:3:MAN:O3	11:b:4:MAN:H61	2.16	0.46
1:A:34:THR:HG22	1:A:51:LYS:HE3	1.97	0.46
2:B:733:ILE:HG12	2:B:734:ILE:N	2.26	0.46
2:B:990:GLU:O	2:B:994:ILE:HG13	2.16	0.46
1:E:80:ARG:HD2	2:F:1010:GLU:HG3	1.97	0.46
1:E:166:VAL:O	1:E:168:PRO:HD3	2.15	0.46
3:K:361:LEU:O	3:K:402:VAL:HA	2.14	0.46
3:L:378:ASP:HA	3:L:381:ARG:HB2	1.96	0.46
4:Q:10:TYR:HE2	4:Q:14:LYS:HE3	1.79	0.46
4:Q:73:ILE:O	4:Q:77:ILE:HG13	2.16	0.46
2:F:740:VAL:CB	4:P:42:ARG:HB2	2.43	0.46
1:G:154:LYS:HD2	1:G:171:TRP:CD1	2.51	0.46
2:H:833:ARG:CG	2:H:833:ARG:NH1	2.75	0.46
3:I:236:ILE:HG21	3:I:443:MET:O	2.15	0.46
3:I:363:THR:HG23	3:I:365:GLY:H	1.80	0.46
3:I:539:LYS:HD2	3:I:539:LYS:N	2.30	0.46
3:J:236:ILE:HG23	3:J:236:ILE:O	2.15	0.46
3:J:352:TRP:CD1	3:J:352:TRP:H	2.33	0.46
3:K:349:PRO:O	3:K:352:TRP:HD1	1.98	0.46
3:L:349:PRO:O	3:L:352:TRP:HD1	1.98	0.46
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.51	0.46
1:C:213:ILE:HG22	1:C:215:GLU:HG3	1.97	0.46
1:C:639:GLN:NE2	1:C:639:GLN:H	2.14	0.46
2:F:1172:TYR:CE1	2:F:1216:LEU:HB3	2.51	0.46
1:G:6:ILE:HD12	1:G:21:VAL:O	2.15	0.46
3:I:531:HIS:HD2	3:I:533:ASN:H	1.64	0.46
3:K:236:ILE:HG23	3:K:236:ILE:O	2.15	0.46
3:K:352:TRP:CD1	3:K:352:TRP:H	2.32	0.46
4:M:73:ILE:O	4:M:77:ILE:HG13	2.16	0.46
8:X:3:MAN:H62	8:X:4:MAN:H2	1.43	0.46
1:C:606:THR:HB	1:C:619:ASP:HB3	1.96	0.46
1:E:342:PHE:CE1	1:E:391:THR:HG21	2.50	0.46
2:F:932:ARG:O	2:F:933:GLU:C	2.58	0.46
2:F:1494:GLU:HB2	2:F:1602:LYS:HB3	1.97	0.46
1:G:247:ALA:HB2	1:G:308:VAL:HG22	1.97	0.46
2:H:837:GLU:HB3	2:H:868:PRO:HD3	1.97	0.46
3:J:531:HIS:HD2	3:J:533:ASN:H	1.64	0.46
3:K:292:TYR:CD1	3:K:325:LYS:HD3	2.51	0.46
3:L:363:THR:HG23	3:L:365:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.97	0.46
2:B:1147:ILE:HG23	2:B:1177:MET:HE2	1.96	0.46
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.16	0.46
1:C:47:LEU:HD13	1:C:66:PHE:HB2	1.97	0.46
1:C:154:LYS:HD2	1:C:171:TRP:CD1	2.51	0.46
2:D:1357:ASP:C	2:D:1359:LYS:H	2.24	0.46
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.16	0.46
2:F:1386:MET:O	2:F:1387:THR:C	2.58	0.46
1:G:218:GLU:C	1:G:220:PHE:H	2.23	0.46
1:G:354:VAL:HG11	1:G:365:VAL:HG11	1.98	0.46
3:J:363:THR:HG23	3:J:365:GLY:H	1.80	0.46
3:K:261:PHE:HB3	3:K:319:TYR:HD1	1.81	0.46
3:K:679:ILE:HG21	3:K:686:PHE:HB3	1.97	0.46
3:L:345:ASP:HB3	3:L:346:ASP:H	1.49	0.46
3:L:531:HIS:HD2	3:L:533:ASN:H	1.64	0.46
4:N:73:ILE:O	4:N:77:ILE:HG13	2.15	0.46
1:A:639:GLN:NE2	1:A:639:GLN:H	2.14	0.46
1:C:6:ILE:HG22	1:C:625:THR:O	2.16	0.46
2:F:811:LEU:HG	2:F:813:LEU:HD13	1.98	0.46
2:F:1290:HIS:O	2:F:1291:TRP:O	2.34	0.46
2:H:1268:GLN:CG	2:H:1269:GLU:N	2.70	0.46
3:I:700:CYS:HA	3:I:704:LYS:O	2.16	0.46
3:J:334:LEU:HD12	3:J:373:PRO:HB3	1.97	0.46
3:L:261:PHE:HB3	3:L:319:TYR:HD1	1.81	0.46
4:P:73:ILE:O	4:P:77:ILE:HG13	2.16	0.46
7:V:4:BMA:H62	7:V:6:BMA:H2	1.36	0.46
11:b:1:NAG:H61	11:b:2:NAG:C7	2.45	0.46
1:E:147:ASN:HB2	1:E:148:PRO:CD	2.46	0.46
1:E:218:GLU:C	1:E:220:PHE:H	2.23	0.46
1:E:354:VAL:HG11	1:E:365:VAL:HG11	1.98	0.46
1:G:47:LEU:HD13	1:G:66:PHE:HB2	1.97	0.46
1:G:144:ASN:HD22	1:G:144:ASN:N	2.14	0.46
1:G:166:VAL:O	1:G:168:PRO:HD3	2.15	0.46
4:M:66:ALA:HA	4:M:69:GLN:HB2	1.98	0.46
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.22	0.45
1:C:34:THR:HG22	1:C:51:LYS:HE3	1.97	0.45
1:G:213:ILE:HG22	1:G:215:GLU:HG3	1.97	0.45
3:J:679:ILE:HG21	3:J:686:PHE:HB3	1.97	0.45
3:K:646:ASP:OD2	3:K:648:SER:HB3	2.17	0.45
4:N:66:ALA:HA	4:N:69:GLN:HB2	1.98	0.45
4:P:10:TYR:HE2	4:P:14:LYS:HE3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG12	1:A:370:GLN:N	2.31	0.45
1:A:426:THR:HG22	1:A:427:VAL:N	2.31	0.45
1:E:351:MET:HE1	1:E:386:LYS:HD2	1.98	0.45
3:I:646:ASP:OD2	3:I:648:SER:HB3	2.16	0.45
3:L:653:PRO:CD	3:L:654:ARG:HH12	2.27	0.45
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.99	0.45
1:A:538:VAL:HB	2:B:791:LYS:O	2.16	0.45
1:E:47:LEU:HD13	1:E:66:PHE:HB2	1.97	0.45
1:E:351:MET:SD	1:E:440:ARG:HD2	2.57	0.45
1:G:639:GLN:NE2	1:G:639:GLN:H	2.14	0.45
2:H:1524:LYS:HB3	2:H:1545:GLN:HG2	1.97	0.45
3:I:261:PHE:HB3	3:I:319:TYR:HD1	1.81	0.45
3:J:700:CYS:HA	3:J:704:LYS:O	2.16	0.45
3:L:292:TYR:CD1	3:L:325:LYS:HD3	2.51	0.45
2:B:819:ARG:O	2:B:820:ASN:HB2	2.17	0.45
2:B:837:GLU:HB3	2:B:868:PRO:HD3	1.97	0.45
1:E:154:LYS:HD2	1:E:171:TRP:CD1	2.51	0.45
2:F:837:GLU:HB3	2:F:868:PRO:HD3	1.97	0.45
2:H:733:ILE:HD13	2:H:841:ARG:HD3	1.98	0.45
3:K:239:ASP:HA	3:K:240:PRO:HD3	1.86	0.45
3:K:702:ASN:O	3:K:703:GLN:HG3	2.17	0.45
3:L:702:ASN:O	3:L:703:GLN:HG3	2.17	0.45
2:B:1264:ALA:HA	2:B:1265:PRO:HD3	1.73	0.45
1:C:248:PHE:CD1	2:D:1378:MET:HE3	2.50	0.45
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.17	0.45
2:D:1288:ARG:HD3	2:D:1290:HIS:NE2	2.32	0.45
2:D:1364:LEU:HD23	2:D:1439:PHE:CZ	2.52	0.45
1:E:569:ALA:HB2	2:F:788:SER:HB2	1.99	0.45
1:G:100:LEU:HD21	1:G:638:LEU:CD2	2.44	0.45
1:G:567:HIS:CG	2:H:760:PRO:HG3	2.52	0.45
3:I:679:ILE:HG21	3:I:686:PHE:HB3	1.97	0.45
3:J:646:ASP:OD2	3:J:648:SER:HB3	2.17	0.45
3:J:705:ARG:O	3:J:706:GLN:CB	2.60	0.45
5:T:1:NAG:H61	5:T:2:NAG:C7	2.46	0.45
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.45
2:B:1288:ARG:HD3	2:B:1290:HIS:NE2	2.32	0.45
1:C:342:PHE:CE1	1:C:391:THR:HG21	2.52	0.45
1:C:392:HIS:C	1:C:394:SER:H	2.25	0.45
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.99	0.45
2:D:1192:ALA:HB2	2:D:1198:TRP:CZ2	2.52	0.45
1:E:510:VAL:HG12	1:E:528:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:TYR:OH	1:G:613:TYR:HB3	2.16	0.45
3:I:292:TYR:CD1	3:I:325:LYS:HD3	2.51	0.45
3:J:261:PHE:HB3	3:J:319:TYR:HD1	1.81	0.45
3:L:646:ASP:OD2	3:L:648:SER:HB3	2.16	0.45
2:B:1192:ALA:HB2	2:B:1198:TRP:CZ2	2.52	0.45
2:B:1203:LYS:HD2	2:B:1206:TYR:CE2	2.52	0.45
2:F:1470:PHE:CB	2:F:1478:GLY:HA3	2.47	0.45
2:H:819:ARG:O	2:H:820:ASN:HB2	2.17	0.45
3:I:653:PRO:CD	3:I:654:ARG:HH12	2.27	0.45
3:K:428:PHE:CE1	4:P:31:LEU:HD11	2.52	0.45
3:K:653:PRO:CD	3:K:654:ARG:HH12	2.27	0.45
4:P:66:ALA:HA	4:P:69:GLN:HB2	1.98	0.45
1:A:354:VAL:HG11	1:A:365:VAL:HG11	1.98	0.45
1:A:392:HIS:C	1:A:394:SER:H	2.25	0.45
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.98	0.45
2:B:729:LEU:O	2:B:729:LEU:HD22	2.17	0.45
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.90	0.45
2:B:1501:SER:O	2:B:1502:ASP:C	2.59	0.45
2:D:811:LEU:HG	2:D:813:LEU:HD13	1.98	0.45
2:D:837:GLU:HB3	2:D:868:PRO:HD3	1.97	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.17	0.45
2:F:1182:GLY:HA3	2:F:1183:PRO:HD2	1.82	0.45
1:G:516:ILE:N	1:G:516:ILE:HD12	2.32	0.45
3:J:292:TYR:CD1	3:J:325:LYS:HD3	2.51	0.45
13:A:701:MAN:C1	6:W:3:BMA:H3	2.46	0.45
2:D:937:LYS:HD2	2:D:937:LYS:O	2.17	0.45
1:E:213:ILE:HG22	1:E:215:GLU:HG3	1.97	0.45
1:E:639:GLN:NE2	1:E:639:GLN:H	2.14	0.45
2:F:1203:LYS:HD2	2:F:1206:TYR:CE2	2.52	0.45
2:F:1288:ARG:HD3	2:F:1290:HIS:NE2	2.32	0.45
2:F:1364:LEU:HD23	2:F:1439:PHE:CZ	2.52	0.45
2:H:811:LEU:HG	2:H:813:LEU:HD13	1.98	0.45
2:H:932:ARG:O	2:H:933:GLU:C	2.58	0.45
1:A:369:VAL:HG12	1:A:370:GLN:H	1.82	0.45
2:D:733:ILE:HD13	2:D:841:ARG:HD3	1.98	0.45
2:D:1444:TYR:HB2	4:P:10:TYR:CE1	2.52	0.45
2:D:1501:SER:O	2:D:1502:ASP:C	2.59	0.45
2:F:1506:THR:OG1	2:F:1509:GLU:HG2	2.17	0.45
2:H:734:ILE:N	2:H:734:ILE:HD12	2.32	0.45
2:H:1498:ILE:HD13	2:H:1498:ILE:N	2.32	0.45
3:J:702:ASN:O	3:J:703:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:554:LEU:H	3:K:726:TRP:HH2	1.65	0.45
3:L:272:ILE:HG12	3:L:284:TYR:CE1	2.52	0.45
3:L:432:ASP:HA	4:N:27:ASN:HD21	1.82	0.45
1:A:193:GLN:CD	1:A:193:GLN:H	2.25	0.44
2:B:729:LEU:C	2:B:729:LEU:HD13	2.41	0.44
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.44
1:C:193:GLN:CD	1:C:193:GLN:H	2.25	0.44
1:C:344:PRO:HD2	1:C:433:TYR:CE1	2.51	0.44
1:C:354:VAL:HG11	1:C:365:VAL:HG11	1.98	0.44
1:E:477:ARG:CG	1:E:477:ARG:NH1	2.76	0.44
2:F:1192:ALA:HB2	2:F:1198:TRP:CZ2	2.52	0.44
2:H:1290:HIS:O	2:H:1291:TRP:O	2.34	0.44
3:K:238:LEU:HD22	3:K:280:VAL:HG21	1.99	0.44
3:K:531:HIS:HD2	3:K:533:ASN:H	1.64	0.44
3:L:700:CYS:HA	3:L:704:LYS:O	2.16	0.44
3:L:705:ARG:O	3:L:706:GLN:CB	2.60	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.46	0.44
1:A:516:ILE:N	1:A:516:ILE:HD12	2.32	0.44
1:C:369:VAL:HG12	1:C:370:GLN:H	1.82	0.44
2:F:1126:LEU:O	2:F:1130:GLN:HG3	2.17	0.44
2:F:1223:ASP:O	2:F:1227:VAL:HG23	2.17	0.44
1:G:392:HIS:C	1:G:394:SER:H	2.25	0.44
1:G:526:ALA:HB2	1:G:617:PHE:CE2	2.52	0.44
3:J:272:ILE:HG12	3:J:284:TYR:CE1	2.52	0.44
3:J:554:LEU:H	3:J:726:TRP:HH2	1.65	0.44
3:K:491:VAL:HB	3:K:572:LEU:HD11	1.99	0.44
3:L:554:LEU:H	3:L:726:TRP:HH2	1.65	0.44
1:A:100:LEU:HD21	1:A:638:LEU:HD23	2.00	0.44
2:B:734:ILE:N	2:B:734:ILE:HD12	2.33	0.44
2:B:1126:LEU:O	2:B:1130:GLN:HG3	2.17	0.44
2:B:1283:SER:O	2:B:1284:LYS:HG2	2.18	0.44
2:D:819:ARG:O	2:D:820:ASN:HB2	2.17	0.44
2:D:1203:LYS:HD2	2:D:1206:TYR:CE2	2.52	0.44
1:E:392:HIS:C	1:E:394:SER:H	2.25	0.44
2:F:1360:ASN:O	2:F:1361:THR:O	2.36	0.44
2:H:1470:PHE:CB	2:H:1478:GLY:HA3	2.47	0.44
3:K:489:ALA:HB2	3:K:677:PRO:CG	2.45	0.44
6:W:2:NAG:H3	6:W:4:BMA:O3	2.17	0.44
1:A:459:ARG:HH21	1:G:459:ARG:HE	1.66	0.44
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.83	0.44
1:C:250:ILE:HG22	1:C:305:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:ALA:HB2	1:E:308:VAL:HG22	1.98	0.44
1:E:427:VAL:HB	1:E:523:GLU:HG3	1.99	0.44
2:F:734:ILE:N	2:F:734:ILE:HD12	2.33	0.44
2:F:943:ALA:O	2:F:1305:ASN:ND2	2.49	0.44
2:H:943:ALA:O	2:H:1305:ASN:ND2	2.49	0.44
2:H:1288:ARG:HD3	2:H:1290:HIS:NE2	2.32	0.44
2:H:1360:ASN:O	2:H:1361:THR:O	2.36	0.44
2:H:1364:LEU:HD23	2:H:1439:PHE:CZ	2.52	0.44
1:A:342:PHE:CE1	1:A:391:THR:HG21	2.53	0.44
1:A:555:PRO:HB3	2:B:775:ASP:HA	1.98	0.44
2:B:1364:LEU:HD23	2:B:1439:PHE:CZ	2.52	0.44
2:B:1639:CYS:HB2	3:L:368:ASN:OD1	2.18	0.44
1:E:144:ASN:HD22	1:E:144:ASN:N	2.14	0.44
1:E:193:GLN:H	1:E:193:GLN:CD	2.25	0.44
2:H:847:ASN:HA	2:H:848:PRO:HD2	1.83	0.44
2:H:1336:CYS:O	2:H:1337:ASN:C	2.60	0.44
3:I:272:ILE:HG12	3:I:284:TYR:CE1	2.52	0.44
3:I:554:LEU:H	3:I:726:TRP:HH2	1.65	0.44
3:K:238:LEU:HD11	3:K:278:TYR:CB	2.46	0.44
3:L:491:VAL:HB	3:L:572:LEU:HD11	1.99	0.44
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.44
2:D:1265:PRO:O	2:D:1266:ASP:CB	2.65	0.44
2:D:1292:GLU:HG2	2:D:1293:SER:H	1.83	0.44
2:D:1639:CYS:HB2	3:I:368:ASN:OD1	2.18	0.44
2:F:847:ASN:HA	2:F:848:PRO:HD2	1.83	0.44
2:F:937:LYS:HD2	2:F:937:LYS:C	2.43	0.44
3:I:375:THR:O	3:I:379:GLU:HG3	2.18	0.44
3:K:446:GLU:OE2	3:K:457:TRP:NE1	2.50	0.44
3:L:375:THR:O	3:L:379:GLU:HG3	2.18	0.44
4:Q:66:ALA:HA	4:Q:69:GLN:HB2	1.98	0.44
1:A:459:ARG:HE	1:G:459:ARG:NH2	2.16	0.44
2:B:840:VAL:HG22	2:B:894:VAL:HG12	2.00	0.44
2:B:937:LYS:O	2:B:937:LYS:HD2	2.17	0.44
1:C:22:LEU:HD13	1:C:33:VAL:HG11	2.00	0.44
2:D:1446:ASN:HB2	4:P:4:LEU:HB2	1.99	0.44
1:E:516:ILE:HD12	1:E:516:ILE:N	2.32	0.44
1:E:558:GLN:HB3	2:F:770:ASN:HD21	1.82	0.44
1:E:567:HIS:CG	2:F:760:PRO:HG3	2.53	0.44
2:F:758:GLU:CD	2:F:758:GLU:H	2.26	0.44
2:F:1370:TYR:CD1	2:F:1376:ALA:HB2	2.52	0.44
1:G:147:ASN:HB2	1:G:148:PRO:CD	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:375:THR:O	3:J:379:GLU:HG3	2.18	0.44
1:A:144:ASN:HD22	1:A:144:ASN:N	2.14	0.44
1:A:329:SER:HA	1:A:330:PRO:HD3	1.78	0.44
2:B:1292:GLU:N	2:B:1292:GLU:CD	2.76	0.44
2:D:1283:SER:O	2:D:1284:LYS:HG2	2.18	0.44
2:F:1264:ALA:HA	2:F:1265:PRO:HD3	1.74	0.44
2:F:1375:ASP:OD1	2:F:1431:HIS:HD2	2.01	0.44
2:H:1283:SER:O	2:H:1284:LYS:HG2	2.18	0.44
2:H:1375:ASP:OD1	2:H:1431:HIS:HD2	2.01	0.44
3:I:543:GLY:O	3:I:545:PRO:HD3	2.18	0.44
3:J:366:LEU:HB2	17:J:2002:HOH:O	2.18	0.44
3:K:245:ASN:OD1	3:K:283:ARG:HB2	2.18	0.44
1:C:10:ASN:HB2	1:C:621:GLY:CA	2.48	0.44
2:D:734:ILE:N	2:D:734:ILE:HD12	2.33	0.44
2:D:1338:LYS:H	2:D:1371:ARG:HD2	1.83	0.44
2:D:1375:ASP:OD1	2:D:1431:HIS:HD2	2.01	0.44
2:D:1462:ASN:HD21	2:D:1464:GLU:HB2	1.83	0.44
2:F:1123:ALA:O	2:F:1127:ILE:HG13	2.17	0.44
1:G:510:VAL:HG12	1:G:528:SER:HB3	1.99	0.44
2:H:937:LYS:HD2	2:H:937:LYS:C	2.43	0.44
2:H:1292:GLU:HG2	2:H:1293:SER:H	1.83	0.44
3:I:702:ASN:O	3:I:703:GLN:HG3	2.17	0.44
3:J:238:LEU:HD22	3:J:280:VAL:HG21	1.99	0.44
3:J:491:VAL:HB	3:J:572:LEU:HD11	1.99	0.44
3:J:654:ARG:HG3	3:J:722:GLN:CB	2.48	0.44
3:K:272:ILE:HG12	3:K:284:TYR:CE1	2.52	0.44
3:K:375:THR:O	3:K:379:GLU:HG3	2.18	0.44
1:A:207:LEU:HA	1:A:208:PRO:HD2	1.81	0.43
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.18	0.43
2:D:1126:LEU:O	2:D:1130:GLN:HG3	2.17	0.43
2:F:819:ARG:O	2:F:820:ASN:HB2	2.17	0.43
2:F:1497:PHE:CZ	2:F:1572:LEU:HD23	2.52	0.43
1:G:193:GLN:H	1:G:193:GLN:CD	2.25	0.43
3:I:491:VAL:HB	3:I:572:LEU:HD11	1.99	0.43
3:K:654:ARG:HG3	3:K:722:GLN:CB	2.48	0.43
3:K:700:CYS:HA	3:K:704:LYS:O	2.16	0.43
1:A:19:THR:HB	1:A:478:LEU:HB2	1.99	0.43
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.99	0.43
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.33	0.43
1:E:343:LYS:HB2	1:E:346:MET:HB2	2.00	0.43
2:F:1283:SER:O	2:F:1284:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1359:LYS:HB2	4:M:4:LEU:HD21	2.00	0.43
2:F:1462:ASN:HD21	2:F:1464:GLU:HB2	1.84	0.43
2:H:840:VAL:HG22	2:H:894:VAL:HG12	2.00	0.43
2:H:1370:TYR:CD1	2:H:1376:ALA:HB2	2.52	0.43
9:Y:1:NAG:H61	9:Y:2:NAG:C7	2.48	0.43
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.19	0.43
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.19	0.43
2:F:1038:ARG:NH1	2:F:1077:VAL:HG22	2.33	0.43
1:G:343:LYS:N	1:G:343:LYS:HD2	2.33	0.43
2:H:887:GLU:OE2	2:H:904:ARG:HD2	2.18	0.43
3:J:543:GLY:O	3:J:545:PRO:HD3	2.18	0.43
3:J:653:PRO:CD	3:J:654:ARG:HH12	2.27	0.43
3:L:654:ARG:HG3	3:L:722:GLN:CB	2.48	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.43
1:C:577:ASP:CG	2:D:778:THR:HG21	2.43	0.43
1:E:208:PRO:CD	1:E:583:LEU:HD11	2.48	0.43
2:F:833:ARG:CG	2:F:833:ARG:NH1	2.75	0.43
2:F:1639:CYS:HA	2:F:1640:PRO:HD3	1.69	0.43
1:G:341:TYR:CE1	1:G:611:LYS:HB3	2.53	0.43
1:G:427:VAL:HB	1:G:523:GLU:HG3	1.99	0.43
2:H:1292:GLU:N	2:H:1292:GLU:CD	2.77	0.43
3:I:245:ASN:OD1	3:I:283:ARG:HB2	2.18	0.43
6:W:2:NAG:H61	6:W:3:BMA:H2	1.99	0.43
1:A:22:LEU:HD13	1:A:33:VAL:HG11	2.00	0.43
2:B:1338:LYS:H	2:B:1371:ARG:HD2	1.83	0.43
2:B:1482:LYS:HA	2:B:1492:ALA:HB3	2.00	0.43
1:C:516:ILE:HD12	1:C:516:ILE:N	2.32	0.43
1:E:22:LEU:HD13	1:E:33:VAL:HG11	2.00	0.43
1:E:250:ILE:HG12	1:E:251:PHE:H	1.84	0.43
1:E:343:LYS:N	1:E:343:LYS:HD2	2.33	0.43
3:L:238:LEU:HD22	3:L:280:VAL:HG21	1.99	0.43
2:B:1290:HIS:O	2:B:1291:TRP:O	2.37	0.43
2:B:1336:CYS:O	2:B:1337:ASN:O	2.37	0.43
2:B:1375:ASP:OD1	2:B:1431:HIS:HD2	2.01	0.43
2:D:758:GLU:H	2:D:758:GLU:CD	2.26	0.43
2:D:840:VAL:HG22	2:D:894:VAL:HG12	2.00	0.43
2:D:1336:CYS:O	2:D:1337:ASN:O	2.36	0.43
1:G:2:PRO:HA	1:G:25:HIS:O	2.19	0.43
2:H:1506:THR:OG1	2:H:1509:GLU:HG2	2.17	0.43
3:I:654:ARG:HG3	3:I:722:GLN:CB	2.48	0.43
3:J:245:ASN:OD1	3:J:283:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:LYS:HD2	1:C:343:LYS:N	2.33	0.43
2:D:1292:GLU:N	2:D:1292:GLU:CD	2.76	0.43
1:E:282:ARG:CZ	1:E:286:LEU:HD11	2.49	0.43
2:F:840:VAL:HG22	2:F:894:VAL:HG12	2.00	0.43
2:F:974:ASP:C	2:F:976:GLU:H	2.27	0.43
2:F:1078:LEU:HD23	2:F:1135:ILE:HG21	2.01	0.43
1:G:572:VAL:HG23	2:H:785:VAL:HB	2.01	0.43
3:I:238:LEU:HD22	3:I:280:VAL:HG21	1.99	0.43
3:K:543:GLY:O	3:K:545:PRO:HD3	2.18	0.43
3:K:655:PHE:HD2	3:K:716:PHE:HB3	1.84	0.43
3:L:543:GLY:O	3:L:545:PRO:HD3	2.18	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.33	0.43
2:B:974:ASP:C	2:B:976:GLU:H	2.27	0.43
1:C:2:PRO:HA	1:C:25:HIS:O	2.19	0.43
1:E:2:PRO:HA	1:E:25:HIS:O	2.19	0.43
1:E:251:PHE:CG	1:E:280:LEU:HD22	2.54	0.43
1:G:508:ARG:HH12	1:G:602:ASP:CG	2.26	0.43
1:G:526:ALA:O	1:G:616:VAL:HG21	2.19	0.43
3:I:655:PHE:HD2	3:I:716:PHE:HB3	1.84	0.43
1:C:282:ARG:CZ	1:C:286:LEU:HD11	2.49	0.43
1:C:503:PHE:HD1	1:C:507:PHE:CG	2.37	0.43
2:D:974:ASP:C	2:D:976:GLU:H	2.27	0.43
1:G:250:ILE:HG12	1:G:251:PHE:H	1.84	0.43
1:G:343:LYS:HB2	1:G:346:MET:HB2	2.00	0.43
2:H:1528:VAL:HG21	2:H:1559:GLN:HE21	1.84	0.43
3:I:431:LYS:HG3	4:M:27:ASN:ND2	2.34	0.43
3:I:446:GLU:H	3:I:446:GLU:HG3	1.66	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.19	0.43
2:B:887:GLU:OE2	2:B:904:ARG:HD2	2.18	0.43
2:B:896:HIS:HB3	4:Q:61:LYS:HD3	2.00	0.43
2:B:1462:ASN:HD21	2:B:1464:GLU:HB2	1.83	0.43
2:B:1523:TYR:HB3	2:B:1543:ILE:HG23	2.01	0.43
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.27	0.43
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.33	0.43
2:D:1523:TYR:HB3	2:D:1543:ILE:HG23	2.01	0.43
2:F:1056:LEU:O	2:F:1060:VAL:HG23	2.19	0.43
2:F:1227:VAL:HB	2:F:1228:PRO:HD3	2.01	0.43
2:F:1292:GLU:N	2:F:1292:GLU:CD	2.77	0.43
2:H:1376:ALA:HB3	2:H:1429:VAL:CG2	2.49	0.43
3:L:238:LEU:HD11	3:L:278:TYR:CB	2.46	0.43
1:A:251:PHE:CG	1:A:280:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1334:LEU:HA	2:B:1334:LEU:HD13	1.80	0.42
1:C:251:PHE:CG	1:C:280:LEU:HD22	2.54	0.42
1:C:538:VAL:HB	2:D:791:LYS:O	2.18	0.42
1:E:239:TYR:HB2	2:F:804:MET:HE2	2.01	0.42
1:G:282:ARG:CZ	1:G:286:LEU:HD11	2.49	0.42
1:G:644:ALA:O	1:G:645:ALA:C	2.62	0.42
2:H:851:CYS:HB2	2:H:1491:CYS:HB2	1.81	0.42
2:H:1462:ASN:HD21	2:H:1464:GLU:HB2	1.84	0.42
3:J:607:PHE:CE1	3:J:669:THR:HG22	2.54	0.42
3:K:503:PHE:HB2	3:K:530:PHE:CZ	2.54	0.42
3:K:607:PHE:CE1	3:K:669:THR:HG22	2.54	0.42
2:B:758:GLU:H	2:B:758:GLU:CD	2.26	0.42
2:B:772:PHE:CD1	4:N:37:ASN:ND2	2.87	0.42
2:B:1215:LEU:O	2:B:1219:LEU:HG	2.19	0.42
1:C:247:ALA:HB2	1:C:308:VAL:HG22	2.02	0.42
2:D:819:ARG:NH1	2:D:819:ARG:CG	2.80	0.42
2:F:745:PHE:N	2:F:746:PRO:HD3	2.32	0.42
2:F:1292:GLU:HG2	2:F:1293:SER:H	1.83	0.42
2:H:824:GLU:OE2	2:H:875:PRO:HB3	2.19	0.42
3:I:238:LEU:HD11	3:I:278:TYR:CB	2.46	0.42
3:J:446:GLU:H	3:J:446:GLU:HG3	1.66	0.42
3:L:245:ASN:OD1	3:L:283:ARG:HB2	2.18	0.42
4:N:49:GLN:HA	4:N:52:MET:HE2	2.01	0.42
4:Q:49:GLN:HA	4:Q:52:MET:HE2	2.01	0.42
1:A:439:LEU:H	1:A:439:LEU:CD1	2.32	0.42
2:B:1265:PRO:O	2:B:1266:ASP:CB	2.64	0.42
2:B:1292:GLU:HG2	2:B:1293:SER:H	1.83	0.42
1:C:144:ASN:HD22	1:C:144:ASN:N	2.14	0.42
