



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 06:14 AM UTC

PDB ID : 2C11 / pdb_00002c11
Title : Crystal structure of the 2-hydrazinopyridine of semicarbazide- sensitive amine oxidase
Authors : Jakobsson, E.; Kleywegt, G.J.
Deposited on : 2005-09-09
Resolution : 2.90 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

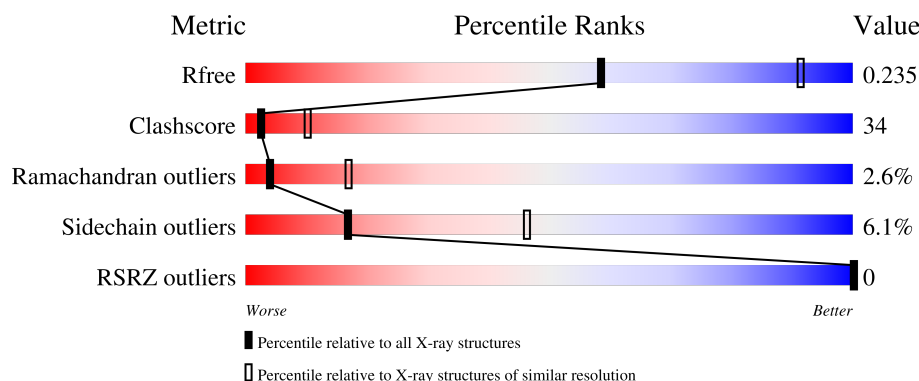
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



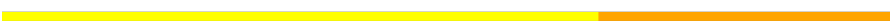
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	735	
1	B	735	
1	C	735	
1	D	735	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
3	F	2	 50% 50%
4	G	3	 33% 67%
4	K	3	 67% 33%
5	H	5	 80% 20%
5	L	5	 20% 80%
6	J	3	 67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PAQ	A	471	X	-	-	-
1	PAQ	B	471	X	-	-	-
1	PAQ	C	471	X	-	-	-
1	PAQ	D	471	X	-	-	-
3	FUC	F	2	X	-	-	-
5	NAG	H	1	X	-	-	-
5	FUC	H	5	X	-	-	-
5	NAG	L	1	X	-	-	-
5	FUC	L	5	X	-	-	-
6	FUC	J	3	X	-	-	-
7	NAG	D	1736	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21917 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 MEMBRANE COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	B	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	C	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	D	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			

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



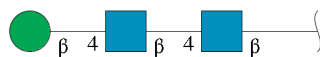
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



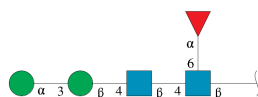
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 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.



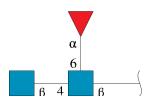
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



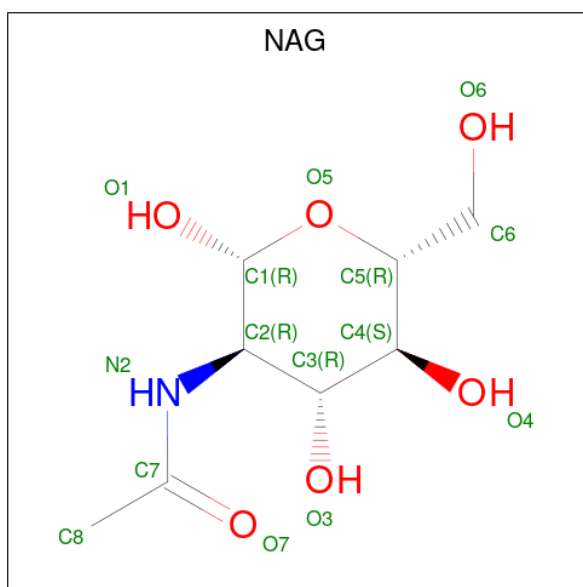
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			
5	L	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Ca	0	0
			2	2		
8	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total 2	Ca 2	0	0
8	D	2	Total 2	Ca 2	0	0

- Molecule 9 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

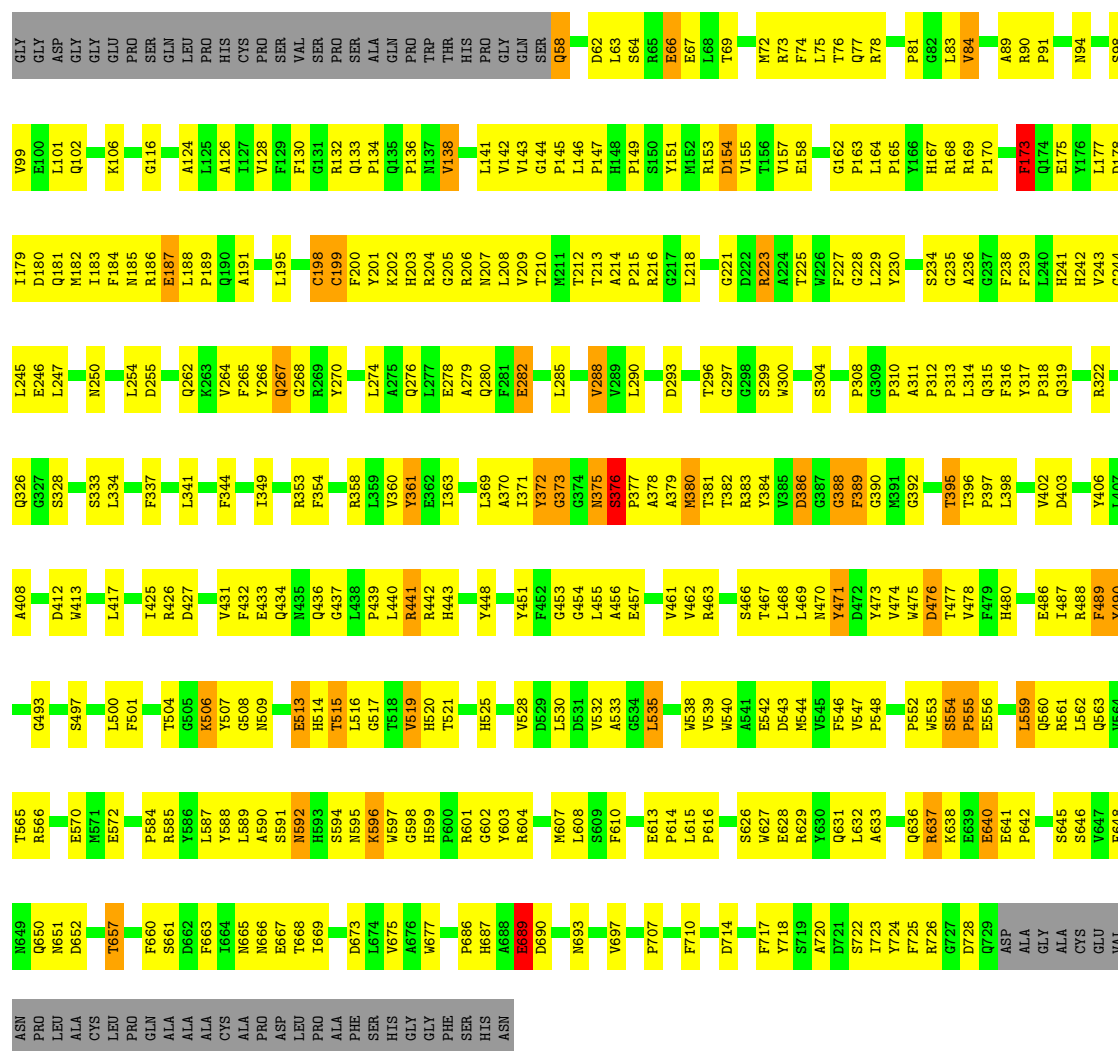
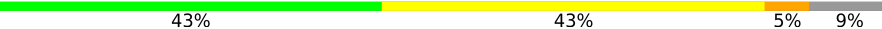
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total 7	Cu 7	0	0
9	B	8	Total 8	Cu 8	0	0
9	C	8	Total 8	Cu 8	0	0
9	D	7	Total 7	Cu 7	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

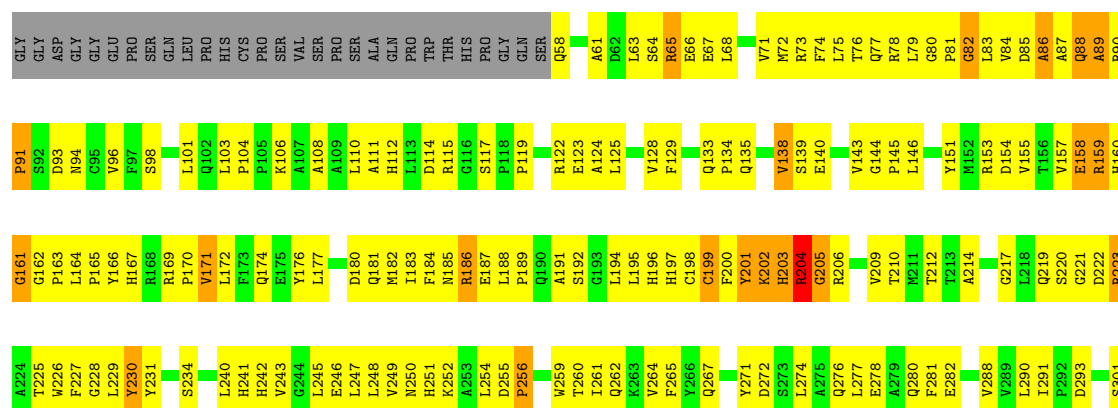
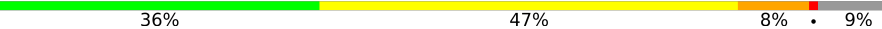
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total 2	Cl 2	0	0
10	C	1	Total 1	Cl 1	0	0
10	D	1	Total 1	Cl 1	0	0

- Molecule 11 is water.

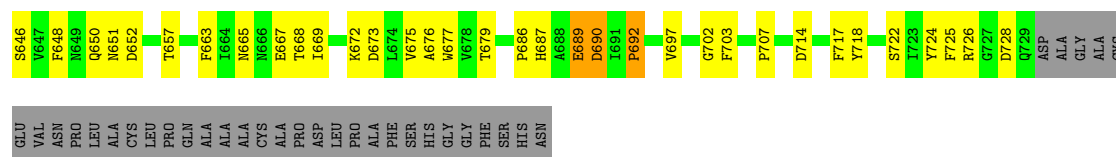
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	19	Total 19	O 19	0	0
11	B	20	Total 20	O 20	0	0
11	C	11	Total 11	O 11	0	0
11	D	9	Total 9	O 9	0	0

Chain B: 

● Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain C: 





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

Chain E: 100%

MAG1
MAG2

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

Chain I: 100%

MAG1
MAG2

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%

MAG1
FUC2

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

Chain G: 33% 67%

MAG1
MAG2
BMA3

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

Chain K: 67% 33%

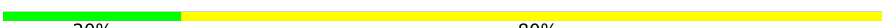
MAG1
MAG2
BMA3

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 80% 20%

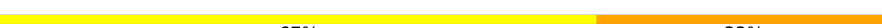


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  20% 80%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	127.40Å 127.40Å 219.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.90) 94.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.276 0.234 , 0.235	Depositor DCC
R_{free} test set	4335 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21917	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: CL, CU, FUC, MAN, PAQ, NAG, CA, 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	0.58	1/5488 (0.0%)	1.09	41/7481 (0.5%)
1	B	0.56	0/5488	1.09	40/7481 (0.5%)
1	C	0.57	1/5488 (0.0%)	1.09	38/7481 (0.5%)
1	D	0.56	1/5488 (0.0%)	1.07	33/7481 (0.4%)
All	All	0.57	3/21952 (0.0%)	1.08	152/29924 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	728	ASP	C-N	-5.28	1.25	1.33
1	C	728	ASP	C-N	-5.27	1.25	1.33
1	D	728	ASP	C-N	-5.06	1.26	1.33

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLY	N-CA-C	11.56	125.24	112.29
1	B	631	GLN	N-CA-C	-10.10	101.09	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	ARG	N-CA-C	9.96	125.78	109.95
1	A	204	ARG	N-CA-C	9.84	125.15	108.23
1	C	631	GLN	N-CA-C	-9.84	100.82	113.12
1	A	631	GLN	N-CA-C	-9.75	100.93	113.12
1	C	103	LEU	CA-C-N	9.51	126.60	119.66
1	C	103	LEU	C-N-CA	9.51	126.60	119.66
1	A	311	ALA	CA-C-N	9.34	126.38	119.66
1	A	311	ALA	C-N-CA	9.34	126.38	119.66
1	B	198	CYS	N-CA-C	8.89	121.78	111.11
1	C	302	LEU	N-CA-C	-8.46	104.09	114.75
1	D	506	LYS	N-CA-C	8.44	122.39	112.93
1	C	365	LEU	N-CA-C	-8.39	99.23	110.55
1	C	317	TYR	CA-C-N	8.07	128.52	119.32
1	C	317	TYR	C-N-CA	8.07	128.52	119.32
1	B	207	ASN	N-CA-C	-8.00	103.63	113.15
1	C	202	LYS	N-CA-C	-7.76	97.43	109.76
1	B	506	LYS	N-CA-C	7.70	121.13	112.97
1	C	255	ASP	CA-C-N	7.69	129.45	119.84
1	C	255	ASP	C-N-CA	7.69	129.45	119.84
1	D	657	THR	N-CA-C	-7.62	103.45	112.89
1	A	317	TYR	CA-C-N	7.61	127.99	119.32
1	A	317	TYR	C-N-CA	7.61	127.99	119.32
1	A	544	MET	N-CA-C	7.59	119.60	110.19
1	A	712	ASP	N-CA-C	-7.57	104.05	113.28
1	C	80	GLY	CA-C-N	7.50	129.22	119.84
1	C	80	GLY	C-N-CA	7.50	129.22	119.84
1	D	205	GLY	N-CA-C	7.47	122.09	112.68
1	C	199	CYS	N-CA-C	7.39	122.29	111.87
1	D	631	GLN	N-CA-C	-7.34	102.25	112.45
1	A	103	LEU	CA-C-N	7.29	124.98	119.66
1	A	103	LEU	C-N-CA	7.29	124.98	119.66
1	D	690	ASP	N-CA-C	-7.28	103.55	113.30
1	A	199	CYS	N-CA-C	7.23	122.06	111.87
1	B	657	THR	N-CA-C	-7.22	103.13	112.23
1	A	335	TRP	N-CA-C	7.07	121.38	110.42
1	D	207	ASN	N-CA-C	-7.06	104.40	113.16
1	D	373	GLY	N-CA-C	-7.06	97.78	111.12
1	D	389	PHE	N-CA-C	-7.04	104.68	113.55
1	A	202	LYS	N-CA-C	-6.96	97.92	109.46
1	C	652	ASP	CA-C-N	6.89	126.60	119.64
1	C	652	ASP	C-N-CA	6.89	126.60	119.64
1	D	717	PHE	N-CA-C	-6.88	103.01	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	ALA	CA-C-N	6.87	124.61	119.66
1	C	311	ALA	C-N-CA	6.87	124.61	119.66
1	B	373	GLY	N-CA-C	-6.82	98.23	111.12
1	A	255	ASP	CA-C-N	6.79	128.32	119.84
1	A	255	ASP	C-N-CA	6.79	128.32	119.84
1	B	268	GLY	N-CA-C	6.75	120.80	113.58
1	C	544	MET	N-CA-C	6.69	118.49	110.19
1	B	690	ASP	N-CA-C	-6.69	104.25	112.88
1	A	365	LEU	N-CA-C	-6.66	99.73	110.32
1	B	610	PHE	N-CA-C	-6.66	103.25	112.30
1	B	436	GLN	N-CA-C	6.66	119.37	111.71
1	C	335	TRP	N-CA-C	6.65	120.73	110.42
1	C	650	GLN	N-CA-C	6.63	119.06	111.11
1	C	361	TYR	N-CA-C	-6.62	103.55	111.69
1	B	162	GLY	CA-C-N	6.58	126.34	119.76
1	B	162	GLY	C-N-CA	6.58	126.34	119.76
1	A	384	TYR	N-CA-C	6.39	118.35	109.15
1	D	311	ALA	CA-C-N	6.39	124.26	119.66
1	D	311	ALA	C-N-CA	6.39	124.26	119.66
1	C	712	ASP	N-CA-C	-6.35	105.54	113.28
1	A	361	TYR	N-CA-C	-6.33	104.46	111.36
1	D	610	PHE	N-CA-C	-6.30	103.03	112.54
1	C	428	ALA	N-CA-C	-6.25	104.39	111.14
1	D	372	TYR	N-CA-C	6.20	120.14	110.17
1	A	372	TYR	N-CA-C	6.15	119.95	110.42
1	B	717	PHE	N-CA-C	-6.14	104.59	111.28
1	A	592	ASN	N-CA-C	-6.11	103.94	111.40
1	A	302	LEU	N-CA-C	-6.09	105.55	114.39
1	D	255	ASP	CA-C-N	6.09	127.45	119.84
1	D	255	ASP	C-N-CA	6.09	127.45	119.84
1	D	388	GLY	N-CA-C	-5.96	108.11	114.67
1	A	396	THR	CA-C-N	5.94	125.70	119.76
1	A	396	THR	C-N-CA	5.94	125.70	119.76
1	D	457	GLU	N-CA-C	5.92	118.84	109.96
1	B	388	GLY	N-CA-C	-5.89	107.03	114.16
1	A	387	GLY	N-CA-C	-5.87	107.06	114.16
1	C	376	SER	CA-C-N	5.85	125.32	119.24
1	C	376	SER	C-N-CA	5.85	125.32	119.24
1	D	446	ASP	N-CA-C	-5.82	106.03	114.12
1	B	116	GLY	N-CA-C	-5.82	106.49	114.64
1	A	665	ASN	N-CA-C	-5.81	100.93	109.81
1	D	592	ASN	N-CA-C	-5.80	104.55	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	437	GLY	N-CA-C	-5.79	108.19	115.08
1	D	198	CYS	N-CA-C	5.78	120.90	111.37
1	B	376	SER	CA-C-N	5.74	125.87	119.32
1	B	376	SER	C-N-CA	5.74	125.87	119.32
1	A	650	GLN	N-CA-C	5.71	117.97	111.11
1	A	80	GLY	CA-C-N	5.68	126.94	119.84
1	A	80	GLY	C-N-CA	5.68	126.94	119.84
1	C	420	GLN	N-CA-C	-5.68	106.23	114.12
1	C	104	PRO	N-CA-C	5.67	115.91	110.47
1	C	435	ASN	N-CA-C	-5.67	101.52	109.96
1	D	199	CYS	N-CA-C	5.66	120.19	112.88
1	B	102	GLN	N-CA-C	-5.66	99.50	108.73
1	D	476	ASP	N-CA-C	5.64	118.14	109.07
1	B	437	GLY	N-CA-C	-5.59	108.42	115.08
1	D	116	GLY	N-CA-C	-5.59	106.81	114.64
1	A	228	GLY	N-CA-C	-5.55	104.19	113.02
1	A	133	GLN	CA-C-N	5.53	125.19	119.05
1	A	133	GLN	C-N-CA	5.53	125.19	119.05
1	C	205	GLY	N-CA-C	-5.52	107.71	115.32
1	D	138	VAL	N-CA-C	-5.51	100.25	108.46
1	C	717	PHE	N-CA-C	-5.49	105.45	111.82
1	B	361	TYR	N-CA-C	-5.48	105.72	112.90
1	B	476	ASP	N-CA-C	5.48	118.17	109.24
1	B	535	LEU	N-CA-C	5.47	118.42	111.69
1	A	428	ALA	N-CA-C	-5.47	104.97	111.69
1	C	602	GLY	N-CA-C	5.46	119.26	111.12
1	B	255	ASP	CA-C-N	5.45	126.65	119.84
1	B	255	ASP	C-N-CA	5.45	126.65	119.84
1	A	610	PHE	N-CA-C	-5.41	103.85	110.61
1	B	372	TYR	N-CA-C	5.38	118.83	110.17
1	A	181	GLN	N-CA-C	-5.38	105.32	111.07
1	C	228	GLY	N-CA-C	-5.37	104.49	113.02
1	A	477	THR	N-CA-C	-5.36	99.38	110.80
1	B	389	PHE	N-CA-C	-5.33	106.45	113.12
1	D	228	GLY	N-CA-C	-5.33	104.35	112.51
1	B	187	GLU	N-CA-C	5.31	120.85	110.56
1	B	138	VAL	N-CA-C	-5.30	100.84	108.48
1	B	592	ASN	N-CA-C	-5.30	105.55	112.23
1	B	288	VAL	N-CA-C	5.28	115.56	108.17
1	D	288	VAL	N-CA-C	5.27	115.55	108.17
1	B	375	ASN	N-CA-C	-5.26	106.54	113.12
1	D	283	ALA	N-CA-C	-5.21	105.77	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	LEU	N-CA-C	5.21	116.64	111.07
1	B	199	CYS	N-CA-C	5.19	119.58	112.88
1	B	199	CYS	N-CA-CB	-5.19	102.68	110.73
1	D	274	LEU	N-CA-C	-5.19	105.62	111.28
1	C	665	ASN	N-CA-C	-5.17	101.89	109.81
1	A	717	PHE	N-CA-C	-5.17	105.77	111.71
1	A	104	PRO	N-CA-C	5.16	115.43	110.47
1	A	445	SER	N-CA-C	5.13	117.09	108.73
1	A	710	PHE	N-CA-C	-5.13	106.18	112.90
1	C	434	GLN	N-CA-C	5.11	117.12	108.02
1	C	199	CYS	N-CA-CB	-5.11	103.42	111.39
1	C	181	GLN	N-CA-C	-5.10	105.61	111.07
1	D	375	ASN	N-CA-C	-5.08	106.76	113.12
1	A	253	ALA	N-CA-C	5.08	117.08	110.43
1	B	457	GLU	N-CA-C	5.05	117.80	109.76
1	D	214	ALA	N-CA-C	5.05	112.77	108.22
1	B	720	ALA	N-CA-C	-5.05	105.67	111.07
1	C	384	TYR	N-CA-C	5.04	117.00	109.59
1	B	480	HIS	N-CA-C	5.04	117.59	110.24
1	A	219	GLN	N-CA-C	-5.02	102.76	110.14
1	B	173	PHE	N-CA-C	-5.02	105.70	111.07
1	D	480	HIS	CA-C-N	5.02	124.68	119.56
1	D	480	HIS	C-N-CA	5.02	124.68	119.56
1	B	663	PHE	N-CA-C	-5.02	107.33	113.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

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	5340	0	5113	432	0
1	B	5340	0	5111	340	0
1	C	5340	0	5113	424	0
1	D	5340	0	5111	364	0
2	E	28	0	25	3	0
2	I	28	0	25	3	0
3	F	24	0	22	4	0
4	G	39	0	34	1	0
4	K	39	0	34	5	0
5	H	60	0	52	3	0
5	L	60	0	52	0	0
6	J	38	0	34	5	0
7	A	28	0	26	4	0
7	B	42	0	39	3	0
7	C	28	0	26	2	0
7	D	42	0	39	2	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	A	7	0	0	0	0
9	B	8	0	0	0	0
9	C	8	0	0	0	0
9	D	7	0	0	0	0
10	A	2	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	19	0	0	5	0
11	B	20	0	0	5	0
11	C	11	0	0	5	0
11	D	9	0	0	4	0
All	All	21917	0	20856	1471	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 34.

