



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:48 AM UTC

PDB ID : 4WJL / pdb_00004wj
Title : Structure of human dipeptidyl peptidase 10 (DPPY): a modulator of neuronal Kv4 channels
Authors : Bezerra, G.A.; Dobrovetsky, E.; Seitova, A.; Fedosyuk, S.; Dhe-Paganon, S.; Gruber, K.
Deposited on : 2014-09-30
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

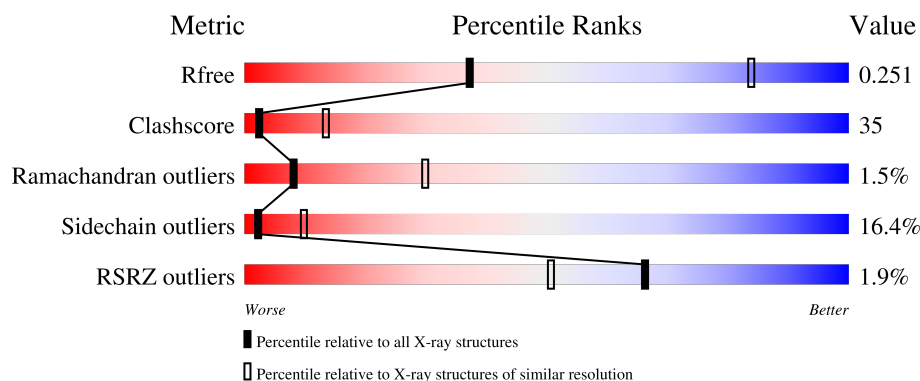
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



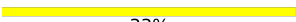
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	719	3% 43% 44% 12% .
1	B	719	3% 42% 44% 12% .
2	C	4	100%
3	D	2	100%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
4	F	3	 33%  67%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11829 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 Inactive dipeptidyl peptidase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	0	0
			5794	3730	959	1080	25			
1	B	719	Total	C	N	O	S	0	0	0
			5806	3736	960	1085	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	MET	VAL	variant	UNP Q8N608
A	401	ILE	VAL	variant	UNP Q8N608
B	288	MET	VAL	variant	UNP Q8N608
B	401	ILE	VAL	variant	UNP Q8N608

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



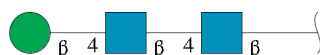
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



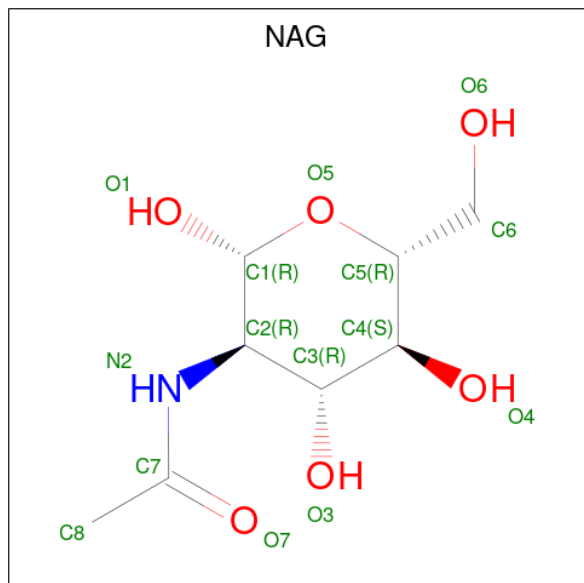
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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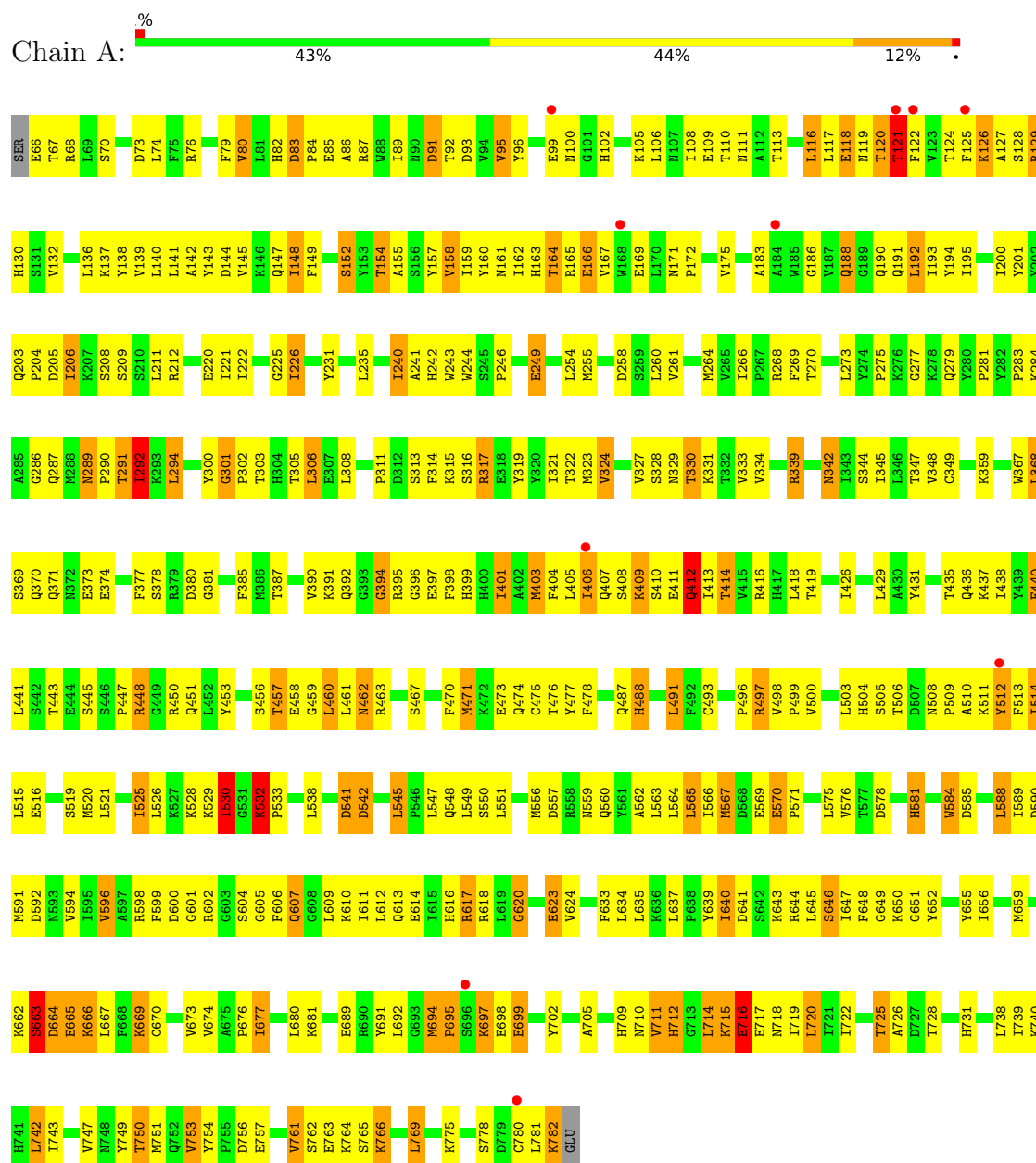
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