1:C:343:LYS:HB2	1:C:346:MET:HB2	2.00	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
2:D:1482:LYS:HA	2:D:1492:ALA:HB3	2.01	0.42
1:E:111:GLN:O	1:E:125:TYR:HA	2.20	0.42
1:G:22:LEU:HD13	1:G:33:VAL:HG11	2.00	0.42
2:H:1500:LYS:NZ	2:H:1504:LYS:HB2	2.34	0.42
3:I:449:SER:HA	3:I:452:LEU:HD13	2.01	0.42
3:J:655:PHE:HD2	3:J:716:PHE:HB3	1.84	0.42
3:K:606:LEU:C	3:K:606:LEU:HD12	2.45	0.42
3:L:655:PHE:HD2	3:L:716:PHE:HB3	1.84	0.42
6:W:2:NAG:N2	6:W:4:BMA:O3	2.52	0.42
1:A:503:PHE:HD1	1:A:507:PHE:CG	2.37	0.42
2:B:1446:ASN:HB2	4:Q:4:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HG12	1:C:20:MET:HE3	2.02	0.42
1:G:127:ILE:N	1:G:127:ILE:HD12	2.35	0.42
3:I:607:PHE:CE1	3:I:669:THR:HG22	2.55	0.42
3:L:607:PHE:CE1	3:L:669:THR:HG22	2.54	0.42
1:A:10:ASN:HB2	1:A:621:GLY:HA2	2.01	0.42
1:A:127:ILE:HD12	1:A:127:ILE:N	2.35	0.42
1:A:282:ARG:CZ	1:A:286:LEU:HD11	2.49	0.42
1:C:111:GLN:O	1:C:125:TYR:HA	2.20	0.42
2:D:1078:LEU:HD23	2:D:1135:ILE:HG21	2.01	0.42
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	2.01	0.42
2:F:959:LEU:HD23	2:F:959:LEU:C	2.45	0.42
2:F:1528:VAL:HG21	2:F:1559:GLN:HE21	1.84	0.42
1:G:424:TYR:CE1	1:G:612:ASP:C	2.97	0.42
2:H:745:PHE:N	2:H:746:PRO:HD3	2.35	0.42
3:I:432:ASP:HA	4:M:27:ASN:HD21	1.84	0.42
3:I:709:VAL:HA	3:I:710:PRO:HD3	1.92	0.42
3:J:606:LEU:C	3:J:606:LEU:HD12	2.45	0.42
3:K:350:GLU:O	3:K:351:GLY:C	2.63	0.42
3:K:354:ARG:HB2	16:K:803:NAG:C8	2.42	0.42
4:M:49:GLN:HA	4:M:52:MET:HE2	2.01	0.42
9:Y:2:NAG:H82	9:Y:2:NAG:H2	1.91	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.84	0.42
2:B:1506:THR:OG1	2:B:1509:GLU:HG2	2.20	0.42
2:D:1215:LEU:O	2:D:1219:LEU:HG	2.19	0.42
2:D:1290:HIS:O	2:D:1291:TRP:O	2.37	0.42
2:D:1437:LEU:C	2:D:1437:LEU:HD12	2.45	0.42
2:D:1506:THR:OG1	2:D:1509:GLU:HG2	2.20	0.42
1:E:454:LEU:HA	1:E:491:ASP:O	2.19	0.42
1:G:251:PHE:CG	1:G:280:LEU:HD22	2.54	0.42
2:H:959:LEU:C	2:H:959:LEU:HD23	2.45	0.42
3:I:289:TYR:HA	3:I:293:PRO:HA	2.01	0.42
3:K:353:ASN:OD1	16:K:803:NAG:C7	2.67	0.42
3:L:489:ALA:HB2	3:L:677:PRO:CG	2.45	0.42
1:A:61:MET:HE1	1:A:482:GLY:HA2	2.01	0.42
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.42
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.46	0.42
1:E:127:ILE:HD12	1:E:127:ILE:N	2.35	0.42
1:G:439:LEU:H	1:G:439:LEU:CD1	2.32	0.42
2:H:758:GLU:H	2:H:758:GLU:CD	2.26	0.42
2:H:1485:ARG:HH21	2:H:1590:TRP:HE1	1.67	0.42
2:H:1516:GLU:HB3	2:H:1517:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:531:HIS:CD2	3:J:533:ASN:HB2	2.55	0.42
1:A:547:GLN:C	1:A:549:GLU:H	2.28	0.42
1:A:549:GLU:O	1:A:550:ASP:HB2	2.20	0.42
2:B:1078:LEU:HD23	2:B:1135:ILE:HG21	2.01	0.42
1:C:127:ILE:HD12	1:C:127:ILE:N	2.35	0.42
2:D:943:ALA:O	2:D:1305:ASN:ND2	2.53	0.42
1:E:6:ILE:HD11	1:E:20:MET:CG	2.50	0.42
1:E:219:LYS:NZ	1:E:356:ASN:ND2	2.68	0.42
2:F:887:GLU:OE2	2:F:904:ARG:HD2	2.19	0.42
2:F:1215:LEU:O	2:F:1219:LEU:HG	2.19	0.42
2:F:1216:LEU:HD21	2:F:1256:ALA:HA	2.02	0.42
1:G:512:TYR:CE1	1:G:624:PHE:HE1	2.37	0.42
3:I:531:HIS:CD2	3:I:533:ASN:HB2	2.55	0.42
3:I:606:LEU:C	3:I:606:LEU:HD12	2.45	0.42
3:L:289:TYR:HA	3:L:293:PRO:HA	2.02	0.42
3:L:503:PHE:HB2	3:L:530:PHE:CZ	2.54	0.42
3:L:531:HIS:CD2	3:L:533:ASN:HB2	2.55	0.42
1:A:250:ILE:HG22	1:A:305:SER:HB3	2.01	0.42
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.49	0.42
1:C:330:PRO:HG2	1:C:409:LEU:HD21	2.01	0.42
1:G:111:GLN:O	1:G:125:TYR:HA	2.20	0.42
1:G:574:VAL:HG13	2:H:783:LEU:HB3	2.01	0.42
2:H:1334:LEU:HA	2:H:1334:LEU:HD13	1.80	0.42
3:I:676:GLY:HA2	3:I:677:PRO:HD3	1.83	0.42
3:I:705:ARG:O	3:I:706:GLN:CB	2.60	0.42
3:K:244:MET:HG2	3:K:245:ASN:N	2.35	0.42
4:Q:84:LYS:O	4:Q:84:LYS:HG3	2.20	0.42
1:C:250:ILE:HG12	1:C:251:PHE:H	1.84	0.42
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.85	0.42
2:D:1518:GLY:CA	2:D:1585:LEU:HD22	2.48	0.42
2:F:1009:THR:HB	2:F:1011:GLN:HE21	1.85	0.42
2:F:1269:GLU:O	2:F:1271:ASN:N	2.52	0.42
2:F:1522:VAL:HG22	2:F:1583:TRP:HB3	2.02	0.42
1:G:19:THR:HG22	1:G:20:MET:N	2.35	0.42
1:G:503:PHE:HD1	1:G:507:PHE:CG	2.37	0.42
3:I:350:GLU:O	3:I:351:GLY:C	2.63	0.42
3:I:503:PHE:HB2	3:I:530:PHE:CZ	2.54	0.42
3:J:503:PHE:HB2	3:J:530:PHE:CZ	2.54	0.42
3:L:298:LYS:HB2	3:L:301:GLU:HG3	2.02	0.42
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	2.02	0.41
1:C:6:ILE:HD11	1:C:20:MET:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:LEU:H	1:C:439:LEU:CD1	2.32	0.41
2:D:1227:VAL:HB	2:D:1228:PRO:HD3	2.01	0.41
2:F:1390:ALA:HA	2:F:1391:PRO:HD3	1.91	0.41
2:F:1437:LEU:C	2:F:1437:LEU:HD12	2.45	0.41
1:G:6:ILE:HD11	1:G:20:MET:CG	2.50	0.41
1:G:526:ALA:CB	1:G:617:PHE:CE2	3.03	0.41
2:H:841:ARG:HH11	2:H:841:ARG:CG	2.23	0.41
2:H:854:ALA:HB2	2:H:860:HIS:HB3	2.02	0.41
2:H:877:VAL:H	2:H:1451:GLN:HE21	1.68	0.41
2:H:1338:LYS:N	2:H:1371:ARG:HB2	2.34	0.41
3:J:319:TYR:CD2	3:J:319:TYR:C	2.98	0.41
3:L:519:GLU:C	3:L:521:ARG:H	2.28	0.41
3:L:606:LEU:C	3:L:606:LEU:HD12	2.45	0.41
4:M:23:LEU:HD21	4:M:51:ALA:HB3	2.02	0.41
4:N:56:LYS:HG3	4:N:57:SER:N	2.34	0.41
1:A:80:ARG:HD2	2:B:1010:GLU:HG3	2.01	0.41
1:A:330:PRO:HG2	1:A:409:LEU:HD21	2.00	0.41
2:B:932:ARG:O	2:B:934:GLY:N	2.53	0.41
2:B:943:ALA:O	2:B:1305:ASN:ND2	2.53	0.41
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.85	0.41
2:D:932:ARG:O	2:D:934:GLY:N	2.53	0.41
2:D:1528:VAL:HG21	2:D:1559:GLN:HE21	1.84	0.41
1:G:350:LEU:CD2	1:G:400:ILE:HG21	2.50	0.41
3:J:489:ALA:HB2	3:J:677:PRO:CG	2.45	0.41
3:K:540:LYS:NZ	3:K:540:LYS:HB2	2.36	0.41
3:L:239:ASP:HA	3:L:240:PRO:HD3	1.86	0.41
3:L:240:PRO:C	3:L:242:GLY:H	2.29	0.41
4:M:56:LYS:HG3	4:M:57:SER:N	2.34	0.41
4:Q:23:LEU:HD21	4:Q:51:ALA:HB3	2.02	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.02	0.41
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.85	0.41
2:B:1528:VAL:HG21	2:B:1559:GLN:HE21	1.84	0.41
1:C:19:THR:HG22	1:C:20:MET:N	2.35	0.41
2:D:1370:TYR:CG	2:D:1376:ALA:HB2	2.55	0.41
2:D:1376:ALA:HB3	2:D:1429:VAL:CG2	2.49	0.41
1:E:126:ARG:CZ	1:E:572:VAL:HB	2.50	0.41
1:E:365:VAL:HA	1:E:366:PRO:HD2	1.80	0.41
1:E:386:LYS:HD3	1:E:440:ARG:HG2	2.02	0.41
2:F:915:ARG:O	2:F:916:MET:HG3	2.21	0.41
2:F:1165:TYR:HD1	2:F:1210:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1472:HIS:HA	2:F:1473:PRO:HD3	1.94	0.41
1:G:341:TYR:CD2	1:G:610:GLY:HA2	2.56	0.41
1:G:481:ALA:O	6:W:1:NAG:H82	2.20	0.41
2:H:1611:GLU:HG3	2:H:1612:GLU:N	2.34	0.41
3:I:519:GLU:C	3:I:521:ARG:H	2.28	0.41
3:I:666:ASP:HA	3:I:667:PRO:HD3	1.95	0.41
3:J:244:MET:HG2	3:J:245:ASN:N	2.35	0.41
3:J:298:LYS:HB2	3:J:301:GLU:HG3	2.02	0.41
3:J:350:GLU:O	3:J:351:GLY:C	2.63	0.41
3:J:519:GLU:C	3:J:521:ARG:H	2.28	0.41
3:K:240:PRO:C	3:K:242:GLY:H	2.29	0.41
3:K:531:HIS:CD2	3:K:533:ASN:HB2	2.55	0.41
3:L:494:TYR:O	3:L:556:LYS:HA	2.21	0.41
3:L:503:PHE:CZ	3:L:555:ILE:HD11	2.55	0.41
3:L:540:LYS:HB2	3:L:540:LYS:NZ	2.36	0.41
4:N:84:LYS:O	4:N:84:LYS:HG3	2.20	0.41
4:Q:56:LYS:HG3	4:Q:57:SER:N	2.34	0.41
7:V:3:BMA:H5	7:V:4:BMA:H2	2.01	0.41
1:A:343:LYS:HB2	1:A:346:MET:HB2	2.00	0.41
1:A:454:LEU:HA	1:A:491:ASP:O	2.21	0.41
2:B:1055:TRP:CD1	2:B:1111:LEU:HD22	2.56	0.41
1:C:100:LEU:HD12	1:C:101:VAL:H	1.86	0.41
2:D:1336:CYS:O	2:D:1337:ASN:C	2.63	0.41
2:F:932:ARG:HH11	3:L:339:SER:CB	2.34	0.41
2:F:937:LYS:HG2	3:L:345:ASP:CG	2.45	0.41
2:F:1055:TRP:CD1	2:F:1111:LEU:HD22	2.56	0.41
2:F:1518:GLY:CA	2:F:1585:LEU:HD22	2.48	0.41
1:G:547:GLN:C	1:G:549:GLU:H	2.28	0.41
2:H:740:VAL:CB	4:Q:42:ARG:HB2	2.45	0.41
2:H:1514:ALA:O	2:H:1519:VAL:HG11	2.20	0.41
3:I:503:PHE:CZ	3:I:555:ILE:HD11	2.55	0.41
3:J:494:TYR:O	3:J:556:LYS:HA	2.21	0.41
3:K:259:SER:HB3	11:b:1:NAG:O7	2.20	0.41
3:L:278:TYR:CE2	3:L:455:MET:SD	3.13	0.41
3:L:350:GLU:O	3:L:351:GLY:C	2.63	0.41
4:N:41:LYS:O	4:N:45:LYS:HG3	2.21	0.41
4:P:84:LYS:O	4:P:84:LYS:HG3	2.20	0.41
11:b:3:MAN:H62	11:b:5:MAN:H2	1.74	0.41
1:A:2:PRO:HA	1:A:25:HIS:O	2.19	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.35	0.41
1:A:250:ILE:HG12	1:A:251:PHE:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1336:CYS:O	2:B:1337:ASN:C	2.63	0.41
2:B:1451:GLN:HA	2:B:1452:PRO:HD3	1.94	0.41
2:D:1055:TRP:CD1	2:D:1111:LEU:HD22	2.56	0.41
2:D:1516:GLU:HB3	2:D:1517:PRO:CD	2.50	0.41
2:F:759:PRO:HA	2:F:760:PRO:HD3	1.84	0.41
2:F:1082:VAL:HG13	2:F:1129:LEU:HD22	2.02	0.41
2:H:1359:LYS:CB	4:N:4:LEU:HD21	2.50	0.41
3:I:244:MET:HG2	3:I:245:ASN:N	2.35	0.41
3:J:289:TYR:HA	3:J:293:PRO:HA	2.02	0.41
3:J:461:LYS:HG2	4:Q:28:VAL:HG12	2.03	0.41
3:J:676:GLY:HA2	3:J:677:PRO:HD3	1.83	0.41
3:K:446:GLU:H	3:K:446:GLU:HG3	1.66	0.41
3:K:503:PHE:CZ	3:K:555:ILE:HD11	2.55	0.41
2:B:813:LEU:HD23	2:B:907:LEU:HD22	2.02	0.41
1:C:549:GLU:O	1:C:550:ASP:HB2	2.20	0.41
2:F:824:GLU:OE2	2:F:875:PRO:HB3	2.19	0.41
2:F:1334:LEU:HD13	2:F:1334:LEU:HA	1.80	0.41
1:G:549:GLU:O	1:G:550:ASP:HB2	2.20	0.41
2:H:1500:LYS:HE3	2:H:1504:LYS:O	2.21	0.41
3:I:319:TYR:C	3:I:319:TYR:CD2	2.98	0.41
3:J:368:ASN:ND2	3:J:368:ASN:N	2.69	0.41
3:J:540:LYS:NZ	3:J:540:LYS:HB2	2.35	0.41
4:M:84:LYS:O	4:M:84:LYS:HG3	2.20	0.41
4:P:49:GLN:HA	4:P:52:MET:HE2	2.01	0.41
4:P:56:LYS:HG3	4:P:57:SER:N	2.34	0.41
1:A:10:ASN:HA	1:A:623:THR:HG23	2.03	0.41
1:A:459:ARG:NH2	1:G:459:ARG:HE	2.19	0.41
2:B:854:ALA:HB2	2:B:860:HIS:HB3	2.02	0.41
2:B:1522:VAL:HG22	2:B:1583:TRP:HB3	2.02	0.41
2:D:851:CYS:HB2	2:D:1491:CYS:HB2	1.78	0.41
2:D:1522:VAL:HG22	2:D:1583:TRP:HB3	2.02	0.41
2:D:1611:GLU:HG3	2:D:1612:GLU:N	2.34	0.41
1:E:481:ALA:N	5:U:1:NAG:H81	2.35	0.41
1:E:503:PHE:HD1	1:E:507:PHE:CG	2.37	0.41
2:F:1514:ALA:O	2:F:1519:VAL:HG11	2.20	0.41
1:G:7:ILE:HG21	1:G:471:LEU:HD22	2.02	0.41
2:H:1500:LYS:HZ1	2:H:1504:LYS:HB2	1.85	0.41
2:H:1518:GLY:CA	2:H:1585:LEU:HD22	2.48	0.41
3:I:494:TYR:O	3:I:556:LYS:HA	2.21	0.41
3:K:298:LYS:HB2	3:K:301:GLU:HG3	2.02	0.41
1:A:6:ILE:HD11	1:A:20:MET:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TYR:CD2	1:A:381:GLY:HA2	2.56	0.41
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.23	0.41
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	2.02	0.41
2:B:1444:TYR:HB2	4:Q:10:TYR:CE1	2.55	0.41
2:B:1522:VAL:HG12	2:B:1547:ILE:HD12	2.03	0.41
1:C:207:LEU:HA	1:C:208:PRO:HD2	1.82	0.41
1:E:549:GLU:O	1:E:550:ASP:HB2	2.20	0.41
2:F:1338:LYS:N	2:F:1371:ARG:HB2	2.36	0.41
1:G:23:GLU:OE1	1:G:469:THR:HG21	2.21	0.41
1:G:249:VAL:HG13	1:G:267:LYS:HB2	2.02	0.41
2:H:813:LEU:HA	2:H:814:PRO:HD3	1.97	0.41
2:H:1639:CYS:HA	2:H:1640:PRO:HD3	1.76	0.41
3:K:319:TYR:CD2	3:K:319:TYR:C	2.98	0.41
3:L:428:PHE:CE1	3:L:439:VAL:HG13	2.56	0.41
1:A:24:ALA:HB3	1:A:60:HIS:HB3	2.03	0.41
1:A:250:ILE:HG12	1:A:251:PHE:N	2.36	0.41
1:A:506:SER:HB2	1:A:530:TRP:NE1	2.27	0.41
1:A:552:GLN:HA	1:A:553:PRO:HD3	1.81	0.41
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.56	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.55	0.41
2:B:1437:LEU:C	2:B:1437:LEU:HD12	2.45	0.41
2:B:1611:GLU:HB3	2:B:1614:GLU:HG3	2.03	0.41
1:C:10:ASN:HB2	1:C:622:LEU:N	2.36	0.41
1:C:454:LEU:HA	1:C:491:ASP:O	2.21	0.41
2:D:1165:TYR:HD1	2:D:1210:ALA:HB2	1.85	0.41
2:D:1611:GLU:HB3	2:D:1614:GLU:HG3	2.03	0.41
1:E:6:ILE:HG12	1:E:20:MET:HE3	2.02	0.41
1:E:19:THR:HG22	1:E:20:MET:N	2.35	0.41
1:E:250:ILE:HG12	1:E:251:PHE:N	2.36	0.41
1:E:250:ILE:HG22	1:E:305:SER:HB3	2.03	0.41
1:E:324:ILE:HA	1:E:325:PRO:HD3	1.89	0.41
1:E:547:GLN:C	1:E:549:GLU:H	2.28	0.41
1:E:640:CYS:HB3	1:E:641:PRO:CD	2.51	0.41
2:F:745:PHE:HA	2:F:776:SER:OG	2.21	0.41
2:F:1376:ALA:HB3	2:F:1429:VAL:CG2	2.49	0.41
1:G:3:MET:HE2	1:G:626:SER:HB2	2.02	0.41
1:G:207:LEU:HA	1:G:208:PRO:HD2	1.82	0.41
2:H:1437:LEU:C	2:H:1437:LEU:HD12	2.45	0.41
2:H:1522:VAL:HG22	2:H:1583:TRP:HB3	2.02	0.41
2:H:1523:TYR:HB3	2:H:1543:ILE:HG23	2.02	0.41
3:I:239:ASP:HA	3:I:240:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:238:LEU:HD11	3:J:278:TYR:CB	2.46	0.41
3:J:423:ASN:N	3:J:423:ASN:ND2	2.68	0.41
3:J:428:PHE:CE1	4:Q:31:LEU:HD11	2.55	0.41
3:J:503:PHE:CZ	3:J:555:ILE:HD11	2.55	0.41
3:J:638:ALA:HA	3:J:639:PRO:HD3	1.98	0.41
3:K:289:TYR:HA	3:K:293:PRO:HA	2.02	0.41
3:K:519:GLU:C	3:K:521:ARG:H	2.28	0.41
3:K:676:GLY:HA2	3:K:677:PRO:HD3	1.83	0.41
3:L:319:TYR:CD2	3:L:319:TYR:C	2.98	0.41
4:M:69:GLN:HE21	4:M:69:GLN:HB3	1.68	0.41
4:P:23:LEU:HD21	4:P:51:ALA:HB3	2.02	0.41
9:a:2:NAG:H82	9:a:2:NAG:H2	1.91	0.41
1:A:6:ILE:HG12	1:A:20:MET:HE3	2.02	0.41
1:A:19:THR:HG22	1:A:20:MET:N	2.35	0.41
1:A:100:LEU:HD12	1:A:101:VAL:H	1.86	0.41
2:B:1229:PRO:HA	2:B:1232:ARG:NH1	2.36	0.41
2:B:1582:MET:HE3	2:B:1606:VAL:HG22	2.03	0.41
1:C:477:ARG:HG2	1:C:477:ARG:NH1	2.21	0.41
2:D:745:PHE:N	2:D:746:PRO:HD3	2.35	0.41
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	2.02	0.41
1:E:438:VAL:HG13	1:E:449:LEU:HD11	2.03	0.41
1:E:439:LEU:H	1:E:439:LEU:CD1	2.32	0.41
2:F:813:LEU:HD23	2:F:907:LEU:HD22	2.02	0.41
2:F:1522:VAL:HG12	2:F:1547:ILE:HD12	2.03	0.41
1:G:391:THR:HG22	1:G:392:HIS:N	2.36	0.41
2:H:1635:VAL:HG23	2:H:1636:VAL:N	2.36	0.41
3:I:503:PHE:HB2	3:I:530:PHE:HZ	1.86	0.41
3:J:428:PHE:CE1	3:J:439:VAL:HG13	2.56	0.41
3:K:244:MET:HG2	3:K:245:ASN:H	1.86	0.41
1:A:400:ILE:N	1:A:400:ILE:HD12	2.36	0.40
2:B:917:ASN:OD1	5:R:1:NAG:O5	2.38	0.40
1:C:365:VAL:HA	1:C:366:PRO:HD2	1.81	0.40
1:C:547:GLN:C	1:C:549:GLU:H	2.28	0.40
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.56	0.40
1:E:249:VAL:HG13	1:E:267:LYS:HB2	2.03	0.40
1:E:541:LEU:HD22	2:F:786:SER:HB3	2.02	0.40
2:F:819:ARG:CG	2:F:819:ARG:NH1	2.80	0.40
2:F:854:ALA:HB2	2:F:860:HIS:HB3	2.02	0.40
2:F:1229:PRO:HA	2:F:1232:ARG:NH1	2.36	0.40
2:F:1516:GLU:HB3	2:F:1517:PRO:CD	2.50	0.40
1:G:400:ILE:HD12	1:G:400:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:915:ARG:O	2:H:916:MET:HG3	2.21	0.40
2:H:965:VAL:HG23	2:H:1268:GLN:OE1	2.22	0.40
2:H:1522:VAL:HG12	2:H:1547:ILE:HD12	2.03	0.40
3:K:428:PHE:CE1	3:K:439:VAL:HG13	2.56	0.40
3:K:439:VAL:HA	4:P:31:LEU:HD21	2.02	0.40
4:M:41:LYS:O	4:M:45:LYS:HG3	2.21	0.40
4:P:41:LYS:O	4:P:45:LYS:HG3	2.21	0.40
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.02	0.40
2:D:1582:MET:HE3	2:D:1606:VAL:HG22	2.03	0.40
1:E:24:ALA:HB3	1:E:60:HIS:HB3	2.03	0.40
1:E:391:THR:HG22	1:E:392:HIS:N	2.36	0.40
1:E:552:GLN:HA	1:E:553:PRO:HD3	1.81	0.40
2:F:1000:VAL:HG22	2:F:1027:ILE:HG23	2.04	0.40
2:F:1192:ALA:HB2	2:F:1198:TRP:CE2	2.56	0.40
2:F:1370:TYR:CE2	2:F:1372:GLY:HA3	2.56	0.40
2:F:1611:GLU:HB3	2:F:1614:GLU:HG3	2.03	0.40
1:G:6:ILE:HG12	1:G:20:MET:HE3	2.02	0.40
1:G:558:GLN:HB3	2:H:770:ASN:HD21	1.86	0.40
2:H:757:LYS:HZ3	2:H:757:LYS:HA	1.86	0.40
2:H:813:LEU:HD23	2:H:907:LEU:HD22	2.02	0.40
2:H:877:VAL:HG22	2:H:1451:GLN:NE2	2.28	0.40
2:H:1370:TYR:CG	2:H:1376:ALA:HB2	2.56	0.40
2:H:1503:ASP:O	2:H:1504:LYS:HG3	2.21	0.40
1:C:109:PHE:CZ	1:C:594:ILE:HG23	2.56	0.40
2:D:813:LEU:HD23	2:D:907:LEU:HD22	2.02	0.40
1:E:480:LYS:HG2	1:E:481:ALA:N	2.36	0.40
2:F:757:LYS:HA	2:F:757:LYS:HZ3	1.86	0.40
2:F:1523:TYR:HB3	2:F:1543:ILE:HG23	2.02	0.40
1:G:126:ARG:HG3	2:H:751:TRP:CZ2	2.56	0.40
1:G:480:LYS:HG2	1:G:481:ALA:N	2.37	0.40
1:G:505:PRO:O	1:G:533:VAL:HB	2.21	0.40
1:G:506:SER:HB2	1:G:530:TRP:NE1	2.27	0.40
2:H:809:ILE:HD11	2:H:892:ALA:CB	2.52	0.40
2:H:1527:LEU:HD22	2:H:1574:LEU:HB3	2.04	0.40
3:I:345:ASP:HB3	3:I:346:ASP:H	1.49	0.40
3:I:654:ARG:HG3	3:I:722:GLN:HB3	2.03	0.40
5:U:3:BMA:H62	5:U:4:BMA:H2	1.58	0.40
1:A:342:PHE:CZ	1:A:423:PRO:HG3	2.56	0.40
1:A:363:TYR:HD2	1:A:381:GLY:HA2	1.86	0.40
2:B:1446:ASN:HB2	4:Q:4:LEU:HD12	2.03	0.40
1:C:391:THR:HG22	1:C:392:HIS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:LEU:HD12	1:C:583:LEU:N	2.36	0.40
2:D:776:SER:HB2	2:D:780:TRP:HZ2	1.86	0.40
2:D:1229:PRO:HA	2:D:1232:ARG:NH1	2.36	0.40
1:E:100:LEU:HD12	1:E:101:VAL:H	1.86	0.40
1:E:577:ASP:CG	2:F:778:THR:HG21	2.45	0.40
1:E:583:LEU:HD12	1:E:583:LEU:N	2.36	0.40
2:F:1269:GLU:CD	2:F:1315:LYS:HB3	2.46	0.40
2:H:1370:TYR:CE2	2:H:1372:GLY:HA3	2.56	0.40
2:H:1609:TRP:HD1	2:H:1610:PRO:O	2.04	0.40
3:I:298:LYS:HB2	3:I:301:GLU:HG3	2.02	0.40
3:I:402:VAL:HG11	3:I:414:ILE:HG23	2.04	0.40
3:I:428:PHE:CE1	3:I:439:VAL:HG13	2.56	0.40
3:I:461:LYS:CG	4:M:28:VAL:HG12	2.51	0.40
3:I:540:LYS:HB2	3:I:540:LYS:NZ	2.35	0.40
3:J:240:PRO:C	3:J:242:GLY:H	2.29	0.40
3:J:364:ASP:C	3:J:366:LEU:H	2.30	0.40
3:K:328:THR:N	3:K:368:ASN:HD21	2.20	0.40
3:K:364:ASP:C	3:K:366:LEU:H	2.30	0.40
3:K:494:TYR:O	3:K:556:LYS:HA	2.21	0.40
3:L:244:MET:HG2	3:L:245:ASN:N	2.35	0.40
2:B:1609:TRP:HD1	2:B:1610:PRO:O	2.04	0.40
1:C:24:ALA:HB3	1:C:60:HIS:HB3	2.03	0.40
1:C:199:GLU:HB2	1:C:587:ASN:OD1	2.22	0.40
1:C:400:ILE:HD12	1:C:400:ILE:N	2.36	0.40
1:C:480:LYS:HG2	1:C:481:ALA:N	2.37	0.40
2:D:1527:LEU:HD22	2:D:1574:LEU:HB3	2.04	0.40
1:E:642:GLN:O	1:E:644:ALA:N	2.54	0.40
2:F:1143:LEU:O	2:F:1147:ILE:HG13	2.22	0.40
2:F:1632:GLU:HA	2:F:1635:VAL:HG22	2.04	0.40
1:G:220:PHE:CZ	1:G:330:PRO:HB3	2.56	0.40
2:H:1582:MET:HE3	2:H:1606:VAL:HG22	2.03	0.40
3:J:292:TYR:HA	3:J:293:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	21	55
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	21	55
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	21	55
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	21	55
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	3	25
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	3	26
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	3	24
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	2	22
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	7	36
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	7	36
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	7	36
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	7	36
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	10	41
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	10	41
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	10	41
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	10	41
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	6	32