All (1471) 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:B:360:VAL:HG11	1:B:363:ILE:HG13	1.37	1.04
1:C:90:ARG:HG2	1:C:91:PRO:HD2	1.42	1.02
1:B:106:LYS:HB2	1:B:637:ARG:HH21	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HG2	1:A:91:PRO:HD2	1.43	0.96
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.45	0.95
1:D:360:VAL:HG11	1:D:363:ILE:HG13	1.49	0.94
1:C:441:ARG:HD2	11:C:2006:HOH:O	1.70	0.92
1:D:195:LEU:HB3	1:D:201:TYR:HB2	1.51	0.92
1:C:587:LEU:HD12	1:C:588:TYR:N	1.86	0.91
1:C:344:PHE:HA	1:C:390:GLY:HA2	1.50	0.90
1:C:278:GLU:O	1:C:282:GLU:HG3	1.72	0.90
4:K:2:NAG:O3	4:K:3:BMA:H2	1.72	0.90
1:D:225:THR:HB	1:D:227:PHE:CE1	2.07	0.89
6:J:1:NAG:H61	6:J:2:NAG:C1	2.02	0.89
1:B:242:HIS:HD2	1:B:244:GLY:H	1.17	0.89
1:A:187:GLU:HB3	1:A:274:LEU:HD12	1.55	0.89
1:B:187:GLU:HB3	1:B:274:LEU:HD11	1.56	0.88
1:C:192:SER:HB2	1:C:203:HIS:HE1	1.39	0.88
1:C:315:GLN:HG3	1:D:315:GLN:HE21	1.38	0.88
1:D:187:GLU:HB3	1:D:274:LEU:HD11	1.54	0.88
1:D:548:PRO:HG3	1:D:560:GLN:HE22	1.37	0.88
1:C:360:VAL:HG22	1:C:530:LEU:HD23	1.56	0.87
3:F:1:NAG:H4	3:F:2:FUC:H61	1.55	0.87
1:B:184:PHE:CD2	1:B:206:ARG:HD2	2.11	0.86
1:D:242:HIS:HD2	1:D:244:GLY:H	1.21	0.85
1:B:548:PRO:HG3	1:B:560:GLN:HE22	1.40	0.85
1:A:587:LEU:HD12	1:A:588:TYR:N	1.93	0.84
1:B:225:THR:HB	1:B:227:PHE:CE1	2.13	0.84
1:C:608:LEU:HD11	1:C:704:PHE:CE1	2.13	0.84
1:B:195:LEU:HB3	1:B:201:TYR:HB2	1.59	0.84
1:D:180:ASP:HB3	1:D:206:ARG:HH12	1.42	0.84
1:C:187:GLU:HB3	1:C:274:LEU:HD12	1.58	0.83
1:B:360:VAL:HG11	1:B:363:ILE:CG1	2.08	0.83
1:A:315:GLN:HG3	1:B:315:GLN:NE2	1.92	0.83
1:A:329:ARG:HH21	1:A:336:THR:HG23	1.44	0.83
1:B:134:PRO:O	1:B:136:PRO:HD3	1.77	0.83
1:C:315:GLN:HG3	1:D:315:GLN:NE2	1.93	0.83
1:A:278:GLU:O	1:A:282:GLU:HG3	1.79	0.82
1:D:134:PRO:O	1:D:136:PRO:HD3	1.80	0.82
1:A:315:GLN:HG3	1:B:315:GLN:HE21	1.44	0.82
1:B:441:ARG:HD2	11:B:2011:HOH:O	1.77	0.82
1:C:439:PRO:HA	1:C:456:ALA:HA	1.61	0.82
1:A:441:ARG:HG2	1:A:441:ARG:HH11	1.43	0.81
1:A:198:CYS:HB3	1:A:288:VAL:HG11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:ND2	1:B:132:ARG:HB3	1.95	0.81
1:B:173:PHE:HE2	1:B:177:LEU:HD11	1.45	0.81
1:D:210:THR:HG22	1:D:229:LEU:HD22	1.62	0.80
1:D:94:ASN:ND2	1:D:132:ARG:HB3	1.96	0.80
1:D:163:PRO:HB3	4:K:1:NAG:H82	1.63	0.80
1:B:106:LYS:HB2	1:B:637:ARG:NH2	1.97	0.79
1:A:58:GLN:HE22	1:A:327:GLY:HA3	1.47	0.79
1:B:469:LEU:HD12	1:B:471:PAQ:H3	1.65	0.78
1:A:360:VAL:HG21	1:A:363:ILE:HD11	1.65	0.78
1:D:225:THR:HB	1:D:227:PHE:HE1	1.47	0.78
1:A:588:TYR:HB3	1:A:604:ARG:HA	1.66	0.77
1:C:544:MET:HE2	1:D:613:GLU:HB2	1.66	0.77
1:A:546:PHE:CD1	1:B:616:PRO:HD3	2.20	0.77
1:C:264:VAL:HG13	1:C:271:TYR:HB2	1.66	0.77
1:A:202:LYS:C	1:A:204:ARG:H	1.92	0.77
1:A:264:VAL:CG1	1:A:271:TYR:HB2	2.15	0.77
1:A:608:LEU:HD11	1:A:704:PHE:CE1	2.19	0.77
1:A:588:TYR:HB2	1:A:603:TYR:O	1.85	0.76
1:C:198:CYS:HB3	1:C:288:VAL:HG11	1.67	0.76
1:C:157:VAL:O	1:C:161:GLY:HA2	1.84	0.76
1:B:216:ARG:HD2	1:B:225:THR:OG1	1.86	0.76
1:C:514:HIS:HE1	11:C:2007:HOH:O	1.65	0.76
1:C:329:ARG:HH21	1:C:336:THR:HG23	1.51	0.76
1:C:361:TYR:HB2	1:C:531:ASP:OD2	1.86	0.76
1:A:111:ALA:O	1:A:115:ARG:HB2	1.86	0.76
1:C:587:LEU:HD12	1:C:588:TYR:H	1.49	0.76
1:A:264:VAL:HG13	1:A:271:TYR:HB2	1.68	0.76
1:A:145:PRO:HD3	1:A:151:TYR:CE2	2.20	0.75
1:C:588:TYR:HB3	1:C:604:ARG:HA	1.67	0.75
1:D:360:VAL:HG11	1:D:363:ILE:CG1	2.17	0.75
1:A:182:MET:HE1	1:A:260:THR:HA	1.69	0.74
1:A:335:TRP:CE2	1:A:479:PHE:HB3	2.21	0.74
1:A:647:VAL:HG12	11:A:2015:HOH:O	1.88	0.74
1:B:636:GLN:NE2	1:B:667:GLU:HB3	2.02	0.74
1:C:192:SER:CB	1:C:203:HIS:HE1	1.99	0.74
1:D:636:GLN:NE2	1:D:667:GLU:HB3	2.02	0.74
1:C:360:VAL:HG22	1:C:530:LEU:CD2	2.18	0.74
1:D:544:MET:HE3	1:D:562:LEU:HD11	1.69	0.74
1:A:157:VAL:O	1:A:161:GLY:HA2	1.87	0.74
1:A:375:ASN:HD22	1:A:376:SER:N	1.85	0.74
1:C:125:LEU:HD11	1:C:140:GLU:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HB3	1:A:201:TYR:CB	2.18	0.73
1:A:198:CYS:HA	1:A:290:LEU:CD2	2.18	0.73
1:B:344:PHE:HA	1:B:390:GLY:HA2	1.69	0.73
1:A:106:LYS:HB2	1:A:637:ARG:NH1	2.03	0.73
1:C:195:LEU:HB3	1:C:201:TYR:CB	2.18	0.73
1:C:360:VAL:HG11	1:C:363:ILE:HG13	1.71	0.73
1:C:588:TYR:HB2	1:C:603:TYR:O	1.88	0.73
1:D:389:PHE:HE1	1:D:650:GLN:HE21	1.37	0.72
1:A:198:CYS:HA	1:A:290:LEU:HD23	1.71	0.72
1:B:687:HIS:ND1	1:B:689:GLU:HG2	2.04	0.72
1:C:264:VAL:CG1	1:C:271:TYR:HB2	2.19	0.72
1:C:546:PHE:CD1	1:D:616:PRO:HD3	2.23	0.72
1:C:58:GLN:HE22	1:C:327:GLY:HA3	1.55	0.72
1:A:88:GLN:O	1:A:174:GLN:HG2	1.90	0.72
1:B:229:LEU:HD12	1:B:245:LEU:HD23	1.70	0.72
1:D:369:LEU:HD11	1:D:371:ILE:HG13	1.70	0.72
1:B:544:MET:HE3	1:B:562:LEU:HD11	1.71	0.72
2:I:1:NAG:H61	2:I:2:NAG:H82	1.70	0.72
1:A:184:PHE:CE2	1:A:206:ARG:HG3	2.25	0.72
1:A:588:TYR:CB	1:A:604:ARG:HA	2.19	0.72
1:C:234:SER:HB3	7:C:1735:NAG:O6	1.89	0.72
1:C:212:THR:HG22	11:C:2001:HOH:O	1.90	0.71
1:C:98:SER:HB3	1:C:417:LEU:HD23	1.73	0.71
1:A:76:THR:HG22	1:A:83:LEU:HD23	1.72	0.71
1:D:185:ASN:O	1:D:189:PRO:HG2	1.91	0.71
1:C:111:ALA:O	1:C:115:ARG:HB2	1.91	0.71
1:C:335:TRP:CE2	1:C:479:PHE:HB3	2.26	0.71
3:F:2:FUC:H63	3:F:2:FUC:H2	1.73	0.71
1:A:468:LEU:HD12	1:A:473:TYR:HE1	1.56	0.70
1:A:317:TYR:CD2	1:A:321:PRO:HA	2.26	0.70
1:A:441:ARG:HG2	1:A:441:ARG:NH1	2.06	0.70
1:D:141:LEU:HD23	1:D:154:ASP:HA	1.72	0.70
1:A:374:GLY:HA2	1:A:507:TYR:HB3	1.73	0.70
1:B:209:VAL:HG12	7:B:1735:NAG:H82	1.72	0.70
1:C:475:TRP:CE3	1:C:489:PHE:HB2	2.27	0.70
1:D:228:GLY:O	1:D:229:LEU:HD23	1.91	0.70
1:C:469:LEU:HG	1:C:471:PAQ:C4	2.21	0.70
1:B:225:THR:HB	1:B:227:PHE:HE1	1.55	0.70
1:C:360:VAL:HG21	1:C:363:ILE:HD11	1.73	0.70
1:A:272:ASP:HB2	1:A:276:GLN:NE2	2.07	0.70
1:A:475:TRP:CE3	1:A:489:PHE:HB2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:TRP:CZ3	1:B:592:ASN:HB2	2.25	0.70
1:D:596:LYS:HD3	1:D:597:TRP:CZ2	2.27	0.69
1:B:185:ASN:O	1:B:189:PRO:HG2	1.92	0.69
1:A:361:TYR:HB2	1:A:531:ASP:OD2	1.92	0.69
1:A:587:LEU:HD12	1:A:588:TYR:H	1.55	0.69
1:A:636:GLN:NE2	1:A:667:GLU:HB3	2.06	0.69
1:B:588:TYR:HB3	1:B:604:ARG:HA	1.73	0.69
1:C:229:LEU:O	1:C:243:VAL:HG22	1.92	0.69
1:C:532:VAL:HB	1:C:537:ASN:ND2	2.06	0.69
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.57	0.69
1:C:73:ARG:O	1:C:77:GLN:HG3	1.93	0.69
1:C:192:SER:HB2	1:C:203:HIS:CE1	2.26	0.69
1:C:220:SER:HB2	1:C:654:TRP:HB2	1.74	0.69
1:D:234:SER:HB3	7:D:1735:NAG:O6	1.92	0.69
1:B:170:PRO:HA	1:B:651:ASN:ND2	2.07	0.68
1:B:469:LEU:HD12	1:B:471:PAQ:C3	2.23	0.68
1:C:242:HIS:CD2	1:C:498:ALA:HA	2.28	0.68
1:C:251:HIS:CD2	1:C:251:HIS:H	2.11	0.68
1:C:198:CYS:HA	1:C:290:LEU:CD2	2.23	0.68
1:B:187:GLU:HB3	1:B:274:LEU:CD1	2.23	0.68
1:B:468:LEU:HB2	1:B:471:PAQ:HN1	1.58	0.68
1:D:468:LEU:HB2	1:D:471:PAQ:HN1	1.57	0.68
1:A:229:LEU:O	1:A:243:VAL:HG22	1.93	0.68
1:C:198:CYS:HA	1:C:290:LEU:HD23	1.74	0.68
1:A:82:GLY:O	1:A:94:ASN:HB2	1.94	0.68
1:A:468:LEU:HB2	1:A:471:PAQ:HN1	1.57	0.68
1:B:360:VAL:HG22	1:B:530:LEU:HD23	1.76	0.68
1:C:608:LEU:HD11	1:C:704:PHE:HE1	1.56	0.68
1:B:632:LEU:HD12	1:B:633:ALA:H	1.59	0.68
1:C:612:GLY:HA2	1:D:585:ARG:NE	2.09	0.68
1:C:392:GLY:O	1:C:395:THR:HG22	1.93	0.67
1:A:376:SER:HB2	11:A:2002:HOH:O	1.93	0.67
1:C:306:VAL:HG21	1:D:718:TYR:O	1.95	0.67
1:D:147:PRO:O	1:D:149:PRO:HD3	1.95	0.67
1:A:202:LYS:C	1:A:204:ARG:N	2.50	0.67
1:A:350:PHE:CD2	1:A:362:GLU:HB2	2.30	0.67
1:C:380:MET:HG3	1:D:561:ARG:NE	2.09	0.67
1:A:360:VAL:HG22	1:A:530:LEU:HD23	1.77	0.67
1:C:169:ARG:HH11	1:C:169:ARG:HG2	1.59	0.67
1:C:315:GLN:HA	1:D:314:LEU:O	1.95	0.67
1:C:432:PHE:O	1:C:460:LEU:HD12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:CD2	1:A:251:HIS:H	2.11	0.66
1:D:106:LYS:HB2	1:D:637:ARG:HH21	1.60	0.66
1:C:588:TYR:CB	1:C:604:ARG:HA	2.24	0.66
1:B:242:HIS:CD2	1:B:244:GLY:H	2.07	0.66
1:C:76:THR:HG22	1:C:83:LEU:HD23	1.77	0.66
1:A:195:LEU:HB3	1:A:201:TYR:HB3	1.77	0.66
1:B:67:GLU:HG2	1:B:146:LEU:HD13	1.78	0.66
1:B:334:LEU:HB3	1:B:354:PHE:CE1	2.30	0.66
1:C:360:VAL:HG11	1:C:363:ILE:CG1	2.26	0.66
1:A:198:CYS:CB	1:A:288:VAL:HG11	2.25	0.66
1:C:225:THR:HB	1:C:227:PHE:CE1	2.30	0.66
1:D:360:VAL:HG22	1:D:530:LEU:HD23	1.78	0.66
1:A:182:MET:HE1	1:A:260:THR:CA	2.26	0.66
1:C:242:HIS:HD2	1:C:498:ALA:HA	1.61	0.66
1:D:276:GLN:O	1:D:280:GLN:HG3	1.96	0.66
1:B:369:LEU:HD12	1:B:370:ALA:H	1.61	0.66
1:C:317:TYR:CD2	1:C:321:PRO:HA	2.31	0.66
1:C:539:VAL:O	1:C:568:LEU:HD12	1.96	0.66
1:B:376:SER:O	1:B:380:MET:HB2	1.96	0.65
1:D:210:THR:HG22	1:D:229:LEU:CD2	2.26	0.65
1:D:334:LEU:HB3	1:D:354:PHE:CE1	2.31	0.65
1:A:140:GLU:OE1	1:A:160:HIS:CD2	2.50	0.65
1:A:403:ASP:OD1	1:B:442:ARG:HG3	1.97	0.65
1:B:182:MET:HG3	1:B:186:ARG:HH21	1.60	0.65
1:C:468:LEU:HB2	1:C:471:PAQ:HN1	1.62	0.65
1:A:507:TYR:O	1:A:519:VAL:HG12	1.96	0.65
1:C:640:GLU:C	1:C:642:PRO:HD3	2.22	0.65
1:A:67:GLU:O	1:A:71:VAL:HG23	1.95	0.65
1:B:180:ASP:HB3	1:B:206:ARG:HH12	1.62	0.65
1:C:195:LEU:HB3	1:C:201:TYR:HB3	1.79	0.65
1:C:539:VAL:CG1	1:C:569:LEU:HD12	2.27	0.65
1:B:595:ASN:HB3	1:B:601:ARG:HG2	1.79	0.65
1:C:183:ILE:HG22	1:C:188:LEU:HG	1.78	0.65
1:D:198:CYS:SG	1:D:199:CYS:N	2.68	0.65
1:D:584:PRO:HG2	1:D:587:LEU:HB2	1.79	0.65
5:H:2:NAG:O3	5:H:2:NAG:H83	1.97	0.65
1:B:596:LYS:HD3	1:B:597:TRP:CZ2	2.32	0.65
1:C:398:LEU:HD13	1:C:404:CYS:SG	2.37	0.65
1:C:455:LEU:HD13	1:C:722:SER:HA	1.78	0.65
1:A:517:GLY:HA3	1:A:686:PRO:HB2	1.77	0.65
1:D:588:TYR:HB3	1:D:604:ARG:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HH21	1:A:256:PRO:HD2	1.62	0.65
1:C:226:TRP:CD1	1:C:248:LEU:HD13	2.30	0.65
1:D:687:HIS:ND1	1:D:689:GLU:HG2	2.12	0.65
1:A:542:GLU:HA	1:A:565:THR:O	1.96	0.65
1:B:370:ALA:HA	1:B:521:THR:O	1.96	0.65
1:C:375:ASN:HD22	1:C:376:SER:N	1.93	0.64
1:A:445:SER:O	1:A:450:HIS:HA	1.97	0.64
1:D:451:TYR:HA	1:D:726:ARG:HA	1.80	0.64
1:A:402:VAL:HA	1:B:456:ALA:HB2	1.80	0.64
1:C:76:THR:HA	1:C:83:LEU:CD2	2.27	0.64
1:D:317:TYR:HE1	1:D:433:GLU:HB2	1.61	0.64
1:B:478:VAL:HB	1:B:486:GLU:HB3	1.79	0.64
1:C:370:ALA:HA	1:C:521:THR:O	1.98	0.64
1:D:170:PRO:HA	1:D:651:ASN:ND2	2.12	0.64
1:A:220:SER:HB2	1:A:654:TRP:HB2	1.80	0.64
1:C:573:GLU:CG	1:C:666:ASN:ND2	2.60	0.64
1:D:539:VAL:HG22	1:D:589:LEU:HD22	1.79	0.64
1:B:106:LYS:CB	1:B:637:ARG:HH21	2.08	0.64
1:C:537:ASN:HA	1:C:590:ALA:O	1.97	0.64
1:C:539:VAL:HB	1:C:569:LEU:HB2	1.79	0.64
1:D:187:GLU:HB3	1:D:274:LEU:CD1	2.26	0.64
1:B:179:ILE:O	1:B:183:ILE:HG13	1.98	0.64
1:C:187:GLU:HB3	1:C:274:LEU:CD1	2.27	0.64
1:D:344:PHE:HA	1:D:390:GLY:HA2	1.80	0.64
1:A:573:GLU:HG3	1:A:666:ASN:ND2	2.13	0.63
1:C:462:VAL:HB	1:C:477:THR:HG23	1.80	0.63
1:C:646:SER:HB2	1:C:658:VAL:HG23	1.79	0.63
1:D:106:LYS:HB2	1:D:637:ARG:NH2	2.13	0.63
1:D:334:LEU:HB3	1:D:354:PHE:HE1	1.63	0.63
1:D:329:ARG:NH2	1:D:336:THR:HB	2.14	0.63
1:D:570:GLU:O	1:D:668:THR:HA	1.98	0.63
1:C:143:VAL:HG12	1:C:144:GLY:N	2.14	0.63
1:B:141:LEU:HD23	1:B:154:ASP:HA	1.80	0.63
1:B:173:PHE:CE2	1:B:177:LEU:HD11	2.31	0.63
1:B:334:LEU:HB3	1:B:354:PHE:HE1	1.64	0.63
1:C:542:GLU:HA	1:C:565:THR:O	1.99	0.63
1:A:649:ASN:HA	11:A:2016:HOH:O	1.98	0.63
1:B:198:CYS:HB3	1:B:288:VAL:HG11	1.80	0.63
1:C:225:THR:HB	1:C:227:PHE:HE1	1.64	0.63
1:D:216:ARG:HD2	1:D:225:THR:OG1	1.99	0.63
1:D:369:LEU:HD11	1:D:371:ILE:CG1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:CG	1:A:91:PRO:HD2	2.26	0.62
1:A:206:ARG:O	7:A:1734:NAG:H81	1.99	0.62
1:A:640:GLU:CD	1:A:640:GLU:H	2.06	0.62
1:A:536:GLU:N	1:A:536:GLU:CD	2.58	0.62
1:B:687:HIS:CE1	1:B:689:GLU:HG2	2.34	0.62
1:A:157:VAL:HG23	1:A:158:GLU:H	1.65	0.62
1:C:636:GLN:NE2	1:C:667:GLU:HB3	2.15	0.62
1:A:245:LEU:HD12	1:A:265:PHE:O	1.99	0.62
1:B:389:PHE:HE1	1:B:650:GLN:HE21	1.47	0.62
1:B:509:ASN:ND2	1:B:686:PRO:O	2.29	0.62
1:A:183:ILE:HG22	1:A:188:LEU:HG	1.81	0.62
1:B:632:LEU:HD12	1:B:633:ALA:N	2.14	0.62
1:C:334:LEU:HD13	1:C:481:PRO:HA	1.81	0.62
1:D:441:ARG:HG2	1:D:441:ARG:HH11	1.64	0.62
1:A:67:GLU:HB3	1:A:146:LEU:CD2	2.29	0.62
1:A:392:GLY:O	1:A:395:THR:HG22	1.99	0.62
1:C:640:GLU:CD	1:C:640:GLU:H	2.07	0.62
1:D:242:HIS:CD2	1:D:244:GLY:H	2.11	0.62
1:A:536:GLU:CD	1:A:536:GLU:H	2.08	0.61
1:A:539:VAL:O	1:A:568:LEU:HD12	1.99	0.61
1:B:276:GLN:O	1:B:280:GLN:HG3	1.99	0.61
1:B:539:VAL:HG22	1:B:589:LEU:HD22	1.82	0.61
1:C:78:ARG:NH1	1:C:78:ARG:HB3	2.15	0.61
1:D:468:LEU:HD12	1:D:473:TYR:CE1	2.35	0.61
1:A:182:MET:HE2	1:A:261:ILE:HD11	1.82	0.61
1:B:316:PHE:HE1	1:B:318:PRO:HA	1.65	0.61
1:A:125:LEU:HD22	1:A:159:ARG:HH12	1.65	0.61
1:A:369:LEU:HA	1:A:384:TYR:O	2.00	0.61
1:A:439:PRO:HA	1:A:456:ALA:HA	1.80	0.61
1:B:210:THR:HG22	1:B:229:LEU:CD2	2.29	0.61
1:B:451:TYR:HA	1:B:726:ARG:HA	1.82	0.61
1:A:608:LEU:HD11	1:A:704:PHE:HE1	1.62	0.61
1:C:90:ARG:O	1:C:93:ASP:HB2	2.00	0.61
1:D:98:SER:O	1:D:126:ALA:HA	2.00	0.61
1:A:138:VAL:O	1:A:164:LEU:HB2	2.00	0.61
1:B:239:PHE:CD2	1:B:470:ASN:HB3	2.36	0.61
1:B:595:ASN:O	1:B:597:TRP:N	2.34	0.61
1:D:386:ASP:HB3	1:D:468:LEU:HD13	1.82	0.61
1:A:75:LEU:O	1:A:79:LEU:HB2	2.00	0.61
1:A:316:PHE:HA	1:A:407:LEU:HD12	1.82	0.61
1:B:497:SER:HB2	1:B:515:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ILE:O	1:C:702:GLY:HA3	2.00	0.61
1:C:619:SER:HB2	1:D:560:GLN:HG3	1.82	0.61
1:C:106:LYS:HE2	1:C:110:LEU:HD11	1.83	0.61
1:C:184:PHE:CD2	1:C:206:ARG:HG3	2.36	0.61
1:A:432:PHE:O	1:A:460:LEU:HD12	2.00	0.61
1:C:402:VAL:HA	1:D:456:ALA:HB2	1.82	0.61
1:A:467:THR:HG23	1:A:472:ASP:OD2	2.00	0.61
1:C:316:PHE:HA	1:C:407:LEU:HD12	1.82	0.61
1:D:538:TRP:CZ3	1:D:592:ASN:HB2	2.36	0.61
1:A:472:ASP:OD1	1:A:493:GLY:HA3	2.01	0.60
1:C:153:ARG:NH1	1:C:153:ARG:HB3	2.15	0.60
1:C:573:GLU:HG2	1:C:666:ASN:ND2	2.15	0.60
1:A:310:PRO:HA	1:B:319:GLN:NE2	2.16	0.60
1:A:360:VAL:HG11	1:A:363:ILE:CG1	2.31	0.60
1:B:209:VAL:HG12	7:B:1735:NAG:C8	2.30	0.60
1:C:85:ASP:OD2	1:C:420:GLN:HG3	2.01	0.60
1:C:167:HIS:CD2	1:C:221:GLY:HA2	2.35	0.60
1:A:157:VAL:HG23	1:A:158:GLU:N	2.16	0.60
1:A:315:GLN:HE22	1:A:434:GLN:HA	1.66	0.60
1:A:584:PRO:HG2	1:A:587:LEU:HB2	1.83	0.60
1:C:184:PHE:CE2	1:C:206:ARG:HG3	2.36	0.60
1:C:468:LEU:HD12	1:C:473:TYR:HE1	1.66	0.60
1:C:525:HIS:HB2	1:C:627:TRP:CE3	2.36	0.60
1:C:561:ARG:NH2	1:D:380:MET:HE2	2.16	0.60
1:A:90:ARG:HG2	1:A:91:PRO:CD	2.25	0.60
1:A:225:THR:HB	1:A:227:PHE:HE1	1.66	0.60
1:A:232:ASN:HB2	7:A:1734:NAG:H83	1.83	0.60
1:A:468:LEU:HD12	1:A:473:TYR:CE1	2.35	0.60
1:B:72:MET:O	1:B:76:THR:HG23	2.00	0.60
1:B:517:GLY:HA3	1:B:686:PRO:HB2	1.83	0.60
1:D:153:ARG:O	1:D:155:VAL:HG13	2.01	0.60
1:A:487:ILE:O	1:A:702:GLY:HA3	2.02	0.60
1:C:180:ASP:O	1:C:184:PHE:HD1	1.84	0.60
1:A:187:GLU:HB3	1:A:274:LEU:CD1	2.29	0.60
1:A:532:VAL:HB	1:A:537:ASN:ND2	2.16	0.60
1:B:507:TYR:O	1:B:519:VAL:HG12	2.01	0.60
1:C:329:ARG:HH21	1:C:336:THR:CG2	2.13	0.60
1:D:296:THR:HG22	1:D:297:GLY:N	2.16	0.60
1:A:110:LEU:O	1:A:114:ASP:OD2	2.20	0.60
1:A:225:THR:HB	1:A:227:PHE:CE1	2.36	0.60
1:A:380:MET:HE3	1:B:559:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:HE3	1:A:561:ARG:HB3	1.84	0.60
1:B:468:LEU:HD12	1:B:473:TYR:CE1	2.35	0.60
1:D:497:SER:HB2	1:D:515:THR:HG22	1.83	0.60
1:A:133:GLN:HB2	1:A:134:PRO:HD2	1.82	0.60
1:A:167:HIS:CD2	1:A:221:GLY:HA2	2.37	0.60
1:C:110:LEU:HD21	1:C:361:TYR:CD1	2.37	0.60
1:D:381:THR:HG22	1:D:381:THR:O	2.02	0.60
1:B:386:ASP:HB3	1:B:468:LEU:HD13	1.84	0.60
1:C:353:ARG:HA	1:C:357:GLU:O	2.01	0.60
1:D:67:GLU:HG2	1:D:146:LEU:HD13	1.82	0.60
1:A:640:GLU:C	1:A:642:PRO:HD3	2.27	0.59
1:B:349:ILE:HD12	1:B:477:THR:HG21	1.82	0.59
1:A:544:MET:HE2	1:B:613:GLU:HB2	1.83	0.59
1:A:564:VAL:HG22	1:B:506:LYS:HA	1.84	0.59
1:D:198:CYS:HB3	1:D:288:VAL:HG11	1.84	0.59
1:A:170:PRO:HA	1:A:651:ASN:HD21	1.67	0.59
1:A:317:TYR:CD1	1:A:317:TYR:N	2.69	0.59
1:D:469:LEU:HD12	1:D:471:PAQ:H3	1.82	0.59
1:A:315:GLN:HA	1:B:314:LEU:O	2.03	0.59
1:A:395:THR:HA	1:A:466:SER:HA	1.83	0.59
1:A:576:ALA:HA	1:A:633:ALA:HA	1.83	0.59
1:B:98:SER:O	1:B:126:ALA:HA	2.02	0.59
1:C:157:VAL:HA	1:C:162:GLY:H	1.65	0.59
1:C:191:ALA:HA	1:C:278:GLU:HB2	1.85	0.59
1:C:217:GLY:HA3	1:C:222:ASP:CB	2.31	0.59
1:C:231:TYR:CE1	1:C:293:ASP:HA	2.38	0.59
1:D:687:HIS:CE1	1:D:689:GLU:HG2	2.37	0.59
1:C:125:LEU:HD22	1:C:159:ARG:HH12	1.67	0.59
1:C:133:GLN:NE2	1:C:135:GLN:O	2.32	0.59
1:A:469:LEU:HG	1:A:471:PAQ:C4	2.32	0.59
1:B:181:GLN:O	1:B:185:ASN:HB2	2.02	0.59
1:C:67:GLU:O	1:C:71:VAL:HG23	2.03	0.59
1:C:369:LEU:HD12	1:C:384:TYR:O	2.03	0.59
1:A:272:ASP:HB2	1:A:276:GLN:HE22	1.66	0.59
1:A:537:ASN:HA	1:A:590:ALA:O	2.03	0.59
1:C:352:VAL:O	1:C:358:ARG:HA	2.01	0.59
1:C:474:VAL:O	1:C:489:PHE:HA	2.03	0.59
1:A:724:TYR:O	1:A:725:PHE:HB3	2.03	0.59
1:B:646:SER:OG	1:B:648:PHE:HD1	1.86	0.59
1:C:85:ASP:CG	1:C:420:GLN:HG3	2.28	0.59
1:D:182:MET:HG3	1:D:186:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:VAL:O	1:D:489:PHE:HA	2.03	0.59
1:C:530:LEU:HD21	1:C:705:LEU:HD13	1.85	0.59
1:A:579:VAL:HA	1:A:631:GLN:HG3	1.85	0.58
1:D:223:ARG:HG2	1:D:223:ARG:HH11	1.67	0.58
1:D:130:PHE:CE1	4:K:1:NAG:H62	2.37	0.58
1:A:247:LEU:HD23	1:A:264:VAL:HG23	1.85	0.58
1:B:198:CYS:SG	1:B:199:CYS:N	2.76	0.58
1:D:360:VAL:HG22	1:D:530:LEU:CD2	2.33	0.58
1:B:299:SER:HG	1:B:300:TRP:CD1	2.21	0.58
1:C:549:MET:HE3	1:C:561:ARG:HB3	1.85	0.58
1:B:58:GLN:OE1	1:B:328:SER:HB2	2.04	0.58
1:B:200:PHE:CD2	1:B:200:PHE:N	2.70	0.58
1:B:312:PRO:O	1:B:313:PRO:C	2.47	0.58
1:C:588:TYR:HB3	1:C:604:ARG:CA	2.34	0.58
1:D:90:ARG:HH12	1:D:178:ASP:CG	2.12	0.58
1:A:360:VAL:HG22	1:A:530:LEU:CD2	2.34	0.58
1:B:229:LEU:O	1:B:243:VAL:HG22	2.04	0.58
1:B:466:SER:HB3	1:B:475:TRP:HE1	1.68	0.58
1:C:138:VAL:O	1:C:164:LEU:HB2	2.03	0.58
1:C:462:VAL:HB	1:C:477:THR:CG2	2.33	0.58
1:C:623:ARG:HB3	1:C:656:PRO:HG2	1.85	0.58
1:A:163:PRO:O	1:A:165:PRO:HD3	2.04	0.58
1:B:170:PRO:HA	1:B:651:ASN:HD22	1.67	0.58
1:C:374:GLY:HA2	1:C:507:TYR:HB3	1.86	0.58
4:K:1:NAG:H61	4:K:2:NAG:C1	2.34	0.58
1:A:125:LEU:HD22	1:A:159:ARG:NH1	2.18	0.58
1:A:334:LEU:HD13	1:A:481:PRO:HA	1.85	0.58
1:B:570:GLU:O	1:B:668:THR:HA	2.04	0.58
1:D:509:ASN:ND2	1:D:686:PRO:O	2.30	0.58
1:A:180:ASP:O	1:A:184:PHE:HD1	1.87	0.57
1:B:106:LYS:HE3	1:B:361:TYR:CG	2.39	0.57
1:B:584:PRO:HG2	1:B:587:LEU:HB2	1.86	0.57
1:C:507:TYR:O	1:C:519:VAL:HG12	2.04	0.57
1:A:90:ARG:O	1:A:93:ASP:HB2	2.04	0.57
1:A:588:TYR:HB3	1:A:604:ARG:CA	2.33	0.57
1:C:376:SER:O	1:C:380:MET:HB2	2.04	0.57
1:A:386:ASP:OD1	1:A:471:PAQ:N3	2.36	0.57
1:B:525:HIS:HE2	1:B:677:TRP:HB3	1.69	0.57
1:C:366:GLN:OE1	1:C:643:SER:HA	2.05	0.57
1:C:561:ARG:CZ	1:D:380:MET:HE2	2.35	0.57
1:D:138:VAL:HG11	1:D:169:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG23	1:A:176:TYR:OH	2.05	0.57
1:A:206:ARG:O	7:A:1734:NAG:C8	2.53	0.57
1:A:548:PRO:HA	1:A:559:LEU:O	2.04	0.57
1:A:145:PRO:HD3	1:A:151:TYR:CD2	2.40	0.57
1:C:536:GLU:CD	1:C:536:GLU:H	2.12	0.57
1:C:573:GLU:HG3	1:C:666:ASN:ND2	2.20	0.57
1:A:157:VAL:O	1:A:161:GLY:CA	2.53	0.57
1:A:455:LEU:HD13	1:A:722:SER:HA	1.87	0.57
1:C:319:GLN:NE2	1:D:311:ALA:H	2.02	0.57
1:C:539:VAL:HG12	1:C:569:LEU:HD12	1.86	0.57
1:C:724:TYR:O	1:C:725:PHE:HB3	2.04	0.57
1:D:195:LEU:HB3	1:D:201:TYR:CB	2.32	0.57
1:D:487:ILE:O	1:D:702:GLY:HA3	2.05	0.57
1:B:296:THR:HG22	1:B:297:GLY:N	2.19	0.57
1:B:369:LEU:HD11	1:B:371:ILE:HG13	1.87	0.57
1:C:722:SER:HB3	1:D:304:SER:HB2	1.87	0.57
1:A:336:THR:HG21	1:A:353:ARG:HD2	1.87	0.57
1:D:200:PHE:N	1:D:200:PHE:CD2	2.70	0.57
1:A:380:MET:HE1	1:B:552:PRO:HD2	1.85	0.57
1:D:181:GLN:O	1:D:185:ASN:HB2	2.04	0.57
1:D:508:GLY:HA3	1:D:517:GLY:O	2.04	0.57
1:D:528:VAL:HG23	1:D:676:ALA:O	2.04	0.57
1:A:184:PHE:O	1:A:189:PRO:HD3	2.05	0.56
1:D:349:ILE:HD12	1:D:477:THR:HG21	1.86	0.56
1:A:133:GLN:NE2	1:A:135:GLN:O	2.30	0.56
1:A:225:THR:HG22	1:A:226:TRP:N	2.21	0.56
1:A:242:HIS:CD2	1:A:498:ALA:HA	2.40	0.56
1:A:242:HIS:HD2	1:A:498:ALA:HA	1.70	0.56
1:A:530:LEU:HD21	1:A:705:LEU:HD13	1.87	0.56
1:B:242:HIS:HD2	1:B:244:GLY:N	1.97	0.56
1:B:395:THR:O	1:B:425:ILE:HD13	2.05	0.56
1:C:106:LYS:HB2	1:C:637:ARG:NH1	2.20	0.56
1:C:372:TYR:CD1	1:C:520:HIS:HB3	2.39	0.56
1:D:142:VAL:CG2	1:D:155:VAL:HG11	2.35	0.56
1:D:242:HIS:HD2	1:D:244:GLY:N	2.00	0.56
1:D:376:SER:O	1:D:380:MET:HB2	2.06	0.56
1:D:500:LEU:HD12	1:D:501:PHE:N	2.19	0.56
1:A:231:TYR:CE1	1:A:293:ASP:HA	2.40	0.56
1:C:72:MET:HE3	1:C:420:GLN:HA	1.87	0.56
1:C:112:HIS:ND1	1:C:117:SER:O	2.35	0.56
1:C:125:LEU:HD22	1:C:159:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:PHE:CD2	1:C:362:GLU:HB2	2.41	0.56
1:B:147:PRO:O	1:B:149:PRO:HD3	2.06	0.56
1:C:240:LEU:O	1:C:515:THR:HG21	2.04	0.56
1:D:590:ALA:HA	1:D:602:GLY:HA2	1.87	0.56
1:C:267:GLN:HG2	1:C:499:PHE:CE1	2.41	0.56
1:C:309:GLY:O	1:C:310:PRO:C	2.48	0.56
1:D:632:LEU:HD12	1:D:633:ALA:N	2.20	0.56
1:A:375:ASN:HA	1:B:561:ARG:HH21	1.71	0.56
1:C:86:ALA:HA	1:C:89:ALA:HB2	1.88	0.56
1:D:439:PRO:HA	1:D:456:ALA:HA	1.88	0.56
1:A:201:TYR:HH	1:A:203:HIS:HD1	1.52	0.56
1:B:614:PRO:HG3	1:B:629:ARG:HA	1.88	0.56
1:D:184:PHE:CD2	1:D:206:ARG:HD2	2.40	0.56
1:D:478:VAL:HB	1:D:486:GLU:HB3	1.86	0.56
1:A:226:TRP:CD1	1:A:248:LEU:HD13	2.41	0.56
1:C:247:LEU:HD23	1:C:264:VAL:HG23	1.87	0.56
1:D:159:ARG:HD3	11:D:2001:HOH:O	2.06	0.56
1:D:455:LEU:HD13	1:D:722:SER:HA	1.86	0.56
1:A:185:ASN:O	1:A:186:ARG:HG3	2.05	0.56
1:B:163:PRO:O	1:B:165:PRO:HD3	2.07	0.56
1:A:63:LEU:HD11	1:A:124:ALA:HB2	1.88	0.55
1:A:198:CYS:SG	1:A:199:CYS:N	2.79	0.55
1:C:372:TYR:HE1	11:C:2009:HOH:O	1.89	0.55
6:J:1:NAG:H5	6:J:2:NAG:H82	1.88	0.55
1:A:309:GLY:O	1:A:310:PRO:C	2.47	0.55
1:B:474:VAL:O	1:B:489:PHE:HA	2.07	0.55
1:B:554:SER:N	1:B:555:PRO:HD3	2.21	0.55
1:C:375:ASN:HD22	1:C:375:ASN:C	2.13	0.55
1:C:632:LEU:HD13	1:C:678:VAL:HG22	1.88	0.55
1:D:440:LEU:HB2	1:D:457:GLU:HB2	1.88	0.55
1:D:554:SER:N	1:D:555:PRO:HD3	2.20	0.55
1:D:632:LEU:HD12	1:D:633:ALA:H	1.71	0.55
1:B:508:GLY:HA3	1:B:517:GLY:O	2.05	0.55
1:C:317:TYR:CD1	1:C:317:TYR:N	2.73	0.55
1:D:58:GLN:OE1	1:D:328:SER:HB2	2.06	0.55