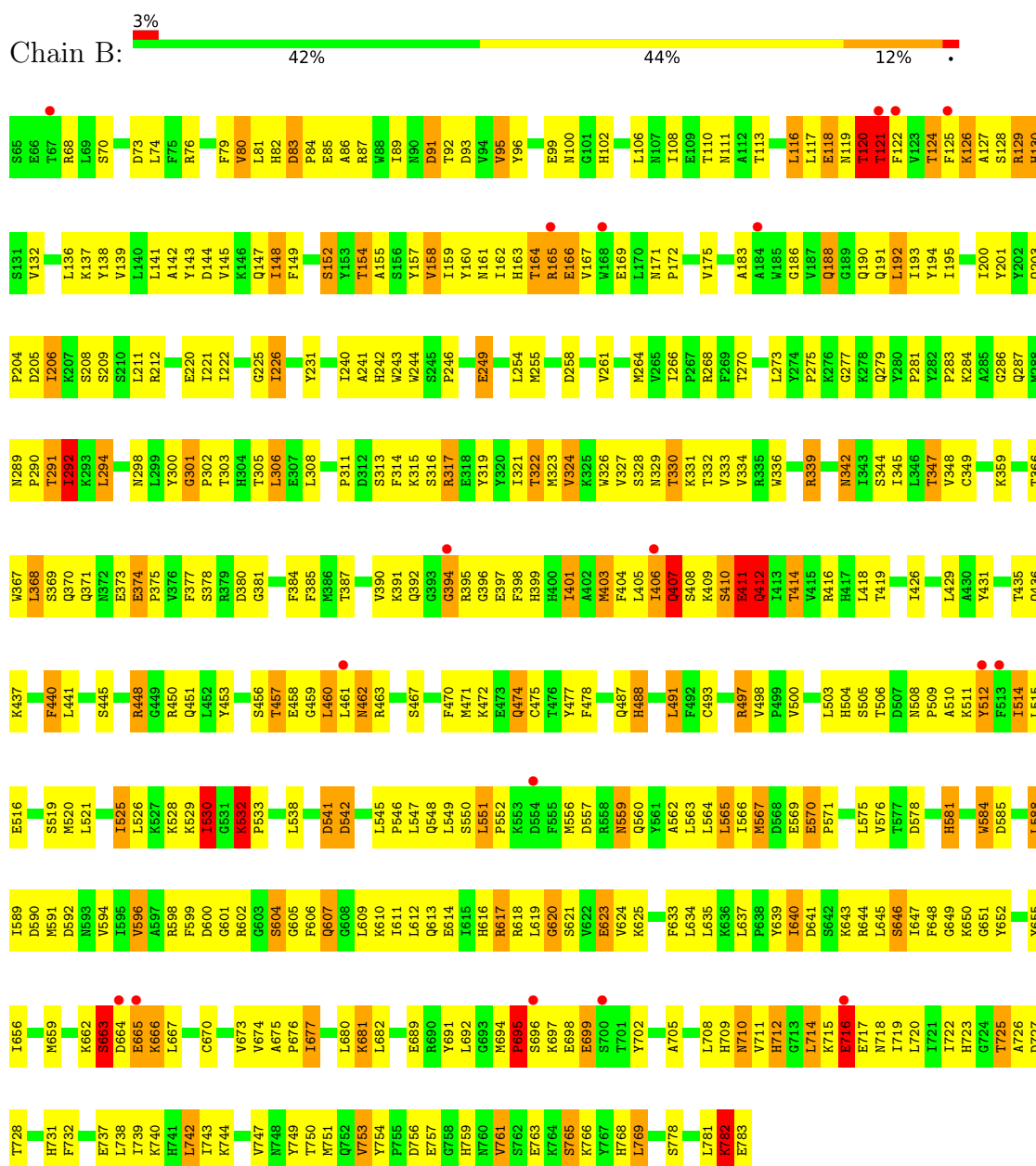
3 Residue-property plots

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

• Molecule 1: Inactive dipeptidyl peptidase 10



• Molecule 1: Inactive dipeptidyl peptidase 10



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

Chain C: 

NAG1
NAG2
BNA3
MAN4

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

Chain D: 

NAG1
NAG2

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain F:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.91Å 143.73Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.55 – 3.40 66.55 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.55-3.40) 99.9 (66.55-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.207 , 0.242 0.223 , 0.251	Depositor DCC
R_{free} test set	1476 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11829	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/5940	0.97	34/8052 (0.4%)
1	B	0.51	1/5952 (0.0%)	0.99	27/8069 (0.3%)
All	All	0.51	1/11892 (0.0%)	0.98	61/16121 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	THR	CA-CB	5.00	1.59	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	696	SER	N-CA-C	-10.25	100.45	113.16
1	A	408	SER	N-CA-C	10.10	123.37	110.24
1	B	716	GLU	N-CA-C	-8.55	102.86	113.20
1	B	120	THR	N-CA-C	-8.02	102.51	113.18
1	B	532	LYS	CA-C-N	8.00	129.84	119.84
1	B	532	LYS	C-N-CA	8.00	129.84	119.84
1	A	532	LYS	CA-C-N	7.86	129.66	119.84
1	A	532	LYS	C-N-CA	7.86	129.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	MET	CA-C-N	7.62	129.37	119.84
1	A	694	MET	C-N-CA	7.62	129.37	119.84
1	A	664	ASP	N-CA-C	-7.24	103.32	111.07
1	B	541	ASP	CB-CA-C	-7.22	108.24	116.54
1	A	541	ASP	CB-CA-C	-7.05	108.43	116.54
1	A	121	THR	N-CA-C	-6.91	98.41	109.39
1	A	620	GLY	N-CA-C	-6.74	107.07	115.08
1	B	620	GLY	N-CA-C	-6.69	107.12	115.08
1	B	121	THR	N-CA-C	-6.64	98.82	109.39
1	A	394	GLY	N-CA-C	-6.30	105.40	112.33
1	B	411	GLU	CA-C-N	-6.22	109.65	121.54
1	B	411	GLU	C-N-CA	-6.22	109.65	121.54
1	A	714	LEU	N-CA-C	-6.22	96.95	108.02
1	B	394	GLY	N-CA-C	-6.16	105.55	112.33
1	A	66	GLU	CA-C-N	-6.11	113.42	122.83
1	A	66	GLU	C-N-CA	-6.11	113.42	122.83
1	B	301	GLY	CA-C-N	6.05	126.21	119.32
1	B	301	GLY	C-N-CA	6.05	126.21	119.32
1	A	67	THR	N-CA-C	5.91	119.25	112.57
1	A	412	GLN	O-C-N	-5.85	114.81	122.59
1	A	301	GLY	CA-C-N	5.84	126.24	119.47
1	A	301	GLY	C-N-CA	5.84	126.24	119.47
1	B	782	LYS	N-CA-C	5.80	118.69	109.24
1	B	342	ASN	N-CA-C	5.78	120.46	113.17
1	B	714	LEU	N-CA-C	-5.77	97.74	108.02
1	A	545	LEU	CA-C-N	5.63	125.39	119.76
1	A	545	LEU	C-N-CA	5.63	125.39	119.76
1	B	374	GLU	CA-C-N	5.63	125.53	119.85
1	B	374	GLU	C-N-CA	5.63	125.53	119.85
1	B	557	ASP	N-CA-C	-5.60	105.94	112.89
1	B	699	GLU	N-CA-C	5.58	118.53	108.48
1	B	121	THR	CB-CA-C	-5.57	103.03	112.00
1	A	663	SER	N-CA-C	5.57	122.66	110.80
1	A	409	LYS	N-CA-C	5.53	122.58	110.80
1	A	292	ILE	N-CA-C	5.50	115.61	108.35
1	B	292	ILE	N-CA-C	5.50	115.61	108.35
1	A	473	GLU	N-CA-C	5.45	119.18	112.54
1	A	699	GLU	N-CA-C	5.38	118.17	108.48
1	A	471	MET	N-CA-C	5.37	119.94	113.17
1	B	474	GLN	N-CA-C	5.36	119.82	113.28
1	A	557	ASP	N-CA-C	-5.35	106.26	112.89
1	B	377	PHE	N-CA-C	5.29	117.31	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	551	LEU	CA-C-N	5.29	125.58	119.92
1	B	551	LEU	C-N-CA	5.29	125.58	119.92
1	A	342	ASN	N-CA-C	5.27	119.81	113.17
1	A	551	LEU	CA-C-N	5.22	125.51	119.92
1	A	551	LEU	C-N-CA	5.22	125.51	119.92
1	A	374	GLU	CA-C-N	5.22	125.12	119.85
1	A	374	GLU	C-N-CA	5.22	125.12	119.85
1	B	437	LYS	N-CA-C	5.20	118.21	109.95
1	A	377	PHE	N-CA-C	5.17	117.13	109.69
1	A	121	THR	CB-CA-C	-5.15	103.70	112.00
1	A	437	LYS	N-CA-C	5.04	117.95	109.95