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	933	GLU
2	B	967	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1291	TRP
2	B	1292	GLU
2	B	1294	ALA
2	B	1337	ASN
2	B	1338	LYS
2	B	1359	LYS
2	B	1377	THR
2	B	1503	ASP

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Mol	Chain	Res	Type
2	D	933	GLU
2	D	967	GLN
2	D	1281	ARG
2	D	1291	TRP
2	D	1292	GLU
2	D	1294	ALA
2	D	1337	ASN
2	D	1338	LYS
2	D	1359	LYS
2	D	1377	THR
2	D	1503	ASP
2	F	933	GLU
2	F	967	GLN
2	F	1269	GLU
2	F	1281	ARG
2	F	1291	TRP
2	F	1292	GLU
2	F	1337	ASN
2	F	1338	LYS
2	F	1361	THR
2	F	1377	THR
2	F	1417	SER
2	F	1446	ASN
2	H	933	GLU
2	H	968	MET
2	H	1281	ARG
2	H	1291	TRP
2	H	1292	GLU
2	H	1337	ASN
2	H	1338	LYS
2	H	1361	THR
2	H	1377	THR
2	H	1417	SER
2	H	1446	ASN
2	H	1493	GLU
3	I	236	ILE
3	I	407	PRO
3	I	701	LYS
3	I	706	GLN
3	J	236	ILE
3	J	407	PRO
3	J	701	LYS

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Mol	Chain	Res	Type
3	J	706	GLN
3	K	236	ILE
3	K	407	PRO
3	K	701	LYS
3	K	706	GLN
3	L	236	ILE
3	L	407	PRO
3	L	701	LYS
3	L	706	GLN
2	B	911	PRO
2	B	1360	ASN
2	B	1361	THR
2	B	1476	GLU
2	B	1571	ALA
2	D	911	PRO
2	D	1360	ASN
2	D	1361	THR
2	D	1476	GLU
2	D	1480	LEU
2	D	1571	ALA
2	F	911	PRO
2	F	1267	HIS
2	F	1294	ALA
2	F	1476	GLU
2	F	1498	ILE
2	F	1571	ALA
2	H	1266	ASP
2	H	1269	GLU
2	H	1294	ALA
2	H	1476	GLU
2	H	1496	CYS
2	H	1498	ILE
2	H	1571	ALA
1	A	442	GLU
1	A	643	PRO
2	B	1387	THR
2	B	1502	ASP
2	B	1573	LYS
1	C	442	GLU
1	C	643	PRO
2	D	1387	THR
2	D	1502	ASP

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Mol	Chain	Res	Type
2	D	1573	LYS
1	E	442	GLU
1	E	643	PRO
2	F	1387	THR
2	F	1573	LYS
1	G	442	GLU
2	H	911	PRO
2	H	1387	THR
2	H	1573	LYS
3	I	707	LYS
3	J	516	VAL
3	J	707	LYS
3	K	516	VAL
3	K	707	LYS
3	L	707	LYS
1	A	505	PRO
2	B	1196	ASN
2	B	1265	PRO
2	B	1480	LEU
1	C	505	PRO
2	D	1196	ASN
2	D	1265	PRO
2	D	1269	GLU
1	E	505	PRO
2	F	1196	ASN
2	F	1265	PRO
2	F	1268	GLN
2	F	1331	LYS
2	F	1637	PHE
1	G	505	PRO
2	H	967	GLN
2	H	1267	HIS
2	H	1486	ASP
2	H	1495	ASN
2	H	1502	ASP
3	I	516	VAL
3	L	516	VAL
4	M	7	SER
4	N	7	SER
4	P	7	SER
4	Q	7	SER
2	B	834	GLN

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Mol	Chain	Res	Type
2	B	1201	PRO
2	B	1267	HIS
2	B	1536	PHE
2	D	834	GLN
2	D	1201	PRO
2	D	1536	PHE
2	F	834	GLN
2	F	1201	PRO
2	F	1270	LEU
2	F	1536	PHE
1	G	643	PRO
2	H	834	GLN
2	H	1196	ASN
2	H	1201	PRO
2	H	1264	ALA
2	H	1536	PHE
3	I	268	LEU
3	J	268	LEU
3	K	268	LEU
3	L	268	LEU
3	I	482	GLY
3	J	482	GLY
3	K	482	GLY
3	L	482	GLY
2	B	1517	PRO
2	D	1517	PRO
2	F	1517	PRO
2	H	1517	PRO
1	A	208	PRO
1	C	208	PRO
1	E	208	PRO
1	G	208	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	558/567 (98%)	549 (98%)	9 (2%)	55	69
1	C	558/567 (98%)	549 (98%)	9 (2%)	55	69
1	E	558/567 (98%)	549 (98%)	9 (2%)	55	69
1	G	558/567 (98%)	550 (99%)	8 (1%)	59	71
2	B	793/810 (98%)	769 (97%)	24 (3%)	36	57
2	D	790/810 (98%)	767 (97%)	23 (3%)	37	58
2	F	793/810 (98%)	772 (97%)	21 (3%)	40	60
2	H	793/810 (98%)	769 (97%)	24 (3%)	36	57
3	I	442/446 (99%)	430 (97%)	12 (3%)	39	60
3	J	442/446 (99%)	430 (97%)	12 (3%)	39	60
3	K	442/446 (99%)	430 (97%)	12 (3%)	39	60
3	L	442/446 (99%)	430 (97%)	12 (3%)	39	60
4	M	76/84 (90%)	73 (96%)	3 (4%)	28	52
4	N	76/84 (90%)	73 (96%)	3 (4%)	28	52
4	P	76/84 (90%)	73 (96%)	3 (4%)	28	52
4	Q	76/84 (90%)	73 (96%)	3 (4%)	28	52
All	All	7473/7628 (98%)	7286 (98%)	187 (2%)	42	62

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	81	ASN
1	A	144	ASN
1	A	155	GLN
1	A	289	VAL
1	A	365	VAL
1	A	398	LEU
1	A	404	THR
1	A	406	LYS
2	B	729	LEU
2	B	757	LYS
2	B	833	ARG
2	B	834	GLN
2	B	841	ARG
2	B	937	LYS
2	B	945	LEU

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Mol	Chain	Res	Type
2	B	953	GLU
2	B	960	LEU
2	B	978	LEU
2	B	1018	GLU
2	B	1196	ASN
2	B	1292	GLU
2	B	1334	LEU
2	B	1335	THR
2	B	1342	LYS
2	B	1361	THR
2	B	1433	GLU
2	B	1447	VAL
2	B	1520	ASP
2	B	1535	ASP
2	B	1536	PHE
2	B	1569	ARG
2	B	1637	PHE
1	C	31	VAL
1	C	81	ASN
1	C	144	ASN
1	C	155	GLN
1	C	289	VAL
1	C	365	VAL
1	C	398	LEU
1	C	404	THR
1	C	406	LYS
2	D	757	LYS
2	D	833	ARG
2	D	834	GLN
2	D	841	ARG
2	D	937	LYS
2	D	945	LEU
2	D	953	GLU
2	D	960	LEU
2	D	978	LEU
2	D	1018	GLU
2	D	1196	ASN
2	D	1292	GLU
2	D	1334	LEU
2	D	1335	THR
2	D	1342	LYS
2	D	1361	THR