1:C:344:PHE:HB3	1:C:387:GLY:O	2.06	0.55
1:D:198:CYS:HA	1:D:290:LEU:HD23	1.89	0.55
1:A:139:SER:HB3	1:A:154:ASP:OD1	2.07	0.55
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.71	0.55
1:C:157:VAL:HG23	1:C:158:GLU:N	2.22	0.55
1:D:152:MET:CE	4:K:2:NAG:H81	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLN:CG	1:D:315:GLN:HE21	2.16	0.55
1:D:72:MET:HE3	1:D:420:GLN:HA	1.89	0.55
1:D:94:ASN:CG	1:D:132:ARG:HB3	2.30	0.55
1:A:499:PHE:CE2	1:A:514:HIS:HB3	2.41	0.55
1:D:91:PRO:HB2	1:D:254:LEU:O	2.06	0.55
1:D:316:PHE:HE1	1:D:318:PRO:HA	1.71	0.55
1:A:306:VAL:HG21	1:B:718:TYR:O	2.06	0.55
1:B:67:GLU:HG2	1:B:146:LEU:HD22	1.87	0.55
1:B:210:THR:HG22	1:B:229:LEU:HD22	1.89	0.55
1:B:247:LEU:HD22	1:B:264:VAL:HG22	1.89	0.55
1:B:468:LEU:HD12	1:B:473:TYR:HE1	1.71	0.55
1:C:140:GLU:OE1	1:C:160:HIS:CD2	2.60	0.55
1:B:216:ARG:HB2	1:B:223:ARG:HA	1.87	0.55
1:C:71:VAL:HG13	1:C:143:VAL:HG11	1.89	0.55
1:D:141:LEU:CD2	1:D:154:ASP:HA	2.37	0.55
1:A:98:SER:HB3	1:A:417:LEU:HD23	1.88	0.54
1:A:612:GLY:HA2	1:B:585:ARG:NE	2.22	0.54
1:C:133:GLN:HB2	1:C:134:PRO:HD2	1.89	0.54
1:C:334:LEU:HD22	1:C:354:PHE:CZ	2.42	0.54
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.89	0.54
1:A:267:GLN:HG2	1:A:499:PHE:CE1	2.42	0.54
1:A:386:ASP:CG	1:A:468:LEU:HD13	2.32	0.54
1:C:88:GLN:O	1:C:174:GLN:HG2	2.07	0.54
1:C:223:ARG:HB3	1:C:252:LYS:HA	1.88	0.54
1:C:584:PRO:HG2	1:C:587:LEU:HB2	1.89	0.54
1:A:709:ASN:N	1:B:689:GLU:OE1	2.35	0.54
1:C:182:MET:HE2	1:C:261:ILE:HD11	1.90	0.54
1:C:184:PHE:O	1:C:189:PRO:HD3	2.07	0.54
1:C:517:GLY:HA3	1:C:686:PRO:HB2	1.88	0.54
1:D:129:PHE:CE1	1:D:169:ARG:HG3	2.42	0.54
1:D:138:VAL:HG23	1:D:164:LEU:CB	2.37	0.54
1:B:173:PHE:CD2	1:B:173:PHE:C	2.85	0.54
1:C:220:SER:HA	1:C:654:TRP:CE3	2.42	0.54
1:C:442:ARG:HG3	1:D:403:ASP:OD1	2.07	0.54
1:A:317:TYR:HD2	1:A:321:PRO:HA	1.73	0.54
1:A:372:TYR:CD1	1:A:520:HIS:HB3	2.43	0.54
1:D:469:LEU:HD12	1:D:471:PAQ:C3	2.38	0.54
5:H:1:NAG:H61	5:H:2:NAG:C1	2.37	0.54
1:B:628:GLU:O	1:B:628:GLU:HG2	2.08	0.54
1:C:322:ARG:NH1	1:D:310:PRO:O	2.40	0.54
1:C:544:MET:CE	1:D:613:GLU:H	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ARG:HH22	1:D:234:SER:HB2	1.73	0.54
1:D:614:PRO:CG	1:D:629:ARG:HG2	2.37	0.54
1:A:76:THR:HG22	1:A:83:LEU:CD2	2.37	0.54
1:A:280:GLN:HE21	1:A:285:LEU:HD23	1.72	0.54
1:B:388:GLY:HA3	1:B:650:GLN:HB2	1.90	0.54
1:B:548:PRO:HG3	1:B:560:GLN:NE2	2.17	0.54
1:C:188:LEU:N	1:C:189:PRO:HD2	2.23	0.54
1:C:500:LEU:HD12	1:C:516:LEU:HB2	1.89	0.54
1:D:91:PRO:CB	1:D:254:LEU:HA	2.38	0.54
1:A:209:VAL:HB	1:B:448:TYR:CE1	2.42	0.54
1:C:67:GLU:HB3	1:C:146:LEU:CD2	2.38	0.54
1:C:445:SER:O	1:C:450:HIS:HA	2.07	0.54
1:D:229:LEU:HD12	1:D:245:LEU:HD23	1.89	0.54
1:A:160:HIS:CE1	1:A:657:THR:HG22	2.43	0.54
1:A:249:VAL:O	1:A:251:HIS:HD2	1.91	0.54
1:A:535:LEU:O	1:A:673:ASP:HA	2.08	0.54
1:B:344:PHE:HA	1:B:390:GLY:CA	2.38	0.54
1:C:536:GLU:CD	1:C:536:GLU:N	2.66	0.54
1:D:229:LEU:O	1:D:243:VAL:HG22	2.06	0.54
1:D:513:GLU:H	1:D:513:GLU:CD	2.15	0.54
1:A:628:GLU:O	1:A:628:GLU:HG2	2.06	0.54
1:C:159:ARG:HG2	1:C:160:HIS:CD2	2.43	0.54
1:A:188:LEU:N	1:A:189:PRO:HD2	2.23	0.53
1:B:381:THR:O	1:B:381:THR:HG22	2.08	0.53
1:C:442:ARG:C	1:C:442:ARG:HD3	2.33	0.53
1:C:616:PRO:HD3	1:D:546:PHE:CD1	2.44	0.53
1:D:517:GLY:HA3	1:D:686:PRO:HB2	1.90	0.53
1:A:601:ARG:NH1	1:A:710:PHE:O	2.41	0.53
1:A:637:ARG:HG3	1:A:637:ARG:O	2.08	0.53
1:C:86:ALA:HA	1:C:89:ALA:CB	2.37	0.53
1:C:441:ARG:HH11	1:C:441:ARG:HG2	1.74	0.53
1:D:329:ARG:HH21	1:D:336:THR:HB	1.73	0.53
1:D:614:PRO:HG3	1:D:629:ARG:HA	1.90	0.53
1:A:85:ASP:CG	1:A:420:GLN:HG3	2.34	0.53
1:B:689:GLU:H	1:B:689:GLU:CD	2.15	0.53
1:C:74:PHE:CZ	1:C:78:ARG:HG3	2.43	0.53
1:C:198:CYS:SG	1:C:199:CYS:N	2.81	0.53
1:C:548:PRO:HA	1:C:559:LEU:O	2.07	0.53
1:C:549:MET:O	1:C:559:LEU:HB3	2.09	0.53
1:D:167:HIS:CD2	1:D:221:GLY:HA2	2.44	0.53
1:A:322:ARG:NH1	1:B:310:PRO:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:VAL:CG1	1:A:569:LEU:HD12	2.38	0.53
1:A:630:TYR:O	1:A:679:THR:HB	2.09	0.53
1:C:576:ALA:HA	1:C:633:ALA:HA	1.91	0.53
1:D:125:LEU:HD11	1:D:140:GLU:HB3	1.90	0.53
1:A:329:ARG:HH21	1:A:336:THR:CG2	2.19	0.53
1:B:382:THR:HG21	1:B:384:TYR:CE2	2.43	0.53
1:B:642:PRO:HB3	11:B:2017:HOH:O	2.09	0.53
1:C:573:GLU:HG2	1:C:666:ASN:HD22	1.73	0.53
1:A:85:ASP:OD2	1:A:420:GLN:HG3	2.08	0.53
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.24	0.53
1:C:96:VAL:HG22	1:C:128:VAL:HG22	1.91	0.53
1:C:311:ALA:HB3	1:D:318:PRO:HG2	1.90	0.53
1:B:212:THR:OG1	1:B:216:ARG:NH1	2.41	0.53
1:C:722:SER:HB3	1:D:304:SER:CB	2.39	0.53
1:D:388:GLY:HA3	1:D:650:GLN:HB2	1.89	0.53
1:D:388:GLY:HA3	1:D:650:GLN:CB	2.38	0.53
1:A:182:MET:HE2	1:A:261:ILE:CD1	2.39	0.53
1:C:139:SER:HB3	1:C:154:ASP:OD1	2.08	0.53
1:A:232:ASN:CB	7:A:1734:NAG:H83	2.39	0.53
1:B:500:LEU:HB3	1:B:514:HIS:HA	1.92	0.53
1:D:133:GLN:HB2	1:D:134:PRO:HD2	1.91	0.53
1:A:141:LEU:HD23	1:A:154:ASP:HA	1.91	0.52
1:C:163:PRO:O	1:C:165:PRO:HD3	2.08	0.52
1:C:395:THR:HA	1:C:466:SER:HA	1.92	0.52
1:D:184:PHE:CD1	1:D:206:ARG:NH1	2.77	0.52
1:A:160:HIS:ND1	1:A:657:THR:HG22	2.23	0.52
1:A:183:ILE:HD12	1:A:210:THR:HG21	1.91	0.52
1:A:352:VAL:O	1:A:358:ARG:HA	2.09	0.52
1:A:386:ASP:HB3	1:A:468:LEU:CD1	2.40	0.52
1:A:386:ASP:HB3	1:A:468:LEU:HD13	1.91	0.52
1:B:540:TRP:O	1:B:587:LEU:HD12	2.09	0.52
1:C:157:VAL:HG23	1:C:158:GLU:H	1.73	0.52
1:C:540:TRP:CZ3	1:C:568:LEU:HB2	2.44	0.52
1:B:195:LEU:HB3	1:B:201:TYR:CB	2.34	0.52
1:C:411:VAL:HG12	1:C:412:ASP:N	2.24	0.52
1:A:170:PRO:HA	1:A:651:ASN:ND2	2.24	0.52
1:A:329:ARG:NH2	1:A:336:THR:HG23	2.19	0.52
1:A:539:VAL:HB	1:A:569:LEU:HB2	1.91	0.52
1:B:134:PRO:C	1:B:136:PRO:HD3	2.35	0.52
1:B:206:ARG:C	1:B:208:LEU:H	2.16	0.52
1:C:61:ALA:O	1:C:122:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:VAL:HG21	1:B:563:GLN:OE1	2.09	0.52
1:C:88:GLN:O	1:C:89:ALA:C	2.51	0.52
1:C:342:GLY:O	1:C:392:GLY:HA3	2.10	0.52
1:D:367:GLU:HG3	1:D:368:ALA:H	1.73	0.52
1:A:88:GLN:O	1:A:89:ALA:C	2.52	0.52
1:A:366:GLN:OE1	1:A:643:SER:HA	2.10	0.52
1:A:540:TRP:HB2	1:A:588:TYR:CZ	2.45	0.52
1:C:230:TYR:HB3	1:C:241:HIS:O	2.10	0.52
1:C:362:GLU:HG2	1:C:363:ILE:N	2.25	0.52
1:A:84:VAL:HG12	1:A:85:ASP:N	2.24	0.52
1:A:217:GLY:HA3	1:A:222:ASP:CB	2.39	0.52
1:A:610:PHE:N	1:A:610:PHE:CD1	2.77	0.52
1:B:228:GLY:O	1:B:229:LEU:HD23	2.09	0.52
1:B:513:GLU:H	1:B:513:GLU:CD	2.17	0.52
1:D:138:VAL:HG23	1:D:164:LEU:HB2	1.92	0.52
1:D:224:ALA:HA	1:D:249:VAL:O	2.10	0.52
1:A:195:LEU:CB	1:A:201:TYR:HB3	2.40	0.52
1:C:153:ARG:HB3	1:C:153:ARG:HH11	1.74	0.52
1:C:171:VAL:HG23	1:C:176:TYR:OH	2.10	0.52
1:C:199:CYS:C	1:C:201:TYR:H	2.18	0.52
1:C:468:LEU:HD12	1:C:473:TYR:CE1	2.44	0.52
1:B:94:ASN:CG	1:B:132:ARG:HB3	2.35	0.52
1:C:138:VAL:HG21	1:C:648:PHE:HE2	1.74	0.52
1:C:441:ARG:NH1	1:C:716:SER:OG	2.43	0.52
1:C:647:VAL:HG13	1:C:648:PHE:CD1	2.45	0.52
1:D:167:HIS:NE2	1:D:221:GLY:HA2	2.24	0.52
1:D:488:ARG:NH1	1:D:608:LEU:HD13	2.25	0.52
1:D:500:LEU:HB3	1:D:514:HIS:HA	1.92	0.52
1:A:189:PRO:HA	1:A:203:HIS:CE1	2.44	0.52
1:A:561:ARG:NH2	1:B:380:MET:HE2	2.25	0.52
1:B:91:PRO:HB2	1:B:254:LEU:O	2.10	0.52
1:B:145:PRO:HD3	1:B:151:TYR:CE2	2.45	0.52
1:C:630:TYR:O	1:C:679:THR:HB	2.10	0.52
1:D:347:PRO:HG2	1:D:475:TRP:CG	2.45	0.52
1:D:553:TRP:O	1:D:554:SER:HB2	2.09	0.52
1:D:595:ASN:O	1:D:598:GLY:N	2.42	0.52
1:A:350:PHE:CE2	1:A:362:GLU:HB2	2.45	0.51
1:B:412:ASP:OD1	1:B:426:ARG:HA	2.10	0.51
1:C:379:ALA:O	1:C:381:THR:N	2.43	0.51
1:A:90:ARG:NH2	1:A:256:PRO:HD2	2.25	0.51
1:A:319:GLN:HE21	1:B:311:ALA:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:HIS:NE2	1:A:677:TRP:HB3	2.25	0.51
1:D:140:GLU:O	1:D:155:VAL:HG22	2.11	0.51
1:D:299:SER:HG	1:D:300:TRP:CD1	2.28	0.51
1:D:628:GLU:O	1:D:628:GLU:HG2	2.10	0.51
1:A:74:PHE:CZ	1:A:78:ARG:HG3	2.45	0.51
1:A:225:THR:O	1:A:248:LEU:HD12	2.11	0.51
1:C:322:ARG:NH2	1:D:312:PRO:HB3	2.26	0.51
1:D:312:PRO:O	1:D:313:PRO:C	2.53	0.51
1:A:454:GLY:HA3	1:B:402:VAL:HG11	1.93	0.51
1:B:525:HIS:NE2	1:B:677:TRP:HB3	2.25	0.51
1:A:398:LEU:HD22	1:A:403:ASP:HB3	1.93	0.51
1:B:167:HIS:CD2	1:B:221:GLY:HA2	2.45	0.51
1:B:431:VAL:HG22	1:B:462:VAL:HG22	1.91	0.51
1:C:329:ARG:NH2	1:C:336:THR:HG23	2.22	0.51
1:C:380:MET:HE3	1:D:559:LEU:HD21	1.90	0.51
1:C:500:LEU:O	1:C:501:PHE:HB3	2.09	0.51
1:C:689:GLU:O	1:D:714:ASP:HB2	2.09	0.51
1:D:134:PRO:C	1:D:136:PRO:HD3	2.35	0.51
1:D:378:ALA:O	1:D:379:ALA:C	2.54	0.51
1:D:640:GLU:CD	1:D:640:GLU:H	2.18	0.51
1:A:64:SER:O	1:A:65:ARG:C	2.53	0.51
1:A:315:GLN:O	1:A:316:PHE:HB3	2.10	0.51
1:A:315:GLN:CG	1:B:315:GLN:HE21	2.20	0.51
1:A:689:GLU:O	1:B:714:ASP:HB2	2.11	0.51
1:B:168:ARG:HG2	1:B:652:ASP:CB	2.41	0.51
1:B:636:GLN:HE21	1:B:667:GLU:HB3	1.73	0.51
1:C:138:VAL:HG13	1:C:164:LEU:HB3	1.92	0.51
1:B:360:VAL:HG22	1:B:530:LEU:CD2	2.41	0.51
1:C:442:ARG:HD3	1:C:442:ARG:O	2.11	0.51
1:D:212:THR:OG1	1:D:216:ARG:NH1	2.44	0.51
1:D:413:TRP:HE3	1:D:425:ILE:HD12	1.76	0.51
1:C:75:LEU:O	1:C:79:LEU:HB2	2.10	0.51
1:A:375:ASN:HD22	1:A:375:ASN:C	2.18	0.51
1:C:198:CYS:CB	1:C:288:VAL:HG11	2.38	0.51
1:D:142:VAL:HG23	1:D:155:VAL:HG11	1.92	0.51
2:I:1:NAG:H61	2:I:2:NAG:C8	2.41	0.51
1:A:214:ALA:HB1	1:A:650:GLN:NE2	2.25	0.51
1:B:285:LEU:HG	1:B:285:LEU:O	2.11	0.51
1:C:579:VAL:HA	1:C:631:GLN:HG3	1.93	0.51
1:C:628:GLU:HG2	1:C:628:GLU:O	2.10	0.51
1:A:549:MET:O	1:A:559:LEU:HB3	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:HD12	1:A:633:ALA:H	1.76	0.50
1:A:678:VAL:HG11	1:A:703:PHE:CD2	2.45	0.50
1:C:329:ARG:NH2	1:C:336:THR:CG2	2.75	0.50
1:A:91:PRO:HB2	1:A:254:LEU:O	2.10	0.50
1:B:138:VAL:HG11	1:B:169:ARG:HB3	1.92	0.50
1:B:378:ALA:O	1:B:379:ALA:C	2.53	0.50
1:C:225:THR:HG22	1:C:226:TRP:N	2.26	0.50
1:C:539:VAL:HG11	1:C:569:LEU:HD12	1.94	0.50
1:D:183:ILE:HA	1:D:187:GLU:HB2	1.93	0.50
1:A:334:LEU:HD22	1:A:354:PHE:CZ	2.46	0.50
1:C:82:GLY:O	1:C:94:ASN:HB2	2.11	0.50
1:D:367:GLU:HG3	1:D:368:ALA:N	2.26	0.50
1:D:572:GLU:HA	1:D:669:ILE:HD13	1.93	0.50
6:J:1:NAG:H62	6:J:3:FUC:O2	2.11	0.50
1:A:157:VAL:HA	1:A:162:GLY:H	1.73	0.50
1:B:360:VAL:HG21	1:B:363:ILE:HD11	1.93	0.50
1:C:322:ARG:HG2	1:C:322:ARG:HH11	1.77	0.50
1:C:386:ASP:OD1	1:C:471:PAQ:N3	2.44	0.50
1:D:588:TYR:CB	1:D:604:ARG:HA	2.42	0.50
1:B:588:TYR:CB	1:B:604:ARG:HA	2.41	0.50
1:D:441:ARG:HG2	1:D:441:ARG:NH1	2.26	0.50
1:A:199:CYS:C	1:A:201:TYR:N	2.69	0.50
1:B:202:LYS:C	1:B:204:ARG:H	2.19	0.50
1:B:542:GLU:HA	1:B:565:THR:O	2.12	0.50
1:C:314:LEU:HD22	1:D:318:PRO:HD3	1.94	0.50
1:C:337:PHE:HA	1:C:351:ASP:O	2.11	0.50
1:D:90:ARG:NH1	1:D:178:ASP:OD2	2.44	0.50
1:D:125:LEU:HD22	1:D:159:ARG:HH12	1.76	0.50
1:A:223:ARG:HB3	1:A:252:LYS:HA	1.93	0.50
1:A:317:TYR:N	1:A:317:TYR:HD1	2.08	0.50
1:B:81:PRO:C	1:B:83:LEU:H	2.20	0.50
1:B:133:GLN:HB2	1:B:134:PRO:HD2	1.92	0.50
1:B:561:ARG:HH11	1:B:561:ARG:HG2	1.77	0.50
1:C:58:GLN:NE2	1:C:326:GLN:O	2.44	0.50
1:D:471:PAQ:OH	1:D:471:PAQ:N2	2.45	0.50
1:A:341:LEU:HB2	1:A:429:PHE:HZ	1.75	0.50
1:B:184:PHE:CD1	1:B:206:ARG:NH1	2.80	0.50
1:C:538:TRP:O	1:C:589:LEU:HA	2.12	0.50
1:B:191:ALA:HA	1:B:278:GLU:HB2	1.92	0.50
1:C:369:LEU:HA	1:C:384:TYR:O	2.11	0.50
1:C:375:ASN:HA	1:D:561:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:TRP:HZ3	1:D:592:ASN:HB2	1.76	0.50
1:D:540:TRP:O	1:D:587:LEU:HD12	2.12	0.50
2:E:1:NAG:O6	2:E:2:NAG:H82	2.12	0.50
5:H:1:NAG:H62	5:H:5:FUC:O2	2.12	0.50
1:A:184:PHE:CD2	1:A:206:ARG:HG3	2.46	0.49
1:A:317:TYR:HD1	1:A:317:TYR:H	1.58	0.49
1:A:474:VAL:O	1:A:489:PHE:HA	2.12	0.49
1:A:624:GLY:HA2	1:A:656:PRO:HG3	1.92	0.49
1:B:90:ARG:HH12	1:B:178:ASP:CG	2.20	0.49
1:B:553:TRP:O	1:B:554:SER:HB2	2.11	0.49
1:B:640:GLU:H	1:B:640:GLU:CD	2.19	0.49
1:B:697:VAL:O	1:B:697:VAL:HG23	2.12	0.49
1:D:238:PHE:CD1	1:D:238:PHE:C	2.90	0.49
1:D:561:ARG:HH11	1:D:561:ARG:HG2	1.76	0.49
1:A:113:LEU:HD21	1:A:351:ASP:OD1	2.12	0.49
1:A:316:PHE:O	1:A:318:PRO:HD3	2.11	0.49
1:A:370:ALA:HA	1:A:521:THR:O	2.13	0.49
1:B:141:LEU:CD2	1:B:154:ASP:HA	2.42	0.49
1:B:554:SER:C	1:B:556:GLU:H	2.21	0.49
1:D:341:LEU:HD23	1:D:413:TRP:CD2	2.47	0.49
1:D:370:ALA:HA	1:D:521:THR:O	2.12	0.49
1:D:445:SER:O	1:D:450:HIS:HA	2.12	0.49
1:A:646:SER:HB2	1:A:658:VAL:HG23	1.93	0.49
1:A:342:GLY:O	1:A:392:GLY:HA3	2.12	0.49
1:A:353:ARG:HA	1:A:357:GLU:O	2.12	0.49
1:A:411:VAL:O	1:A:428:ALA:N	2.42	0.49
1:C:64:SER:O	1:C:65:ARG:C	2.55	0.49
1:A:315:GLN:OE1	1:A:435:ASN:HB3	2.12	0.49
1:A:546:PHE:CE2	1:B:615:LEU:HD23	2.47	0.49
1:A:640:GLU:CD	1:A:640:GLU:N	2.70	0.49
1:C:155:VAL:O	1:C:159:ARG:N	2.41	0.49
1:C:169:ARG:HG2	1:C:169:ARG:NH1	2.27	0.49
1:C:373:GLY:HA3	1:D:562:LEU:HB3	1.94	0.49
1:C:386:ASP:CG	1:C:468:LEU:HD13	2.37	0.49
1:D:285:LEU:O	1:D:285:LEU:HG	2.11	0.49
1:A:73:ARG:O	1:A:77:GLN:HG3	2.12	0.49
1:A:187:GLU:CB	1:A:274:LEU:HD12	2.34	0.49
1:B:184:PHE:CE2	1:B:206:ARG:HA	2.48	0.49
1:B:488:ARG:NH1	1:B:608:LEU:HD13	2.28	0.49
1:B:538:TRP:CH2	1:B:592:ASN:HB2	2.47	0.49
1:C:63:LEU:HD23	1:C:122:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ALA:HA	1:C:278:GLU:OE1	2.13	0.49
1:D:431:VAL:HG22	1:D:462:VAL:HG22	1.93	0.49
1:D:697:VAL:HG23	1:D:697:VAL:O	2.12	0.49
1:A:525:HIS:HB2	1:A:627:TRP:CE3	2.48	0.49
1:B:106:LYS:HG3	1:B:361:TYR:CE1	2.48	0.49
1:B:178:ASP:O	1:B:181:GLN:HB3	2.13	0.49
1:D:226:TRP:CD1	1:D:248:LEU:HD13	2.47	0.49
1:D:573:GLU:C	1:D:575:ALA:H	2.20	0.49
1:B:191:ALA:HA	1:B:278:GLU:CG	2.43	0.49
1:C:199:CYS:C	1:C:201:TYR:N	2.71	0.49
1:C:317:TYR:HB3	1:C:320:GLY:O	2.13	0.49
1:A:84:VAL:HG12	1:A:85:ASP:H	1.77	0.49
1:A:106:LYS:HE2	1:A:110:LEU:HD11	1.94	0.49
1:A:490:TYR:CE2	1:A:700:GLY:HA3	2.48	0.49
1:C:90:ARG:NH2	1:C:256:PRO:HD2	2.28	0.49
1:D:78:ARG:HH11	1:D:78:ARG:HG2	1.78	0.49
1:A:66:GLU:H	1:A:66:GLU:CD	2.20	0.48
1:A:100:GLU:HG2	1:A:101:LEU:H	1.77	0.48
1:A:314:LEU:HD22	1:B:318:PRO:HD3	1.95	0.48
1:A:369:LEU:HD12	1:A:384:TYR:O	2.12	0.48
1:B:626:SER:HB2	1:B:661:SER:OG	2.13	0.48
1:C:157:VAL:O	1:C:161:GLY:CA	2.56	0.48
1:D:83:LEU:HD12	1:D:94:ASN:O	2.13	0.48
1:A:58:GLN:NE2	1:A:326:GLN:O	2.46	0.48
1:A:314:LEU:HD23	1:A:314:LEU:N	2.28	0.48
1:A:573:GLU:HG3	1:A:666:ASN:HD21	1.76	0.48
1:A:578:LEU:HD23	1:A:630:TYR:CE2	2.47	0.48
1:B:388:GLY:HA3	1:B:650:GLN:CB	2.43	0.48
1:C:160:HIS:CE1	1:C:657:THR:HG22	2.48	0.48
1:C:403:ASP:OD1	1:D:442:ARG:HG3	2.12	0.48
1:A:579:VAL:HA	1:A:631:GLN:CG	2.43	0.48
1:B:554:SER:H	1:B:555:PRO:HD3	1.78	0.48
1:C:106:LYS:HE3	1:C:361:TYR:CG	2.48	0.48
1:C:315:GLN:HE22	1:C:434:GLN:HA	1.78	0.48
1:C:398:LEU:HD22	1:C:403:ASP:HB3	1.94	0.48
1:A:195:LEU:HB2	1:A:201:TYR:CD2	2.48	0.48
1:C:184:PHE:CD2	1:C:188:LEU:HD12	2.48	0.48
1:C:272:ASP:HB2	1:C:276:GLN:NE2	2.28	0.48
1:C:612:GLY:HA2	1:D:585:ARG:HE	1.78	0.48
1:C:709:ASN:N	1:D:689:GLU:OE1	2.41	0.48
1:D:495:ILE:HG12	11:D:2008:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:HIS:HA	1:C:259:TRP:CD1	2.49	0.48
1:A:341:LEU:HB2	1:A:429:PHE:CZ	2.48	0.48
1:A:360:VAL:HG11	1:A:363:ILE:HG13	1.95	0.48
1:A:471:PAQ:OH	1:A:471:PAQ:N2	2.47	0.48
1:B:157:VAL:HG13	4:G:1:NAG:C8	2.43	0.48
1:C:646:SER:HB2	1:C:658:VAL:CG2	2.43	0.48
1:D:595:ASN:O	1:D:597:TRP:N	2.47	0.48
1:A:245:LEU:HB2	1:A:266:TYR:HD1	1.78	0.48
1:C:336:THR:HG21	1:C:353:ARG:HD2	1.95	0.48
1:C:619:SER:HB2	1:D:560:GLN:CG	2.44	0.48
1:D:371:ILE:HD13	1:D:615:LEU:HG	1.95	0.48
1:B:440:LEU:HD23	1:B:455:LEU:HD23	1.95	0.48
1:B:533:ALA:HB3	1:B:591:SER:HB2	1.96	0.48
1:B:637:ARG:O	1:B:637:ARG:HG3	2.13	0.48
1:C:160:HIS:ND1	1:C:657:THR:HG22	2.28	0.48
1:C:182:MET:HE1	1:C:260:THR:HA	1.96	0.48
1:A:347:PRO:HG2	1:A:475:TRP:CG	2.48	0.48
1:B:183:ILE:HA	1:B:187:GLU:HB2	1.96	0.48
1:C:145:PRO:HD3	1:C:151:TYR:CE2	2.49	0.48
1:C:174:GLN:O	1:C:177:LEU:N	2.46	0.48
1:C:398:LEU:HG	11:C:2003:HOH:O	2.14	0.48
1:D:81:PRO:C	1:D:83:LEU:H	2.21	0.48
1:D:200:PHE:O	1:D:202:LYS:HG3	2.14	0.48
1:D:298:GLY:O	1:D:692:PRO:HB3	2.14	0.48
1:D:369:LEU:CD1	1:D:371:ILE:HG13	2.40	0.48
1:D:637:ARG:HB2	1:D:675:VAL:HB	1.96	0.48
1:A:546:PHE:CZ	1:B:615:LEU:HD23	2.49	0.48
1:B:371:ILE:HG23	1:B:383:ARG:NH1	2.29	0.48
1:D:117:SER:HB3	1:D:118:PRO:HD2	1.96	0.48
1:D:577:PHE:CD2	1:D:583:THR:HG22	2.49	0.48
1:B:473:TYR:HB3	1:B:475:TRP:CZ2	2.49	0.47
1:D:166:TYR:O	1:D:169:ARG:HB3	2.14	0.47
1:D:554:SER:H	1:D:555:PRO:HD3	1.79	0.47
1:D:595:ASN:HB3	1:D:601:ARG:HG2	1.94	0.47
1:A:344:PHE:HB3	1:A:387:GLY:O	2.14	0.47
1:A:442:ARG:HG3	1:B:403:ASP:OD1	2.15	0.47
1:B:546:PHE:CE2	1:B:562:LEU:HD13	2.49	0.47
1:D:67:GLU:O	1:D:71:VAL:HG23	2.13	0.47
1:D:143:VAL:HG12	1:D:144:GLY:N	2.28	0.47
1:D:395:THR:O	1:D:425:ILE:HD13	2.14	0.47
1:B:132:ARG:O	1:B:132:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:HG23	1:B:164:LEU:CB	2.44	0.47
1:B:488:ARG:NH1	1:B:608:LEU:CD1	2.77	0.47
1:B:540:TRP:HB2	1:B:588:TYR:CZ	2.49	0.47
1:B:666:ASN:ND2	7:B:1738:NAG:H82	2.29	0.47
1:D:142:VAL:HG23	1:D:155:VAL:CG1	2.43	0.47
1:D:216:ARG:HB2	1:D:223:ARG:HA	1.96	0.47
1:B:278:GLU:O	1:B:282:GLU:HG2	2.14	0.47
1:C:306:VAL:HG23	1:C:306:VAL:O	2.14	0.47
1:D:614:PRO:CB	1:D:629:ARG:HG2	2.45	0.47
1:C:58:GLN:OE1	1:C:61:ALA:HB2	2.14	0.47
1:C:564:VAL:HG22	1:D:506:LYS:HA	1.96	0.47
1:D:490:TYR:CD1	1:D:490:TYR:N	2.82	0.47
1:A:466:SER:O	1:A:472:ASP:HA	2.14	0.47
1:A:588:TYR:HB2	1:A:603:TYR:C	2.40	0.47
1:B:142:VAL:CG2	1:B:155:VAL:HG11	2.44	0.47
1:C:570:GLU:O	1:C:668:THR:HA	2.15	0.47
1:D:170:PRO:HA	1:D:651:ASN:HD22	1.78	0.47
1:D:535:LEU:HD22	1:D:673:ASP:OD2	2.14	0.47
1:A:106:LYS:HB2	1:A:637:ARG:HH12	1.78	0.47
1:A:112:HIS:ND1	1:A:117:SER:O	2.42	0.47
1:A:199:CYS:O	1:A:201:TYR:N	2.47	0.47
1:A:636:GLN:HE21	1:A:667:GLU:HB3	1.77	0.47
1:B:188:LEU:N	1:B:189:PRO:CD	2.78	0.47
1:B:317:TYR:HE1	1:B:433:GLU:HB2	1.79	0.47
1:B:601:ARG:HB3	1:B:710:PHE:HA	1.96	0.47
1:D:78:ARG:HG2	1:D:78:ARG:NH1	2.29	0.47
1:D:468:LEU:HD12	1:D:473:TYR:HE1	1.78	0.47
1:D:523:SER:O	1:D:627:TRP:HH2	1.98	0.47
1:D:585:ARG:HG3	1:D:585:ARG:HH11	1.79	0.47
1:A:539:VAL:HG12	1:A:569:LEU:HD12	1.95	0.47
1:A:607:MET:HE1	1:A:631:GLN:HB3	1.96	0.47
1:C:195:LEU:CB	1:C:201:TYR:HB3	2.44	0.47
1:C:490:TYR:CE2	1:C:700:GLY:HA3	2.49	0.47
1:A:376:SER:O	1:A:380:MET:HB2	2.15	0.47
1:C:220:SER:HA	1:C:654:TRP:HE3	1.79	0.47
1:C:317:TYR:N	1:C:317:TYR:HD1	2.12	0.47
1:D:91:PRO:HB3	1:D:254:LEU:HA	1.96	0.47
1:D:173:PHE:CE2	1:D:177:LEU:HD11	2.50	0.47
1:D:191:ALA:HA	1:D:278:GLU:HB2	1.97	0.47
1:A:63:LEU:HD23	1:A:122:ARG:NH2	2.31	0.47
1:A:157:VAL:O	1:A:161:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HG	1:B:392:GLY:HA2	1.97	0.47
1:B:493:GLY:O	1:B:693:ASN:HA	2.14	0.47
1:C:71:VAL:O	1:C:75:LEU:HG	2.14	0.47
1:C:101:LEU:HD12	1:C:123:GLU:O	2.15	0.47
1:C:129:PHE:CE1	1:C:172:LEU:HD21	2.50	0.47
1:C:360:VAL:HA	1:C:530:LEU:HA	1.97	0.47
1:C:587:LEU:HD12	1:C:587:LEU:C	2.37	0.47
1:C:632:LEU:HD12	1:C:677:TRP:O	2.14	0.47
1:D:441:ARG:NH2	1:D:722:SER:OG	2.46	0.47
1:D:466:SER:HB3	1:D:475:TRP:HE1	1.79	0.47
1:B:99:VAL:HG22	1:B:126:ALA:HB2	1.97	0.46
1:C:490:TYR:CD2	1:C:696:THR:HB	2.50	0.46
1:D:440:LEU:HD22	1:D:481:PRO:HG2	1.97	0.46
1:A:138:VAL:HG21	1:A:648:PHE:HE2	1.80	0.46
1:A:213:THR:O	1:A:214:ALA:HB2	2.15	0.46
1:A:217:GLY:HA3	1:A:222:ASP:HB2	1.96	0.46
1:A:493:GLY:HA2	1:B:443:HIS:HB2	1.97	0.46
1:B:84:VAL:CG2	1:B:89:ALA:HB2	2.44	0.46
1:B:200:PHE:HE1	1:B:293:ASP:OD1	1.98	0.46
1:C:143:VAL:CG1	1:C:144:GLY:N	2.79	0.46
1:C:551:VAL:HG21	1:D:218:LEU:HD22	1.97	0.46
1:D:296:THR:CG2	1:D:297:GLY:N	2.78	0.46
6:J:1:NAG:O4	6:J:2:NAG:C7	2.62	0.46
1:A:395:THR:HG23	1:A:395:THR:O	2.14	0.46
1:C:315:GLN:OE1	1:C:435:ASN:HB3	2.15	0.46
1:D:168:ARG:HG2	1:D:652:ASP:CB	2.46	0.46
1:A:86:ALA:HA	1:A:89:ALA:CB	2.46	0.46
1:C:546:PHE:CZ	1:D:615:LEU:HD23	2.50	0.46
1:C:666:ASN:HD22	1:C:666:ASN:HA	1.53	0.46
1:D:200:PHE:HE1	1:D:293:ASP:OD1	1.98	0.46
1:D:278:GLU:HG3	1:D:282:GLU:OE1	2.16	0.46
1:A:247:LEU:CD2	1:A:264:VAL:HG23	2.45	0.46
1:B:213:THR:HA	1:B:384:TYR:CE1	2.49	0.46
1:C:525:HIS:NE2	1:C:677:TRP:HB3	2.29	0.46
1:D:156:THR:HG23	1:D:164:LEU:HG	1.97	0.46
1:D:328:SER:O	1:D:338:SER:HA	2.15	0.46
1:D:488:ARG:NH1	1:D:608:LEU:CD1	2.78	0.46
1:A:191:ALA:HA	1:A:278:GLU:HB2	1.97	0.46
1:A:240:LEU:O	1:A:515:THR:HG21	2.15	0.46
1:B:94:ASN:OD1	1:B:130:PHE:HA	2.14	0.46
1:C:217:GLY:HA3	1:C:222:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:TYR:HD2	1:C:427:ASP:HB3	1.81	0.46
1:C:710:PHE:CD1	1:C:710:PHE:C	2.94	0.46
1:D:106:LYS:O	1:D:110:LEU:HG	2.14	0.46
1:D:191:ALA:HA	1:D:278:GLU:CG	2.45	0.46
1:A:129:PHE:CE1	1:A:172:LEU:HD21	2.51	0.46
1:A:353:ARG:HH21	1:A:358:ARG:HH12	1.62	0.46
1:C:395:THR:HG23	1:C:395:THR:O	2.15	0.46
1:D:468:LEU:O	1:D:469:LEU:HB2	2.16	0.46
1:A:159:ARG:HG2	1:A:160:HIS:CD2	2.50	0.46
1:A:187:GLU:C	1:A:189:PRO:HD2	2.40	0.46
1:A:201:TYR:CE2	1:A:203:HIS:ND1	2.78	0.46
1:C:98:SER:CB	1:C:417:LEU:HD23	2.43	0.46
1:C:451:TYR:HB3	1:D:235:GLY:HA2	1.98	0.46
1:C:471:PAQ:N2	1:C:471:PAQ:OH	2.49	0.46
1:A:76:THR:HA	1:A:83:LEU:CD2	2.46	0.46
1:A:199:CYS:C	1:A:201:TYR:H	2.23	0.46
1:A:220:SER:HA	1:A:654:TRP:CE3	2.51	0.46
1:A:231:TYR:CD1	1:A:293:ASP:HA	2.51	0.46
1:A:477:THR:HG23	1:A:477:THR:O	2.15	0.46
1:C:90:ARG:HH21	1:C:256:PRO:HD2	1.81	0.46
1:C:183:ILE:HD12	1:C:210:THR:HG21	1.97	0.46
1:C:219:GLN:NE2	1:D:557:HIS:CE1	2.84	0.46
1:C:361:TYR:HB3	1:C:529:ASP:OD2	2.16	0.46
1:D:593:HIS:CE1	11:D:2006:HOH:O	2.68	0.46
1:D:614:PRO:HB2	1:D:629:ARG:HG2	1.98	0.46
1:B:395:THR:O	1:B:395:THR:HG22	2.15	0.46
1:B:413:TRP:HE3	1:B:425:ILE:HD12	1.81	0.46
1:B:490:TYR:CD1	1:B:490:TYR:N	2.84	0.46
1:C:187:GLU:CB	1:C:274:LEU:HD12	2.36	0.46
1:C:578:LEU:HD23	1:C:630:TYR:CE2	2.51	0.46
1:A:214:ALA:HA	1:A:215:PRO:C	2.42	0.45
1:A:386:ASP:CB	1:A:468:LEU:HD13	2.46	0.45
1:A:499:PHE:HE2	1:A:514:HIS:HB3	1.81	0.45
1:A:500:LEU:O	1:A:501:PHE:HB3	2.17	0.45
1:A:551:VAL:HG21	1:B:218:LEU:HD22	1.97	0.45
1:B:99:VAL:HG22	1:B:126:ALA:CB	2.46	0.45