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	GLN	Peptide,Mainchain
1	B	407	GLN	Peptide
1	B	412	GLN	Mainchain
1	B	695	PRO	Mainchain
1	B	710	ASN	Peptide,Mainchain

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	5794	0	5719	413	0
1	B	5806	0	5720	415	0
2	C	50	0	43	4	0
3	D	28	0	25	4	0
3	E	28	0	25	3	0
3	G	28	0	25	4	0
4	F	39	0	34	4	0
5	A	28	0	26	1	0
5	B	28	0	26	6	0
All	All	11829	0	11643	827	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 35.

All (827) 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:A:165:ARG:CD	1:A:165:ARG:H	1.60	1.14
1:A:165:ARG:H	1:A:165:ARG:HD2	1.08	1.08
1:A:488:HIS:HB3	1:A:505:SER:HA	1.38	1.05
1:A:644:ARG:HD2	1:A:781:LEU:O	1.57	1.04
1:B:488:HIS:HB3	1:B:505:SER:HA	1.39	1.03
1:B:165:ARG:H	1:B:165:ARG:HD2	1.18	1.03
1:A:165:ARG:HD2	1:A:165:ARG:N	1.72	1.02
1:B:644:ARG:HD2	1:B:781:LEU:O	1.58	1.02
1:B:165:ARG:HD2	1:B:165:ARG:N	1.72	1.01
1:A:118:GLU:HG3	1:A:119:ASN:H	1.28	0.98
1:B:118:GLU:HG3	1:B:119:ASN:N	1.80	0.95
1:A:602:ARG:HD2	1:A:614:GLU:HG2	1.47	0.94
1:B:118:GLU:HG3	1:B:119:ASN:H	1.33	0.94
1:B:602:ARG:HD2	1:B:614:GLU:HG2	1.48	0.94
1:A:775:LYS:NZ	5:B:809:NAG:H62	1.83	0.93
1:A:118:GLU:HG3	1:A:119:ASN:N	1.82	0.92
1:B:710:ASN:O	1:B:712:HIS:N	2.01	0.91
1:A:201:TYR:CE1	1:A:212:ARG:HG3	2.05	0.91
1:A:570:GLU:HG3	1:A:571:PRO:HD2	1.52	0.91
1:A:710:ASN:C	1:A:712:HIS:H	1.78	0.90
1:B:201:TYR:CE1	1:B:212:ARG:HG3	2.10	0.87
1:A:409:LYS:HG2	1:A:410:SER:H	1.40	0.87
1:A:775:LYS:CE	5:B:809:NAG:H62	2.05	0.86
1:B:570:GLU:HG3	1:B:571:PRO:HD2	1.57	0.85
1:B:742:LEU:HD23	1:B:747:VAL:HB	1.58	0.85
1:A:399:HIS:CE1	1:A:609:LEU:HD21	2.12	0.85
1:A:742:LEU:HD23	1:A:747:VAL:HB	1.59	0.84
1:A:695:PRO:HA	1:A:702:TYR:CD2	2.13	0.84
1:A:440:PHE:HE1	1:A:453:TYR:HB3	1.43	0.83
1:B:399:HIS:HE1	1:B:609:LEU:HD21	1.43	0.83
1:B:195:ILE:HD12	1:B:226:ILE:HG23	1.61	0.83
1:B:440:PHE:HE1	1:B:453:TYR:HB3	1.43	0.82
1:B:440:PHE:CE1	1:B:453:TYR:CB	2.63	0.82
1:A:609:LEU:HB3	1:A:613:GLN:HE21	1.45	0.82
1:B:399:HIS:CE1	1:B:609:LEU:HD21	2.14	0.82
1:A:440:PHE:CE1	1:A:453:TYR:CB	2.63	0.82
1:A:195:ILE:HD12	1:A:226:ILE:HG23	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HE1	1:A:609:LEU:HD21	1.44	0.81
1:A:753:VAL:HG11	1:B:753:VAL:HG11	1.63	0.81
1:B:411:GLU:O	1:B:412:GLN:HB2	1.80	0.80
1:B:673:VAL:HG11	1:B:676:PRO:HB3	1.64	0.80
1:A:460:LEU:HD13	1:A:460:LEU:H	1.47	0.79
1:B:609:LEU:HB3	1:B:613:GLN:HE21	1.46	0.78
1:B:460:LEU:HD13	1:B:460:LEU:H	1.47	0.78
1:B:644:ARG:HD3	1:B:783:GLU:OE2	1.83	0.78
1:B:448:ARG:HG3	1:B:448:ARG:HH11	1.48	0.78
1:B:287:GLN:HE21	1:B:287:GLN:HA	1.49	0.78
1:B:695:PRO:HA	1:B:702:TYR:CD2	2.18	0.78
1:B:440:PHE:HE1	1:B:453:TYR:CB	1.96	0.78
1:A:673:VAL:HG11	1:A:676:PRO:HB3	1.66	0.78
1:A:607:GLN:HG3	1:A:611:ILE:HD12	1.66	0.78
1:B:145:VAL:HA	1:B:155:ALA:HB2	1.64	0.78
1:A:145:VAL:HA	1:A:155:ALA:HB2	1.64	0.77
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.46	0.77
1:B:673:VAL:CG1	1:B:676:PRO:HB3	2.14	0.77
1:A:440:PHE:CE1	1:A:453:TYR:HB2	2.20	0.76
1:A:83:ASP:OD2	1:A:85:GLU:HG3	1.84	0.76
1:B:607:GLN:HG3	1:B:611:ILE:HD12	1.67	0.76
1:B:440:PHE:CE1	1:B:453:TYR:HB2	2.19	0.76
1:A:260:LEU:HD11	2:C:1:NAG:H62	1.67	0.76
1:A:287:GLN:HE21	1:A:287:GLN:HA	1.49	0.76
1:A:333:VAL:HG12	1:A:348:VAL:HG22	1.68	0.76
1:B:710:ASN:C	1:B:712:HIS:N	2.44	0.76
1:A:514:ILE:HD12	1:A:514:ILE:H	1.50	0.75
1:B:460:LEU:HD23	1:B:462:ASN:H	1.52	0.75
1:B:761:VAL:HG21	1:B:769:LEU:HD12	1.67	0.75
1:B:411:GLU:O	1:B:412:GLN:CB	2.28	0.75
1:A:270:THR:HG21	1:B:740:LYS:HD2	1.68	0.75
1:A:270:THR:CG2	1:B:740:LYS:HD2	2.17	0.74
1:B:514:ILE:HD12	1:B:514:ILE:H	1.52	0.74
1:A:440:PHE:HE1	1:A:453:TYR:CB	1.97	0.74
1:B:333:VAL:HG12	1:B:348:VAL:HG22	1.68	0.74
1:A:403:MET:HG3	1:A:418:LEU:HD21	1.70	0.74