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Mol	Chain	Res	Type
2	D	1433	GLU
2	D	1447	VAL
2	D	1520	ASP
2	D	1535	ASP
2	D	1536	PHE
2	D	1569	ARG
2	D	1637	PHE
1	E	31	VAL
1	E	81	ASN
1	E	144	ASN
1	E	155	GLN
1	E	289	VAL
1	E	365	VAL
1	E	398	LEU
1	E	404	THR
1	E	406	LYS
2	F	757	LYS
2	F	833	ARG
2	F	834	GLN
2	F	841	ARG
2	F	937	LYS
2	F	945	LEU
2	F	953	GLU
2	F	978	LEU
2	F	1018	GLU
2	F	1196	ASN
2	F	1268	GLN
2	F	1292	GLU
2	F	1334	LEU
2	F	1335	THR
2	F	1342	LYS
2	F	1433	GLU
2	F	1520	ASP
2	F	1535	ASP
2	F	1536	PHE
2	F	1569	ARG
2	F	1572	LEU
1	G	31	VAL
1	G	81	ASN
1	G	144	ASN
1	G	155	GLN
1	G	289	VAL

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Mol	Chain	Res	Type
1	G	398	LEU
1	G	404	THR
1	G	406	LYS
2	H	757	LYS
2	H	833	ARG
2	H	834	GLN
2	H	841	ARG
2	H	937	LYS
2	H	945	LEU
2	H	953	GLU
2	H	968	MET
2	H	969	THR
2	H	1018	GLU
2	H	1196	ASN
2	H	1267	HIS
2	H	1292	GLU
2	H	1334	LEU
2	H	1335	THR
2	H	1342	LYS
2	H	1433	GLU
2	H	1498	ILE
2	H	1499	GLN
2	H	1520	ASP
2	H	1535	ASP
2	H	1536	PHE
2	H	1569	ARG
2	H	1572	LEU
3	I	237	VAL
3	I	255	SER
3	I	322	HIS
3	I	368	ASN
3	I	381	ARG
3	I	423	ASN
3	I	429	LYS
3	I	446	GLU
3	I	540	LYS
3	I	654	ARG
3	I	702	ASN
3	I	703	GLN
3	J	237	VAL
3	J	255	SER
3	J	322	HIS

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Mol	Chain	Res	Type
3	J	368	ASN
3	J	381	ARG
3	J	423	ASN
3	J	429	LYS
3	J	446	GLU
3	J	540	LYS
3	J	654	ARG
3	J	702	ASN
3	J	703	GLN
3	K	237	VAL
3	K	255	SER
3	K	322	HIS
3	K	368	ASN
3	K	381	ARG
3	K	423	ASN
3	K	429	LYS
3	K	446	GLU
3	K	540	LYS
3	K	654	ARG
3	K	702	ASN
3	K	703	GLN
3	L	237	VAL
3	L	255	SER
3	L	322	HIS
3	L	368	ASN
3	L	381	ARG
3	L	423	ASN
3	L	429	LYS
3	L	446	GLU
3	L	540	LYS
3	L	654	ARG
3	L	702	ASN
3	L	703	GLN
4	M	11	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	69	GLN
4	P	71	GLN

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Mol	Chain	Res	Type
4	Q	11	GLN
4	Q	69	GLN
4	Q	71	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (269) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	104	GLN
1	A	144	ASN
1	A	155	GLN
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	332	GLN
1	A	334	HIS
1	A	370	GLN
1	A	380	GLN
1	A	390	ASN
1	A	414	GLN
1	A	490	GLN
1	A	558	GLN
1	A	567	HIS
1	A	587	ASN
1	A	634	GLN
1	A	639	GLN
2	B	738	ASN
2	B	752	ASN
2	B	762	ASN
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	860	HIS
2	B	896	HIS
2	B	897	HIS
2	B	980	HIS
2	B	1069	ASN
2	B	1076	GLN
2	B	1114	ASN
2	B	1130	GLN
2	B	1139	GLN
2	B	1141	ASN

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Mol	Chain	Res	Type
2	B	1160	ASN
2	B	1196	ASN
2	B	1204	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1333	GLN
2	B	1337	ASN
2	B	1401	ASN
2	B	1431	HIS
2	B	1451	GLN
2	B	1462	ASN
2	B	1559	GLN
2	B	1579	HIS
2	B	1608	HIS
2	B	1620	ASN
1	C	10	ASN
1	C	60	HIS
1	C	87	GLN
1	C	104	GLN
1	C	132	HIS
1	C	144	ASN
1	C	155	GLN
1	C	161	GLN
1	C	162	ASN
1	C	163	GLN
1	C	356	ASN
1	C	370	GLN
1	C	380	GLN
1	C	390	ASN
1	C	414	GLN
1	C	490	GLN
1	C	558	GLN
1	C	567	HIS
1	C	587	ASN
1	C	634	GLN
1	C	639	GLN
2	D	738	ASN
2	D	752	ASN
2	D	762	ASN
2	D	770	ASN
2	D	820	ASN
2	D	834	GLN

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Mol	Chain	Res	Type
2	D	860	HIS
2	D	897	HIS
2	D	980	HIS
2	D	1069	ASN
2	D	1076	GLN
2	D	1097	GLN
2	D	1114	ASN
2	D	1130	GLN
2	D	1141	ASN
2	D	1160	ASN
2	D	1196	ASN
2	D	1204	GLN
2	D	1267	HIS
2	D	1277	GLN
2	D	1333	GLN
2	D	1337	ASN
2	D	1401	ASN
2	D	1431	HIS
2	D	1451	GLN
2	D	1462	ASN
2	D	1559	GLN
2	D	1579	HIS
2	D	1608	HIS
2	D	1620	ASN
1	E	60	HIS
1	E	87	GLN
1	E	104	GLN
1	E	132	HIS
1	E	144	ASN
1	E	155	GLN
1	E	161	GLN
1	E	162	ASN
1	E	163	GLN
1	E	332	GLN
1	E	334	HIS
1	E	356	ASN
1	E	370	GLN
1	E	380	GLN
1	E	390	ASN
1	E	414	GLN
1	E	450	ASN
1	E	490	GLN

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Mol	Chain	Res	Type
1	E	558	GLN
1	E	567	HIS
1	E	639	GLN
2	F	738	ASN
2	F	752	ASN
2	F	762	ASN
2	F	770	ASN
2	F	820	ASN
2	F	834	GLN
2	F	860	HIS
2	F	897	HIS
2	F	980	HIS
2	F	1069	ASN
2	F	1076	GLN
2	F	1097	GLN
2	F	1114	ASN
2	F	1130	GLN
2	F	1141	ASN
2	F	1160	ASN
2	F	1196	ASN
2	F	1204	GLN
2	F	1248	GLN
2	F	1267	HIS
2	F	1277	GLN
2	F	1333	GLN
2	F	1337	ASN
2	F	1360	ASN
2	F	1401	ASN
2	F	1431	HIS
2	F	1443	GLN
2	F	1451	GLN
2	F	1462	ASN
2	F	1559	GLN
2	F	1579	HIS
2	F	1608	HIS
2	F	1620	ASN
2	F	1641	ASN
1	G	60	HIS
1	G	87	GLN
1	G	104	GLN
1	G	132	HIS
1	G	144	ASN

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Mol	Chain	Res	Type
1	G	155	GLN
1	G	161	GLN
1	G	162	ASN
1	G	163	GLN
1	G	178	ASN
1	G	356	ASN
1	G	370	GLN
1	G	380	GLN
1	G	390	ASN
1	G	414	GLN
1	G	490	GLN
1	G	558	GLN
1	G	567	HIS
1	G	587	ASN
1	G	634	GLN
1	G	639	GLN
2	H	738	ASN
2	H	752	ASN
2	H	762	ASN
2	H	770	ASN
2	H	820	ASN
2	H	834	GLN
2	H	860	HIS
2	H	896	HIS
2	H	897	HIS
2	H	1277	GLN
2	H	1333	GLN
2	H	1337	ASN
2	H	1360	ASN
2	H	1401	ASN
2	H	1431	HIS
2	H	1443	GLN
2	H	1451	GLN
2	H	1462	ASN
2	H	1559	GLN
2	H	1579	HIS
2	H	1608	HIS
2	H	1620	ASN
2	H	1641	ASN
3	I	270	ASN
3	I	368	ASN
3	I	392	ASN

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Mol	Chain	Res	Type
3	I	411	GLN
3	I	423	ASN
3	I	466	HIS
3	I	531	HIS
3	I	533	ASN
3	I	591	GLN
3	I	681	HIS
3	I	703	GLN
3	J	270	ASN
3	J	367	HIS
3	J	368	ASN
3	J	392	ASN
3	J	411	GLN
3	J	415	ASN
3	J	423	ASN
3	J	435	ASN
3	J	466	HIS
3	J	531	HIS
3	J	533	ASN
3	J	591	GLN
3	J	681	HIS
3	J	703	GLN
3	K	270	ASN
3	K	329	ASN
3	K	368	ASN
3	K	392	ASN
3	K	411	GLN
3	K	423	ASN
3	K	435	ASN
3	K	466	HIS
3	K	531	HIS
3	K	533	ASN
3	K	591	GLN
3	K	681	HIS
3	K	703	GLN
3	L	270	ASN
3	L	368	ASN
3	L	392	ASN
3	L	411	GLN
3	L	423	ASN
3	L	466	HIS
3	L	531	HIS

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Mol	Chain	Res	Type
3	L	533	ASN
3	L	591	GLN
3	L	681	HIS
3	L	703	GLN
4	M	11	GLN
4	M	27	ASN
4	M	49	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	27	ASN
4	N	49	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	27	ASN
4	P	49	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	27	ASN
4	Q	49	GLN
4	Q	69	GLN
4	Q	71	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

52 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	$\# Z > 2$
5	NAG	O	1	1,5	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
5	NAG	O	2	5	14,14,15	0.64	0	17,19,21	1.80	4 (23%)
5	BMA	O	3	5	11,11,12	0.55	0	15,15,17	1.23	2 (13%)
5	BMA	O	4	5	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
5	NAG	R	1	2,5	14,14,15	0.54	0	17,19,21	1.10	2 (11%)
5	NAG	R	2	5	14,14,15	0.53	0	17,19,21	2.21	2 (11%)
5	BMA	R	3	5	11,11,12	0.93	0	15,15,17	1.82	4 (26%)
5	BMA	R	4	5	11,11,12	0.71	0	15,15,17	0.68	0
6	NAG	S	1	1,6	14,14,15	0.60	0	17,19,21	1.17	2 (11%)
6	NAG	S	2	6	14,14,15	0.66	0	17,19,21	1.13	2 (11%)
6	BMA	S	3	6	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
6	BMA	S	4	6	11,11,12	0.74	0	15,15,17	1.45	3 (20%)
6	BMA	S	5	6	11,11,12	0.65	0	15,15,17	1.52	3 (20%)
5	NAG	T	1	2,5	14,14,15	0.49	0	17,19,21	0.80	0
5	NAG	T	2	5	14,14,15	0.58	0	17,19,21	1.05	2 (11%)
5	BMA	T	3	5	11,11,12	0.62	0	15,15,17	1.24	2 (13%)
5	BMA	T	4	5	11,11,12	0.65	0	15,15,17	1.06	1 (6%)
5	NAG	U	1	1,5	14,14,15	0.55	0	17,19,21	0.86	0
5	NAG	U	2	5	14,14,15	0.60	0	17,19,21	1.16	2 (11%)
5	BMA	U	3	5	11,11,12	0.68	0	15,15,17	0.98	1 (6%)
5	BMA	U	4	5	11,11,12	0.91	1 (9%)	15,15,17	1.53	2 (13%)
7	NAG	V	1	2,7	14,14,15	0.39	0	17,19,21	1.27	3 (17%)
7	NAG	V	2	7	14,14,15	0.45	0	17,19,21	1.61	3 (17%)
7	BMA	V	3	7	11,11,12	0.57	0	15,15,17	1.33	3 (20%)
7	BMA	V	4	7	11,11,12	0.98	1 (9%)	15,15,17	1.56	4 (26%)
7	BMA	V	5	7	11,11,12	0.65	0	15,15,17	1.59	4 (26%)
7	BMA	V	6	7	11,11,12	0.69	0	15,15,17	0.89	0
6	NAG	W	1	1,6	14,14,15	0.43	0	17,19,21	1.16	1 (5%)
6	NAG	W	2	6	14,14,15	0.52	0	17,19,21	2.18	4 (23%)
6	BMA	W	3	6	11,11,12	0.51	0	15,15,17	2.61	6 (40%)
6	BMA	W	4	6	11,11,12	0.55	0	15,15,17	4.11	6 (40%)
6	BMA	W	5	6	11,11,12	0.63	0	15,15,17	1.14	1 (6%)
8	NAG	X	1	2,8	14,14,15	0.58	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	X	2	8	14,14,15	0.47	0	17,19,21	0.75	0
8	MAN	X	3	8	11,11,12	0.77	0	15,15,17	1.21	1 (6%)
8	MAN	X	4	8	11,11,12	0.75	0	15,15,17	0.92	1 (6%)
9	NAG	Y	1	9,3	14,14,15	0.55	0	17,19,21	1.00	2 (11%)
9	NAG	Y	2	9	14,14,15	0.62	0	17,19,21	1.02	1 (5%)
9	MAN	Y	3	9	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
10	NAG	Z	1	3,10	14,14,15	0.53	0	17,19,21	1.11	2 (11%)
10	NAG	Z	2	10	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
9	NAG	a	1	9,3	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
9	NAG	a	2	9	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
9	MAN	a	3	9	11,11,12	0.63	0	15,15,17	0.89	1 (6%)
11	NAG	b	1	11,3	14,14,15	0.61	0	17,19,21	1.03	2 (11%)
11	NAG	b	2	11	14,14,15	0.69	0	17,19,21	1.37	3 (17%)
11	MAN	b	3	11	11,11,12	0.56	0	15,15,17	1.69	5 (33%)
11	MAN	b	4	11	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
11	MAN	b	5	11	11,11,12	0.73	0	15,15,17	1.49	2 (13%)
12	NAG	c	1	3,12	14,14,15	0.48	0	17,19,21	0.87	0
12	NAG	c	2	12	14,14,15	0.61	0	17,19,21	1.05	1 (5%)
12	BMA	c	3	12	11,11,12	0.63	0	15,15,17	0.81	1 (6%)

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
5	NAG	O	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	BMA	O	4	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	BMA	R	4	5	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	S	4	6	-	0/2/19/22	0/1/1/1
6	BMA	S	5	6	-	0/2/19/22	0/1/1/1
5	NAG	T	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	BMA	T	4	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
5	BMA	U	4	5	-	0/2/19/22	0/1/1/1
7	NAG	V	1	2,7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	V	2	7	-	4/6/23/26	0/1/1/1
7	BMA	V	3	7	-	2/2/19/22	0/1/1/1
7	BMA	V	4	7	-	2/2/19/22	0/1/1/1
7	BMA	V	5	7	-	1/2/19/22	0/1/1/1
7	BMA	V	6	7	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	BMA	W	4	6	-	0/2/19/22	0/1/1/1
6	BMA	W	5	6	-	0/2/19/22	0/1/1/1
8	NAG	X	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	MAN	X	3	8	1/1/4/5	2/2/19/22	0/1/1/1
8	MAN	X	4	8	1/1/4/5	2/2/19/22	0/1/1/1
9	NAG	Y	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	MAN	Y	3	9	1/1/4/5	0/2/19/22	0/1/1/1
10	NAG	Z	1	3,10	1/1/5/7	3/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
9	NAG	a	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	MAN	a	3	9	1/1/4/5	0/2/19/22	0/1/1/1
11	NAG	b	1	11,3	1/1/5/7	5/6/23/26	0/1/1/1
11	NAG	b	2	11	-	4/6/23/26	0/1/1/1
11	MAN	b	3	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	b	4	11	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	b	5	11	1/1/4/5	2/2/19/22	0/1/1/1
12	NAG	c	1	3,12	-	3/6/23/26	0/1/1/1
12	NAG	c	2	12	-	2/6/23/26	0/1/1/1
12	BMA	c	3	12	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	4	BMA	O5-C1	-2.21	1.40	1.43
7	V	4	BMA	O5-C1	-2.09	1.40	1.43

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	4	BMA	C1-C2-C3	-9.00	96.54	109.64
5	R	2	NAG	C1-O5-C5	7.17	121.79	112.19
6	W	4	BMA	C1-O5-C5	-7.05	102.74	112.19
6	W	4	BMA	C3-C4-C5	-6.98	97.58	110.23
6	W	2	NAG	C1-O5-C5	6.03	120.26	112.19
6	W	4	BMA	O3-C3-C4	6.01	124.55	110.38
6	W	4	BMA	O5-C5-C6	5.29	117.96	107.66
6	W	3	BMA	O5-C5-C6	5.09	117.57	107.66
5	O	2	NAG	C4-C3-C2	4.96	118.29	111.02
6	W	3	BMA	C1-C2-C3	-4.64	102.89	109.64
5	U	4	BMA	C1-O5-C5	-4.50	106.16	112.19
6	W	3	BMA	C6-C5-C4	-4.17	102.77	113.02
6	W	3	BMA	C1-O5-C5	-4.07	106.73	112.19
5	R	2	NAG	O5-C1-C2	3.87	117.27	111.29
5	R	3	BMA	C1-O5-C5	-3.78	107.13	112.19
5	R	3	BMA	C1-C2-C3	3.76	115.13	109.64
5	T	3	BMA	C1-O5-C5	-3.76	107.14	112.19
11	b	3	MAN	C1-O5-C5	-3.75	107.16	112.19
7	V	5	BMA	C1-C2-C3	-3.74	104.20	109.64
11	b	2	NAG	C4-C3-C2	3.67	116.40	111.02
11	b	5	MAN	C3-C4-C5	3.66	116.87	110.23
7	V	2	NAG	C1-O5-C5	3.57	116.97	112.19
6	S	5	BMA	C1-C2-C3	-3.56	104.46	109.64
6	W	2	NAG	C4-C3-C2	-3.48	105.92	111.02
5	O	2	NAG	C1-O5-C5	3.32	116.63	112.19
8	X	3	MAN	C1-C2-C3	3.31	114.46	109.64
7	V	2	NAG	C4-C3-C2	-3.30	106.18	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	4	BMA	C1-C2-C3	3.29	114.44	109.64
6	S	4	BMA	O3-C3-C4	-3.22	102.78	110.38
6	W	2	NAG	O4-C4-C5	3.22	117.25	109.32
11	b	3	MAN	O5-C5-C6	3.17	113.83	107.66
5	O	3	BMA	C1-O5-C5	-3.13	107.99	112.19
6	W	3	BMA	C3-C4-C5	3.10	115.85	110.23
6	S	4	BMA	C3-C4-C5	3.02	115.70	110.23
5	R	1	NAG	C1-O5-C5	2.97	116.17	112.19
9	Y	3	MAN	C1-O5-C5	-2.94	108.24	112.19
6	S	1	NAG	C3-C4-C5	2.93	115.54	110.23
7	V	4	BMA	C2-C3-C4	2.87	115.91	110.86
6	W	1	NAG	C4-C3-C2	2.82	115.15	111.02
7	V	2	NAG	O4-C4-C3	2.75	116.87	110.38
11	b	2	NAG	C3-C4-C5	2.74	115.19	110.23
6	W	5	BMA	C1-C2-C3	-2.73	105.68	109.64
6	S	5	BMA	C1-O5-C5	-2.72	108.54	112.19
5	O	3	BMA	O5-C5-C6	2.69	112.90	107.66
11	b	1	NAG	C3-C4-C5	2.66	115.05	110.23
9	a	1	NAG	C1-O5-C5	2.65	115.73	112.19
12	c	2	NAG	C4-C3-C2	2.64	114.89	111.02
6	S	3	BMA	C1-O5-C5	-2.58	108.72	112.19
9	a	3	MAN	C1-O5-C5	-2.58	108.73	112.19
9	a	2	NAG	C4-C3-C2	2.58	114.79	111.02
7	V	5	BMA	C3-C4-C5	2.57	114.89	110.23
7	V	4	BMA	C1-O5-C5	-2.56	108.75	112.19
5	O	2	NAG	C3-C4-C5	2.56	114.87	110.23
9	Y	2	NAG	C4-C3-C2	2.55	114.76	111.02
11	b	3	MAN	O3-C3-C2	2.55	115.25	110.05
10	Z	1	NAG	C3-C4-C5	2.54	114.84	110.23
7	V	1	NAG	O5-C1-C2	-2.53	107.37	111.29
6	W	2	NAG	O5-C1-C2	2.53	115.21	111.29
5	O	4	BMA	C1-C2-C3	-2.50	106.00	109.64
6	W	3	BMA	O6-C6-C5	2.50	119.86	111.33
5	U	2	NAG	C1-O5-C5	2.49	115.53	112.19
10	Z	2	NAG	C1-O5-C5	2.49	115.53	112.19
7	V	5	BMA	C1-O5-C5	-2.48	108.87	112.19
5	U	2	NAG	O5-C1-C2	2.47	115.11	111.29
6	S	4	BMA	C1-O5-C5	-2.47	108.88	112.19
5	U	3	BMA	C1-O5-C5	-2.44	108.92	112.19
10	Z	1	NAG	C4-C3-C2	2.43	114.57	111.02
5	U	4	BMA	C1-C2-C3	-2.41	106.13	109.64
8	X	4	MAN	C1-O5-C5	-2.36	109.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	3	BMA	O5-C1-C2	-2.36	105.17	110.79
6	S	5	BMA	C3-C4-C5	2.35	114.50	110.23
5	R	3	BMA	C2-C3-C4	2.34	114.97	110.86
5	T	4	BMA	C1-C2-C3	-2.33	106.25	109.64
11	b	3	MAN	C1-C2-C3	-2.32	106.26	109.64
6	S	1	NAG	C1-O5-C5	2.32	115.30	112.19
5	T	2	NAG	C1-O5-C5	2.32	115.29	112.19
6	S	2	NAG	C4-C3-C2	2.31	114.41	111.02
7	V	3	BMA	C2-C3-C4	-2.30	106.81	110.86
7	V	1	NAG	O4-C4-C5	2.30	114.99	109.32
5	R	3	BMA	O5-C5-C4	-2.28	105.29	110.83
5	O	2	NAG	O4-C4-C3	-2.24	105.10	110.38
7	V	1	NAG	C4-C3-C2	-2.21	107.77	111.02
7	V	5	BMA	O5-C1-C2	-2.20	105.53	110.79
5	T	3	BMA	O5-C5-C6	2.19	111.93	107.66
9	Y	1	NAG	C1-O5-C5	2.18	115.11	112.19
12	c	3	BMA	C1-O5-C5	-2.17	109.27	112.19
9	Y	1	NAG	C3-C4-C5	2.14	114.11	110.23
6	S	2	NAG	O5-C1-C2	2.13	114.58	111.29
11	b	5	MAN	C6-C5-C4	-2.12	107.81	113.02
7	V	4	BMA	C3-C4-C5	2.09	114.02	110.23
5	R	1	NAG	C3-C4-C5	2.07	113.99	110.23
11	b	4	MAN	C1-O5-C5	2.07	114.96	112.19
11	b	3	MAN	C2-C3-C4	-2.05	107.26	110.86
11	b	4	MAN	C3-C4-C5	2.04	113.94	110.23
6	W	4	BMA	O3-C3-C2	2.03	114.21	110.05
5	O	4	BMA	O5-C1-C2	-2.03	105.94	110.79
7	V	3	BMA	C6-C5-C4	-2.03	108.03	113.02
5	T	2	NAG	C4-C3-C2	2.03	114.00	111.02
11	b	1	NAG	C4-C3-C2	2.02	113.98	111.02
5	O	1	NAG	C1-O5-C5	2.02	114.89	112.19
11	b	2	NAG	O4-C4-C3	-2.02	105.62	110.38