1:B:375:ASN:ND2	1:B:501:PHE:CE1	2.84	0.45
1:B:559:LEU:C	1:B:559:LEU:HD12	2.41	0.45
1:D:106:LYS:HG3	1:D:361:TYR:CE1	2.51	0.45
1:A:597:TRP:CZ3	1:B:513:GLU:N	2.84	0.45
1:C:63:LEU:HG	1:C:101:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:VAL:HG12	1:C:85:ASP:N	2.30	0.45
1:C:640:GLU:CD	1:C:640:GLU:N	2.73	0.45
1:D:228:GLY:C	1:D:229:LEU:HD23	2.41	0.45
1:D:247:LEU:HD22	1:D:264:VAL:HG22	1.98	0.45
1:D:366:GLN:OE1	1:D:643:SER:HA	2.16	0.45
1:D:527:LYS:NZ	1:D:642:PRO:HA	2.31	0.45
1:D:554:SER:C	1:D:556:GLU:H	2.24	0.45
1:B:250:ASN:ND2	1:B:262:GLN:OE1	2.50	0.45
1:C:191:ALA:C	1:C:278:GLU:OE1	2.59	0.45
1:C:462:VAL:O	1:C:477:THR:HG22	2.17	0.45
1:C:646:SER:HB3	1:C:649:ASN:OD1	2.15	0.45
1:D:110:LEU:O	1:D:111:ALA:C	2.59	0.45
1:D:316:PHE:CE1	1:D:318:PRO:HA	2.50	0.45
1:D:341:LEU:HB3	1:D:413:TRP:CE2	2.52	0.45
1:D:636:GLN:NE2	1:D:668:THR:O	2.48	0.45
1:C:170:PRO:HA	1:C:651:ASN:ND2	2.31	0.45
1:C:535:LEU:O	1:C:673:ASP:HA	2.17	0.45
1:D:187:GLU:C	1:D:189:PRO:HD2	2.41	0.45
1:D:561:ARG:HG2	1:D:561:ARG:NH1	2.31	0.45
1:D:646:SER:OG	1:D:648:PHE:HD1	2.00	0.45
2:E:1:NAG:O4	2:E:2:NAG:C7	2.63	0.45
1:A:246:GLU:OE1	1:A:377:PRO:HD2	2.15	0.45
1:B:84:VAL:HG23	1:B:89:ALA:HB2	1.97	0.45
1:B:153:ARG:O	1:B:155:VAL:HG13	2.16	0.45
1:C:182:MET:HE1	1:C:260:THR:CA	2.47	0.45
1:C:681:GLY:O	1:C:682:PHE:HB3	2.17	0.45
1:C:722:SER:CB	1:D:304:SER:HB2	2.46	0.45
1:A:184:PHE:CD2	1:A:188:LEU:HD12	2.52	0.45
1:A:230:TYR:HB3	1:A:241:HIS:O	2.16	0.45
1:A:410:TYR:HD2	1:A:427:ASP:HB3	1.81	0.45
1:B:175:GLU:OE2	1:B:223:ARG:NH1	2.50	0.45
1:B:471:PAQ:OH	1:B:471:PAQ:N2	2.48	0.45
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.70	0.45
1:D:389:PHE:HE1	1:D:650:GLN:NE2	2.11	0.45
1:A:63:LEU:HG	1:A:101:LEU:HB2	1.99	0.45
1:A:317:TYR:HB3	1:A:320:GLY:O	2.17	0.45
1:B:67:GLU:CG	1:B:146:LEU:HD13	2.45	0.45
1:B:230:TYR:N	1:B:230:TYR:CD1	2.84	0.45
1:C:380:MET:HE1	1:D:552:PRO:HG2	1.99	0.45
1:C:562:LEU:HB3	1:D:373:GLY:CA	2.46	0.45
1:C:632:LEU:HA	1:C:677:TRP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:PHE:CD2	1:D:470:ASN:HB3	2.51	0.45
1:A:202:LYS:O	1:A:204:ARG:N	2.50	0.45
1:A:546:PHE:CE1	1:B:615:LEU:HA	2.52	0.45
1:B:250:ASN:HB2	1:B:262:GLN:HG3	1.98	0.45
1:B:561:ARG:HG2	1:B:561:ARG:NH1	2.31	0.45
1:B:572:GLU:HA	1:B:669:ILE:HD13	1.99	0.45
1:C:214:ALA:CB	1:C:650:GLN:NE2	2.80	0.45
1:C:251:HIS:HA	1:C:259:TRP:CG	2.51	0.45
1:C:322:ARG:NH1	1:C:322:ARG:HG2	2.30	0.45
1:D:188:LEU:N	1:D:189:PRO:CD	2.80	0.45
1:D:488:ARG:HH11	1:D:608:LEU:CD1	2.30	0.45
1:D:540:TRP:HB2	1:D:588:TYR:CZ	2.52	0.45
1:A:441:ARG:HH11	1:A:441:ARG:CG	2.20	0.45
1:A:462:VAL:HB	1:A:477:THR:CG2	2.46	0.45
1:B:276:GLN:O	1:B:279:ALA:HB3	2.16	0.45
1:B:488:ARG:HH11	1:B:608:LEU:CD1	2.29	0.45
1:C:66:GLU:H	1:C:66:GLU:CD	2.25	0.45
1:C:205:GLY:O	1:C:206:ARG:C	2.60	0.45
1:C:230:TYR:CD1	1:C:230:TYR:N	2.84	0.45
1:C:305:PRO:HD2	1:D:718:TYR:HD2	1.81	0.45
1:A:280:GLN:HG2	1:A:285:LEU:HB3	1.97	0.45
1:A:678:VAL:HG11	1:A:703:PHE:HD2	1.82	0.45
1:A:726:ARG:HH22	1:B:234:SER:HB2	1.82	0.45
1:B:106:LYS:HG3	1:B:361:TYR:CZ	2.51	0.45
1:B:398:LEU:HD22	1:B:403:ASP:HB3	1.98	0.45
1:D:178:ASP:O	1:D:181:GLN:HB3	2.17	0.45
1:D:277:LEU:O	1:D:278:GLU:C	2.60	0.45
1:A:137:ASN:CG	2:E:1:NAG:H82	2.42	0.44
1:A:314:LEU:CD2	1:B:318:PRO:HD3	2.47	0.44
1:A:484:ALA:HA	1:A:705:LEU:O	2.18	0.44
1:B:157:VAL:HG23	1:B:158:GLU:N	2.32	0.44
1:C:540:TRP:HB2	1:C:588:TYR:CZ	2.52	0.44
1:C:632:LEU:HD12	1:C:633:ALA:H	1.82	0.44
1:D:90:ARG:NH1	1:D:178:ASP:CG	2.75	0.44
1:D:110:LEU:HD21	1:D:361:TYR:CD1	2.52	0.44
1:D:578:LEU:HD21	1:D:629:ARG:HH12	1.82	0.44
1:A:366:GLN:HB3	1:A:644:SER:OG	2.18	0.44
1:B:168:ARG:HG2	1:B:652:ASP:HB3	1.98	0.44
1:C:593:HIS:O	1:C:601:ARG:HG3	2.17	0.44
1:D:163:PRO:O	1:D:165:PRO:HD3	2.17	0.44
1:A:306:VAL:HG23	1:A:306:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLN:CB	1:B:78:ARG:NH1	2.80	0.44
1:B:439:PRO:HA	1:B:456:ALA:HA	1.98	0.44
1:B:614:PRO:O	1:B:615:LEU:C	2.57	0.44
1:C:217:GLY:HA3	1:C:222:ASP:HB3	1.97	0.44
1:C:231:TYR:CD1	1:C:293:ASP:HA	2.52	0.44
1:C:489:PHE:CD1	1:C:489:PHE:C	2.96	0.44
1:D:202:LYS:C	1:D:204:ARG:H	2.24	0.44
1:D:539:VAL:HB	1:D:569:LEU:HB2	1.98	0.44
1:C:159:ARG:HE	1:C:159:ARG:HB2	1.66	0.44
1:D:72:MET:O	1:D:76:THR:HG23	2.16	0.44
1:D:513:GLU:CD	1:D:513:GLU:N	2.76	0.44
1:A:106:LYS:HE3	1:A:361:TYR:CG	2.53	0.44
1:A:191:ALA:O	1:A:195:LEU:HG	2.17	0.44
1:A:335:TRP:CH2	1:A:485:ILE:HG12	2.52	0.44
1:A:375:ASN:HA	1:B:561:ARG:NH2	2.32	0.44
1:A:438:LEU:HA	1:B:463:ARG:HH12	1.83	0.44
1:A:538:TRP:O	1:A:589:LEU:HA	2.18	0.44
1:A:632:LEU:HD13	1:A:678:VAL:HG22	2.00	0.44
1:B:641:GLU:N	1:B:642:PRO:CD	2.80	0.44
1:C:317:TYR:HD1	1:C:317:TYR:H	1.65	0.44
1:C:466:SER:O	1:C:472:ASP:HA	2.17	0.44
1:C:597:TRP:CZ3	1:D:513:GLU:N	2.85	0.44
1:D:125:LEU:CD2	1:D:159:ARG:HH12	2.29	0.44
1:D:374:GLY:HA3	1:D:379:ALA:HB3	1.99	0.44
1:A:702:GLY:O	1:A:703:PHE:HB3	2.18	0.44
1:C:400:ARG:H	1:C:400:ARG:HG2	1.32	0.44
1:C:416:LEU:HD13	1:C:422:PRO:N	2.32	0.44
1:D:412:ASP:OD1	1:D:426:ARG:HA	2.17	0.44
1:A:61:ALA:O	1:A:122:ARG:NH2	2.51	0.44
1:A:191:ALA:HA	1:A:278:GLU:OE1	2.18	0.44
1:A:546:PHE:CE2	1:A:562:LEU:HD13	2.53	0.44
1:B:77:GLN:CB	1:B:78:ARG:HH12	2.31	0.44
1:B:187:GLU:C	1:B:189:PRO:HD2	2.43	0.44
1:C:143:VAL:HG12	1:C:144:GLY:H	1.81	0.44
1:C:192:SER:CB	1:C:203:HIS:CE1	2.90	0.44
1:C:588:TYR:HB2	1:C:603:TYR:C	2.41	0.44
1:C:637:ARG:O	1:C:637:ARG:HG3	2.18	0.44
1:C:689:GLU:HG2	1:D:707:PRO:HG2	1.99	0.44
1:A:360:VAL:HG13	1:A:530:LEU:HA	2.00	0.44
1:A:490:TYR:CD1	1:A:490:TYR:N	2.86	0.44
1:A:646:SER:HB3	1:A:649:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLY:HA2	11:B:2011:HOH:O	2.17	0.44
1:B:535:LEU:HD22	1:B:673:ASP:OD2	2.17	0.44
1:B:585:ARG:HG3	1:B:585:ARG:HH11	1.83	0.44
1:B:637:ARG:HB2	1:B:675:VAL:HB	1.99	0.44
1:C:108:ALA:HA	1:C:111:ALA:HB3	1.98	0.44
1:C:312:PRO:HA	1:D:322:ARG:CZ	2.47	0.44
1:D:404:CYS:HB2	1:D:410:TYR:OH	2.17	0.44
1:D:559:LEU:C	1:D:559:LEU:HD12	2.42	0.44
2:I:1:NAG:C6	2:I:2:NAG:H82	2.45	0.44
1:A:551:VAL:O	1:A:552:PRO:C	2.60	0.44
1:A:637:ARG:HG3	1:A:637:ARG:HH21	1.81	0.44
1:B:369:LEU:HG	11:B:2014:HOH:O	2.18	0.44
1:C:245:LEU:HD12	1:C:265:PHE:O	2.18	0.44
1:C:385:VAL:O	1:C:387:GLY:N	2.51	0.44
1:C:386:ASP:HB3	1:C:468:LEU:HD13	2.00	0.44
1:C:538:TRP:CD1	1:C:670:ALA:HA	2.53	0.44
1:D:223:ARG:HG2	1:D:223:ARG:NH1	2.32	0.44
1:A:157:VAL:O	1:A:158:GLU:C	2.61	0.43
1:B:143:VAL:HG12	1:B:144:GLY:N	2.33	0.43
1:B:595:ASN:O	1:B:598:GLY:N	2.50	0.43
1:B:607:MET:O	1:B:608:LEU:HD23	2.17	0.43
1:C:472:ASP:OD1	1:C:493:GLY:HA3	2.18	0.43
1:D:138:VAL:HG23	1:D:164:LEU:HB3	1.99	0.43
3:F:1:NAG:H4	3:F:2:FUC:C6	2.37	0.43
1:A:483:GLY:O	1:A:707:PRO:HD3	2.18	0.43
1:C:647:VAL:HG13	1:C:648:PHE:CE1	2.53	0.43
1:D:106:LYS:HE3	1:D:361:TYR:CG	2.53	0.43
1:D:614:PRO:O	1:D:615:LEU:C	2.61	0.43
1:A:155:VAL:O	1:A:159:ARG:N	2.41	0.43
1:A:167:HIS:CD2	1:A:221:GLY:CA	3.02	0.43
1:A:303:LYS:HB2	1:B:724:TYR:CD2	2.52	0.43
1:A:500:LEU:HD22	1:A:510:GLN:HG3	2.00	0.43
1:B:77:GLN:HB3	1:B:78:ARG:HH12	1.83	0.43
1:B:723:ILE:CG2	1:B:724:TYR:N	2.80	0.43
1:C:170:PRO:HA	1:C:651:ASN:HD21	1.83	0.43
1:C:199:CYS:O	1:C:201:TYR:N	2.50	0.43
1:C:316:PHE:O	1:C:318:PRO:HD3	2.19	0.43
1:C:365:LEU:HD12	1:C:366:GLN:H	1.82	0.43
1:C:395:THR:O	1:C:425:ILE:HD13	2.18	0.43
1:C:653:PRO:HD2	1:C:654:TRP:CE3	2.54	0.43
1:D:475:TRP:CE3	1:D:489:PHE:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:THR:HG22	1:D:504:THR:O	2.17	0.43
1:A:67:GLU:HB3	1:A:146:LEU:HD22	1.98	0.43
1:A:132:ARG:HH11	1:A:132:ARG:HG3	1.83	0.43
1:A:360:VAL:HG11	1:A:363:ILE:HG12	2.00	0.43
1:B:184:PHE:CB	1:B:206:ARG:HH11	2.31	0.43
1:C:85:ASP:O	1:C:87:ALA:N	2.51	0.43
1:C:195:LEU:HB2	1:C:201:TYR:CD2	2.54	0.43
1:C:400:ARG:HA	1:C:410:TYR:OH	2.19	0.43
1:D:90:ARG:HB3	1:D:91:PRO:HD2	2.00	0.43
1:D:525:HIS:HB2	1:D:627:TRP:CE3	2.53	0.43
1:A:108:ALA:HA	1:A:111:ALA:HB3	2.01	0.43
1:A:379:ALA:O	1:A:381:THR:N	2.51	0.43
1:A:647:VAL:HG13	1:A:648:PHE:CD1	2.54	0.43
1:B:69:THR:O	1:B:73:ARG:HG3	2.17	0.43
1:B:728:ASP:HB2	11:B:2018:HOH:O	2.18	0.43
1:C:187:GLU:C	1:C:189:PRO:HD2	2.43	0.43
1:D:317:TYR:CE1	1:D:433:GLU:HB2	2.48	0.43
1:D:382:THR:HG21	1:D:384:TYR:CE2	2.54	0.43
1:D:702:GLY:O	1:D:703:PHE:HB3	2.19	0.43
1:A:313:PRO:HB3	1:B:317:TYR:CD1	2.53	0.43
1:A:319:GLN:NE2	1:B:311:ALA:H	2.16	0.43
1:B:270:TYR:OH	1:B:377:PRO:HG3	2.17	0.43
1:C:90:ARG:HG2	1:C:91:PRO:CD	2.29	0.43
1:C:384:TYR:HA	1:C:650:GLN:HE22	1.83	0.43
1:C:441:ARG:HG2	1:C:441:ARG:NH1	2.32	0.43
1:D:89:ALA:HB1	1:D:93:ASP:HB2	2.00	0.43
1:A:90:ARG:O	1:A:91:PRO:C	2.62	0.43
1:A:549:MET:HE3	1:A:561:ARG:CB	2.48	0.43
1:A:563:GLN:HB3	1:B:506:LYS:HB2	2.00	0.43
1:B:296:THR:CG2	1:B:297:GLY:N	2.82	0.43
1:C:319:GLN:HE21	1:D:311:ALA:HB2	1.83	0.43
1:C:552:PRO:HB2	1:C:553:TRP:CE3	2.54	0.43
1:D:184:PHE:HA	1:D:188:LEU:HD12	2.00	0.43
1:D:347:PRO:HG2	1:D:475:TRP:CB	2.48	0.43
1:D:386:ASP:HB3	1:D:468:LEU:CD1	2.47	0.43
1:A:562:LEU:HB3	1:B:373:GLY:CA	2.49	0.43
1:B:184:PHE:CG	1:B:206:ARG:NH1	2.80	0.43
1:C:632:LEU:HD11	1:C:676:ALA:HB1	2.01	0.43
1:D:84:VAL:HG23	1:D:89:ALA:HB2	2.00	0.43
1:D:129:PHE:CZ	1:D:169:ARG:HG3	2.54	0.43
1:D:689:GLU:H	1:D:689:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:FUC:H63	3:F:2:FUC:C2	2.46	0.43
1:A:129:PHE:CD1	1:A:169:ARG:HD2	2.53	0.43
1:A:144:GLY:HA3	1:A:150:SER:H	1.84	0.43
1:A:508:GLY:HA3	1:A:517:GLY:O	2.18	0.43
1:A:689:GLU:OE2	1:B:707:PRO:HB2	2.18	0.43
1:B:198:CYS:HA	1:B:290:LEU:HD23	2.00	0.43
1:B:316:PHE:CE1	1:B:318:PRO:HA	2.48	0.43
1:B:386:ASP:HB3	1:B:468:LEU:CD1	2.47	0.43
1:C:621:MET:HB2	1:C:653:PRO:HB2	2.01	0.43
1:D:106:LYS:HG3	1:D:361:TYR:CZ	2.54	0.43
1:D:132:ARG:O	1:D:132:ARG:HG3	2.18	0.43
1:D:630:TYR:O	1:D:679:THR:HB	2.19	0.43
1:A:110:LEU:HD21	1:A:361:TYR:CD1	2.53	0.43
1:A:441:ARG:HB2	1:B:693:ASN:HB2	1.99	0.43
1:A:653:PRO:HD2	1:A:654:TRP:CE3	2.54	0.43
1:B:566:ARG:HH11	1:B:566:ARG:HB3	1.84	0.43
1:C:112:HIS:CE1	1:C:119:PRO:HD3	2.54	0.43
1:C:249:VAL:O	1:C:251:HIS:HD2	2.02	0.43
1:C:641:GLU:OE2	1:C:663:PHE:HA	2.18	0.43
1:A:153:ARG:NH1	1:A:153:ARG:HB3	2.34	0.42
1:A:616:PRO:HD3	1:B:546:PHE:CD1	2.54	0.42
1:B:487:ILE:C	1:B:488:ARG:HG2	2.43	0.42
1:B:539:VAL:HG22	1:B:589:LEU:CD2	2.48	0.42
1:C:441:ARG:HH12	1:C:716:SER:C	2.27	0.42
1:D:142:VAL:HG21	1:D:155:VAL:HG11	2.00	0.42
1:D:369:LEU:HD21	1:D:371:ILE:HD11	2.01	0.42
1:D:539:VAL:CG1	1:D:569:LEU:HD12	2.49	0.42
1:A:138:VAL:HG13	1:A:164:LEU:HB3	2.00	0.42
1:A:314:LEU:N	1:A:314:LEU:CD2	2.82	0.42
1:A:322:ARG:CZ	1:B:312:PRO:HA	2.48	0.42
1:A:621:MET:HB2	1:A:653:PRO:HB2	2.00	0.42
1:B:238:PHE:CD1	1:B:238:PHE:C	2.97	0.42
1:B:473:TYR:HB3	1:B:475:TRP:CE2	2.53	0.42
1:C:526:PHE:N	1:C:526:PHE:CD1	2.87	0.42
1:D:427:ASP:OD2	1:D:427:ASP:N	2.52	0.42
1:A:189:PRO:HA	1:A:203:HIS:HE1	1.83	0.42
1:A:194:LEU:HA	1:A:281:PHE:CE2	2.55	0.42
1:B:614:PRO:CG	1:B:629:ARG:HG2	2.49	0.42
1:C:67:GLU:HB3	1:C:146:LEU:HD22	2.01	0.42
1:C:202:LYS:C	1:C:204:ARG:N	2.77	0.42
1:C:246:GLU:OE1	1:C:377:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:GLY:O	1:C:707:PRO:HD3	2.20	0.42
1:C:551:VAL:O	1:C:552:PRO:C	2.62	0.42
1:D:61:ALA:O	1:D:62:ASP:C	2.61	0.42
1:D:63:LEU:HD11	1:D:124:ALA:CB	2.50	0.42
1:D:536:GLU:HA	1:D:672:LYS:O	2.19	0.42
1:D:573:GLU:C	1:D:575:ALA:N	2.78	0.42
1:B:371:ILE:O	1:B:520:HIS:HA	2.20	0.42
1:B:590:ALA:HA	1:B:602:GLY:HA2	2.01	0.42
1:C:166:TYR:O	1:C:169:ARG:HG2	2.20	0.42
1:C:636:GLN:HE21	1:C:667:GLU:HB3	1.84	0.42
1:D:173:PHE:CD2	1:D:173:PHE:C	2.97	0.42
1:D:395:THR:HA	1:D:466:SER:HA	2.00	0.42
1:C:229:LEU:HD11	1:C:247:LEU:HD12	2.01	0.42
1:C:615:LEU:O	1:C:616:PRO:O	2.37	0.42
1:D:396:THR:CG2	1:D:467:THR:HB	2.50	0.42
1:D:725:PHE:CD1	1:D:725:PHE:C	2.98	0.42
1:A:147:PRO:O	1:A:149:PRO:HD3	2.19	0.42
1:A:442:ARG:C	1:A:442:ARG:HD3	2.45	0.42
1:A:468:LEU:CB	1:A:471:PAQ:HN1	2.27	0.42
1:B:138:VAL:HG23	1:B:164:LEU:HB3	2.01	0.42
1:B:408:ALA:HB1	1:B:432:PHE:HB3	2.01	0.42
1:C:182:MET:O	1:C:187:GLU:HG2	2.19	0.42
1:C:380:MET:HE1	1:D:552:PRO:HD2	2.02	0.42
1:C:570:GLU:C	1:C:669:ILE:HG12	2.43	0.42
1:D:157:VAL:HG23	1:D:158:GLU:N	2.35	0.42
1:A:86:ALA:HA	1:A:89:ALA:HB2	2.00	0.42
1:A:588:TYR:HB3	1:A:604:ARG:CB	2.50	0.42
1:B:241:HIS:CE1	1:B:299:SER:O	2.73	0.42
1:B:265:PHE:CD2	1:B:265:PHE:C	2.97	0.42
1:B:441:ARG:HG2	1:B:441:ARG:HH11	1.84	0.42
1:C:366:GLN:HB2	1:C:525:HIS:O	2.20	0.42
1:C:433:GLU:HG2	1:C:458:THR:CG2	2.50	0.42
1:C:601:ARG:NH1	1:C:710:PHE:O	2.53	0.42
1:C:668:THR:O	1:C:668:THR:HG23	2.20	0.42
1:A:155:VAL:O	1:A:159:ARG:HB3	2.20	0.42
1:A:263:LYS:HE2	11:A:2004:HOH:O	2.19	0.42
1:B:64:SER:OG	1:B:67:GLU:HB2	2.20	0.42
1:C:198:CYS:HB3	1:C:288:VAL:CG1	2.44	0.42
1:D:83:LEU:HA	1:D:94:ASN:O	2.20	0.42
1:D:459:VAL:HG11	1:D:480:HIS:CE1	2.55	0.42
1:A:397:PRO:HG3	1:A:425:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD13	1:A:430:CYS:HB3	2.02	0.42
1:A:433:GLU:HG2	1:A:458:THR:CG2	2.50	0.42
1:B:627:TRP:HA	1:B:660:PHE:CD2	2.55	0.42
1:C:68:LEU:HD22	1:C:416:LEU:HB2	2.01	0.42
1:C:538:TRP:CZ2	1:C:671:GLY:CA	3.02	0.42
1:C:723:ILE:HG22	1:C:724:TYR:N	2.34	0.42
1:D:532:VAL:O	1:D:533:ALA:C	2.61	0.42
1:A:315:GLN:HG2	1:B:315:GLN:HG2	2.02	0.42
1:A:668:THR:HG23	1:A:668:THR:O	2.19	0.42
1:B:167:HIS:NE2	1:B:221:GLY:HA2	2.35	0.42
1:B:241:HIS:NE2	1:B:299:SER:O	2.53	0.42
1:B:397:PRO:HB3	1:B:426:ARG:O	2.20	0.42
1:B:513:GLU:CD	1:B:513:GLU:N	2.77	0.42
1:B:725:PHE:CD1	1:B:725:PHE:C	2.98	0.42
1:C:314:LEU:CD2	1:D:318:PRO:HD3	2.50	0.42
1:C:389:PHE:CE1	1:C:650:GLN:OE1	2.73	0.42
1:D:495:ILE:HG22	11:D:2009:HOH:O	2.20	0.42
1:D:607:MET:O	1:D:608:LEU:HD23	2.20	0.42
1:A:88:GLN:HA	1:A:174:GLN:OE1	2.19	0.41
1:A:140:GLU:OE1	1:A:160:HIS:HD2	2.00	0.41
1:A:274:LEU:HA	1:A:274:LEU:HD23	1.65	0.41
1:A:315:GLN:OE1	1:A:435:ASN:N	2.53	0.41
1:B:594:SER:HA	1:B:599:HIS:O	2.19	0.41
1:C:367:GLU:HG3	1:C:368:ALA:N	2.35	0.41
1:C:624:GLY:HA2	1:C:656:PRO:HG3	2.01	0.41
1:D:91:PRO:HB2	1:D:254:LEU:HA	2.02	0.41
1:D:182:MET:O	1:D:187:GLU:HG2	2.20	0.41
1:D:240:LEU:HA	1:D:497:SER:OG	2.19	0.41
1:D:442:ARG:HD3	1:D:442:ARG:C	2.45	0.41
1:D:500:LEU:HD23	1:D:510:GLN:NE2	2.35	0.41
1:A:311:ALA:HB3	1:B:318:PRO:HG2	2.02	0.41
1:A:332:SER:O	1:A:333:SER:C	2.63	0.41
1:A:546:PHE:CG	1:B:616:PRO:HD3	2.55	0.41
1:A:593:HIS:O	1:A:601:ARG:HG3	2.20	0.41
1:B:266:TYR:OH	1:B:267:GLN:NE2	2.54	0.41
1:B:596:LYS:HD3	1:B:597:TRP:CE2	2.55	0.41
1:C:177:LEU:HA	1:C:177:LEU:HD23	1.83	0.41
1:C:479:PHE:CD1	1:C:479:PHE:N	2.88	0.41
1:D:230:TYR:CD1	1:D:230:TYR:N	2.87	0.41
1:D:556:GLU:HG3	1:D:557:HIS:HD1	1.85	0.41
1:D:632:LEU:HA	1:D:677:TRP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.85	0.41
1:B:62:ASP:O	1:B:63:LEU:C	2.63	0.41
1:B:206:ARG:C	1:B:208:LEU:N	2.75	0.41
1:B:461:VAL:HG12	1:B:462:VAL:N	2.35	0.41
1:C:250:ASN:ND2	1:C:262:GLN:NE2	2.68	0.41
1:C:572:GLU:HG2	1:C:669:ILE:CG2	2.51	0.41
1:D:106:LYS:CB	1:D:637:ARG:HH21	2.30	0.41
1:D:134:PRO:HG2	1:D:135:GLN:H	1.85	0.41
1:D:173:PHE:HE2	1:D:177:LEU:HD11	1.84	0.41
1:D:182:MET:CG	1:D:186:ARG:HH21	2.33	0.41
1:D:195:LEU:C	1:D:197:HIS:N	2.77	0.41
1:A:182:MET:CE	1:A:260:THR:HA	2.44	0.41
1:A:195:LEU:C	1:A:197:HIS:N	2.79	0.41
1:A:230:TYR:CD1	1:A:230:TYR:N	2.88	0.41
1:B:63:LEU:HD11	1:B:124:ALA:CB	2.50	0.41
1:B:77:GLN:HB3	1:B:78:ARG:NH1	2.35	0.41
1:B:155:VAL:O	1:B:158:GLU:HB3	2.20	0.41
1:B:214:ALA:HB1	1:B:215:PRO:HA	2.02	0.41
1:C:195:LEU:HB3	1:C:201:TYR:HB2	2.00	0.41
1:C:303:LYS:HB2	1:D:724:TYR:CD2	2.55	0.41
1:C:375:ASN:C	1:C:375:ASN:ND2	2.78	0.41
7:C:1735:NAG:H81	1:D:448:TYR:CD2	2.56	0.41
1:D:144:GLY:C	1:D:149:PRO:HA	2.45	0.41
1:D:341:LEU:HB3	1:D:413:TRP:NE1	2.35	0.41
1:D:455:LEU:HD13	1:D:722:SER:CA	2.50	0.41
1:A:81:PRO:O	1:A:83:LEU:N	2.54	0.41
1:A:130:PHE:HB2	1:A:137:ASN:O	2.20	0.41
1:A:312:PRO:HA	1:B:322:ARG:CZ	2.50	0.41
1:A:364:SER:HB2	11:A:2006:HOH:O	2.20	0.41
1:A:578:LEU:HD23	1:A:630:TYR:CD2	2.55	0.41
1:A:637:ARG:HG2	1:A:673:ASP:OD2	2.20	0.41
1:C:63:LEU:HD11	1:C:124:ALA:HB2	2.01	0.41
1:C:301:SER:OG	1:C:302:LEU:N	2.53	0.41
1:D:184:PHE:CE2	1:D:206:ARG:HA	2.55	0.41
1:D:440:LEU:HD22	1:D:481:PRO:CG	2.49	0.41
1:A:58:GLN:NE2	1:A:327:GLY:HA3	2.27	0.41
1:A:305:PRO:HD2	1:B:718:TYR:HD2	1.85	0.41
1:A:337:PHE:HA	1:A:351:ASP:O	2.20	0.41
1:A:480:HIS:HB3	1:A:481:PRO:HD2	2.02	0.41
1:A:646:SER:HB2	1:A:658:VAL:CG2	2.51	0.41
1:C:91:PRO:HB2	1:C:254:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:PHE:CD1	1:C:610:PHE:N	2.87	0.41
1:D:367:GLU:CG	1:D:368:ALA:H	2.34	0.41
1:A:607:MET:HE2	1:A:607:MET:HB3	1.93	0.41
1:B:66:GLU:O	1:B:69:THR:HB	2.20	0.41
1:B:216:ARG:HD2	1:B:225:THR:HG1	1.79	0.41
1:B:280:GLN:HE21	1:B:280:GLN:HB3	1.63	0.41
1:B:500:LEU:HD12	1:B:501:PHE:N	2.35	0.41
1:B:506:LYS:H	1:B:506:LYS:HG2	1.56	0.41
1:B:543:ASP:OD1	1:B:544:MET:N	2.52	0.41
1:B:636:GLN:O	1:B:638:LYS:HG3	2.20	0.41
1:C:114:ASP:OD2	1:C:358:ARG:NH2	2.54	0.41
1:C:584:PRO:O	1:C:585:ARG:C	2.63	0.41
1:D:329:ARG:HH21	1:D:336:THR:C	2.28	0.41
1:D:460:LEU:HB3	1:D:479:PHE:HB2	2.03	0.41
1:A:143:VAL:HG12	1:A:144:GLY:N	2.36	0.41
1:A:182:MET:O	1:A:186:ARG:HB2	2.20	0.41
1:A:525:HIS:HE2	1:A:677:TRP:HB3	1.85	0.41
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.35	0.41
1:B:246:GLU:OE2	1:B:378:ALA:HB3	2.19	0.41
1:B:426:ARG:HB3	1:B:427:ASP:OD2	2.21	0.41
1:B:432:PHE:HE1	1:B:434:GLN:HB2	1.85	0.41
1:C:191:ALA:O	1:C:195:LEU:HG	2.21	0.41
1:D:473:TYR:HB3	1:D:475:TRP:CZ2	2.56	0.41
6:J:1:NAG:C6	6:J:3:FUC:O2	2.69	0.41
1:A:78:ARG:NH1	1:A:78:ARG:HB3	2.36	0.41
1:A:85:ASP:OD1	1:A:87:ALA:CB	2.69	0.41
1:A:98:SER:O	1:A:126:ALA:HA	2.21	0.41
1:A:225:THR:CG2	1:A:226:TRP:N	2.82	0.41
1:A:302:LEU:HG	1:B:453:GLY:HA3	2.03	0.41
1:A:360:VAL:HG13	1:A:530:LEU:HD23	2.01	0.41
1:B:63:LEU:HG	1:B:101:LEU:N	2.36	0.41
1:B:250:ASN:HD22	1:B:262:GLN:CD	2.29	0.41
1:B:353:ARG:NH2	1:B:358:ARG:NH1	2.69	0.41
1:B:372:TYR:O	1:B:383:ARG:NH1	2.48	0.41
1:B:396:THR:CG2	1:B:467:THR:HB	2.51	0.41
1:B:455:LEU:HD13	1:B:722:SER:HA	2.01	0.41
1:B:504:THR:O	1:B:504:THR:HG22	2.21	0.41
1:C:76:THR:HG22	1:C:83:LEU:CD2	2.49	0.41
1:C:182:MET:HE2	1:C:261:ILE:CD1	2.50	0.41
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.70	0.41
1:C:195:LEU:C	1:C:197:HIS:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:PRO:HG2	1:C:475:TRP:CG	2.56	0.41
1:C:350:PHE:CE2	1:C:362:GLU:HB2	2.55	0.41
1:C:484:ALA:HA	1:C:705:LEU:O	2.21	0.41
1:C:500:LEU:CD2	1:C:510:GLN:HG3	2.51	0.41
1:C:562:LEU:HB3	1:D:373:GLY:HA2	2.03	0.41
1:D:187:GLU:C	1:D:189:PRO:CD	2.93	0.41
1:D:539:VAL:HG22	1:D:589:LEU:CD2	2.49	0.41
1:A:95:CYS:O	1:A:128:VAL:HG13	2.20	0.41
1:A:627:TRP:HB3	1:A:660:PHE:CD2	2.56	0.41
1:A:728:ASP:CG	1:A:729:GLN:N	2.79	0.41
1:B:74:PHE:O	1:B:77:GLN:HB2	2.21	0.41
1:B:235:GLY:O	1:B:236:ALA:HB2	2.20	0.41
1:B:546:PHE:CZ	1:B:562:LEU:HD13	2.56	0.41
1:C:380:MET:HG3	1:D:561:ARG:CD	2.51	0.41
1:D:94:ASN:OD1	1:D:130:PHE:HA	2.21	0.41
1:D:194:LEU:HD12	1:D:194:LEU:O	2.21	0.41
1:D:438:LEU:HD12	1:D:439:PRO:HD2	2.03	0.41
1:D:487:ILE:C	1:D:488:ARG:HG2	2.46	0.41
1:A:85:ASP:O	1:A:87:ALA:N	2.54	0.40
1:A:313:PRO:HB3	1:B:317:TYR:HD1	1.86	0.40
1:A:347:PRO:HG2	1:A:475:TRP:CD1	2.56	0.40
1:B:337:PHE:CD1	1:B:337:PHE:C	2.99	0.40
1:B:471:PAQ:HD2	1:B:471:PAQ:O	2.21	0.40
1:C:157:VAL:O	1:C:158:GLU:C	2.63	0.40
1:C:189:PRO:C	1:C:191:ALA:H	2.29	0.40
1:C:397:PRO:HD2	1:D:444:HIS:CD2	2.56	0.40
1:C:442:ARG:HH11	1:D:472:ASP:HB3	1.86	0.40
1:D:83:LEU:HD11	1:D:96:VAL:HG23	2.03	0.40
1:D:266:TYR:O	1:D:267:GLN:C	2.64	0.40
1:D:330:VAL:HB	1:D:337:PHE:CE1	2.55	0.40
1:D:440:LEU:HD23	1:D:455:LEU:HD23	2.03	0.40
1:A:500:LEU:CD2	1:A:510:GLN:HG3	2.51	0.40
1:A:710:PHE:CD1	1:A:710:PHE:C	2.98	0.40
1:B:90:ARG:NH1	1:B:178:ASP:OD2	2.54	0.40
1:C:129:PHE:HZ	1:C:170:PRO:HD2	1.85	0.40
1:C:194:LEU:HA	1:C:281:PHE:CE2	2.56	0.40
1:C:247:LEU:CD2	1:C:264:VAL:HG23	2.50	0.40
1:D:187:GLU:C	1:D:274:LEU:CD1	2.94	0.40
1:A:84:VAL:HG21	1:A:93:ASP:OD1	2.21	0.40
1:A:722:SER:HB3	1:B:304:SER:CB	2.51	0.40
1:B:538:TRP:O	1:B:589:LEU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:VAL:HG12	1:C:331:ALA:N	2.34	0.40
1:C:492:THR:OG1	1:C:493:GLY:N	2.53	0.40
1:D:369:LEU:HD12	1:D:370:ALA:H	1.86	0.40
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.83	0.40
1:A:215:PRO:HB3	1:A:653:PRO:HG2	2.03	0.40
1:A:240:LEU:N	1:A:240:LEU:HD23	2.37	0.40
1:A:318:PRO:HB2	1:B:311:ALA:HB3	2.03	0.40
1:A:570:GLU:O	1:A:668:THR:HA	2.21	0.40
1:A:623:ARG:HB3	1:A:656:PRO:HG2	2.03	0.40
1:B:369:LEU:HD11	1:B:371:ILE:CG1	2.50	0.40
1:C:90:ARG:O	1:C:91:PRO:C	2.64	0.40
1:C:185:ASN:O	1:C:186:ARG:HG3	2.21	0.40
1:C:315:GLN:O	1:C:316:PHE:HB3	2.20	0.40
1:D:171:VAL:HG13	1:D:175:GLU:CD	2.47	0.40
1:A:72:MET:O	1:A:73:ARG:C	2.64	0.40
1:A:322:ARG:NH1	1:A:322:ARG:HG2	2.36	0.40
1:A:380:MET:CE	1:B:552:PRO:HD2	2.50	0.40
1:A:411:VAL:HG12	1:A:412:ASP:N	2.37	0.40
1:A:489:PHE:CD1	1:A:489:PHE:C	2.98	0.40
1:A:561:ARG:CZ	1:B:380:MET:HE2	2.51	0.40
1:A:614:PRO:HG3	1:A:629:ARG:HA	2.03	0.40
1:B:142:VAL:HG21	1:B:155:VAL:HG11	2.02	0.40
1:B:278:GLU:HG3	1:B:282:GLU:OE1	2.22	0.40
1:B:389:PHE:HE1	1:B:650:GLN:NE2	2.16	0.40
1:B:648:PHE:HB2	1:B:657:THR:OG1	2.22	0.40
1:C:322:ARG:CZ	1:D:312:PRO:HA	2.52	0.40
1:C:368:ALA:HB3	1:C:386:ASP:HB2	2.03	0.40
1:C:448:TYR:CE1	1:D:209:VAL:HB	2.57	0.40
1:C:549:MET:HE3	1:C:561:ARG:CB	2.51	0.40
1:D:234:SER:CB	7:D:1735:NAG:O6	2.66	0.40
1:D:556:GLU:CD	1:D:557:HIS:CE1	2.99	0.40
1:D:663:PHE:N	1:D:663:PHE:CD1	2.88	0.40
1:D:687:HIS:O	1:D:690:ASP:HB2	2.21	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	669/735 (91%)	571 (85%)	72 (11%)	26 (4%)	2	10
1	B	669/735 (91%)	585 (87%)	76 (11%)	8 (1%)	10	34
1	C	669/735 (91%)	575 (86%)	69 (10%)	25 (4%)	2	11
1	D	669/735 (91%)	587 (88%)	71 (11%)	11 (2%)	7	27
All	All	2676/2940 (91%)	2318 (87%)	288 (11%)	70 (3%)	4	17