1:A:761:VAL:HG21	1:A:769:LEU:HD12	1.68	0.74
1:A:460:LEU:HD23	1:A:462:ASN:H	1.53	0.73
1:B:562:ALA:HB1	1:B:781:LEU:HD13	1.71	0.73
1:B:83:ASP:OD2	1:B:85:GLU:HG3	1.88	0.73
1:B:403:MET:HG3	1:B:418:LEU:HD21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:HG2	1:A:410:SER:N	2.02	0.72
1:B:695:PRO:HA	1:B:702:TYR:CE2	2.23	0.72
4:F:1:NAG:H62	4:F:2:NAG:C7	2.19	0.72
1:A:673:VAL:CG1	1:A:676:PRO:HB3	2.17	0.72
1:B:165:ARG:N	1:B:165:ARG:CD	2.49	0.72
1:B:264:MET:HE3	1:B:264:MET:HA	1.72	0.72
1:A:581:HIS:ND1	1:A:581:HIS:C	2.47	0.72
1:A:264:MET:HE3	1:A:264:MET:HA	1.72	0.72
1:A:710:ASN:C	1:A:712:HIS:N	2.46	0.72
1:B:373:GLU:CD	1:B:387:THR:HG22	2.16	0.71
1:B:390:VAL:HG23	1:B:392:GLN:HG2	1.71	0.71
1:B:581:HIS:ND1	1:B:581:HIS:C	2.47	0.71
1:A:562:ALA:HB1	1:A:781:LEU:HD13	1.72	0.71
1:A:662:LYS:HB3	1:A:712:HIS:HE1	1.56	0.71
1:A:373:GLU:CD	1:A:387:THR:HG22	2.16	0.71
1:B:477:TYR:O	1:B:493:CYS:O	2.08	0.71
1:A:160:TYR:HE1	1:A:162:ILE:HD12	1.56	0.70
1:A:493:CYS:HB3	1:A:500:VAL:H	1.56	0.70
1:A:440:PHE:CE1	1:A:453:TYR:HB3	2.24	0.70
1:A:694:MET:HE3	1:A:697:LYS:HG3	1.72	0.70
1:B:478:PHE:CE1	1:B:491:LEU:HD11	2.27	0.70
1:A:201:TYR:HE1	1:A:212:ARG:HG3	1.53	0.70
1:A:292:ILE:HD11	1:A:321:ILE:HG13	1.75	0.69
1:A:695:PRO:HA	1:A:702:TYR:CE2	2.28	0.69
1:A:390:VAL:HG23	1:A:392:GLN:HG2	1.72	0.69
1:B:403:MET:HE2	1:B:403:MET:O	1.92	0.69
1:B:591:MET:O	1:B:592:ASP:HB2	1.93	0.69
1:A:403:MET:HE2	1:A:403:MET:O	1.93	0.69
1:A:478:PHE:CE1	1:A:491:LEU:HD11	2.27	0.69
1:B:246:PRO:HD2	1:B:329:ASN:HA	1.73	0.69
1:B:440:PHE:CE1	1:B:453:TYR:HB3	2.23	0.69
1:B:694:MET:HE3	1:B:697:LYS:HG3	1.75	0.69
1:A:246:PRO:HD2	1:A:329:ASN:HA	1.74	0.69
1:A:695:PRO:HA	1:A:702:TYR:HD2	1.56	0.69
1:B:287:GLN:HA	1:B:287:GLN:NE2	2.08	0.68
1:B:545:LEU:HD13	1:B:601:GLY:HA2	1.75	0.68
1:B:192:LEU:HD23	1:B:203:GLN:HB2	1.76	0.68
1:B:471:MET:HB2	1:B:475:CYS:N	2.09	0.68
1:A:169:GLU:HG2	1:A:171:ASN:HD21	1.57	0.68
1:A:220:GLU:HG3	1:A:281:PRO:HD3	1.76	0.68
1:B:493:CYS:HB3	1:B:500:VAL:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:LYS:HB3	1:B:712:HIS:HE1	1.59	0.68
1:A:192:LEU:HD23	1:A:203:GLN:HB2	1.76	0.68
1:A:287:GLN:HA	1:A:287:GLN:NE2	2.07	0.68
1:A:775:LYS:NZ	5:B:809:NAG:C6	2.56	0.68
2:C:2:NAG:O3	2:C:3:BMA:H2	1.94	0.68
1:B:148:ILE:HG13	1:B:154:THR:HG22	1.76	0.68
1:B:201:TYR:HE1	1:B:212:ARG:HG3	1.57	0.67
1:B:655:TYR:OH	1:B:705:ALA:HB1	1.95	0.67
1:B:677:ILE:HG13	1:B:677:ILE:O	1.93	0.67
1:A:139:VAL:HG23	1:A:162:ILE:HD13	1.75	0.67
1:A:148:ILE:HG13	1:A:154:THR:HG22	1.75	0.67
1:A:324:VAL:HB	1:A:334:VAL:HG22	1.75	0.67
1:B:169:GLU:HG2	1:B:171:ASN:HD21	1.58	0.67
1:A:477:TYR:O	1:A:493:CYS:O	2.11	0.67
1:B:139:VAL:HG23	1:B:162:ILE:HD13	1.77	0.67
1:A:73:ASP:HA	1:A:76:ARG:HG3	1.76	0.66
1:A:270:THR:HG22	1:A:270:THR:O	1.95	0.66
1:A:419:THR:HG21	1:A:440:PHE:HE2	1.61	0.66
1:B:160:TYR:HE1	1:B:162:ILE:HD12	1.59	0.66
1:A:129:ARG:HB3	1:A:142:ALA:HB3	1.77	0.66
1:B:407:GLN:HB3	1:B:408:SER:OG	1.95	0.66
3:D:1:NAG:H4	3:D:2:NAG:C7	2.24	0.66
1:A:591:MET:O	1:A:592:ASP:HB2	1.95	0.66
1:B:84:PRO:HG3	1:B:516:GLU:CB	2.26	0.66
1:B:467:SER:HB2	1:B:478:PHE:CE2	2.31	0.66
1:B:450:ARG:NH2	1:B:606:PHE:CD2	2.64	0.66
1:A:445:SER:OG	1:A:451:GLN:HG3	1.95	0.66
1:A:132:VAL:HG11	1:A:136:LEU:HD23	1.78	0.65
1:B:475:CYS:HB3	1:B:478:PHE:CZ	2.31	0.65
1:A:195:ILE:HG21	1:A:226:ILE:HG12	1.79	0.65
1:A:84:PRO:HG3	1:A:516:GLU:CB	2.25	0.65
1:A:655:TYR:OH	1:A:705:ALA:HB1	1.97	0.65
1:A:545:LEU:HD13	1:A:601:GLY:HA2	1.77	0.65
1:B:292:ILE:HD11	1:B:321:ILE:HG13	1.79	0.65
1:B:549:LEU:HD21	1:B:634:LEU:HD21	1.77	0.65
1:A:68:ARG:HB2	1:A:590:ASP:OD2	1.96	0.65
1:A:467:SER:HB2	1:A:478:PHE:CE2	2.32	0.65
1:A:677:ILE:HG13	1:A:677:ILE:O	1.94	0.65
1:B:220:GLU:HG3	1:B:281:PRO:HD3	1.78	0.65