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	O	1	NAG	C1
7	V	1	NAG	C1
8	X	3	MAN	C1
8	X	4	MAN	C1
9	Y	3	MAN	C1
9	a	3	MAN	C1

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Mol	Chain	Res	Type	Atom
10	Z	1	NAG	C1
11	b	1	NAG	C1
11	b	3	MAN	C1
11	b	4	MAN	C1
11	b	5	MAN	C1

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C1-C2-N2-C7
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C1-C2-N2-C7
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
6	S	1	NAG	C1-C2-N2-C7
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C1-C2-N2-C7
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
7	V	1	NAG	C1-C2-N2-C7
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
8	X	1	NAG	C3-C2-N2-C7
8	X	1	NAG	C8-C7-N2-C2
8	X	1	NAG	O7-C7-N2-C2
9	Y	1	NAG	C1-C2-N2-C7
9	a	1	NAG	C1-C2-N2-C7
10	Z	1	NAG	C1-C2-N2-C7
11	b	1	NAG	C1-C2-N2-C7
12	c	1	NAG	C1-C2-N2-C7
12	c	1	NAG	O7-C7-N2-C2
12	c	2	NAG	C8-C7-N2-C2
9	Y	2	NAG	C8-C7-N2-C2
9	a	2	NAG	C8-C7-N2-C2
12	c	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
12	c	2	NAG	O7-C7-N2-C2
5	U	3	BMA	O5-C5-C6-O6
9	Y	1	NAG	C8-C7-N2-C2
9	Y	1	NAG	O7-C7-N2-C2
9	Y	2	NAG	O7-C7-N2-C2
9	a	2	NAG	O7-C7-N2-C2
10	Z	1	NAG	C8-C7-N2-C2
10	Z	1	NAG	O7-C7-N2-C2
7	V	4	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
7	V	3	BMA	O5-C5-C6-O6
11	b	2	NAG	O5-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
11	b	2	NAG	C4-C5-C6-O6
5	U	3	BMA	C4-C5-C6-O6
5	O	1	NAG	C8-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
11	b	1	NAG	C8-C7-N2-C2
6	S	3	BMA	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
11	b	5	MAN	C4-C5-C6-O6
5	O	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
6	W	2	NAG	C8-C7-N2-C2
6	W	2	NAG	O7-C7-N2-C2
7	V	2	NAG	C8-C7-N2-C2
7	V	2	NAG	O7-C7-N2-C2
8	X	2	NAG	C8-C7-N2-C2
8	X	2	NAG	O7-C7-N2-C2
9	a	1	NAG	C8-C7-N2-C2
10	Z	2	NAG	C8-C7-N2-C2
10	Z	2	NAG	O7-C7-N2-C2
11	b	1	NAG	O7-C7-N2-C2
11	b	2	NAG	C8-C7-N2-C2
11	b	2	NAG	O7-C7-N2-C2
5	O	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	V	3	BMA	C4-C5-C6-O6
9	a	1	NAG	O7-C7-N2-C2
6	S	3	BMA	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
11	b	5	MAN	O5-C5-C6-O6
7	V	4	BMA	C4-C5-C6-O6
8	X	3	MAN	O5-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
8	X	3	MAN	C4-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
8	X	4	MAN	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
8	X	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
11	b	1	NAG	C4-C5-C6-O6
7	V	5	BMA	C4-C5-C6-O6
11	b	1	NAG	O5-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 25 short contacts:

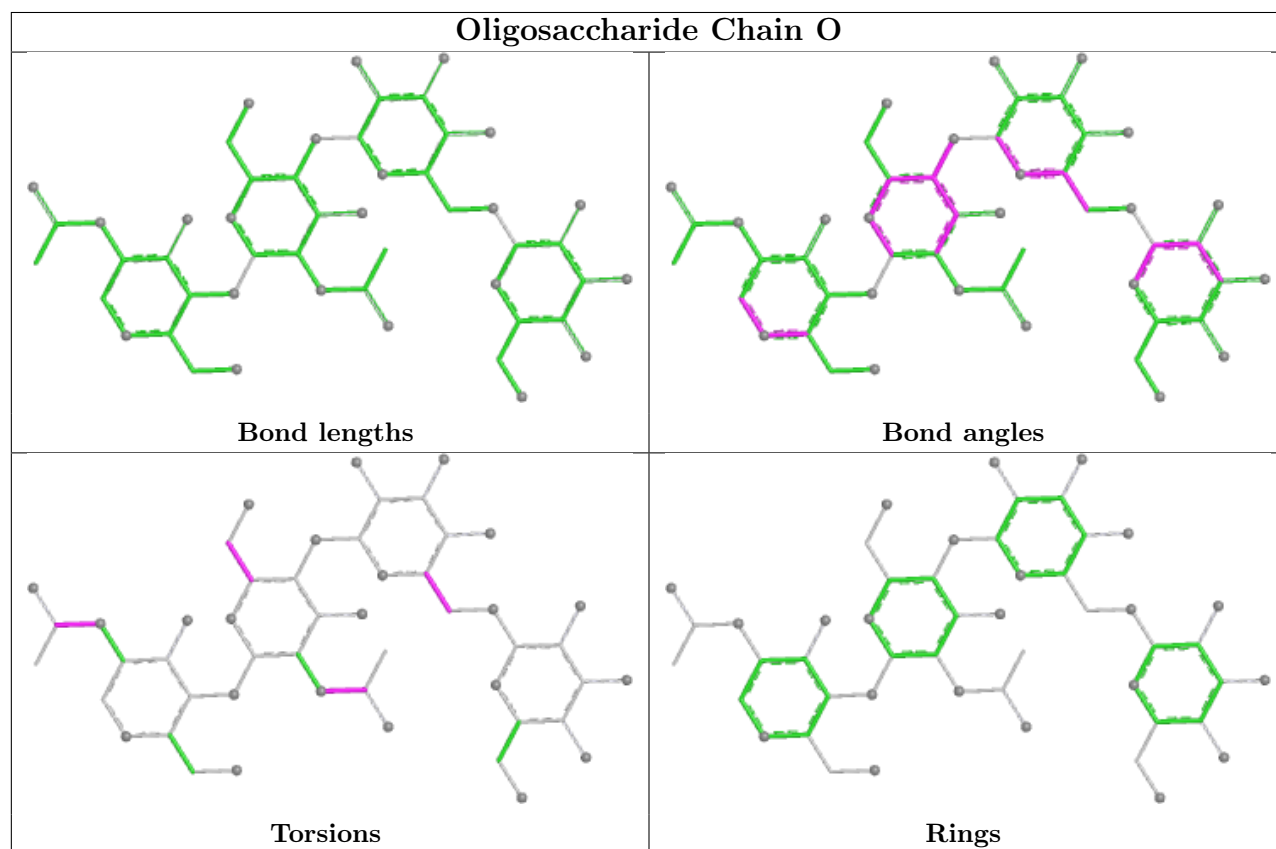
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1	NAG	1	0
6	W	3	BMA	2	0
7	V	4	BMA	2	0
6	S	1	NAG	1	0
11	b	5	MAN	1	0
8	X	4	MAN	1	0
8	X	3	MAN	1	0
5	U	2	NAG	1	0
7	V	6	BMA	1	0
5	U	1	NAG	2	0
5	U	3	BMA	1	0
9	a	2	NAG	2	0
11	b	1	NAG	3	0
9	a	1	NAG	1	0
11	b	4	MAN	1	0
6	W	1	NAG	1	0
5	T	2	NAG	1	0

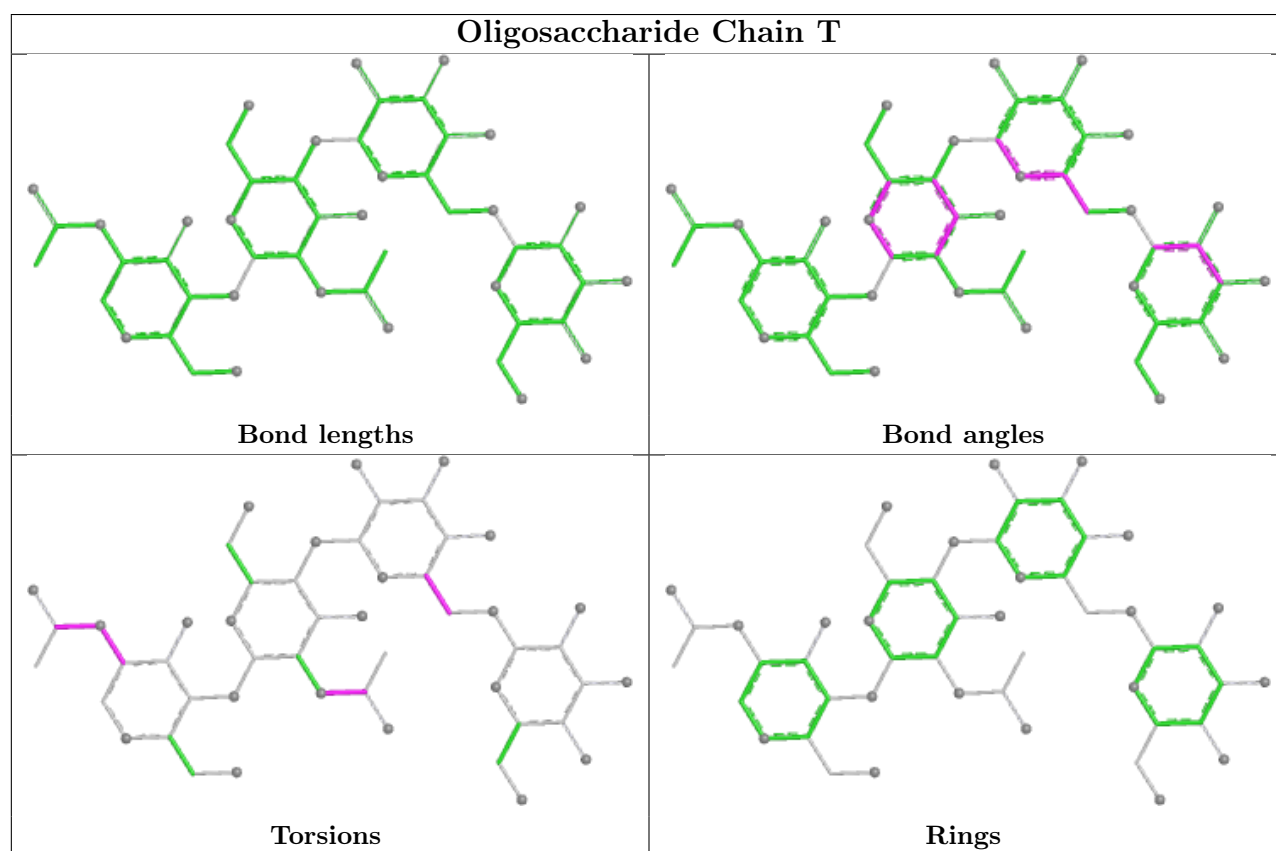
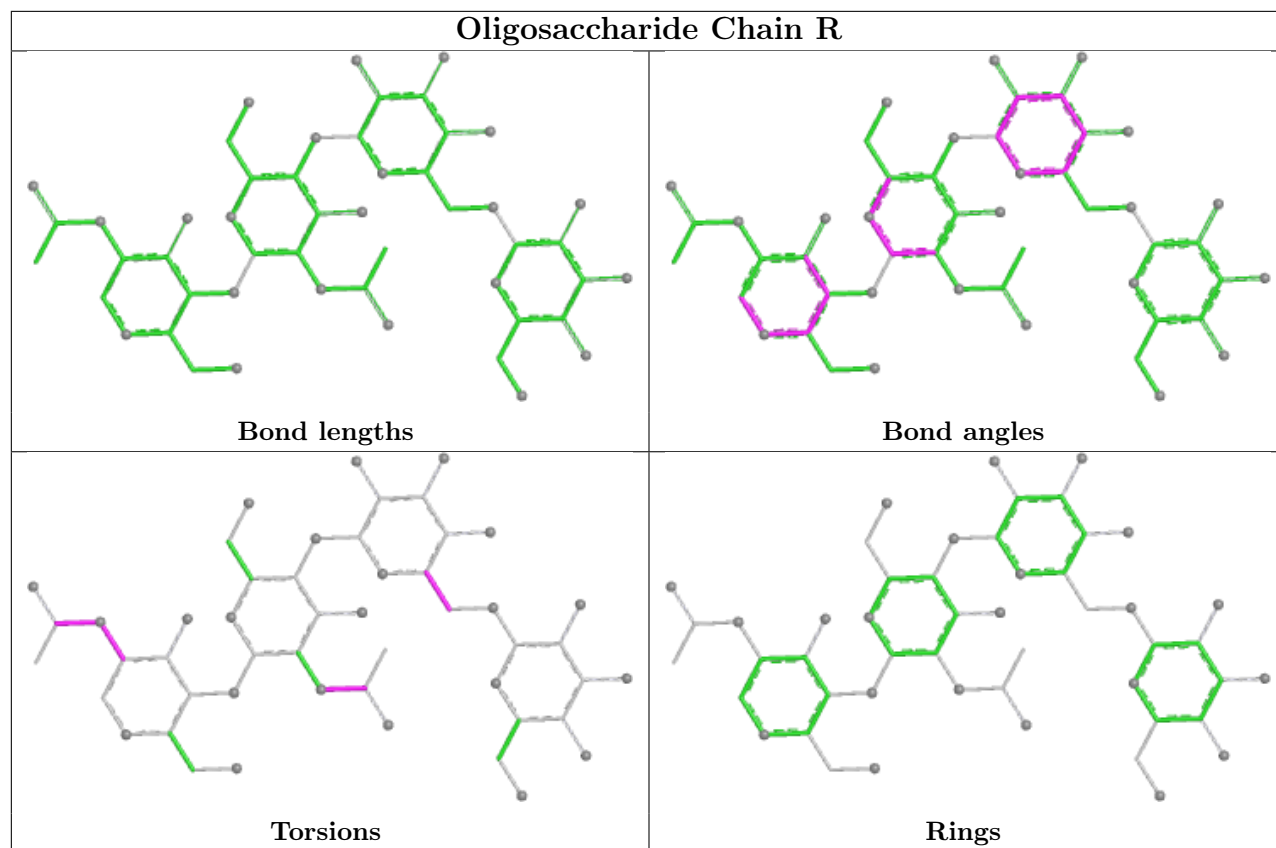
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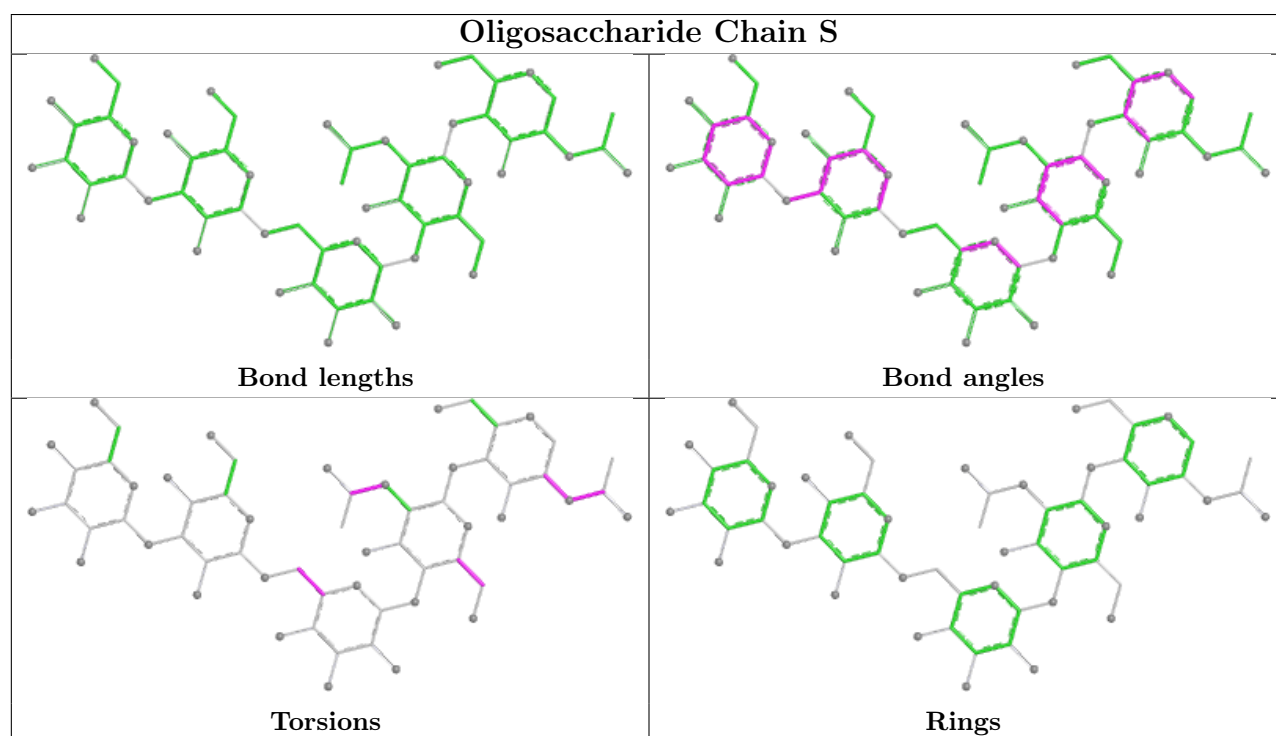
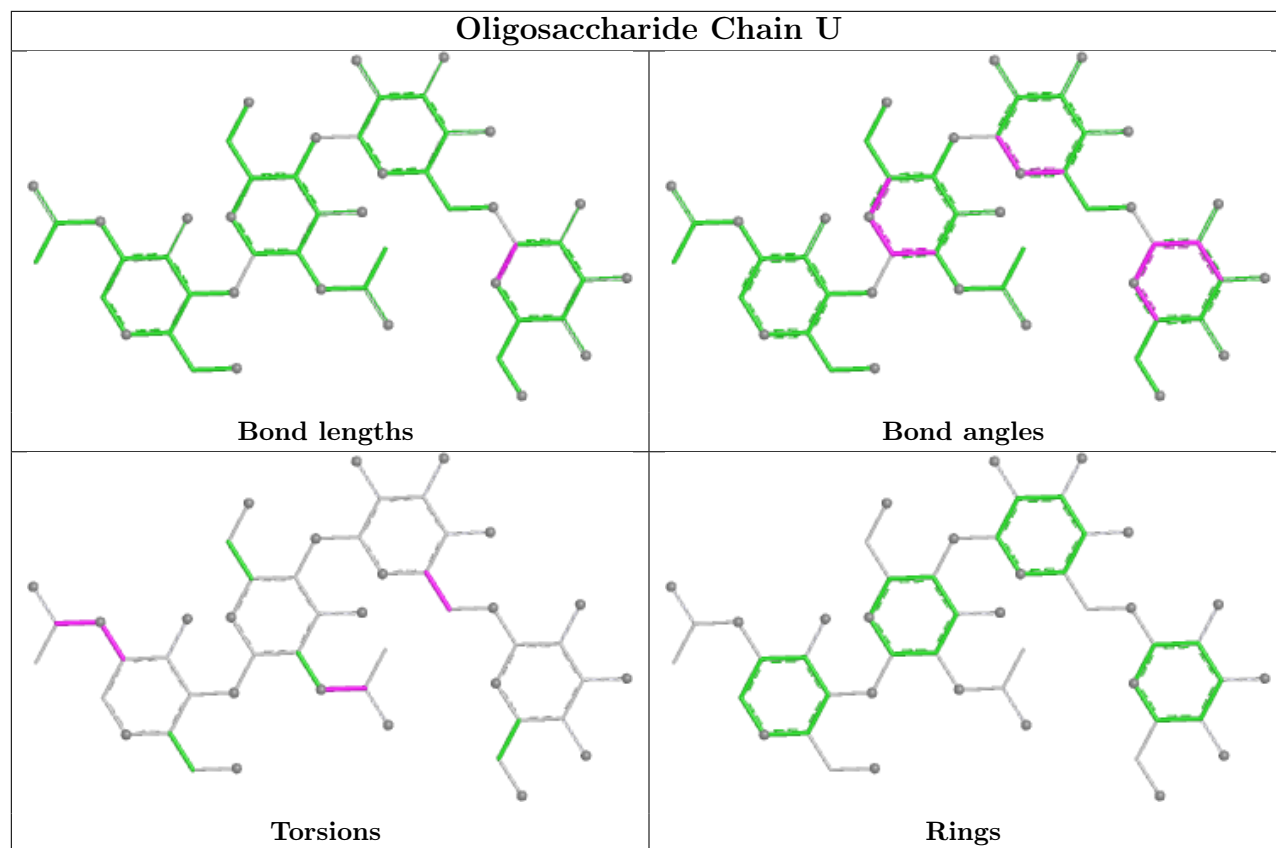
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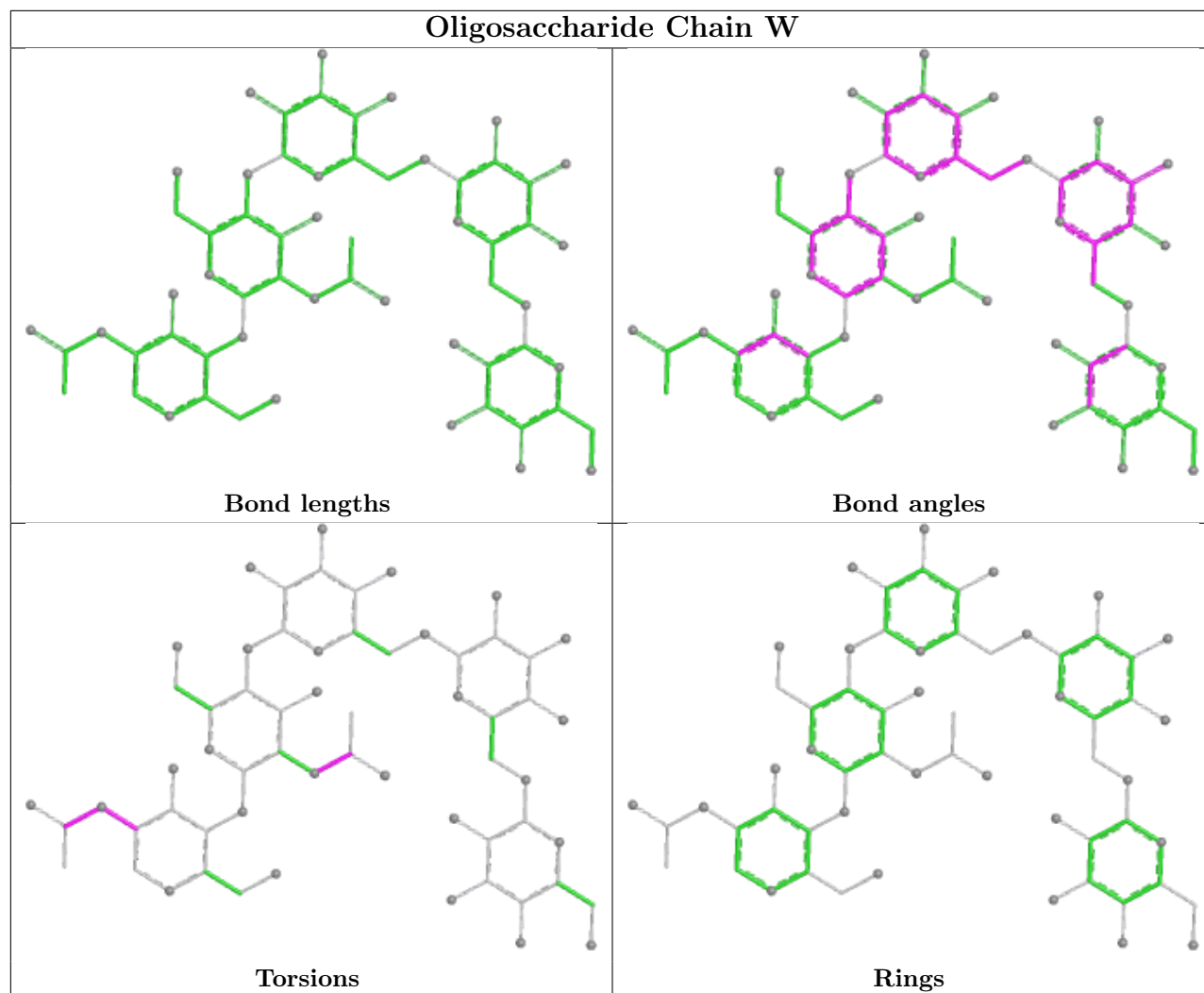
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	2	NAG	1	0
11	b	3	MAN	2	0
5	T	1	NAG	1	0
6	W	4	BMA	2	0
7	V	3	BMA	1	0
9	Y	1	NAG	1	0
11	b	2	NAG	1	0
5	O	2	NAG	1	0
9	Y	2	NAG	2	0
8	X	2	NAG	1	0
6	W	2	NAG	3	0
5	O	1	NAG	1	0
5	U	4	BMA	1	0