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	MET
1	A	637	ARG
1	B	267	GLN
1	B	386	ASP
1	B	596	LYS
1	C	201	TYR
1	C	380	MET
1	D	596	LYS
1	A	65	ARG
1	A	82	GLY
1	A	86	ALA
1	A	186	ARG
1	A	223	ARG
1	A	386	ASP
1	A	616	PRO
1	B	380	MET
1	C	65	ARG
1	C	86	ALA
1	C	386	ASP
1	C	418	GLU
1	C	545	VAL
1	C	616	PRO

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Mol	Chain	Res	Type
1	C	637	ARG
1	D	267	GLN
1	D	380	MET
1	D	386	ASP
1	A	89	ALA
1	A	161	GLY
1	A	267	GLN
1	A	316	PHE
1	A	596	LYS
1	A	697	VAL
1	C	81	PRO
1	C	159	ARG
1	C	186	ARG
1	C	200	PHE
1	C	223	ARG
1	C	725	PHE
1	A	200	PHE
1	A	201	TYR
1	A	455	LEU
1	A	725	PHE
1	B	554	SER
1	B	689	GLU
1	C	82	GLY
1	C	505	GLY
1	D	203	HIS
1	D	406	TYR
1	D	469	LEU
1	D	554	SER
1	A	81	PRO
1	A	145	PRO
1	A	256	PRO
1	A	532	VAL
1	C	89	ALA
1	C	158	GLU
1	C	316	PHE
1	C	448	TYR
1	C	532	VAL
1	D	347	PRO
1	A	545	VAL
1	B	308	PRO
1	C	161	GLY
1	C	310	PRO