1:A:674:VAL:HG22	1:A:722:ILE:HB	1.79	0.65
1:A:538:LEU:HD21	1:A:633:PHE:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG11	1:B:136:LEU:HD23	1.79	0.65
1:A:143:TYR:O	1:A:155:ALA:HB1	1.97	0.65
1:B:129:ARG:HB3	1:B:142:ALA:HB3	1.78	0.65
1:B:419:THR:HG21	1:B:440:PHE:HE2	1.62	0.64
1:B:652:TYR:O	1:B:655:TYR:HB3	1.96	0.64
1:B:102:HIS:HE2	3:E:1:NAG:HO6	1.44	0.64
1:B:324:VAL:HB	1:B:334:VAL:HG22	1.80	0.64
1:A:775:LYS:HE2	5:B:809:NAG:H62	1.80	0.64
1:B:270:THR:O	1:B:270:THR:HG22	1.95	0.64
3:G:1:NAG:H4	3:G:2:NAG:C7	2.27	0.64
1:B:457:THR:HG23	1:B:458:GLU:H	1.63	0.64
1:A:450:ARG:NH2	1:A:606:PHE:CD2	2.66	0.64
1:B:125:PHE:O	1:B:126:LYS:C	2.42	0.63
1:B:445:SER:OG	1:B:451:GLN:HG3	1.97	0.63
1:A:342:ASN:C	1:A:368:LEU:HD23	2.23	0.63
1:A:457:THR:HG23	1:A:458:GLU:H	1.63	0.63
1:A:775:LYS:HZ3	5:B:809:NAG:C6	2.09	0.63
1:A:775:LYS:HZ3	5:B:809:NAG:H62	1.63	0.63
1:A:471:MET:HB2	1:A:475:CYS:N	2.13	0.63
1:B:698:GLU:C	1:B:699:GLU:HG2	2.22	0.63
1:B:609:LEU:HB3	1:B:613:GLN:NE2	2.14	0.63
1:A:475:CYS:HB3	1:A:478:PHE:CZ	2.33	0.63
1:B:73:ASP:HA	1:B:76:ARG:HG3	1.80	0.63
1:A:286:GLY:HA3	1:A:695:PRO:HG3	1.80	0.62
1:B:195:ILE:HG21	1:B:226:ILE:HG12	1.81	0.62
1:B:436:GLN:O	1:B:457:THR:HG22	1.99	0.62
1:A:652:TYR:O	1:A:655:TYR:HB3	1.98	0.62
1:B:407:GLN:O	1:B:409:LYS:O	2.16	0.62
1:B:68:ARG:HB2	1:B:590:ASP:OD2	1.98	0.62
1:B:172:PRO:HG2	1:B:175:VAL:HB	1.82	0.62
1:B:739:ILE:HD13	1:B:751:MET:HE3	1.80	0.62
1:A:416:ARG:HH11	1:A:461:LEU:HD21	1.65	0.62
1:A:694:MET:HB3	1:A:697:LYS:HB2	1.81	0.62
1:A:436:GLN:O	1:A:457:THR:HG22	2.00	0.62
1:A:609:LEU:HB3	1:A:613:GLN:NE2	2.13	0.62
1:A:401:ILE:HD11	1:A:440:PHE:CD2	2.35	0.62
1:A:698:GLU:C	1:A:699:GLU:HG2	2.23	0.62
1:A:549:LEU:HD21	1:A:634:LEU:HD21	1.81	0.61
1:B:530:ILE:HG23	1:B:530:ILE:O	1.98	0.61
1:A:504:HIS:ND1	1:A:511:LYS:HA	2.15	0.61
1:B:342:ASN:C	1:B:368:LEU:HD23	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ASN:O	1:A:712:HIS:N	2.22	0.61
1:B:436:GLN:O	1:B:457:THR:N	2.32	0.61
1:B:530:ILE:O	1:B:530:ILE:CG2	2.48	0.61
1:B:674:VAL:HG22	1:B:722:ILE:HB	1.81	0.61
1:A:378:SER:HB3	1:A:381:GLY:H	1.65	0.61
1:A:715:LYS:C	1:A:717:GLU:H	2.08	0.61
1:B:538:LEU:HD21	1:B:633:PHE:CD2	2.35	0.61
1:A:220:GLU:HG2	1:A:279:GLN:O	2.01	0.61
1:A:739:ILE:HD13	1:A:751:MET:HE3	1.81	0.61
1:B:86:ALA:HA	1:B:96:TYR:HA	1.81	0.61
1:A:172:PRO:HG2	1:A:175:VAL:HB	1.82	0.61
1:B:403:MET:HB2	1:B:416:ARG:O	2.00	0.61
1:B:694:MET:HB3	1:B:697:LYS:HB2	1.82	0.61
1:A:125:PHE:O	1:A:126:LYS:C	2.43	0.61
1:B:416:ARG:HH11	1:B:461:LEU:HD21	1.66	0.61
1:B:225:GLY:C	1:B:241:ALA:HB3	2.25	0.61
1:A:121:THR:HG22	1:A:127:ALA:HB3	1.82	0.60
1:B:120:THR:O	1:B:122:PHE:N	2.32	0.60
1:B:714:LEU:HD13	1:B:719:ILE:HD12	1.82	0.60
1:A:86:ALA:HA	1:A:96:TYR:HA	1.82	0.60
1:A:403:MET:HB2	1:A:416:ARG:O	2.00	0.60
1:A:448:ARG:HD3	1:A:576:VAL:HG12	1.83	0.60
1:B:616:HIS:NE2	1:B:617:ARG:HD2	2.16	0.60
1:A:342:ASN:HA	1:A:368:LEU:HD23	1.84	0.60
1:A:530:ILE:HG23	1:A:530:ILE:O	2.00	0.60
1:A:565:LEU:HD22	1:A:567:MET:HE1	1.83	0.60
1:A:294:LEU:HD23	1:A:308:LEU:HB2	1.84	0.60
1:A:585:ASP:OD2	1:A:598:ARG:NH2	2.35	0.60
1:B:143:TYR:O	1:B:155:ALA:HB1	2.02	0.60
1:B:231:TYR:OH	1:B:292:ILE:HG21	2.01	0.60
1:A:436:GLN:O	1:A:457:THR:N	2.33	0.60
1:A:530:ILE:O	1:A:530:ILE:CG2	2.50	0.60
1:B:695:PRO:CA	1:B:702:TYR:CE2	2.85	0.60
1:A:448:ARG:HB3	1:A:578:ASP:OD1	2.02	0.59
1:A:403:MET:HG2	1:A:418:LEU:HD11	1.83	0.59
1:A:194:TYR:CE2	1:A:201:TYR:HD2	2.20	0.59
1:B:448:ARG:HD3	1:B:576:VAL:HG12	1.84	0.59
1:A:79:PHE:O	1:A:80:VAL:HB	2.00	0.59
1:B:192:LEU:CD2	1:B:203:GLN:HB2	2.33	0.59
1:A:317:ARG:O	1:A:319:TYR:HD1	1.85	0.59
1:B:385:PHE:CE1	1:B:403:MET:HE3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1:NAG:H4	3:D:2:NAG:N2	2.16	0.59