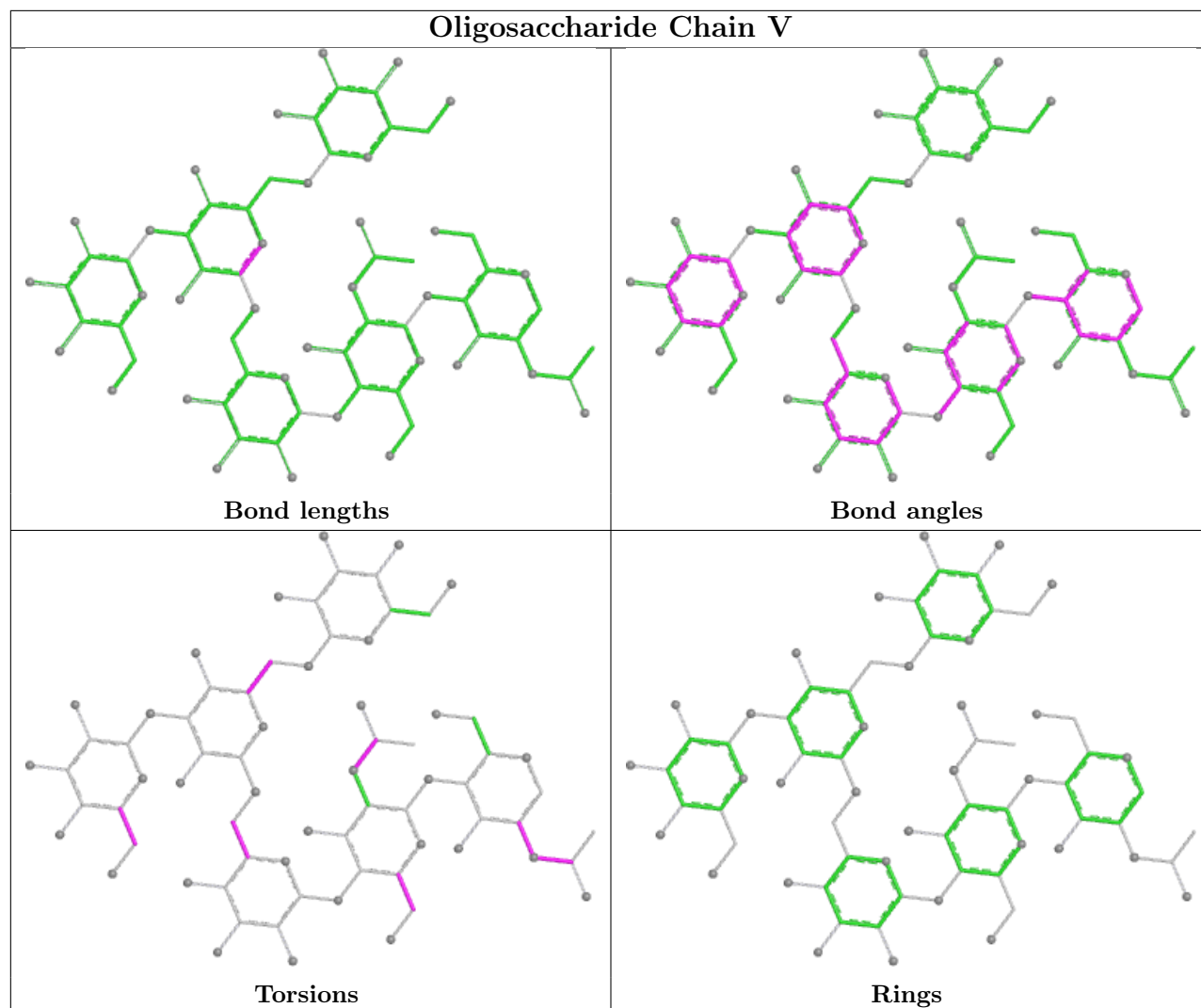
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

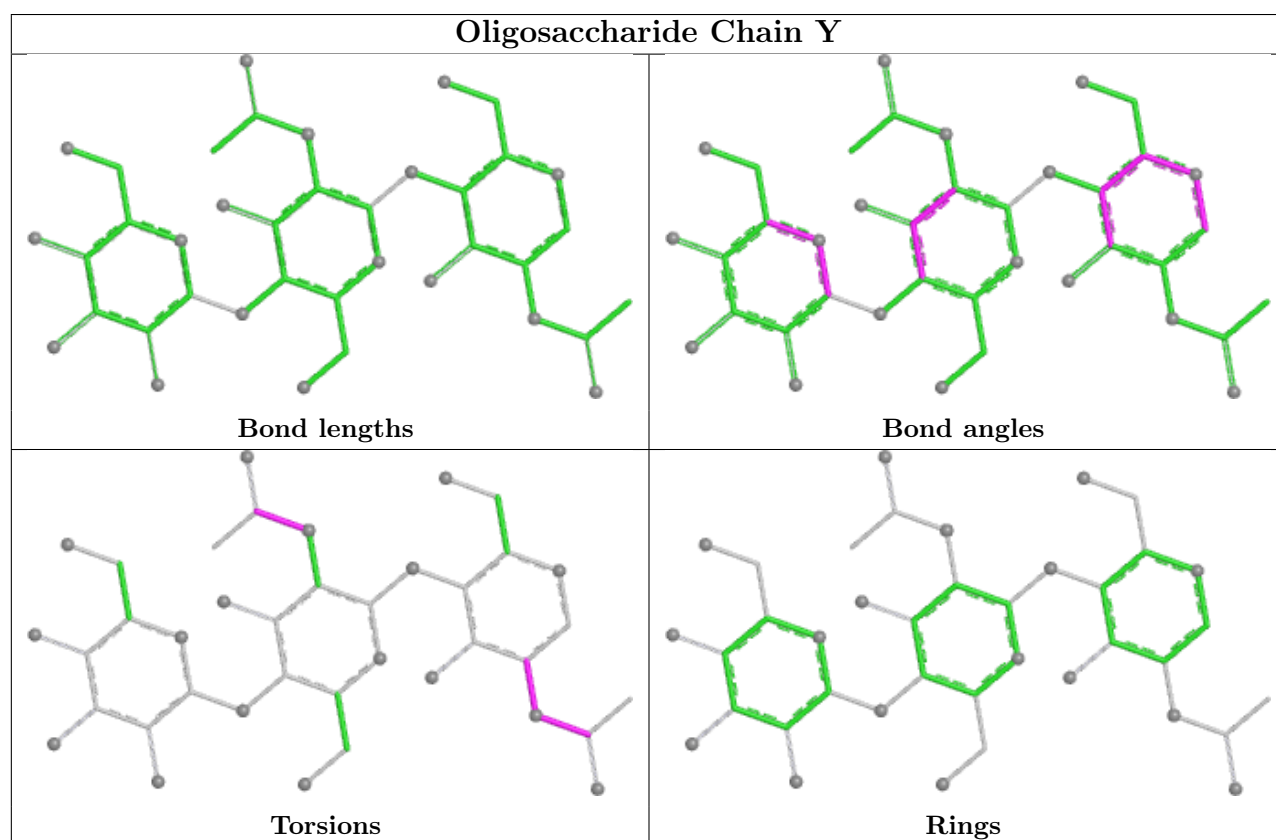
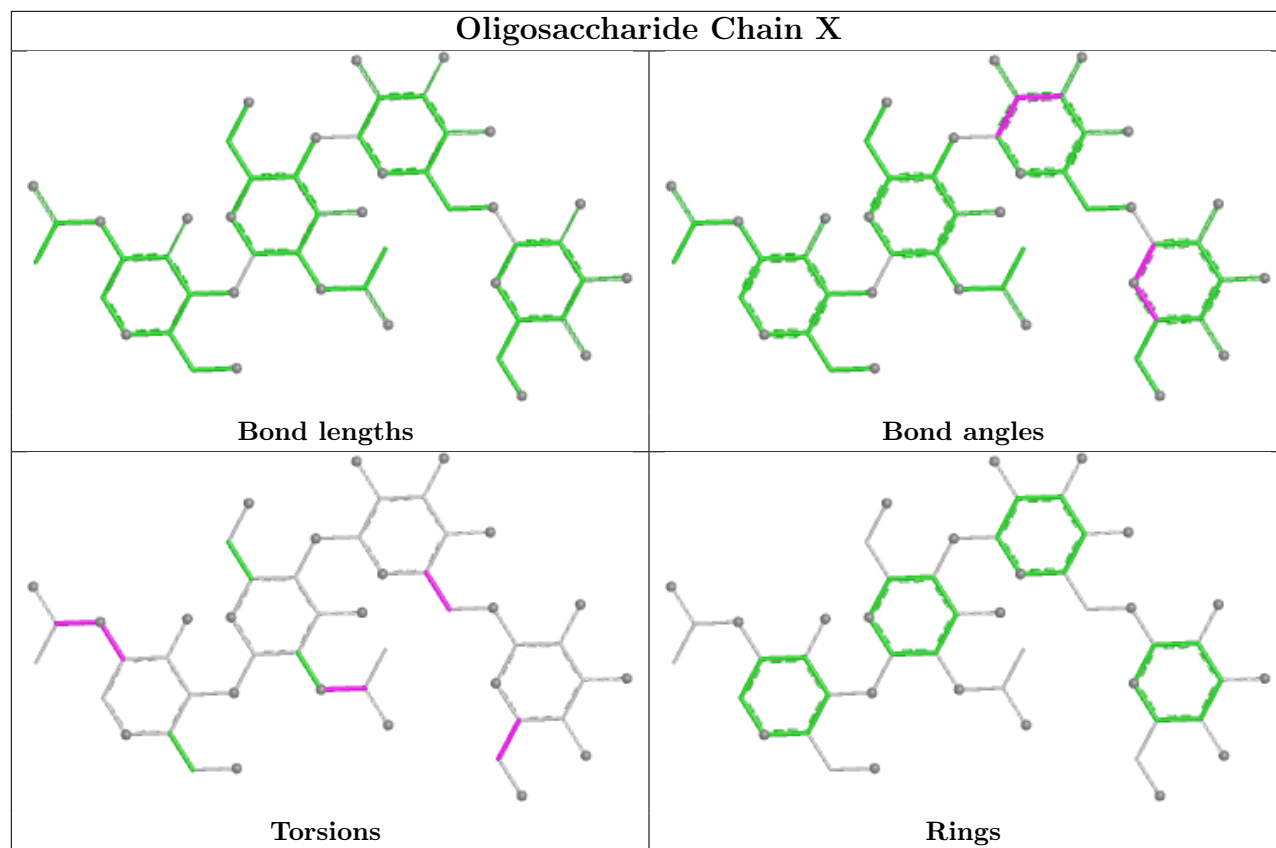