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Mol	Chain	Res	Type
1	D	545	VAL
1	A	495	ILE
1	B	555	PRO
1	C	256	PRO
1	A	286	VAL
1	D	692	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	562/609 (92%)	523 (93%)	39 (7%)	14	41
1	B	562/609 (92%)	530 (94%)	32 (6%)	18	49
1	C	562/609 (92%)	523 (93%)	39 (7%)	14	41
1	D	562/609 (92%)	534 (95%)	28 (5%)	22	53
All	All	2248/2436 (92%)	2110 (94%)	138 (6%)	17	46

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	88	GLN
1	A	91	PRO
1	A	138	VAL
1	A	171	VAL
1	A	196	HIS
1	A	203	HIS
1	A	204	ARG
1	A	209	VAL
1	A	277	LEU
1	A	280	GLN
1	A	291	ILE
1	A	317	TYR
1	A	336	THR
1	A	345	SER

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Mol	Chain	Res	Type
1	A	349	ILE
1	A	360	VAL
1	A	362	GLU
1	A	375	ASN
1	A	427	ASP
1	A	430	CYS
1	A	435	ASN
1	A	441	ARG
1	A	472	ASP
1	A	489	PHE
1	A	490	TYR
1	A	519	VAL
1	A	536	GLU
1	A	552	PRO
1	A	587	LEU
1	A	589	LEU
1	A	610	PHE
1	A	640	GLU
1	A	642	PRO
1	A	645	SER
1	A	647	VAL
1	A	665	ASN
1	A	666	ASN
1	A	675	VAL
1	B	58	GLN
1	B	66	GLU
1	B	84	VAL
1	B	128	VAL
1	B	154	ASP
1	B	173	PHE
1	B	203	HIS
1	B	223	ARG
1	B	282	GLU
1	B	326	GLN
1	B	333	SER
1	B	376	SER
1	B	395	THR
1	B	406	TYR
1	B	417	LEU
1	B	441	ARG
1	B	476	ASP
1	B	489	PHE

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Mol	Chain	Res	Type
1	B	490	TYR
1	B	513	GLU
1	B	515	THR
1	B	516	LEU
1	B	519	VAL
1	B	528	VAL
1	B	532	VAL
1	B	559	LEU
1	B	603	TYR
1	B	637	ARG
1	B	640	GLU
1	B	645	SER
1	B	665	ASN
1	B	689	GLU
1	C	88	GLN
1	C	91	PRO
1	C	138	VAL
1	C	171	VAL
1	C	196	HIS
1	C	203	HIS
1	C	204	ARG
1	C	209	VAL
1	C	230	TYR
1	C	277	LEU
1	C	280	GLN
1	C	291	ILE
1	C	317	TYR
1	C	336	THR
1	C	349	ILE
1	C	360	VAL
1	C	375	ASN
1	C	400	ARG
1	C	427	ASP
1	C	435	ASN
1	C	441	ARG
1	C	489	PHE
1	C	490	TYR
1	C	519	VAL
1	C	523	SER
1	C	536	GLU
1	C	552	PRO
1	C	564	VAL

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Mol	Chain	Res	Type
1	C	587	LEU
1	C	589	LEU
1	C	610	PHE
1	C	640	GLU
1	C	642	PRO
1	C	647	VAL
1	C	650	GLN
1	C	665	ASN
1	C	666	ASN
1	C	675	VAL
1	C	706	ARG
1	D	66	GLU
1	D	154	ASP
1	D	169	ARG
1	D	200	PHE
1	D	203	HIS
1	D	223	ARG
1	D	333	SER
1	D	376	SER
1	D	395	THR
1	D	406	TYR
1	D	441	ARG
1	D	476	ASP
1	D	489	PHE
1	D	490	TYR
1	D	513	GLU
1	D	515	THR
1	D	516	LEU
1	D	519	VAL
1	D	523	SER
1	D	528	VAL
1	D	556	GLU
1	D	559	LEU
1	D	603	TYR
1	D	637	ARG
1	D	640	GLU
1	D	645	SER
1	D	665	ASN
1	D	689	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	A	185	ASN
1	A	241	HIS
1	A	276	GLN
1	A	280	GLN
1	A	319	GLN
1	A	326	GLN
1	A	375	ASN
1	A	444	HIS
1	A	450	HIS
1	A	560	GLN
1	A	593	HIS
1	A	606	GLN
1	A	617	GLN
1	A	618	ASN
1	A	636	GLN
1	A	650	GLN
1	A	666	ASN
1	A	693	ASN
1	B	77	GLN
1	B	181	GLN
1	B	185	ASN
1	B	207	ASN
1	B	242	HIS
1	B	250	ASN
1	B	276	GLN
1	B	280	GLN
1	B	315	GLN
1	B	319	GLN
1	B	420	GLN
1	B	510	GLN
1	B	537	ASN
1	B	560	GLN
1	B	618	ASN
1	B	631	GLN
1	B	693	ASN
1	C	77	GLN
1	C	160	HIS
1	C	185	ASN
1	C	203	HIS
1	C	219	GLN
1	C	262	GLN
1	C	276	GLN

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Mol	Chain	Res	Type
1	C	280	GLN
1	C	287	ASN
1	C	319	GLN
1	C	326	GLN
1	C	375	ASN
1	C	434	GLN
1	C	514	HIS
1	C	537	ASN
1	C	560	GLN
1	C	593	HIS
1	C	606	GLN
1	C	617	GLN
1	C	618	ASN
1	C	636	GLN
1	C	650	GLN
1	C	666	ASN
1	C	693	ASN
1	D	77	GLN
1	D	181	GLN
1	D	185	ASN
1	D	242	HIS
1	D	250	ASN
1	D	280	GLN
1	D	315	GLN
1	D	319	GLN
1	D	420	GLN
1	D	434	GLN
1	D	444	HIS
1	D	510	GLN
1	D	537	ASN
1	D	560	GLN
1	D	606	GLN
1	D	618	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	PAQ	D	471	1	19,22,23	2.01	6 (31%)	18,29,31	2.57	5 (27%)
1	PAQ	B	471	1	19,22,23	2.01	6 (31%)	18,29,31	2.58	5 (27%)
1	PAQ	C	471	1	19,22,23	2.04	6 (31%)	18,29,31	2.64	5 (27%)
1	PAQ	A	471	1	19,22,23	2.01	6 (31%)	18,29,31	2.63	4 (22%)

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
1	PAQ	D	471	1	1/1/5/10	5/8/27/29	0/2/2/2
1	PAQ	B	471	1	1/1/5/10	5/8/27/29	0/2/2/2
1	PAQ	C	471	1	1/1/5/10	6/8/27/29	0/2/2/2
1	PAQ	A	471	1	1/1/5/10	6/8/27/29	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	PAQ	CG-CD2	-5.80	1.39	1.50
1	D	471	PAQ	CG-CD2	-5.77	1.39	1.50
1	C	471	PAQ	CG-CD2	-5.76	1.39	1.50
1	B	471	PAQ	CG-CD2	-5.75	1.39	1.50
1	C	471	PAQ	CE1-CD1	-3.56	1.39	1.46
1	B	471	PAQ	CE1-CD1	-3.53	1.39	1.46
1	D	471	PAQ	CE1-CD1	-3.52	1.39	1.46
1	A	471	PAQ	CE1-CD1	-3.46	1.39	1.46
1	C	471	PAQ	CB-CG	-2.70	1.51	1.54
1	A	471	PAQ	CB-CG	-2.66	1.51	1.54
1	B	471	PAQ	CB-CG	-2.65	1.51	1.54
1	D	471	PAQ	CB-CG	-2.62	1.51	1.54
1	C	471	PAQ	N2-N1	-2.53	1.32	1.39
1	B	471	PAQ	N2-N1	-2.50	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	PAQ	N2-N1	-2.49	1.32	1.39
1	A	471	PAQ	N2-N1	-2.45	1.32	1.39
1	C	471	PAQ	O2-CD1	2.25	1.25	1.22
1	D	471	PAQ	O2-CD1	2.09	1.25	1.22
1	C	471	PAQ	CE1-CZ	2.08	1.39	1.36
1	B	471	PAQ	O2-CD1	2.06	1.25	1.22
1	A	471	PAQ	O2-CD1	2.05	1.25	1.22
1	D	471	PAQ	CE1-CZ	2.03	1.39	1.36
1	B	471	PAQ	CE1-CZ	2.03	1.39	1.36
1	A	471	PAQ	CE1-CZ	2.00	1.39	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	PAQ	CB-CG-CD1	6.79	120.61	111.13
1	A	471	PAQ	CB-CG-CD1	6.72	120.53	111.13
1	B	471	PAQ	CB-CG-CD1	6.39	120.06	111.13
1	D	471	PAQ	CB-CG-CD1	6.32	119.97	111.13
1	D	471	PAQ	CD2-CG-CD1	6.27	119.02	104.64
1	B	471	PAQ	CD2-CG-CD1	6.26	119.01	104.64
1	A	471	PAQ	CD2-CG-CD1	6.23	118.92	104.64
1	C	471	PAQ	CD2-CG-CD1	6.20	118.86	104.64
1	B	471	PAQ	C5-N3-C1	3.56	122.29	117.21
1	D	471	PAQ	C5-N3-C1	3.54	122.26	117.21
1	C	471	PAQ	C5-N3-C1	3.45	122.14	117.21
1	A	471	PAQ	N2-C1-N3	3.35	119.99	114.83
1	C	471	PAQ	N2-C1-N3	3.35	119.98	114.83
1	A	471	PAQ	C5-N3-C1	3.34	121.98	117.21
1	B	471	PAQ	N2-C1-N3	3.34	119.97	114.83
1	D	471	PAQ	N2-C1-N3	3.32	119.95	114.83
1	B	471	PAQ	C4-C5-N3	-2.16	120.00	123.42
1	C	471	PAQ	C4-C5-N3	-2.07	120.14	123.42
1	D	471	PAQ	C4-C5-N3	-2.01	120.24	123.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	PAQ	N-CA-CB-CG
1	A	471	PAQ	CA-CB-CG-CD1
1	A	471	PAQ	C2-C1-N2-N1
1	A	471	PAQ	N3-C1-N2-N1
1	B	471	PAQ	N-CA-CB-CG
1	B	471	PAQ	CA-CB-CG-CD1
1	B	471	PAQ	C2-C1-N2-N1
1	B	471	PAQ	N3-C1-N2-N1
1	C	471	PAQ	N-CA-CB-CG
1	C	471	PAQ	CA-CB-CG-CD1
1	C	471	PAQ	C2-C1-N2-N1
1	C	471	PAQ	N3-C1-N2-N1
1	D	471	PAQ	N-CA-CB-CG
1	D	471	PAQ	CA-CB-CG-CD1
1	D	471	PAQ	C2-C1-N2-N1
1	D	471	PAQ	N3-C1-N2-N1
1	A	471	PAQ	CA-CB-CG-CD2
1	B	471	PAQ	CA-CB-CG-CD2
1	C	471	PAQ	CA-CB-CG-CD2
1	D	471	PAQ	CA-CB-CG-CD2
1	A	471	PAQ	C-CA-CB-CG
1	C	471	PAQ	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	471	PAQ	4	0
1	B	471	PAQ	5	0
1	C	471	PAQ	4	0
1	A	471	PAQ	5	0

5.5 Carbohydrates

25 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	0.85	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	0.98	1 (5%)
3	FUC	F	2	3	10,10,11	0.61	0	14,14,16	0.81	0
4	NAG	G	1	4,1	14,14,15	0.77	0	17,19,21	0.87	0
4	NAG	G	2	4	14,14,15	0.97	0	17,19,21	0.99	2 (11%)
4	BMA	G	3	4	11,11,12	0.91	0	15,15,17	0.55	0
5	NAG	H	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	H	2	5	14,14,15	0.70	0	17,19,21	0.91	0
5	BMA	H	3	5	11,11,12	0.91	0	15,15,17	1.04	1 (6%)
5	MAN	H	4	5	11,11,12	0.72	0	15,15,17	0.84	1 (6%)
5	FUC	H	5	5	10,10,11	0.73	0	14,14,16	0.56	0
2	NAG	I	1	2,1	14,14,15	0.61	0	17,19,21	0.75	1 (5%)
2	NAG	I	2	2	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.65	0	17,19,21	1.22	2 (11%)
6	NAG	J	2	6	14,14,15	0.46	0	17,19,21	0.71	0
6	FUC	J	3	6	10,10,11	0.49	0	14,14,16	0.58	0
4	NAG	K	1	4,1	14,14,15	0.55	0	17,19,21	0.73	0
4	NAG	K	2	4	14,14,15	0.74	0	17,19,21	0.76	0
4	BMA	K	3	4	11,11,12	0.63	0	15,15,17	0.72	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.79	0	17,19,21	1.12	1 (5%)
5	NAG	L	2	5	14,14,15	0.87	1 (7%)	17,19,21	0.92	1 (5%)
5	BMA	L	3	5	11,11,12	1.02	1 (9%)	15,15,17	0.57	0
5	MAN	L	4	5	11,11,12	0.96	1 (9%)	15,15,17	0.65	1 (6%)
5	FUC	L	5	5	10,10,11	0.81	0	14,14,16	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	F	2	3	1/1/4/5	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	FUC	H	5	5	1/1/4/5	-	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	6/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	6/6/23/26	0/1/1/1
6	FUC	J	3	6	1/1/4/5	-	0/1/1/1
4	NAG	K	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	5/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
5	NAG	L	1	1,5	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	1/1/1/1
5	FUC	L	5	5	1/1/4/5	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	3	BMA	C2-C3	2.46	1.56	1.52
3	F	1	NAG	C1-C2	2.33	1.55	1.52
5	L	4	MAN	C2-C3	2.22	1.55	1.52
5	L	2	NAG	C1-C2	2.16	1.55	1.52
5	H	1	NAG	C1-C2	2.01	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C4-C3-C2	-4.13	104.97	111.02
5	H	3	BMA	C1-C2-C3	3.67	114.98	109.64
5	H	1	NAG	C3-C4-C5	-3.17	104.49	110.23
6	J	1	NAG	C4-C3-C2	-3.14	106.42	111.02
5	H	4	MAN	C1-O5-C5	2.96	116.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C4-C3-C2	2.80	115.12	111.02
4	G	2	NAG	C2-N2-C7	-2.77	119.18	122.90
6	J	1	NAG	C2-N2-C7	-2.76	119.20	122.90
2	I	2	NAG	C2-N2-C7	-2.65	119.34	122.90
5	L	1	NAG	C3-C4-C5	-2.55	105.61	110.23
3	F	1	NAG	C2-N2-C7	-2.50	119.55	122.90
2	E	2	NAG	C2-N2-C7	-2.47	119.59	122.90
5	H	1	NAG	C2-N2-C7	-2.37	119.73	122.90
5	L	2	NAG	C2-N2-C7	-2.36	119.73	122.90
4	K	3	BMA	C1-C2-C3	-2.34	106.24	109.64
5	L	4	MAN	C1-O5-C5	2.31	115.28	112.19
4	G	2	NAG	O5-C1-C2	-2.11	108.03	111.29
2	I	1	NAG	C2-N2-C7	-2.00	120.22	122.90