1:B:279:GLN:O	1:B:279:GLN:HG3	2.02	0.59
1:A:331:LYS:HA	1:A:349:CYS:O	2.03	0.59
1:B:317:ARG:O	1:B:319:TYR:HD1	1.85	0.59
1:A:764:LYS:HD3	1:B:744:LYS:HD2	1.85	0.58
1:B:510:ALA:C	1:B:512:TYR:H	2.10	0.58
1:B:339:ARG:HD2	1:B:689:GLU:OE1	2.03	0.58
1:B:342:ASN:HA	1:B:368:LEU:HD23	1.84	0.58
1:B:592:ASP:OD1	1:B:778:SER:HB2	2.04	0.58
1:B:694:MET:HE3	1:B:695:PRO:HD2	1.84	0.58
1:B:589:ILE:HG22	1:B:590:ASP:N	2.17	0.58
1:B:644:ARG:CD	1:B:783:GLU:OE2	2.52	0.58
1:A:225:GLY:C	1:A:241:ALA:HB3	2.27	0.58
1:A:563:LEU:HB3	1:A:645:LEU:HD22	1.85	0.58
1:A:641:ASP:OD1	1:A:643:LYS:HB2	2.04	0.58
1:B:450:ARG:HG3	1:B:450:ARG:HH11	1.69	0.58
1:B:563:LEU:HB3	1:B:645:LEU:HD22	1.85	0.58
1:A:411:GLU:C	1:A:412:GLN:O	2.44	0.57
1:B:448:ARG:HB3	1:B:578:ASP:OD1	2.04	0.57
1:B:270:THR:O	1:B:270:THR:CG2	2.52	0.57
1:A:192:LEU:CD2	1:A:203:GLN:HB2	2.34	0.57
1:B:121:THR:HG22	1:B:127:ALA:HB3	1.84	0.57
1:A:616:HIS:NE2	1:A:617:ARG:HD2	2.20	0.57
1:B:471:MET:HB3	1:B:474:GLN:HB2	1.85	0.57
1:B:401:ILE:HD11	1:B:440:PHE:CD2	2.40	0.57
1:A:714:LEU:HD13	1:A:719:ILE:HD12	1.86	0.57
4:F:2:NAG:H61	4:F:3:BMA:O2	2.05	0.57
1:A:231:TYR:OH	1:A:292:ILE:HG21	2.05	0.57
1:B:504:HIS:ND1	1:B:511:LYS:HA	2.20	0.57
1:A:165:ARG:H	1:A:165:ARG:HD3	1.61	0.56
1:A:270:THR:CG2	1:A:270:THR:O	2.52	0.56
1:A:450:ARG:HH11	1:A:450:ARG:HG3	1.70	0.56
1:A:538:LEU:HD12	1:A:599:PHE:CE1	2.41	0.56
1:B:220:GLU:HG2	1:B:279:GLN:O	2.05	0.56
1:A:339:ARG:HD2	1:A:689:GLU:OE1	2.05	0.56
1:A:740:LYS:HD2	1:B:270:THR:CG2	2.35	0.56
1:A:328:SER:HG	1:A:331:LYS:H	1.52	0.56
1:A:510:ALA:C	1:A:512:TYR:H	2.11	0.56
1:B:79:PHE:O	1:B:80:VAL:HB	2.04	0.56
1:B:511:LYS:O	1:B:512:TYR:C	2.49	0.56
1:A:118:GLU:C	1:A:120:THR:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:MET:HE3	1:A:695:PRO:HD2	1.88	0.56
1:B:378:SER:HB3	1:B:381:GLY:H	1.70	0.56
1:A:89:ILE:HD11	1:A:95:VAL:HB	1.87	0.56
1:A:279:GLN:O	1:A:279:GLN:HG3	2.06	0.56
1:B:331:LYS:HA	1:B:349:CYS:O	2.06	0.56
1:B:448:ARG:HG3	1:B:448:ARG:NH1	2.20	0.56
1:B:488:HIS:ND1	1:B:488:HIS:N	2.53	0.56
1:A:471:MET:HB3	1:A:474:GLN:HB2	1.87	0.56
1:A:589:ILE:HG22	1:A:590:ASP:N	2.20	0.56
1:B:394:GLY:O	1:B:395:ARG:CB	2.52	0.56
1:A:715:LYS:C	1:A:717:GLU:N	2.61	0.56
1:A:394:GLY:O	1:A:395:ARG:CB	2.54	0.55
1:B:186:GLY:HA3	1:B:191:GLN:HG3	1.88	0.55
1:A:575:LEU:HD22	1:A:598:ARG:HD3	1.89	0.55
1:A:589:ILE:HG13	1:A:596:VAL:HG13	1.89	0.55
1:A:663:SER:HB3	1:A:712:HIS:CE1	2.41	0.55
1:B:403:MET:HG2	1:B:418:LEU:HD11	1.88	0.55
1:B:695:PRO:CA	1:B:702:TYR:HE2	2.20	0.55
1:A:563:LEU:HB3	1:A:645:LEU:CD2	2.36	0.55
1:A:385:PHE:CE1	1:A:403:MET:HE3	2.41	0.55
1:B:563:LEU:HB3	1:B:645:LEU:CD2	2.36	0.55
1:A:194:TYR:CE2	1:A:201:TYR:CD2	2.95	0.54
3:D:1:NAG:H2	3:D:2:NAG:O7	2.06	0.54
1:A:110:THR:O	1:A:111:ASN:HB2	2.07	0.54
1:B:89:ILE:HD11	1:B:95:VAL:HB	1.89	0.54
1:B:102:HIS:CD2	3:E:1:NAG:HO6	2.26	0.54
1:B:367:TRP:CD1	1:B:367:TRP:C	2.85	0.54
1:B:471:MET:HG3	1:B:475:CYS:SG	2.46	0.54
1:A:118:GLU:CG	1:A:119:ASN:N	2.64	0.54
1:A:592:ASP:OD1	1:A:778:SER:HB2	2.07	0.54
1:B:84:PRO:HG3	1:B:516:GLU:HB2	1.89	0.54
1:B:194:TYR:CE2	1:B:201:TYR:HD2	2.25	0.54
1:B:575:LEU:HD13	1:B:598:ARG:HB3	1.88	0.54
1:A:511:LYS:O	1:A:512:TYR:C	2.50	0.54
1:A:565:LEU:HD22	1:A:567:MET:CE	2.37	0.54
1:A:695:PRO:CA	1:A:702:TYR:CE2	2.91	0.54
1:B:431:TYR:HE1	1:B:457:THR:HG21	1.73	0.54
1:A:120:THR:O	1:A:122:PHE:N	2.41	0.54
1:A:488:HIS:ND1	1:A:488:HIS:N	2.54	0.54
1:A:575:LEU:HD13	1:A:598:ARG:HB3	1.90	0.54
1:A:323:MET:HE2	1:A:373:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TYR:HE1	1:A:457:THR:HG21	1.73	0.53
1:B:96:TYR:CG	1:B:96:TYR:O	2.59	0.53
1:A:644:ARG:HD2	1:A:781:LEU:C	2.33	0.53
1:B:538:LEU:HD12	1:B:599:PHE:CE1	2.43	0.53
1:A:84:PRO:HG3	1:A:516:GLU:HB2	1.90	0.53
1:B:725:THR:HG22	1:B:756:ASP:H	1.74	0.53