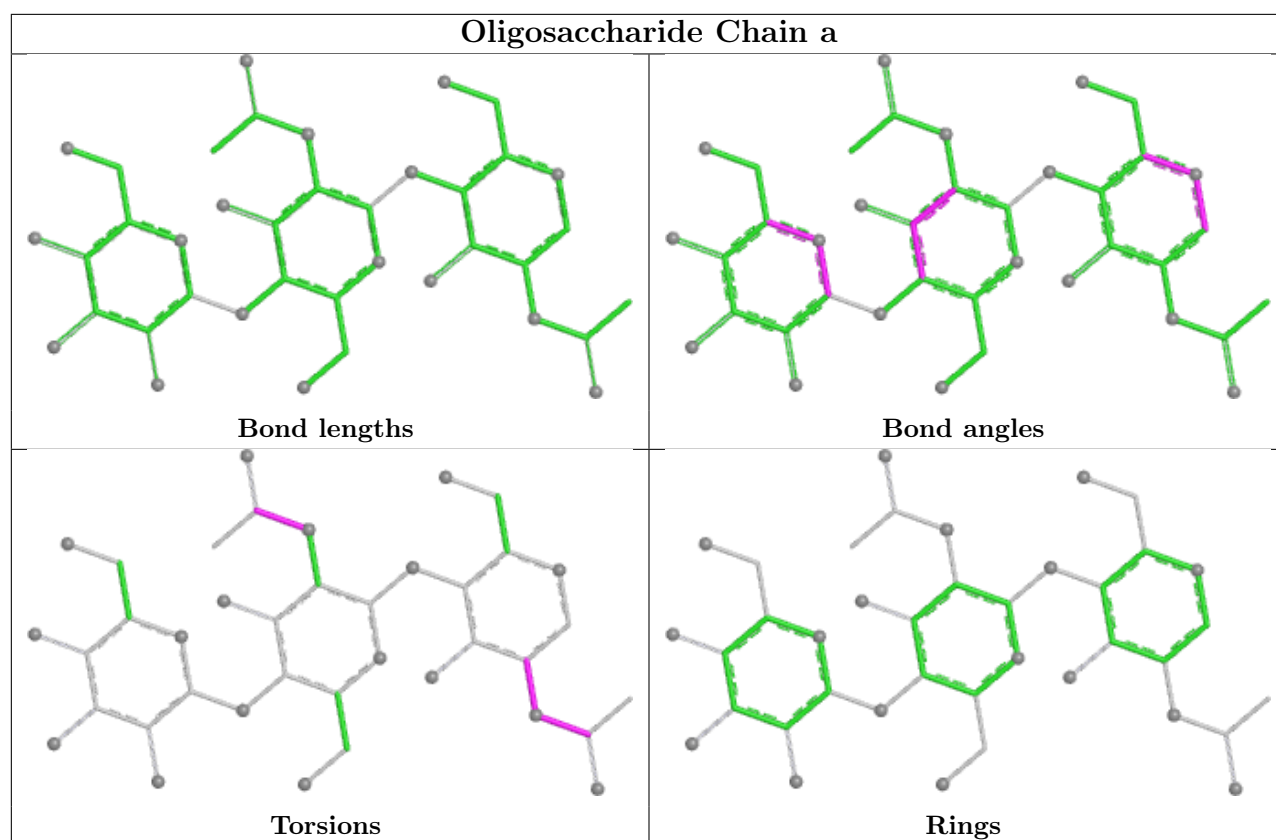


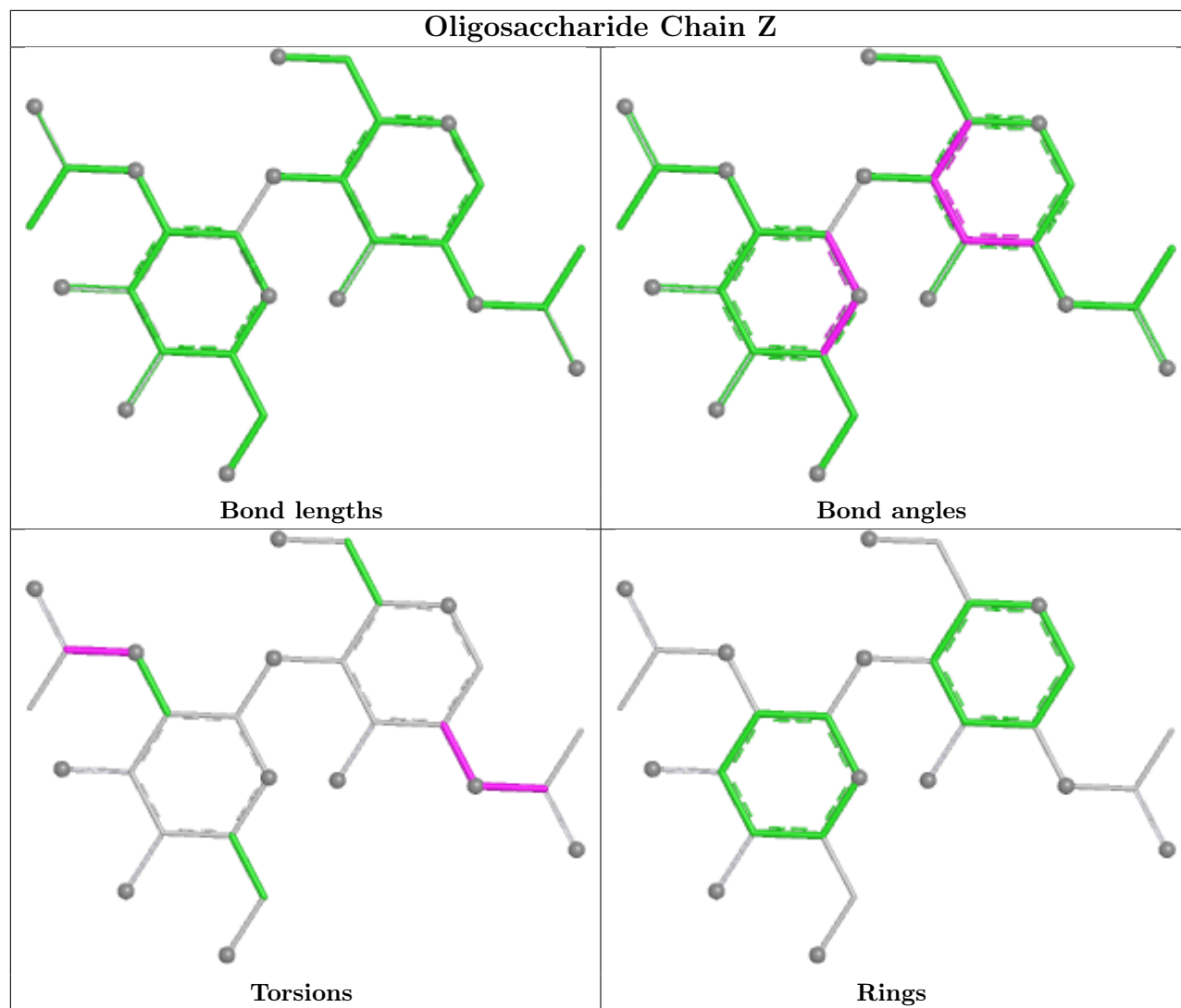


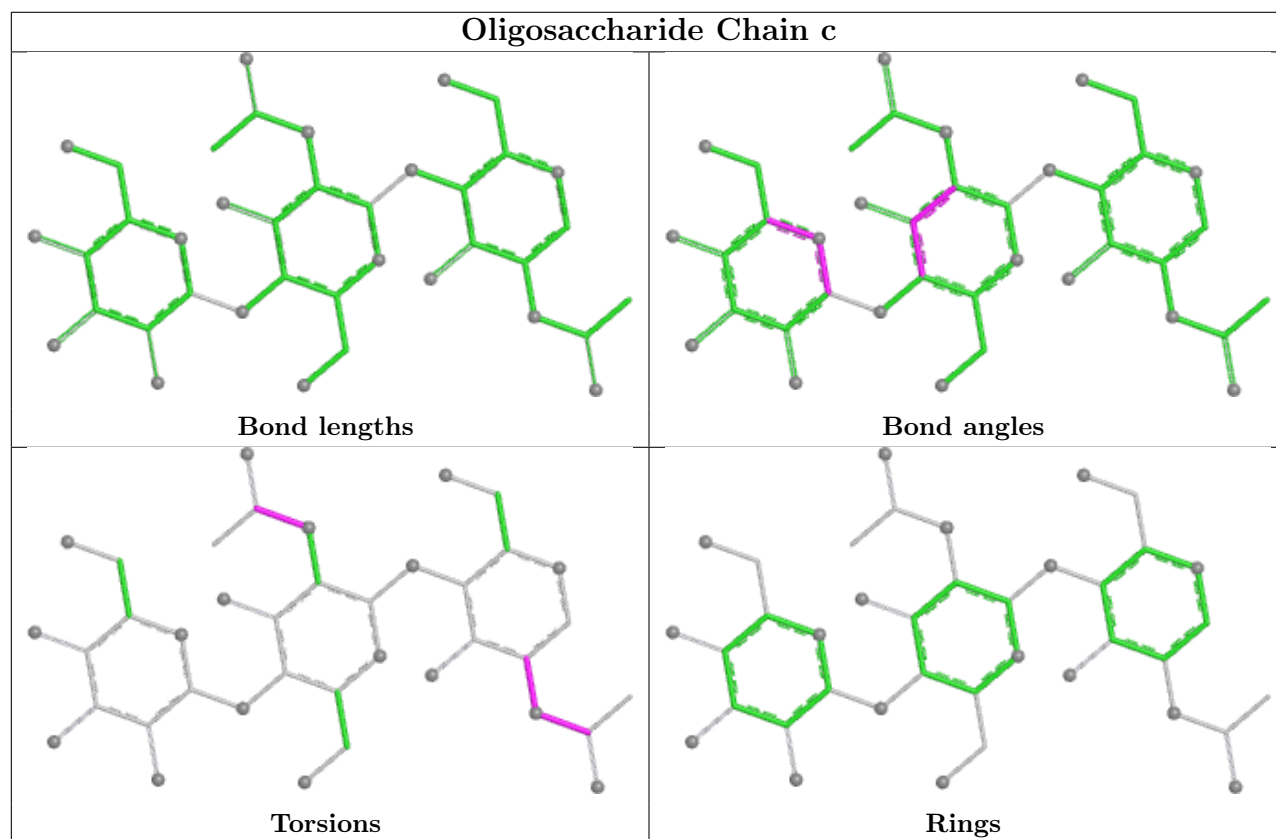
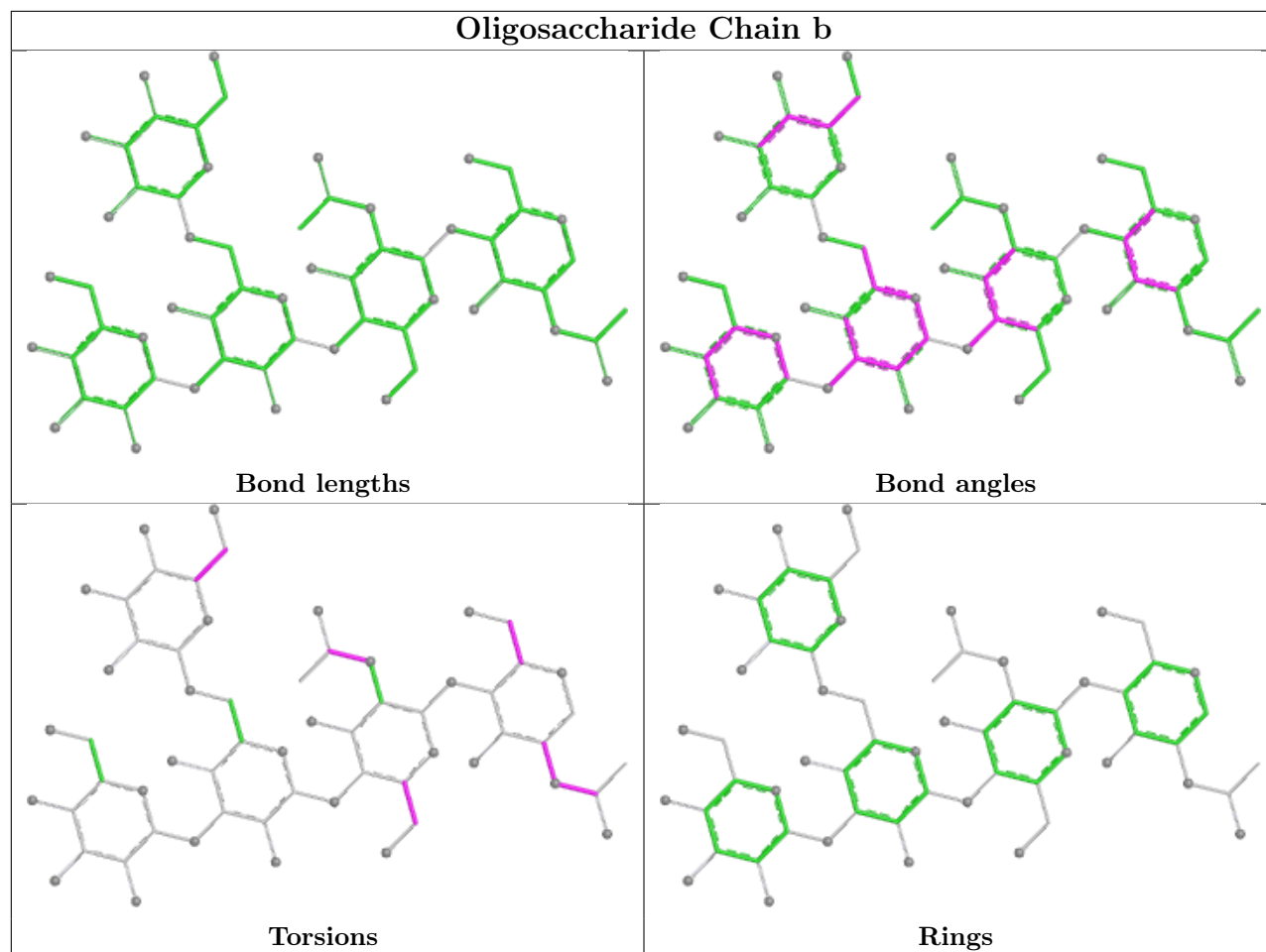












5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
16	NAG	K	803	3	14,14,15	0.51	0	17,19,21	1.85	3 (17%)
13	MAN	A	701	-	11,11,12	0.81	0	15,15,17	1.50	3 (20%)
16	NAG	L	802	3	14,14,15	0.50	0	17,19,21	0.66	0
14	BMA	K	802	-	11,11,12	0.78	0	15,15,17	1.76	3 (20%)
14	BMA	B	1701	-	11,11,12	0.72	0	15,15,17	1.21	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
16	NAG	K	803	3	1/1/5/7	3/6/23/26	0/1/1/1
13	MAN	A	701	-	-	0/2/19/22	0/1/1/1
16	NAG	L	802	3	1/1/5/7	3/6/23/26	0/1/1/1
14	BMA	K	802	-	-	0/2/19/22	0/1/1/1
14	BMA	B	1701	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K	802	BMA	C1-O5-C5	-5.08	105.37	112.19
16	K	803	NAG	O5-C1-C2	-4.85	103.78	111.29
16	K	803	NAG	C1-C2-N2	4.19	117.04	110.43
13	A	701	MAN	C1-C2-C3	-3.39	104.70	109.64
14	K	802	BMA	C1-C2-C3	-3.18	105.01	109.64
13	A	701	MAN	C1-O5-C5	-3.03	108.12	112.19
14	B	1701	BMA	C1-C2-C3	-2.84	105.52	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	701	MAN	C3-C4-C5	2.61	114.96	110.23
14	B	1701	BMA	C1-O5-C5	-2.17	109.28	112.19
14	K	802	BMA	C3-C4-C5	2.10	114.03	110.23
16	K	803	NAG	C2-N2-C7	2.08	125.69	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	K	803	NAG	C1
16	L	802	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	803	NAG	C1-C2-N2-C7
16	K	803	NAG	C8-C7-N2-C2
16	K	803	NAG	O7-C7-N2-C2
16	L	802	NAG	C1-C2-N2-C7
16	L	802	NAG	C8-C7-N2-C2
16	L	802	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	803	NAG	3	0
13	A	701	MAN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1500:LYS	C	1501:SER	N	3.64
1	H	988:CYS	C	989:GLY	N	2.97

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	638/645 (98%)	0.09	7 (1%) 78 57	87, 142, 190, 237	0
1	C	638/645 (98%)	0.14	6 (0%) 81 62	80, 127, 176, 228	0
1	E	638/645 (98%)	0.15	10 (1%) 70 49	84, 142, 196, 245	0
1	G	638/645 (98%)	0.34	25 (3%) 43 31	93, 180, 241, 267	0
2	B	901/915 (98%)	0.18	13 (1%) 73 52	91, 167, 229, 260	0
2	D	901/915 (98%)	0.22	24 (2%) 56 39	81, 155, 216, 266	0
2	F	900/915 (98%)	0.23	15 (1%) 69 48	96, 179, 284, 329	0
2	H	605/915 (66%)	0.25	8 (1%) 75 54	98, 162, 231, 294	0
3	I	507/507 (100%)	0.22	10 (1%) 65 45	93, 142, 197, 240	0
3	J	507/507 (100%)	0.17	11 (2%) 62 44	127, 170, 220, 261	0
3	K	507/507 (100%)	0.21	8 (1%) 70 49	132, 183, 230, 284	0
3	L	507/507 (100%)	0.23	9 (1%) 67 47	101, 144, 194, 239	0
4	M	84/92 (91%)	0.16	2 (2%) 59 42	87, 110, 186, 221	0
4	N	84/92 (91%)	0.15	3 (3%) 46 33	97, 116, 189, 227	0
4	P	84/92 (91%)	0.23	1 (1%) 76 55	100, 124, 176, 211	0
4	Q	84/92 (91%)	0.14	1 (1%) 76 55	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.20	153 (1%) 66 46	80, 154, 228, 329	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	509	LEU	6.7
1	G	529	VAL	6.4
3	L	267	CYS	3.9
1	G	608	GLY	3.8
1	G	421	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
3	J	267	CYS	3.7
3	L	741	ALA	3.6
3	I	366	LEU	3.6
1	G	436	LEU	3.5
2	D	1417	SER	3.4
3	L	693	SER	3.4
2	D	1603	ASP	3.4
1	G	437	SER	3.4
1	E	509	LEU	3.4
2	F	1168	ALA	3.4
2	B	1488	LEU	3.3
1	E	290	GLN	3.3
2	D	1357	ASP	3.2
2	D	1359	LYS	3.2
2	F	1590	TRP	3.2
1	E	436	LEU	3.2
3	K	324	LEU	3.1
2	F	996	MET	3.1
3	L	689	VAL	3.1
2	D	1263	ASP	3.1
1	G	528	SER	3.1
1	G	609	SER	3.0
2	D	1387	THR	3.0
3	I	741	ALA	3.0
3	J	741	ALA	3.0
1	G	340	LYS	2.9
3	I	267	CYS	2.8
2	D	1269	GLU	2.8
2	B	1498	ILE	2.8
1	E	101	VAL	2.8
1	G	427	VAL	2.8
3	K	371	GLY	2.8
1	G	511	ALA	2.8
2	D	1081	ALA	2.8
1	C	19	THR	2.7
4	Q	70	LEU	2.7
1	A	645	ALA	2.7
3	K	607	PHE	2.7
1	C	20	MET	2.7
2	D	1483	LEU	2.7
2	F	1201	PRO	2.6
1	G	336	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	K	699	VAL	2.6
1	G	290	GLN	2.6
2	D	1416	PHE	2.6
3	K	741	ALA	2.6
1	G	610	GLY	2.6
1	G	333	ILE	2.5
4	N	12	ASN	2.5
2	D	1488	LEU	2.5
2	B	1293	SER	2.5
2	F	1466	SER	2.5
1	G	626	SER	2.5
2	F	1632	GLU	2.5
2	H	1411	GLU	2.4
3	L	595	GLU	2.4
1	A	20	MET	2.4
1	A	312	SER	2.4
2	B	1417	SER	2.4
2	B	1439	PHE	2.4
1	G	470	TYR	2.4
2	D	1293	SER	2.4
1	G	453	PHE	2.4
1	C	636	ALA	2.4
2	F	1210	ALA	2.4
3	J	636	GLN	2.4
1	A	99	VAL	2.4
3	I	364	ASP	2.4
2	F	1416	PHE	2.4
2	B	1351	THR	2.4
2	B	1239	TYR	2.4
4	M	85	TYR	2.4
2	D	1356	GLN	2.3
1	A	22	LEU	2.3
2	F	1001	ILE	2.3
2	D	968	MET	2.3
1	E	634	GLN	2.3
3	J	565	GLN	2.3
2	B	838	LEU	2.3
2	B	1572	LEU	2.3
4	M	12	ASN	2.3
3	J	235	LYS	2.3
2	D	925	LEU	2.3
1	E	599	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	675	GLY	2.3
1	G	438	VAL	2.3
3	I	517	GLY	2.3
1	G	352	VAL	2.3
3	J	510	HIS	2.2
3	J	284	TYR	2.2
3	L	449	SER	2.2
3	L	610	GLU	2.2
2	D	978	LEU	2.2
3	J	324	LEU	2.2
2	B	1306	GLU	2.2
3	I	693	SER	2.2
2	H	1572	LEU	2.2
3	K	686	PHE	2.2
3	J	323	LYS	2.2
2	F	1374	GLN	2.2
4	N	85	TYR	2.2
1	G	510	VAL	2.2
1	E	441	THR	2.2
2	H	1416	PHE	2.2
2	F	1062	LYS	2.2
1	G	70	ALA	2.2
2	D	1210	ALA	2.2
3	I	445	ASP	2.2
2	D	1041	SER	2.2
2	D	1158	TYR	2.2
1	G	452	ASN	2.2
3	I	443	MET	2.2
1	E	527	ASP	2.1
2	H	1327	HIS	2.1
2	F	925	LEU	2.1
1	A	485	VAL	2.1
2	D	1445	PHE	2.1
2	H	1377	THR	2.1
2	B	925	LEU	2.1
1	E	636	ALA	2.1
2	B	836	GLN	2.1
1	G	542	VAL	2.1
3	J	699	VAL	2.1
3	K	697	VAL	2.1
2	F	1523	TYR	2.1
2	H	1334	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	633	ARG	2.1
2	F	1169	ILE	2.1
2	B	1606	VAL	2.1
2	D	955	GLU	2.1
2	D	1491	CYS	2.1
3	K	574	CYS	2.1
2	H	1546	THR	2.1
1	C	645	ALA	2.1
2	D	1065	SER	2.1
2	F	1501	SER	2.1
1	E	365	VAL	2.1
3	L	443	MET	2.1
1	C	590	THR	2.0
4	N	84	LYS	2.0
3	L	486	CYS	2.0
1	A	633	ALA	2.0
2	H	1328	ALA	2.0
1	C	190	ASN	2.0
4	P	44	ILE	2.0
1	G	200	PHE	2.0
2	D	1572	LEU	2.0
3	I	361	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
5	NAG	O	1	14/15	-	-	156,185,187,188	0
5	NAG	O	2	14/15	-	-	199,200,201,203	0
5	BMA	O	3	11/12	-	-	212,214,215,216	0
5	BMA	O	4	11/12	-	-	226,227,228,228	0
6	BMA	S	4	11/12	0.06	0.13	235,237,239,240	0
5	BMA	R	4	11/12	0.07	0.14	237,239,240,241	0

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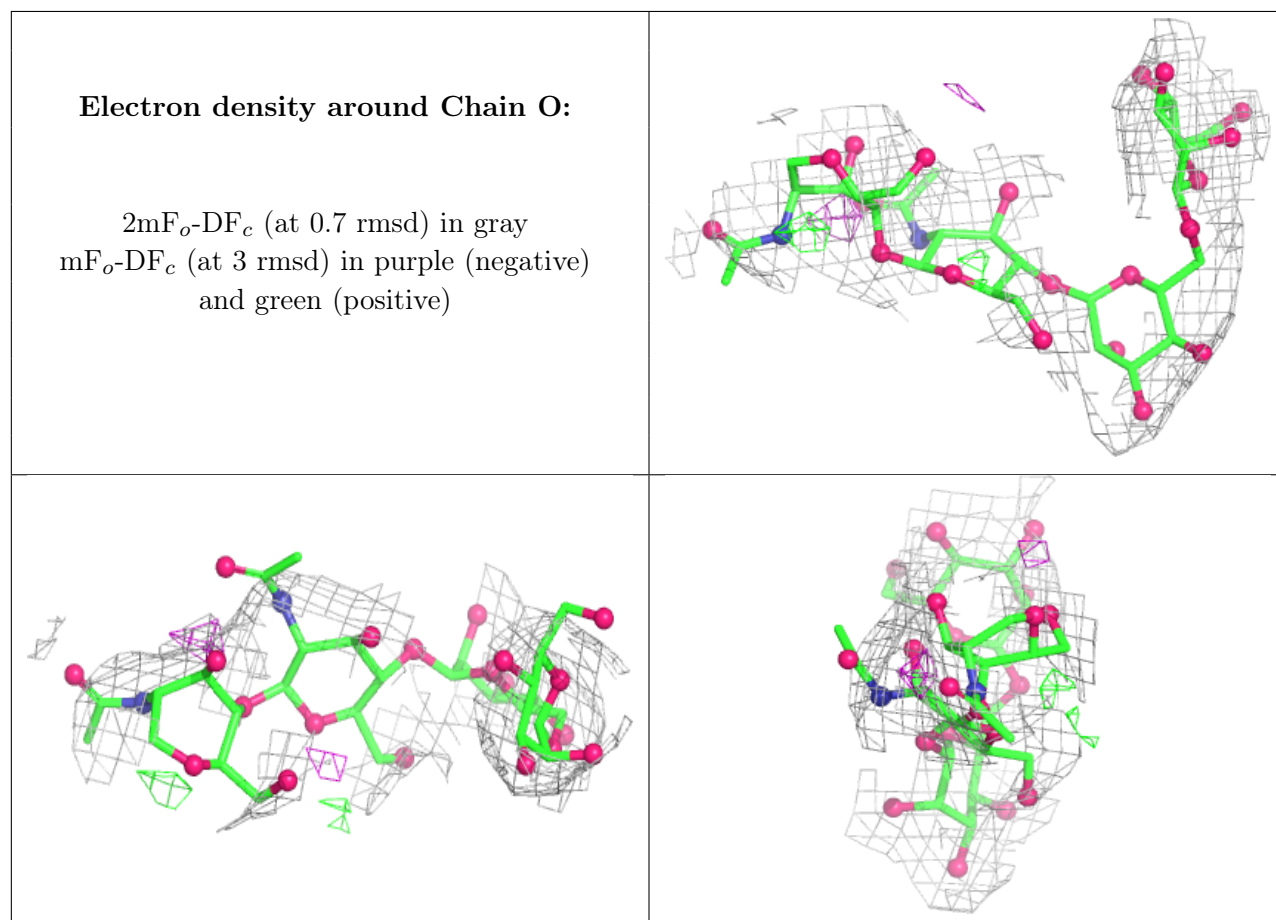
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	S	5	11/12	0.13	0.13	231,233,235,235	0
9	MAN	Y	3	11/12	0.18	0.15	205,207,208,209	0
5	BMA	U	4	11/12	0.19	0.13	209,212,214,215	0
6	BMA	S	3	11/12	0.27	0.10	219,220,222,223	0
5	BMA	T	3	11/12	0.30	0.11	220,221,223,223	0
6	BMA	W	5	11/12	0.31	0.11	229,231,232,232	0
7	BMA	V	5	11/12	0.38	0.16	221,222,224,224	0
5	BMA	T	4	11/12	0.38	0.09	229,232,233,234	0
5	BMA	R	3	11/12	0.40	0.12	218,220,222,223	0
10	NAG	Z	2	14/15	0.41	0.12	222,223,224,224	0
7	BMA	V	3	11/12	0.44	0.09	232,233,234,234	0
6	BMA	W	3	11/12	0.49	0.09	247,249,250,251	0
8	MAN	X	3	11/12	0.50	0.09	229,230,231,232	0
10	NAG	Z	1	14/15	0.52	0.10	198,225,227,227	0
6	NAG	S	2	14/15	0.52	0.12	200,202,203,203	0
5	BMA	U	3	11/12	0.55	0.14	229,230,231,232	0
7	BMA	V	4	11/12	0.61	0.12	248,249,249,250	0
8	MAN	X	4	11/12	0.67	0.08	234,236,237,238	0
8	NAG	X	2	14/15	0.67	0.10	221,222,224,225	0
6	NAG	W	2	14/15	0.68	0.10	213,216,216,217	0
6	BMA	W	4	11/12	0.68	0.07	226,228,229,230	0
7	BMA	V	6	11/12	0.69	0.13	214,215,217,217	0
6	NAG	W	1	14/15	0.70	0.13	198,201,208,215	0
5	NAG	R	2	14/15	0.72	0.10	193,196,196,197	0
9	NAG	Y	2	14/15	0.73	0.12	178,180,181,182	0
7	NAG	V	1	14/15	0.74	0.15	169,193,194,194	0
5	NAG	T	2	14/15	0.74	0.08	200,201,202,203	0
5	NAG	U	2	14/15	0.77	0.10	223,225,227,227	0
7	NAG	V	2	14/15	0.78	0.11	200,202,204,204	0
8	NAG	X	1	14/15	0.82	0.10	183,213,214,215	0
5	NAG	U	1	14/15	0.87	0.10	174,204,206,206	0
5	NAG	T	1	14/15	0.87	0.10	147,176,178,179	0
5	NAG	R	1	14/15	0.87	0.09	163,194,194,195	0
9	NAG	a	1	14/15	-	-	158,188,189,189	0
9	NAG	a	2	14/15	-	-	177,179,180,180	0
9	MAN	a	3	11/12	-	-	206,210,211,212	0
6	NAG	S	1	14/15	0.88	0.14	163,191,192,193	0
9	NAG	Y	1	14/15	0.89	0.12	122,149,151,152	0
11	NAG	b	1	14/15	-	-	174,204,206,207	0
11	NAG	b	2	14/15	-	-	196,199,201,202	0
11	MAN	b	3	11/12	-	-	249,252,253,254	0
11	MAN	b	4	11/12	-	-	230,232,235,235	0

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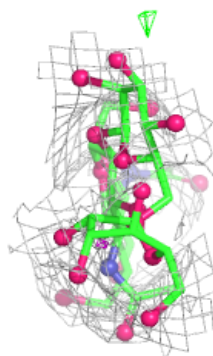
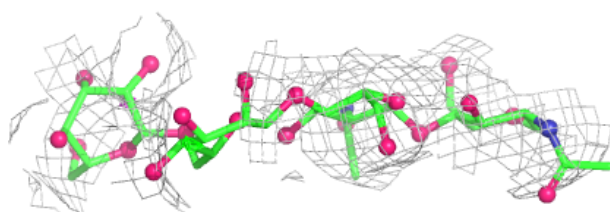
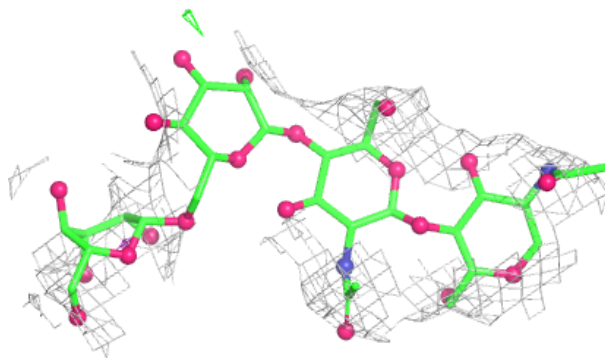
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MAN	b	5	11/12	-	-	229,230,232,232	0
12	NAG	c	1	14/15	-	-	122,147,148,148	0
12	NAG	c	2	14/15	-	-	185,187,189,189	0
12	BMA	c	3	11/12	-	-	197,201,202,202	0

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.