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	2	FUC	C1
5	H	1	NAG	C1
5	H	5	FUC	C1
5	L	1	NAG	C1
5	L	5	FUC	C1
6	J	3	FUC	C1

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	L	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
4	G	3	BMA	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2
6	J	1	NAG	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	K	3	BMA	C4-C5-C6-O6
4	G	2	NAG	O7-C7-N2-C2
5	H	3	BMA	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
2	I	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
5	L	4	MAN	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
6	J	2	NAG	C3-C2-N2-C7
5	L	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O7-C7-N2-C2
6	J	2	NAG	C1-C2-N2-C7
5	H	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	J	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
3	F	1	NAG	O7-C7-N2-C2

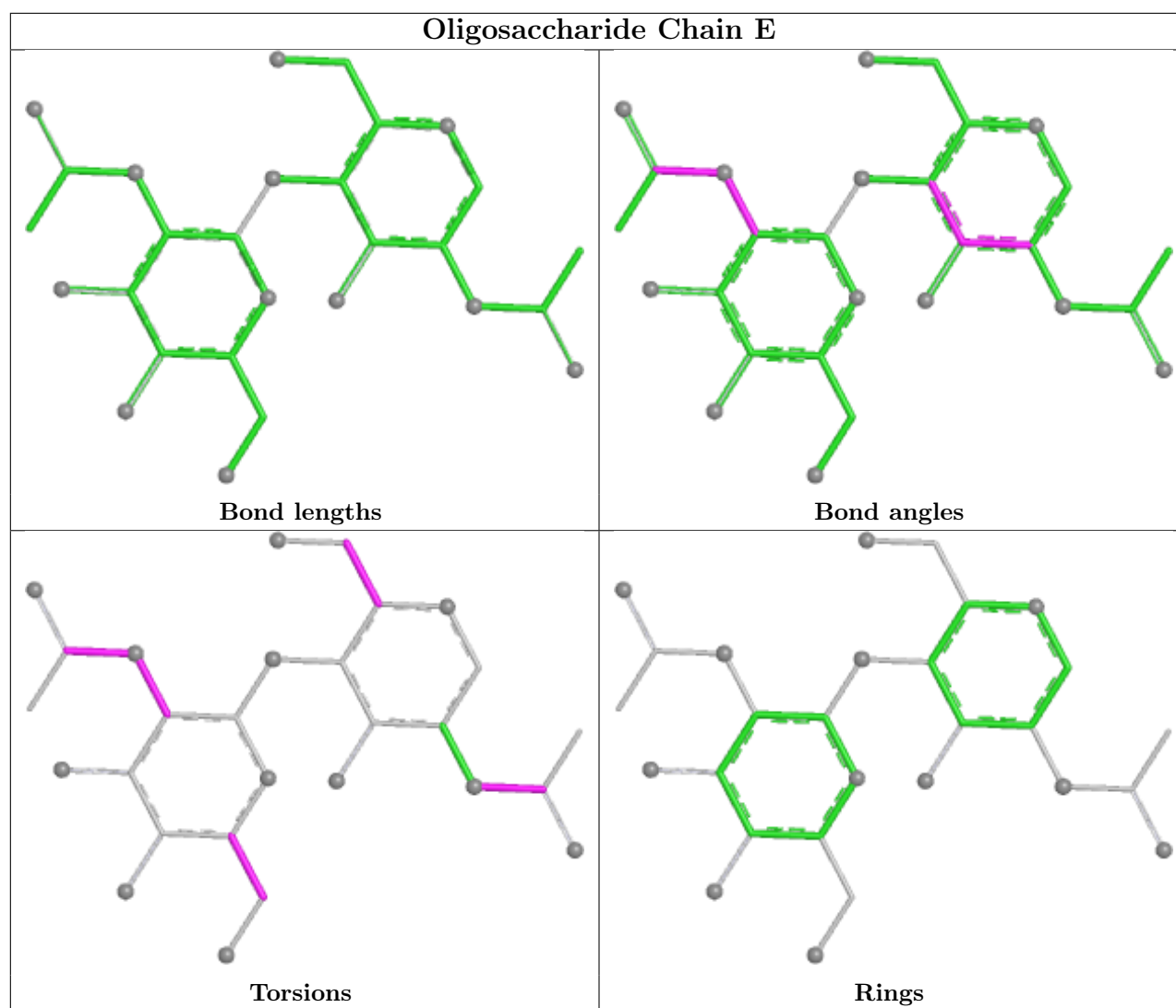
All (1) ring outliers are listed below:

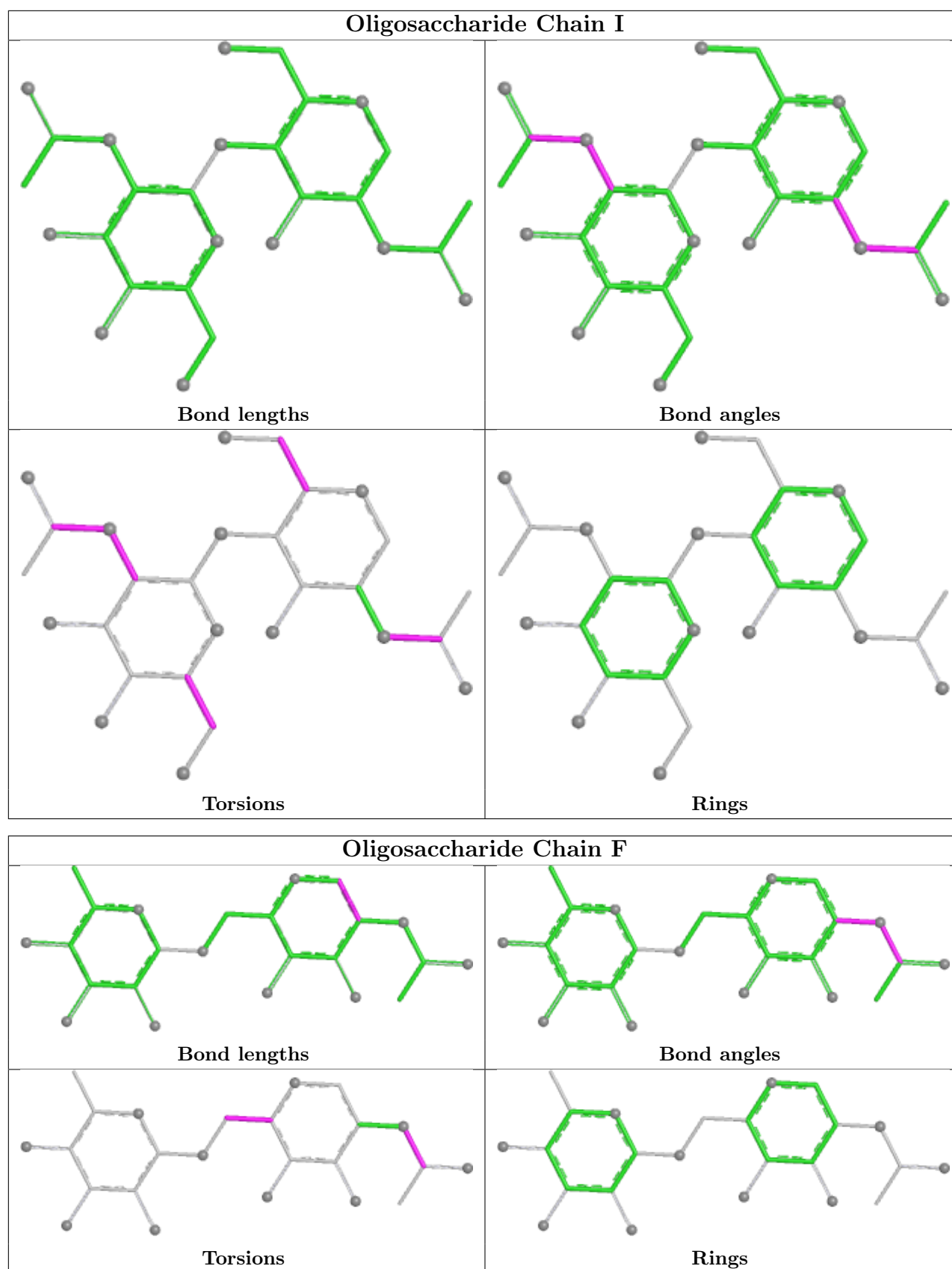
Mol	Chain	Res	Type	Atoms
5	L	4	MAN	C1-C2-C3-C4-C5-O5

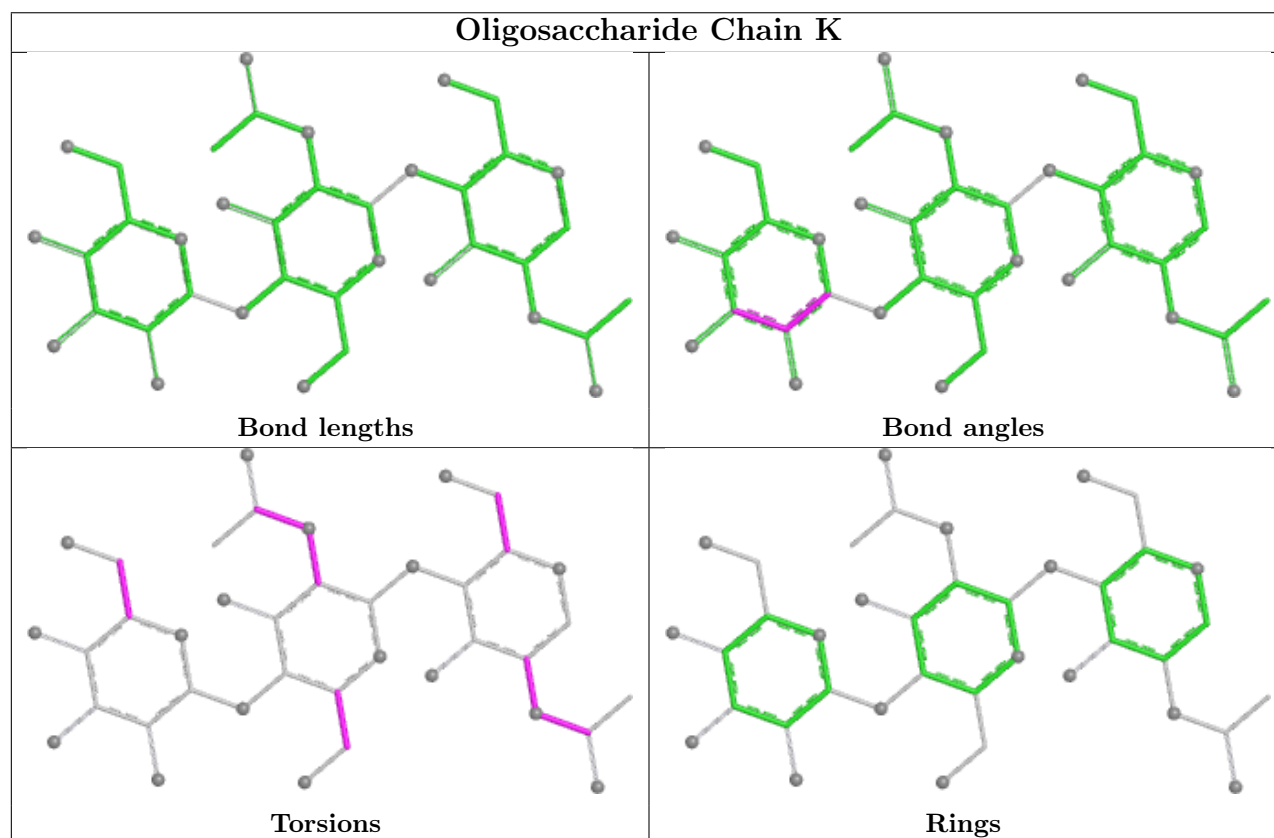
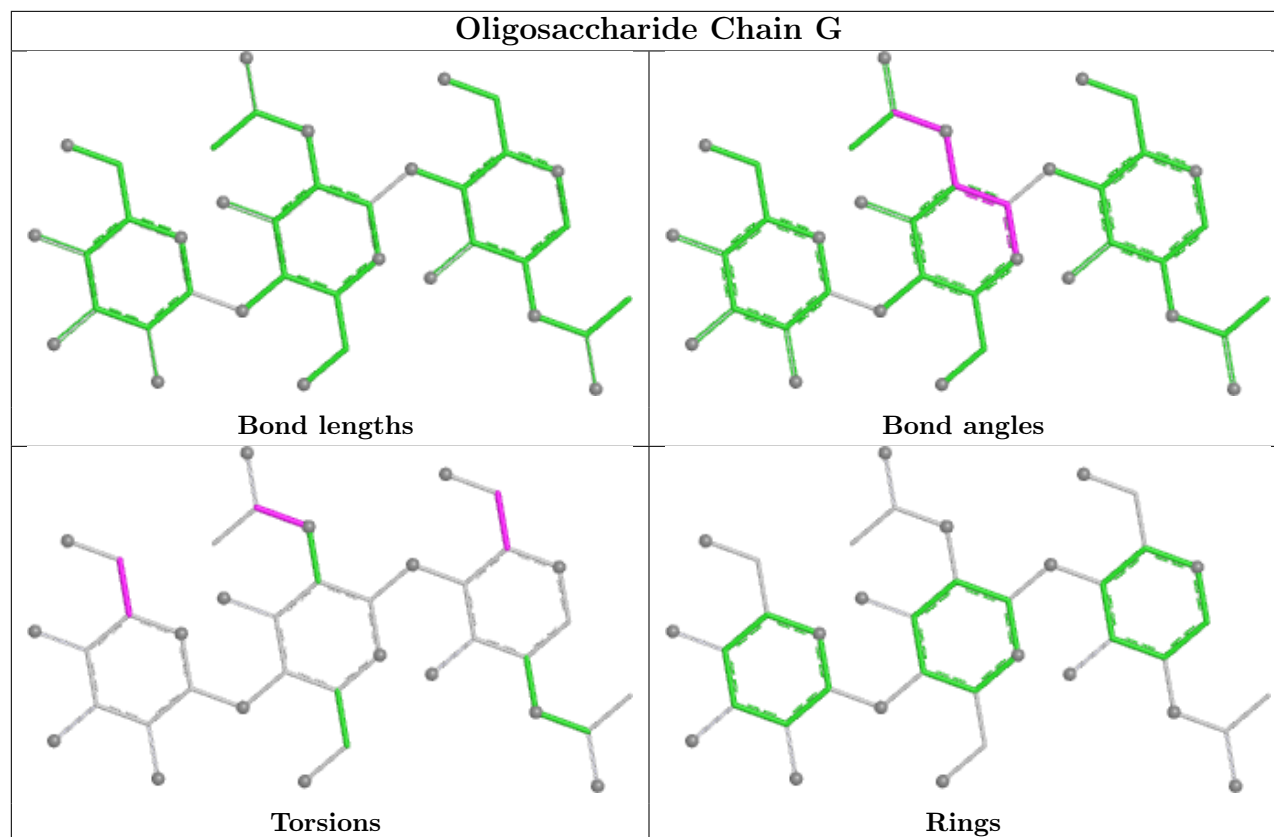
16 monomers are involved in 24 short contacts:

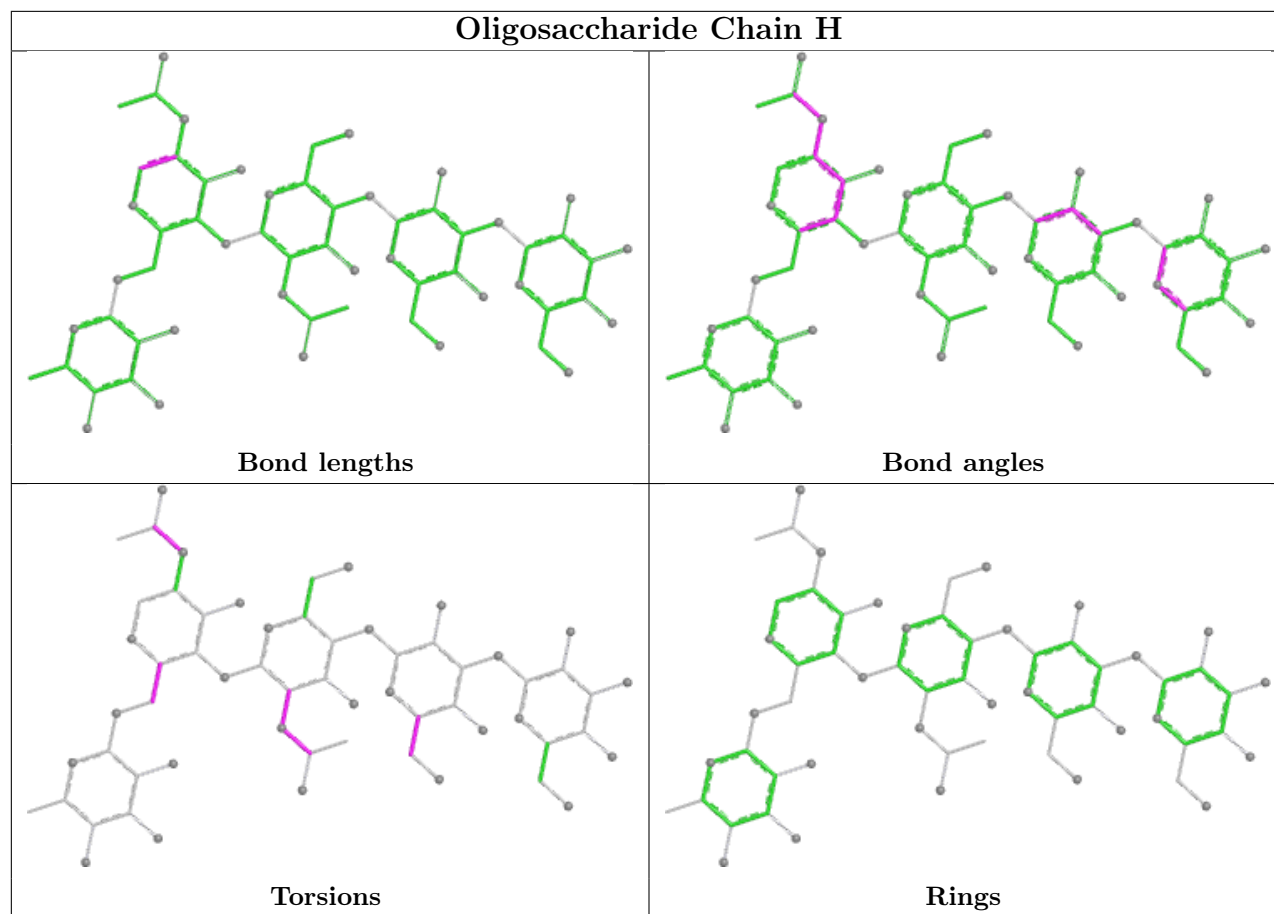
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	FUC	4	0
5	H	2	NAG	2	0
2	E	2	NAG	2	0
6	J	2	NAG	3	0
6	J	3	FUC	2	0
2	I	2	NAG	3	0
2	E	1	NAG	3	0
3	F	1	NAG	2	0
6	J	1	NAG	5	0
2	I	1	NAG	3	0
4	G	1	NAG	1	0
4	K	1	NAG	3	0
4	K	2	NAG	3	0
5	H	1	NAG	2	0
4	K	3	BMA	1	0
5	H	5	FUC	1	0

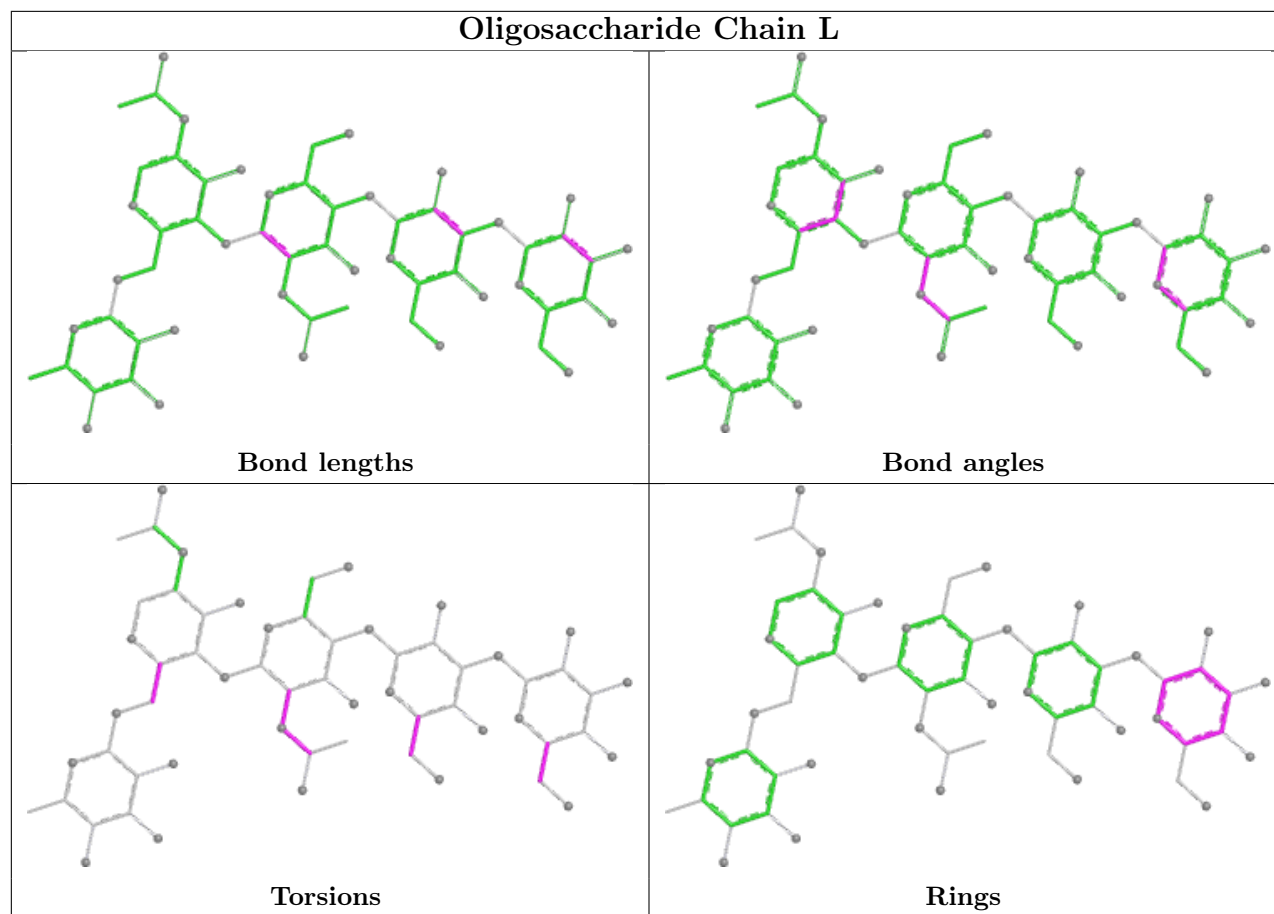
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