1:A:448:ARG:HG3	1:A:448:ARG:NH1	2.18	0.53
1:B:110:THR:O	1:B:111:ASN:HB2	2.08	0.53
1:B:663:SER:HB3	1:B:712:HIS:CE1	2.43	0.53
1:B:739:ILE:HD13	1:B:751:MET:CE	2.38	0.53
1:B:460:LEU:HD23	1:B:462:ASN:HB3	1.89	0.53
1:B:663:SER:O	1:B:664:ASP:C	2.50	0.53
1:B:160:TYR:CE1	1:B:162:ILE:HD12	2.44	0.53
1:B:644:ARG:HD2	1:B:781:LEU:C	2.33	0.53
1:B:450:ARG:HG3	1:B:450:ARG:NH1	2.23	0.53
1:A:165:ARG:CD	1:A:165:ARG:N	2.37	0.53
1:A:378:SER:C	1:A:380:ASP:H	2.17	0.53
1:A:739:ILE:HD13	1:A:751:MET:CE	2.38	0.53
1:B:670:CYS:CB	1:B:718:ASN:HB3	2.39	0.53
1:B:725:THR:CG2	1:B:756:ASP:H	2.22	0.53
1:A:141:LEU:HB2	1:A:158:VAL:HG12	1.91	0.53
1:A:169:GLU:HG2	1:A:171:ASN:ND2	2.24	0.53
1:A:258:ASP:OD1	1:A:290:PRO:HB3	2.09	0.53
1:A:694:MET:CE	1:A:697:LYS:HG3	2.39	0.53
1:B:193:ILE:HD11	1:B:242:HIS:CD2	2.44	0.53
1:B:589:ILE:HG13	1:B:596:VAL:HG13	1.90	0.53
1:B:294:LEU:HD23	1:B:308:LEU:HB2	1.90	0.52
1:B:322:THR:HG21	1:B:371:GLN:OE1	2.07	0.52
1:B:714:LEU:HD13	1:B:719:ILE:CD1	2.38	0.52
1:A:96:TYR:O	1:A:96:TYR:CG	2.62	0.52
1:B:328:SER:HG	1:B:331:LYS:H	1.55	0.52
1:B:709:HIS:O	1:B:710:ASN:HB2	2.09	0.52
1:A:73:ASP:OD1	1:A:76:ARG:NH1	2.43	0.52
1:A:584:TRP:HH2	1:A:648:PHE:CE1	2.28	0.52
1:B:584:TRP:HH2	1:B:648:PHE:CZ	2.27	0.52
1:A:725:THR:CG2	1:A:756:ASP:H	2.22	0.52
1:B:339:ARG:NH1	1:B:689:GLU:OE2	2.43	0.52
1:B:584:TRP:HH2	1:B:648:PHE:CE1	2.27	0.52
1:A:725:THR:HG22	1:A:756:ASP:H	1.74	0.52
1:B:102:HIS:NE2	3:E:1:NAG:O6	2.38	0.52
1:B:695:PRO:HA	1:B:702:TYR:HD2	1.69	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:GLU:HG3	1:B:656:ILE:CD1	2.40	0.52
1:B:648:PHE:CD1	1:B:648:PHE:C	2.87	0.52
1:A:186:GLY:HA3	1:A:191:GLN:HG3	1.90	0.52
1:A:193:ILE:HD11	1:A:242:HIS:CD2	2.44	0.52
1:B:641:ASP:OD1	1:B:643:LYS:HB2	2.09	0.52
1:B:677:ILE:HD11	1:B:680:LEU:HD22	1.90	0.52
1:A:695:PRO:C	1:A:697:LYS:N	2.68	0.52
1:B:323:MET:HE2	1:B:373:GLU:O	2.10	0.52
1:A:520:MET:HG2	1:A:521:LEU:N	2.25	0.51
1:A:623:GLU:HG3	1:A:656:ILE:CD1	2.40	0.51
1:B:694:MET:CE	1:B:697:LYS:HG3	2.41	0.51
3:G:1:NAG:H2	3:G:2:NAG:O7	2.10	0.51
1:A:163:HIS:ND1	1:A:163:HIS:C	2.68	0.51
1:A:188:GLN:O	1:A:191:GLN:HG2	2.09	0.51
1:A:648:PHE:C	1:A:648:PHE:CD1	2.87	0.51
1:B:520:MET:HG2	1:B:521:LEU:N	2.24	0.51
1:B:565:LEU:HD22	1:B:567:MET:HE1	1.92	0.51
1:B:95:VAL:HG13	1:B:95:VAL:O	2.10	0.51
1:A:322:THR:HG21	1:A:371:GLN:OE1	2.10	0.51
1:B:163:HIS:ND1	1:B:163:HIS:C	2.68	0.51
1:A:426:ILE:HD12	1:A:450:ARG:HG2	1.93	0.51
1:A:132:VAL:HG22	1:A:139:VAL:HG22	1.93	0.51
1:A:367:TRP:CD1	1:A:367:TRP:C	2.89	0.51
1:A:670:CYS:CB	1:A:718:ASN:HB3	2.41	0.51
1:A:401:ILE:HD11	1:A:440:PHE:HD2	1.75	0.51
1:A:403:MET:O	1:A:404:PHE:C	2.54	0.51
1:A:403:MET:O	1:A:405:LEU:HD22	2.11	0.51
1:B:169:GLU:HG2	1:B:171:ASN:ND2	2.26	0.51
1:B:584:TRP:CH2	1:B:648:PHE:CZ	2.99	0.51
1:A:193:ILE:HG23	1:A:244:TRP:CH2	2.45	0.51
1:A:588:LEU:HD22	1:A:594:VAL:HB	1.93	0.51
1:B:588:LEU:HD22	1:B:594:VAL:HB	1.93	0.50
1:A:95:VAL:HG13	1:A:95:VAL:O	2.11	0.50
1:A:440:PHE:N	1:A:440:PHE:CD1	2.78	0.50
1:A:644:ARG:CD	1:A:781:LEU:O	2.46	0.50
1:B:141:LEU:HB2	1:B:158:VAL:HG12	1.93	0.50
1:B:161:ASN:OD1	1:B:161:ASN:C	2.55	0.50
1:B:460:LEU:HD22	1:B:460:LEU:N	2.26	0.50
2:C:2:NAG:O3	2:C:4:MAN:H3	2.10	0.50
1:A:159:ILE:HG21	1:A:206:ILE:HD11	1.93	0.50
1:B:508:ASN:OD1	1:B:510:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:CE1	1:A:162:ILE:HD12	2.41	0.50
1:A:450:ARG:HG3	1:A:450:ARG:NH1	2.25	0.50
1:A:567:MET:SD	1:A:647:ILE:HD11	2.51	0.50
1:B:403:MET:O	1:B:405:LEU:HD22	2.10	0.50
1:B:550:SER:HB2	1:B:596:VAL:HG22	1.92	0.50
1:B:73:ASP:OD2	1:B:528:LYS:NZ	2.45	0.50
1:A:460:LEU:N	1:A:460:LEU:HD22	2.26	0.50
1:B:410:SER:C	1:B:411:GLU:O	2.51	0.50
1:A:513:PHE:HB3	5:A:801:NAG:H61	1.93	0.50
1:B:194:TYR:CE2	1:B:201:TYR:CD2	2.99	0.50