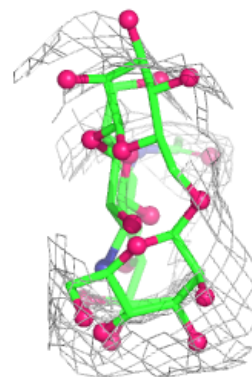
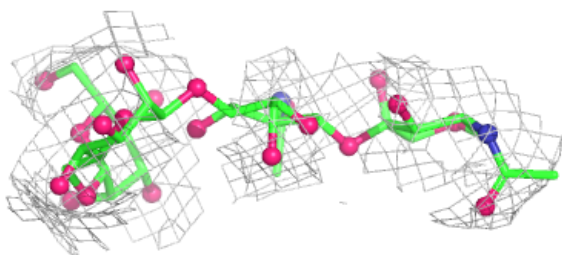
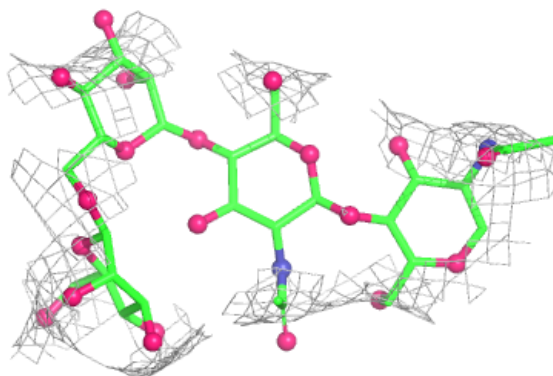


Electron density around Chain R:

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

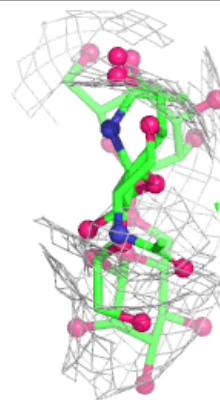
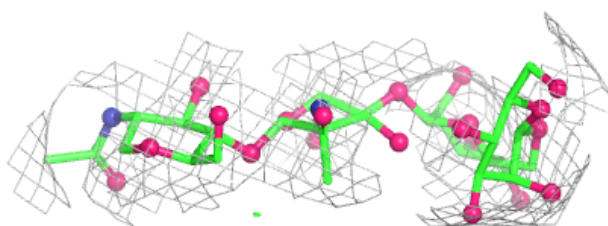
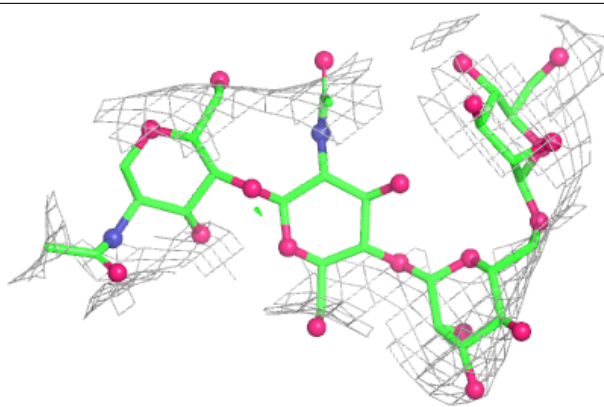
**Electron density around Chain T:**

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



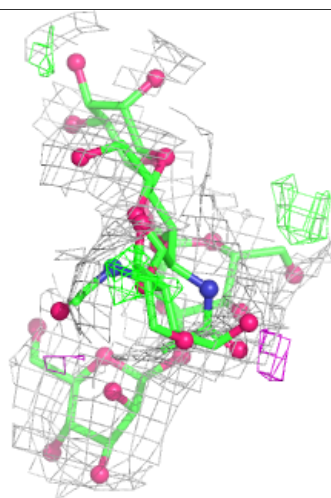
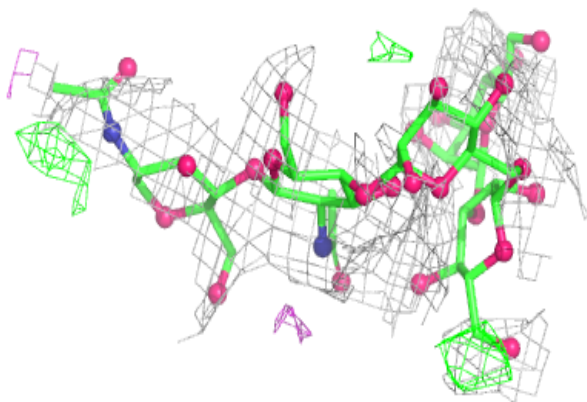
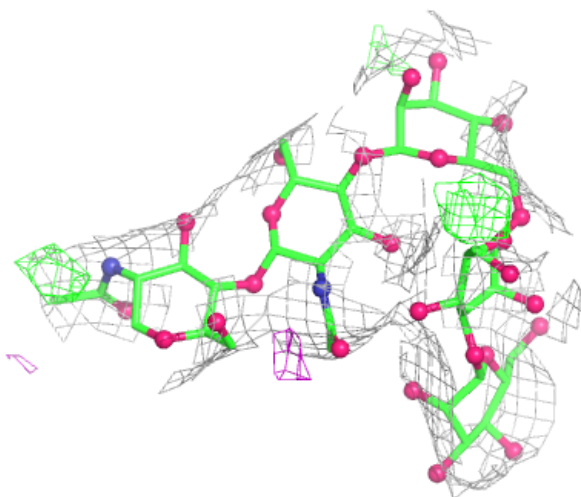
Electron density around Chain U:

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



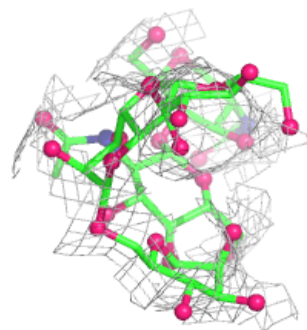
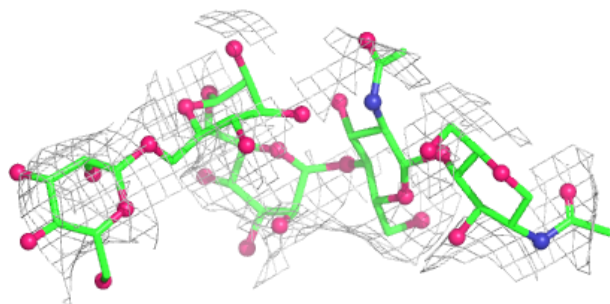
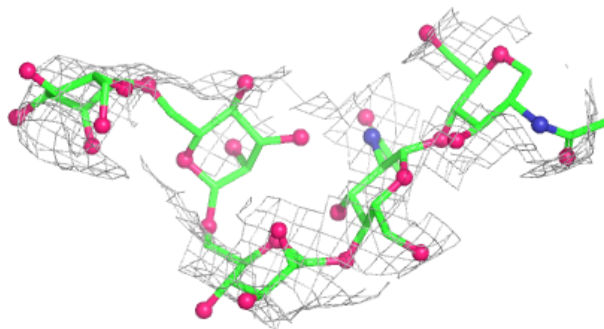
Electron density around Chain S:

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



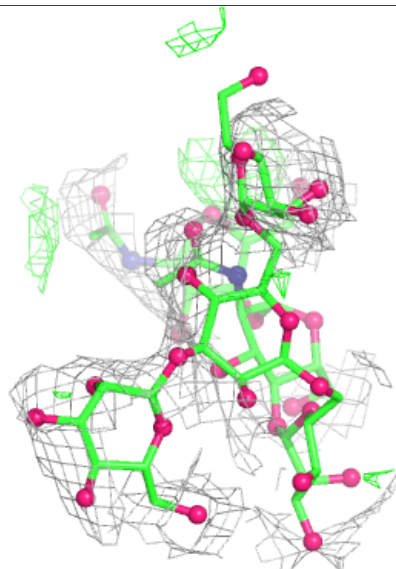
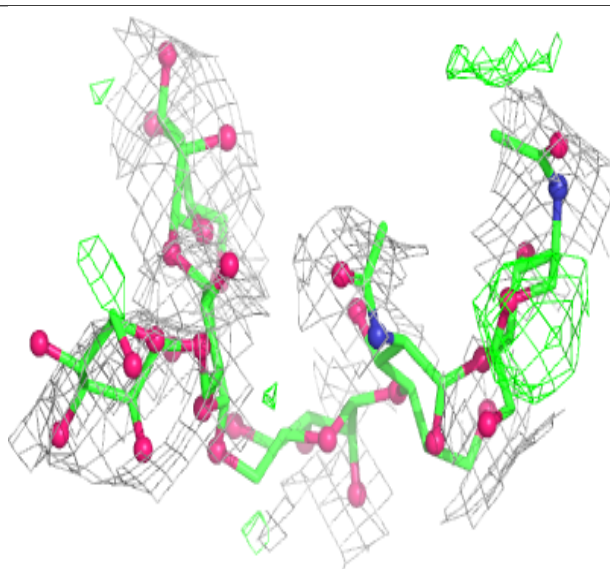
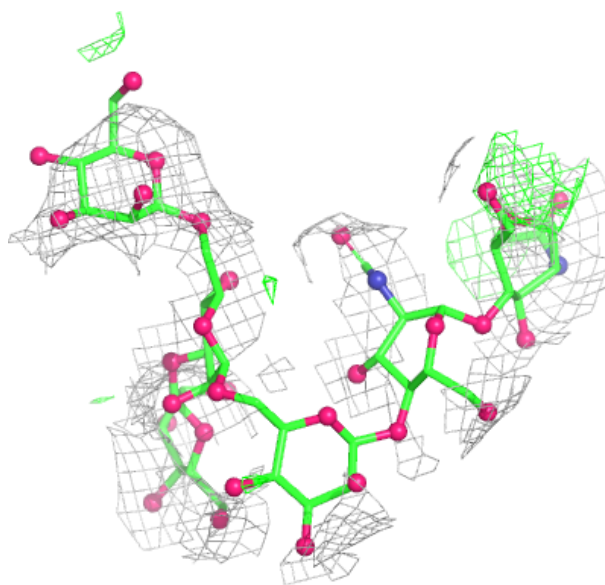
Electron density around Chain W:

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



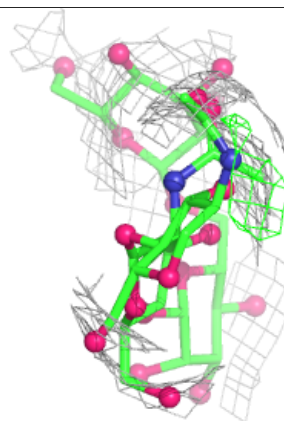
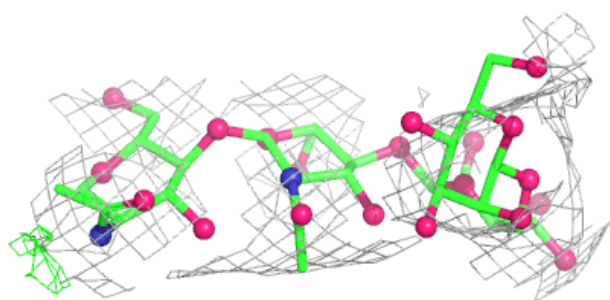
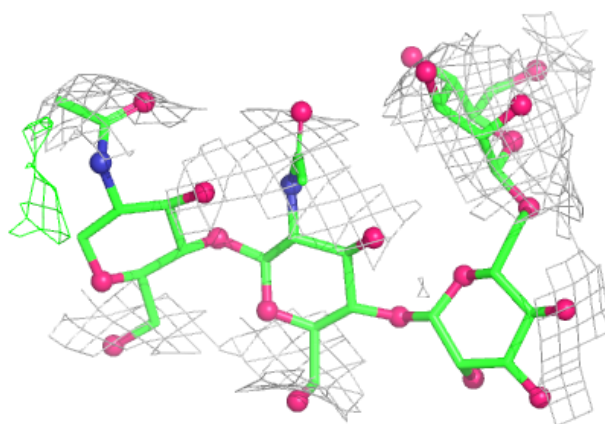
Electron density around Chain V:

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

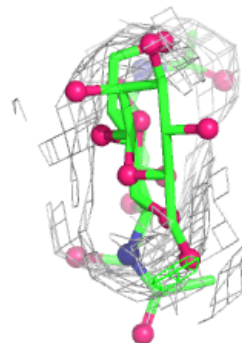
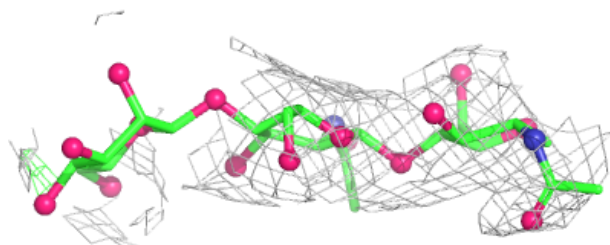
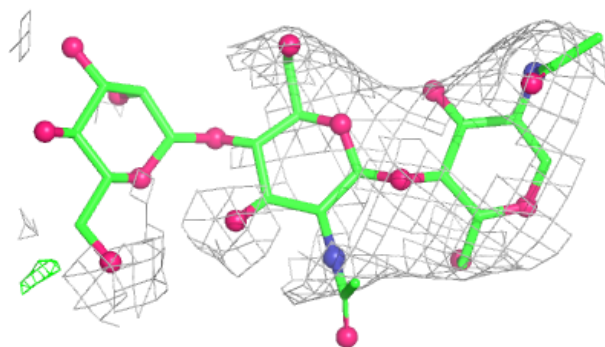


Electron density around Chain X:

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

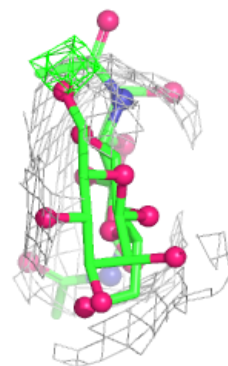
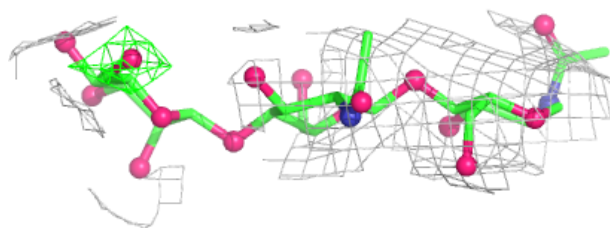
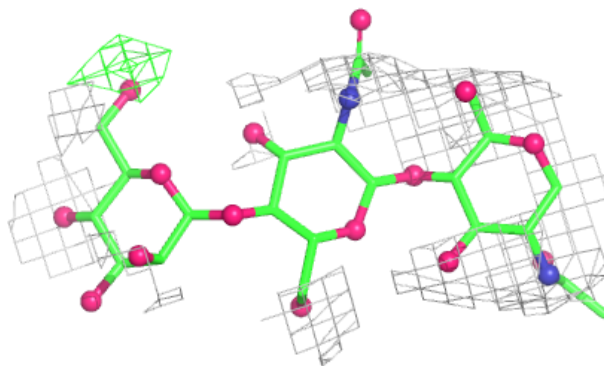
**Electron density around Chain Y:**

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

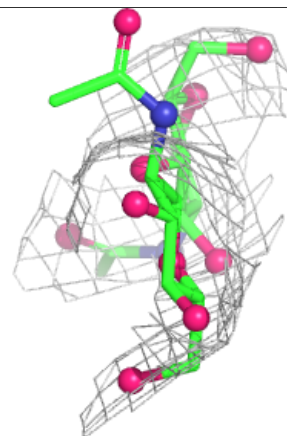
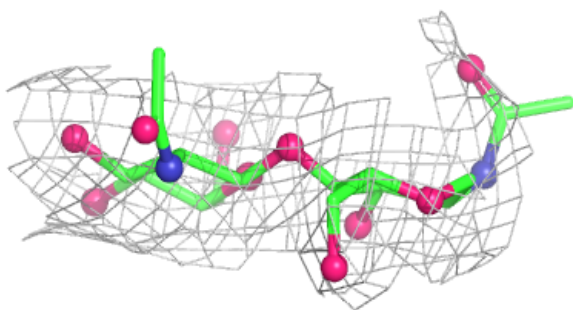
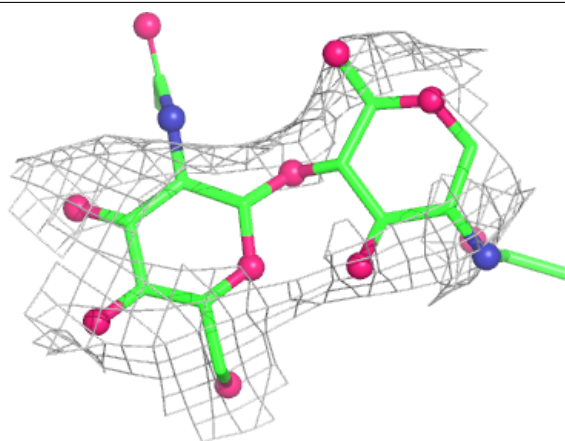


Electron density around Chain a:

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

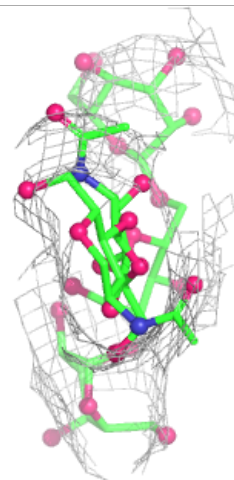
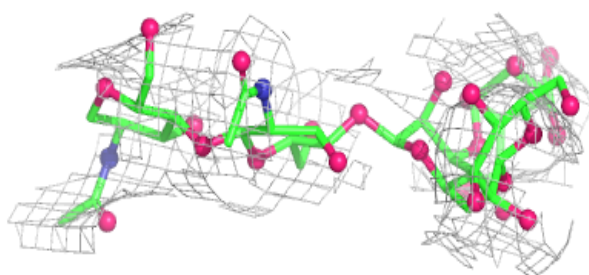
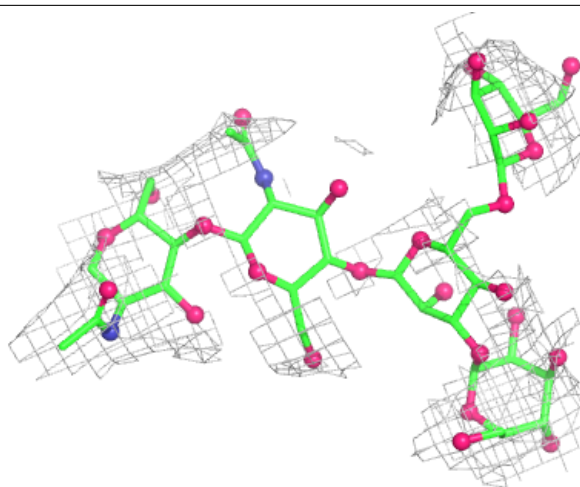
**Electron density around Chain Z:**

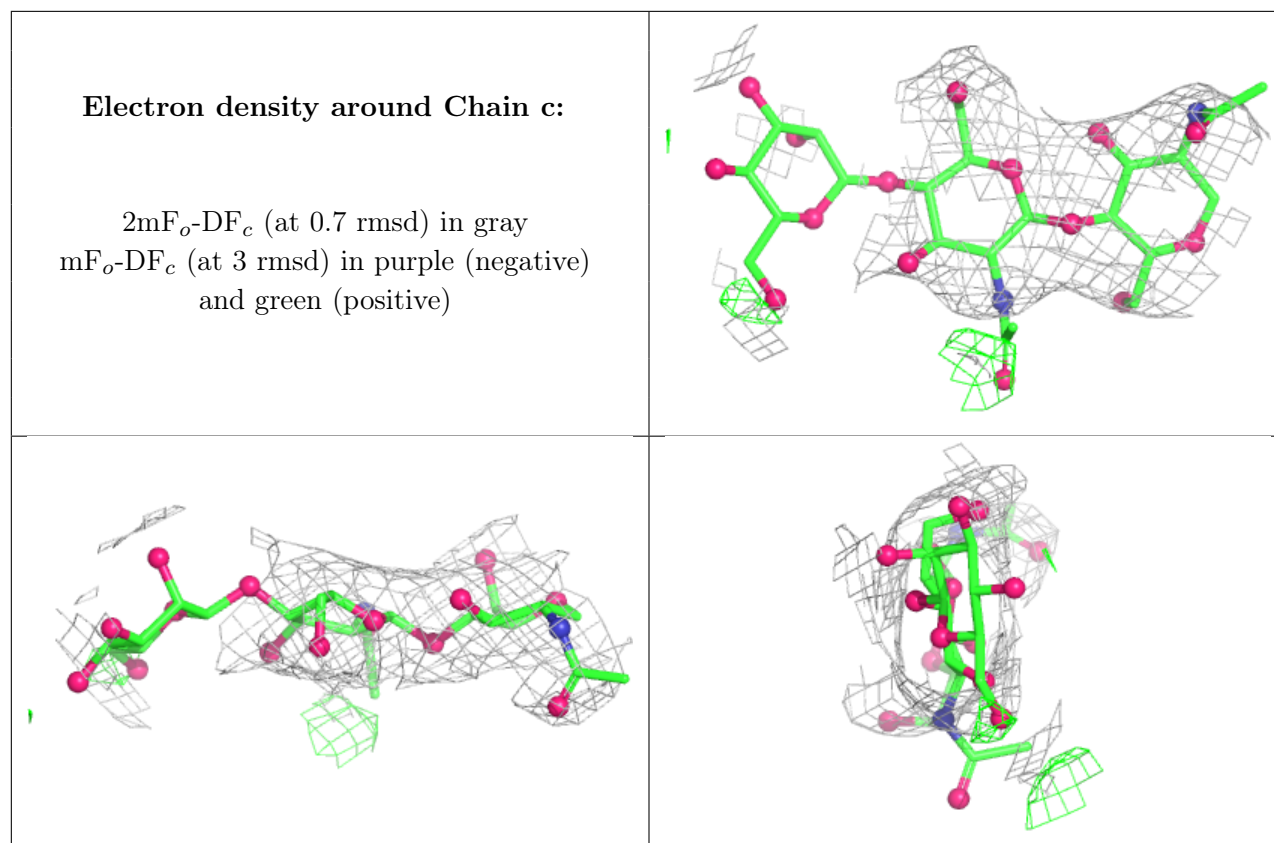
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain b:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	MAN	A	701	11/12	-0.13	0.16	222,225,227,228	0
14	BMA	B	1701	11/12	0.42	0.10	198,200,200,201	0
14	BMA	K	802	11/12	0.46	0.10	194,195,196,196	0
16	NAG	K	803	14/15	0.57	0.10	184,214,216,217	0
16	NAG	L	802	14/15	0.75	0.09	176,204,205,205	0
15	MG	I	801	1/1	0.94	0.06	120,120,120,120	0
15	MG	K	801	1/1	0.94	0.06	138,138,138,138	0
15	MG	J	801	1/1	0.95	0.05	148,148,148,148	0
15	MG	L	801	1/1	0.97	0.08	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.