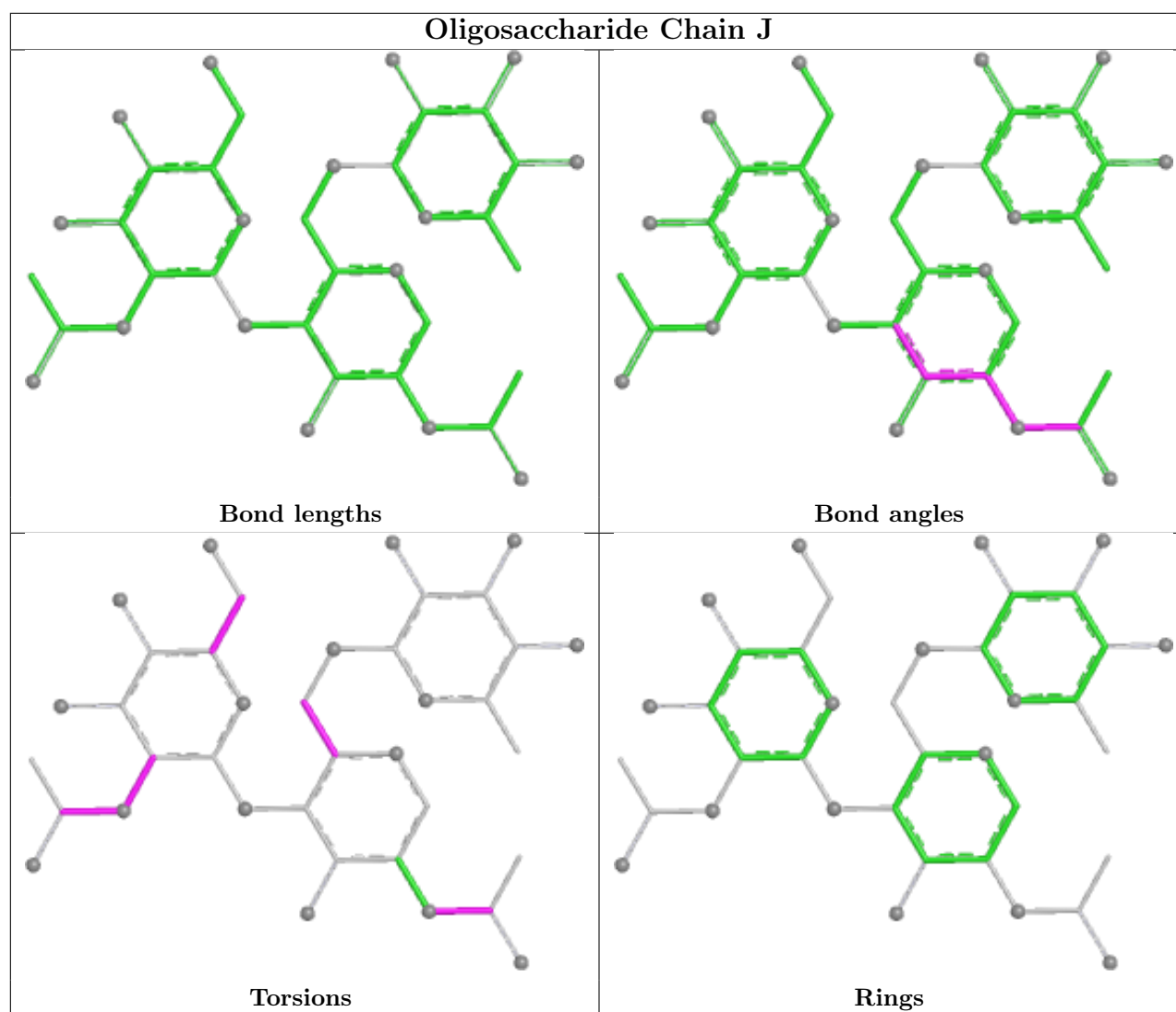












5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 42 are monoatomic - leaving 10 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	$\# Z > 2$
7	NAG	D	1738	1	14,14,15	1.07	1 (7%)	17,19,21	0.85	0
7	NAG	B	1736	1	14,14,15	0.89	1 (7%)	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	1736	1	14,14,15	0.75	0	17,19,21	0.73	1 (5%)
7	NAG	B	1735	1	14,14,15	0.71	0	17,19,21	0.81	0
7	NAG	A	1734	1	14,14,15	0.71	0	17,19,21	0.63	0
7	NAG	A	1735	1	14,14,15	0.66	0	17,19,21	0.68	0
7	NAG	D	1735	1	14,14,15	0.88	1 (7%)	17,19,21	0.67	0
7	NAG	C	1735	1	14,14,15	0.82	1 (7%)	17,19,21	0.67	0
7	NAG	B	1738	1	14,14,15	0.80	1 (7%)	17,19,21	0.58	0
7	NAG	C	1736	1	14,14,15	0.81	1 (7%)	17,19,21	0.75	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	1738	1	-	5/6/23/26	0/1/1/1
7	NAG	B	1736	1	-	5/6/23/26	0/1/1/1
7	NAG	D	1736	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	B	1735	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1734	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1735	1	-	5/6/23/26	0/1/1/1
7	NAG	D	1735	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1735	1	-	6/6/23/26	0/1/1/1
7	NAG	B	1738	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1736	1	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1738	NAG	C1-C2	3.27	1.56	1.52
7	B	1736	NAG	C1-C2	2.77	1.56	1.52
7	C	1735	NAG	C1-C2	2.34	1.55	1.52
7	C	1736	NAG	C1-C2	2.29	1.55	1.52
7	D	1735	NAG	C1-C2	2.26	1.55	1.52
7	B	1738	NAG	C1-C2	2.13	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1736	NAG	C2-N2-C7	-2.16	120.01	122.90
7	D	1736	NAG	C2-N2-C7	-2.06	120.14	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	1736	NAG	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1734	NAG	C8-C7-N2-C2
7	A	1734	NAG	O7-C7-N2-C2
7	A	1735	NAG	C8-C7-N2-C2
7	A	1735	NAG	O7-C7-N2-C2
7	B	1736	NAG	C8-C7-N2-C2
7	B	1736	NAG	O7-C7-N2-C2
7	B	1738	NAG	C8-C7-N2-C2
7	B	1738	NAG	O7-C7-N2-C2
7	C	1735	NAG	C1-C2-N2-C7
7	C	1735	NAG	C8-C7-N2-C2
7	C	1735	NAG	O7-C7-N2-C2
7	C	1736	NAG	O7-C7-N2-C2
7	D	1735	NAG	C8-C7-N2-C2
7	D	1735	NAG	O7-C7-N2-C2
7	D	1736	NAG	C8-C7-N2-C2
7	D	1736	NAG	O7-C7-N2-C2
7	D	1738	NAG	C8-C7-N2-C2
7	D	1738	NAG	O7-C7-N2-C2
7	C	1736	NAG	C8-C7-N2-C2
7	C	1735	NAG	O5-C5-C6-O6
7	B	1736	NAG	O5-C5-C6-O6
7	D	1735	NAG	O5-C5-C6-O6
7	A	1734	NAG	O5-C5-C6-O6
7	C	1735	NAG	C4-C5-C6-O6
7	B	1736	NAG	C4-C5-C6-O6
7	D	1735	NAG	C4-C5-C6-O6
7	A	1735	NAG	C4-C5-C6-O6
7	C	1736	NAG	C4-C5-C6-O6
7	A	1735	NAG	O5-C5-C6-O6
7	B	1735	NAG	O5-C5-C6-O6
7	C	1736	NAG	O5-C5-C6-O6
7	D	1738	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	1735	NAG	C3-C2-N2-C7
7	D	1736	NAG	C4-C5-C6-O6
7	A	1734	NAG	C4-C5-C6-O6
7	D	1738	NAG	O5-C5-C6-O6
7	C	1735	NAG	C3-C2-N2-C7
7	D	1736	NAG	O5-C5-C6-O6
7	D	1738	NAG	C1-C2-N2-C7
7	B	1736	NAG	C3-C2-N2-C7
7	B	1738	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1735	NAG	2	0
7	A	1734	NAG	4	0
7	D	1735	NAG	2	0
7	C	1735	NAG	2	0
7	B	1738	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	671/735 (91%)	-1.48	0 100 100	43, 64, 79, 87	0
1	B	671/735 (91%)	-1.49	0 100 100	41, 60, 75, 81	0
1	C	671/735 (91%)	-1.52	0 100 100	43, 64, 79, 88	0
1	D	671/735 (91%)	-1.53	0 100 100	41, 60, 75, 81	0
All	All	2684/2940 (91%)	-1.51	0 100 100	41, 62, 77, 88	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PAQ	D	471	21/22	0.98	0.06	54,59,60,61	0
1	PAQ	B	471	21/22	0.99	0.07	55,59,61,61	0
1	PAQ	C	471	21/22	0.99	0.03	56,59,61,61	0
1	PAQ	A	471	21/22	0.99	0.04	56,59,60,63	0

6.3 Carbohydrates [i](#)

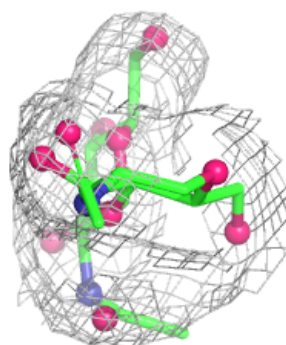
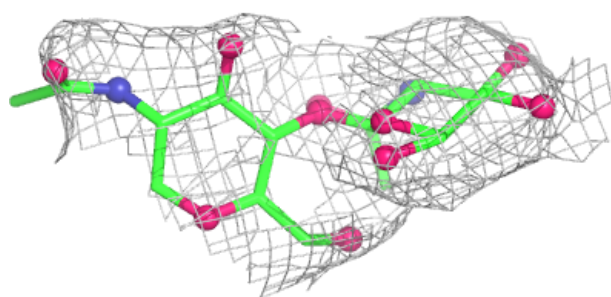
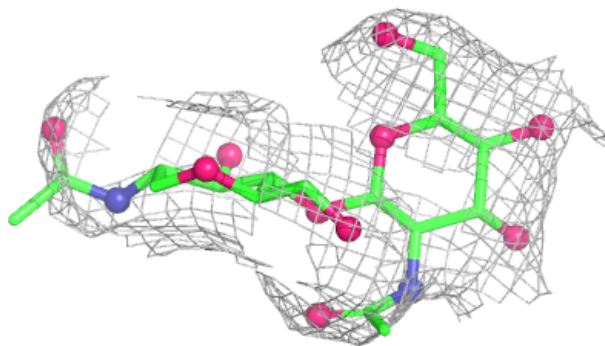
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	G	3	11/12	0.93	0.06	94,94,95,95	0
5	NAG	H	2	14/15	0.97	0.04	95,97,98,98	0
5	BMA	H	3	11/12	0.97	0.03	97,97,98,98	0
5	FUC	H	5	10/11	0.97	0.06	91,93,94,95	0
5	NAG	L	2	14/15	0.97	0.04	92,95,96,97	0
6	NAG	J	2	14/15	0.97	0.05	91,92,93,93	0
4	NAG	K	2	14/15	0.98	0.04	83,85,87,89	0
4	BMA	K	3	11/12	0.98	0.04	89,90,91,91	0
2	NAG	I	1	14/15	0.98	0.05	74,75,77,80	0
2	NAG	I	2	14/15	0.98	0.04	82,84,85,85	0
5	MAN	H	4	11/12	0.98	0.03	96,98,99,99	0
3	NAG	F	1	14/15	0.98	0.05	80,81,83,85	0
5	NAG	L	1	14/15	0.98	0.05	76,79,84,88	0
3	FUC	F	2	10/11	0.98	0.03	78,79,80,80	0
5	BMA	L	3	11/12	0.98	0.04	97,98,98,98	0
5	MAN	L	4	11/12	0.98	0.03	96,98,98,98	0
5	FUC	L	5	10/11	0.98	0.05	84,85,86,86	0
2	NAG	E	2	14/15	0.98	0.04	88,91,92,92	0
2	NAG	E	1	14/15	0.99	0.03	75,77,80,84	0
4	NAG	K	1	14/15	0.99	0.04	75,76,78,81	0
4	NAG	G	1	14/15	0.99	0.04	72,75,77,80	0
4	NAG	G	2	14/15	0.99	0.04	85,86,89,92	0
6	NAG	J	1	14/15	0.99	0.03	80,83,86,89	0
5	NAG	H	1	14/15	0.99	0.03	82,86,91,93	0
6	FUC	J	3	10/11	0.99	0.04	82,83,84,84	0

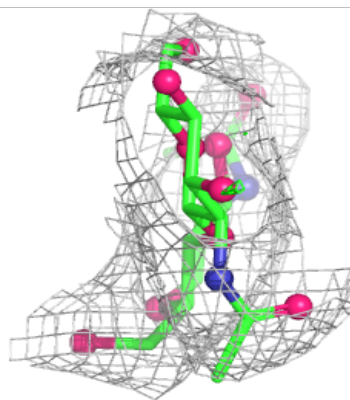
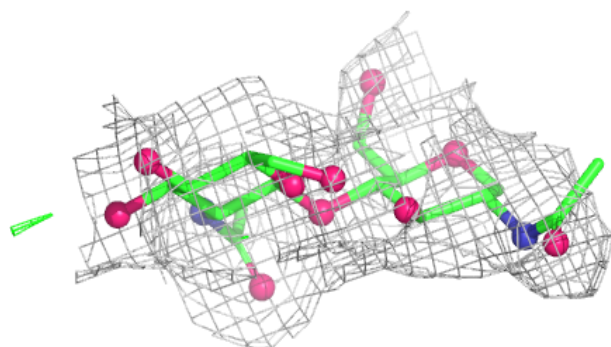
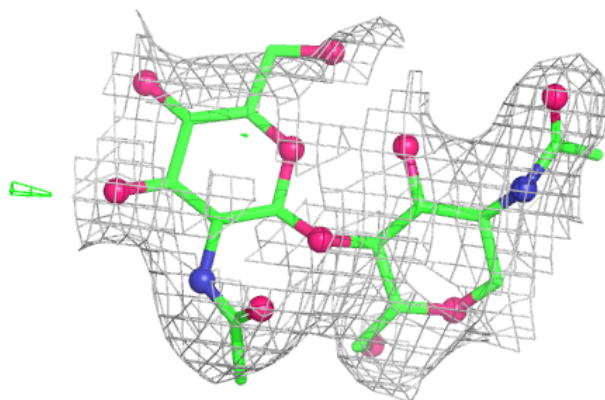
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

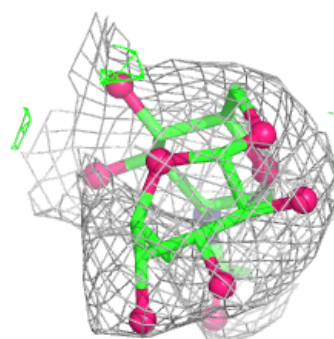
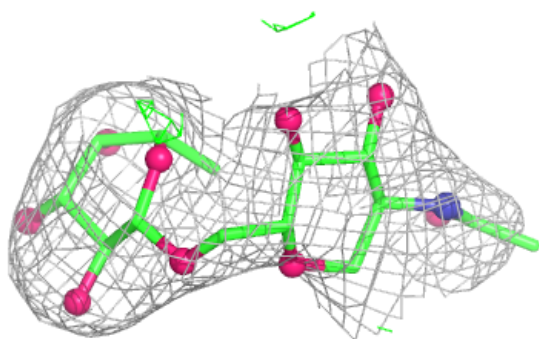
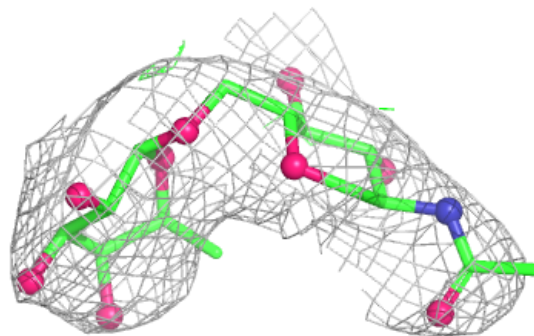
**Electron density around Chain I:**

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

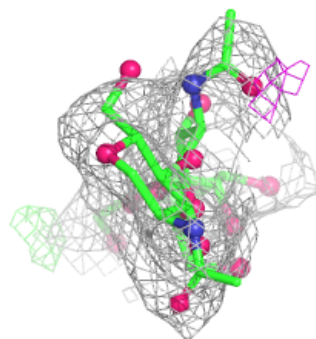
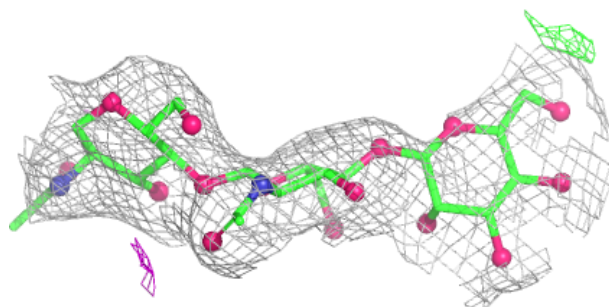
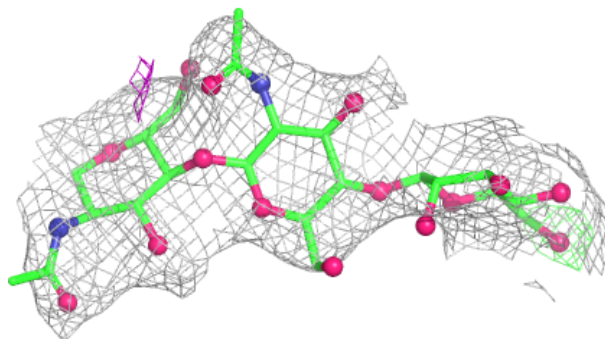


Electron density around Chain F:

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

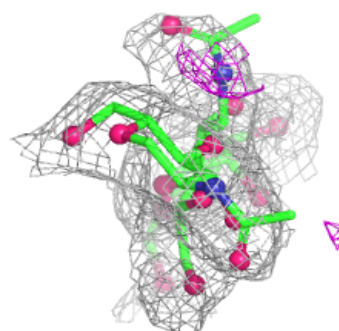
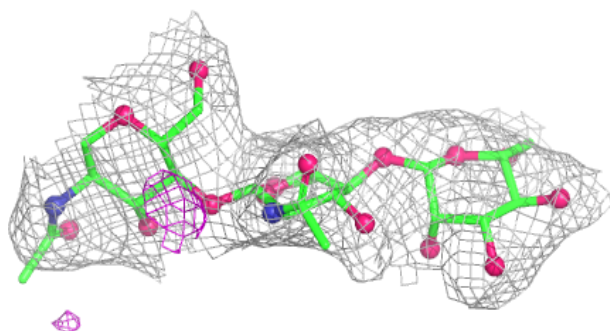
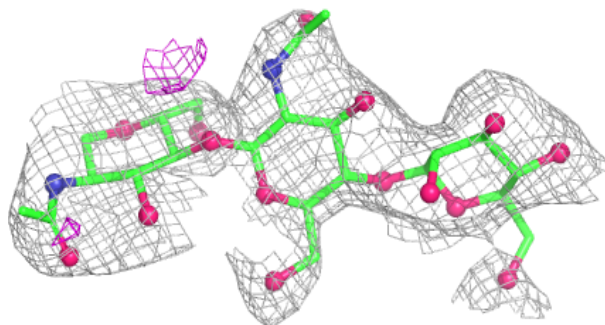
**Electron density around Chain G:**

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

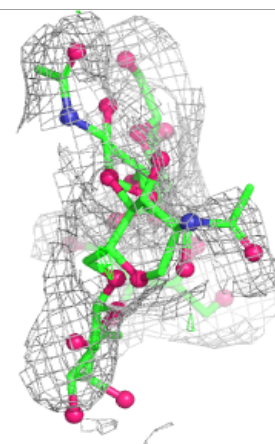
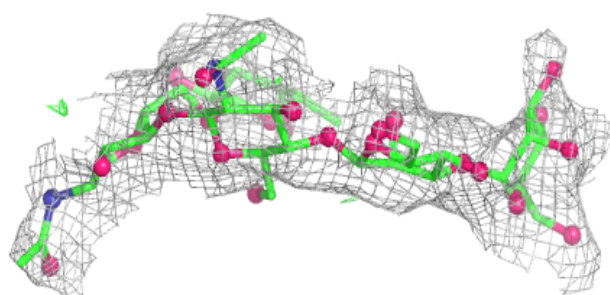
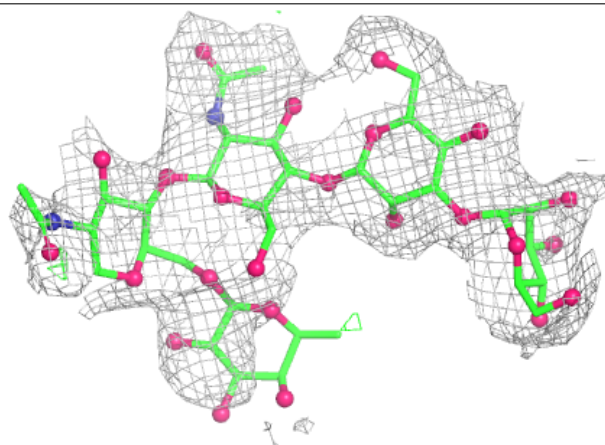


Electron density around Chain K:

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

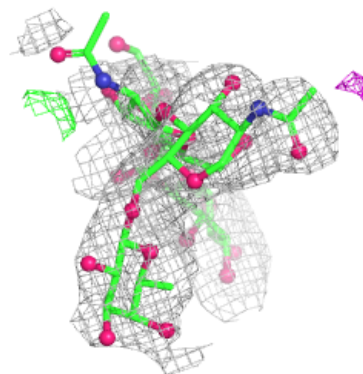
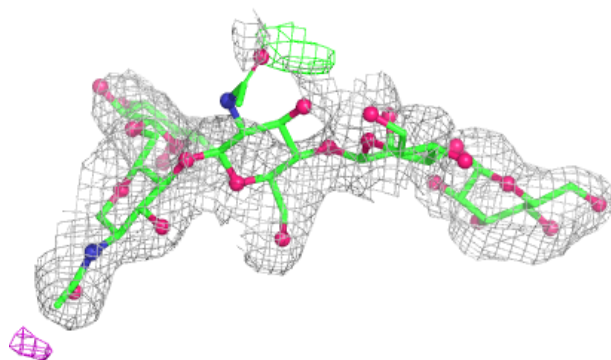
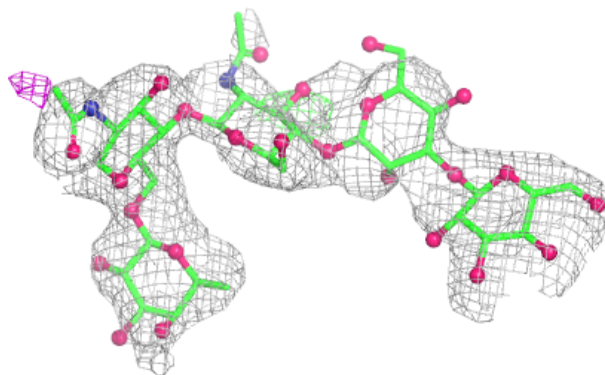
**Electron density around Chain H:**

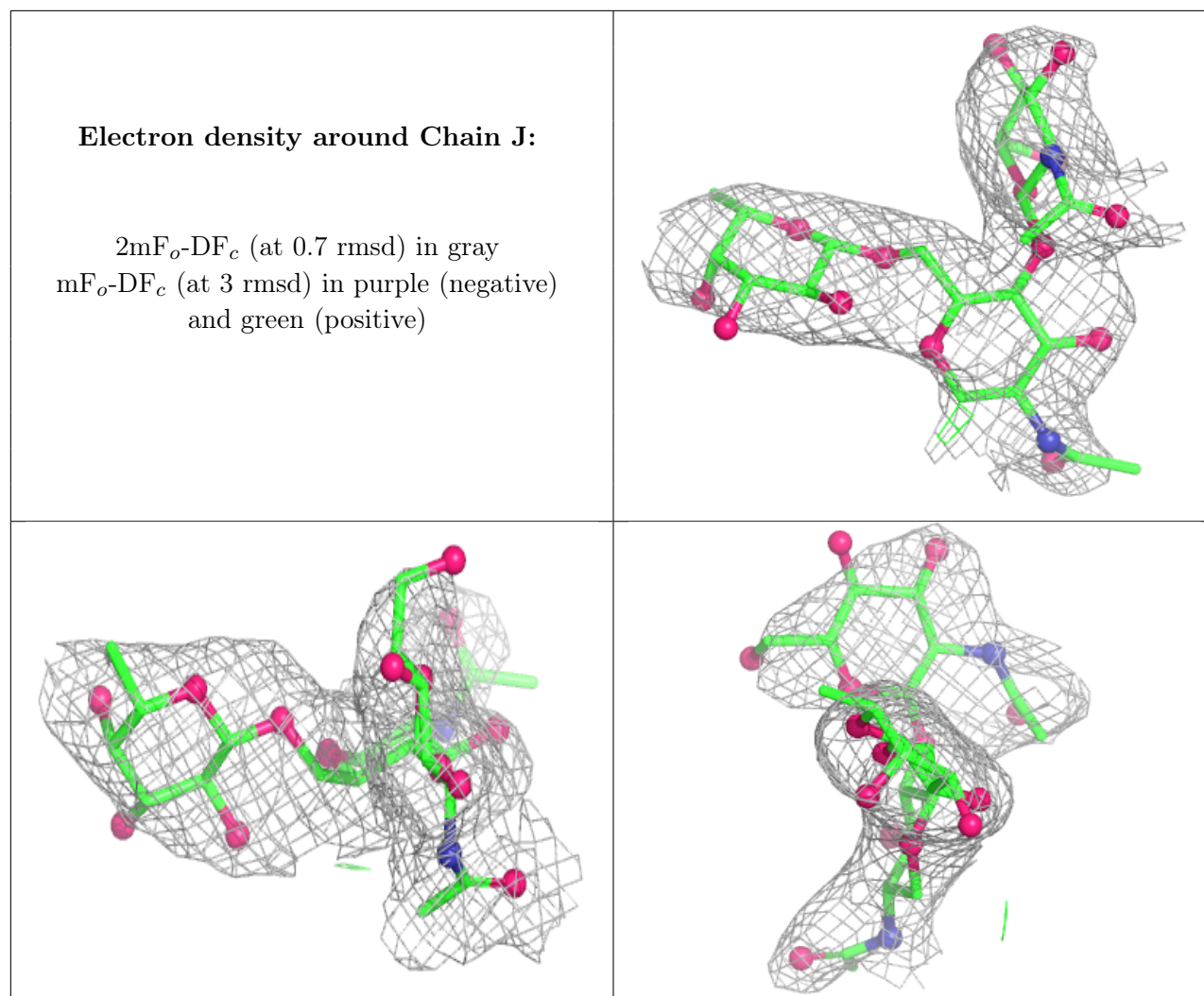
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





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
7	NAG	B	1736	14/15	0.94	0.05	84,86,88,88	0
7	NAG	B	1738	14/15	0.94	0.05	81,83,84,85	0
7	NAG	C	1735	14/15	0.96	0.04	70,72,73,74	0
7	NAG	D	1738	14/15	0.96	0.05	81,83,85,85	0
7	NAG	D	1736	14/15	0.97	0.03	83,84,86,86	0
7	NAG	A	1735	14/15	0.98	0.03	84,86,88,89	0
7	NAG	C	1736	14/15	0.98	0.04	82,85,88,88	0
7	NAG	D	1735	14/15	0.99	0.03	71,74,76,77	0
7	NAG	A	1734	14/15	0.99	0.03	71,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	1735	14/15	0.99	0.04	69,70,73,73	0
8	CA	D	1743	1/1	0.99	0.02	46,46,46,46	0
9	CU	A	1740	1/1	0.99	0.02	81,81,81,81	0
9	CU	A	1743	1/1	0.99	0.02	84,84,84,84	0
9	CU	A	1744	1/1	0.99	0.02	74,74,74,74	0
9	CU	B	1747	1/1	0.99	0.02	81,81,81,81	0
9	CU	B	1748	1/1	0.99	0.02	66,66,66,66	0
9	CU	B	1750	1/1	0.99	0.02	63,63,63,63	0
9	CU	C	1742	1/1	0.99	0.03	84,84,84,84	0
9	CU	C	1744	1/1	0.99	0.03	90,90,90,90	0
9	CU	C	1747	1/1	0.99	0.02	84,84,84,84	0
9	CU	D	1745	1/1	0.99	0.02	79,79,79,79	0
9	CU	D	1746	1/1	0.99	0.02	78,78,78,78	0
9	CU	D	1747	1/1	0.99	0.07	82,82,82,82	0
8	CA	B	1743	1/1	1.00	0.02	47,47,47,47	0
9	CU	A	1745	1/1	1.00	0.02	80,80,80,80	0
9	CU	B	1742	1/1	1.00	0.01	55,55,55,55	0
9	CU	B	1744	1/1	1.00	0.02	76,76,76,76	0
9	CU	B	1745	1/1	1.00	0.01	75,75,75,75	0
9	CU	B	1746	1/1	1.00	0.01	71,71,71,71	0
8	CA	C	1737	1/1	1.00	0.01	50,50,50,50	0
8	CA	C	1739	1/1	1.00	0.01	50,50,50,50	0
9	CU	B	1749	1/1	1.00	0.03	69,69,69,69	0
8	CA	D	1741	1/1	1.00	0.01	47,47,47,47	0
9	CU	C	1738	1/1	1.00	0.01	49,49,49,49	0
9	CU	C	1741	1/1	1.00	0.01	79,79,79,79	0
8	CA	A	1736	1/1	1.00	0.02	52,52,52,52	0
9	CU	C	1743	1/1	1.00	0.02	73,73,73,73	0
9	CU	A	1737	1/1	1.00	0.01	49,49,49,49	0
9	CU	C	1745	1/1	1.00	0.02	77,77,77,77	0
9	CU	C	1746	1/1	1.00	0.03	67,67,67,67	0
8	CA	A	1738	1/1	1.00	0.02	49,49,49,49	0
9	CU	D	1742	1/1	1.00	0.02	52,52,52,52	0
9	CU	A	1741	1/1	1.00	0.02	83,83,83,83	0
9	CU	A	1742	1/1	1.00	0.02	77,77,77,77	0
8	CA	B	1741	1/1	1.00	0.02	46,46,46,46	0
9	CU	D	1748	1/1	1.00	0.01	74,74,74,74	0
9	CU	D	1749	1/1	1.00	0.01	67,67,67,67	0
9	CU	D	1750	1/1	1.00	0.02	67,67,67,67	0
10	CL	A	1739	1/1	1.00	0.03	47,47,47,47	0
10	CL	A	1746	1/1	1.00	0.03	47,47,47,47	0
10	CL	C	1740	1/1	1.00	0.03	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CL	D	1744	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.