1:B:567:MET:SD	1:B:647:ILE:HD11	2.52	0.50
1:A:460:LEU:HD23	1:A:462:ASN:HB3	1.94	0.50
1:A:315:LYS:O	1:A:316:SER:OG	2.27	0.50
1:A:508:ASN:OD1	1:A:510:ALA:HB2	2.12	0.50
1:B:646:SER:HA	1:B:670:CYS:O	2.12	0.50
1:A:264:MET:HG2	1:A:731:HIS:NE2	2.27	0.49
1:A:403:MET:CG	1:A:418:LEU:HD11	2.42	0.49
1:B:188:GLN:O	1:B:191:GLN:HG2	2.12	0.49
1:B:249:GLU:HG3	1:B:300:TYR:CE2	2.47	0.49
1:B:405:LEU:HB2	1:B:414:THR:HG23	1.94	0.49
1:B:73:ASP:OD1	1:B:76:ARG:NH1	2.44	0.49
1:B:403:MET:O	1:B:404:PHE:C	2.53	0.49
1:B:193:ILE:HG23	1:B:244:TRP:CH2	2.46	0.49
1:B:264:MET:HG2	1:B:731:HIS:NE2	2.28	0.49
1:A:373:GLU:OE2	1:A:387:THR:HG22	2.12	0.49
1:B:142:ALA:HB2	1:B:157:TYR:CE2	2.47	0.49
1:B:488:HIS:HB2	1:B:504:HIS:O	2.11	0.49
1:A:488:HIS:HB2	1:A:504:HIS:O	2.12	0.49
1:A:714:LEU:HD13	1:A:719:ILE:CD1	2.43	0.49
1:B:102:HIS:CE1	1:B:119:ASN:OD1	2.66	0.49
1:B:132:VAL:HG22	1:B:139:VAL:HG22	1.95	0.49
1:B:161:ASN:ND2	1:B:164:THR:HG23	2.28	0.49
1:B:620:GLY:N	1:B:623:GLU:OE1	2.40	0.49
1:A:525:ILE:HD13	1:A:526:LEU:N	2.28	0.49
1:A:550:SER:HB2	1:A:596:VAL:HG22	1.95	0.49
1:A:666:LYS:NZ	1:A:666:LYS:HB3	2.27	0.49
1:A:255:MET:SD	1:A:255:MET:C	2.95	0.49
1:B:562:ALA:CB	1:B:781:LEU:HD13	2.41	0.49
1:B:749:TYR:C	1:B:749:TYR:CD1	2.91	0.49
1:A:677:ILE:HD11	1:A:680:LEU:HD22	1.95	0.49
1:A:121:THR:CG2	1:A:127:ALA:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:O	1:B:125:PHE:C	2.55	0.49
1:B:286:GLY:HA3	1:B:695:PRO:HG3	1.93	0.49
1:A:165:ARG:O	1:A:166:GLU:C	2.55	0.49
1:A:339:ARG:NH1	1:A:689:GLU:OE2	2.46	0.49
1:A:670:CYS:HB3	1:A:718:ASN:HB3	1.95	0.49
1:A:739:ILE:CD1	1:A:751:MET:HE3	2.43	0.49
1:A:161:ASN:C	1:A:161:ASN:OD1	2.57	0.48
1:B:373:GLU:OE2	1:B:387:THR:HG22	2.13	0.48
1:A:695:PRO:CA	1:A:702:TYR:HE2	2.27	0.48
1:B:328:SER:HG	1:B:331:LYS:N	2.11	0.48
1:B:450:ARG:H	1:B:477:TYR:HA	1.78	0.48
1:B:710:ASN:O	1:B:712:HIS:CG	2.67	0.48
4:F:1:NAG:H4	4:F:2:NAG:O7	2.14	0.48
1:A:669:LYS:HD2	1:A:780:CYS:O	2.13	0.48
1:B:159:ILE:HG21	1:B:206:ILE:HD11	1.95	0.48
1:A:268:ARG:NH1	1:A:277:GLY:HA2	2.29	0.48
1:A:409:LYS:CG	1:A:410:SER:H	2.10	0.48
1:B:195:ILE:CD1	1:B:226:ILE:HG23	2.38	0.48
1:B:575:LEU:HD22	1:B:598:ARG:HD3	1.95	0.48
1:A:512:TYR:HB3	1:A:513:PHE:H	1.54	0.48
1:A:640:ILE:HD13	1:A:640:ILE:O	2.13	0.48
1:A:751:MET:O	1:A:751:MET:HG2	2.13	0.48
1:B:470:PHE:CE1	1:B:491:LEU:HD12	2.49	0.48
1:A:584:TRP:HH2	1:A:648:PHE:CZ	2.32	0.48
1:B:120:THR:C	1:B:122:PHE:N	2.72	0.48
1:B:143:TYR:O	1:B:144:ASP:HB2	2.14	0.48
1:B:429:LEU:HD11	1:B:441:LEU:CD2	2.44	0.48
1:B:666:LYS:NZ	1:B:666:LYS:HB3	2.29	0.48
1:A:646:SER:HA	1:A:670:CYS:O	2.13	0.48
1:B:159:ILE:HD13	1:B:206:ILE:HD11	1.96	0.48
1:A:471:MET:HG3	1:A:475:CYS:SG	2.54	0.48
1:A:663:SER:O	1:A:664:ASP:C	2.56	0.48
1:B:440:PHE:CD1	1:B:440:PHE:N	2.81	0.48
1:A:243:TRP:HH2	1:A:254:LEU:HG	1.78	0.47
1:A:566:ILE:C	1:A:567:MET:HE3	2.39	0.47
1:B:602:ARG:HA	1:B:611:ILE:HG23	1.96	0.47
1:B:670:CYS:HB3	1:B:718:ASN:HB3	1.96	0.47
1:A:124:THR:O	1:A:125:PHE:C	2.57	0.47
1:B:70:SER:HA	1:B:591:MET:HE2	1.96	0.47
1:B:637:LEU:HD13	1:B:639:TYR:CZ	2.49	0.47
1:A:166:GLU:H	1:A:166:GLU:HG3	1.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ALA:CB	1:A:781:LEU:HD13	2.43	0.47
1:B:525:ILE:HD13	1:B:526:LEU:N	2.29	0.47
1:B:620:GLY:H	1:B:623:GLU:CD	2.22	0.47
1:B:118:GLU:CG	1:B:119:ASN:N	2.64	0.47
3:D:1:NAG:H4	3:D:2:NAG:O7	2.14	0.47
1:A:70:SER:HA	1:A:591:MET:HE2	1.96	0.47
1:A:116:LEU:C	1:A:162:ILE:HD11	2.40	0.47
1:A:436:GLN:C	1:A:457:THR:HG22	2.40	0.47
1:A:488:HIS:CB	1:A:504:HIS:O	2.62	0.47
1:A:749:TYR:CD1	1:A:749:TYR:C	2.92	0.47
1:B:460:LEU:HD23	1:B:462:ASN:N	2.23	0.47
1:A:405:LEU:HB2	1:A:414:THR:HG23	1.97	0.47
1:B:121:THR:CG2	1:B:127:ALA:HB3	2.44	0.47
1:B:738:LEU:HG	1:B:742:LEU:HD12	1.95	0.47
1:B:739:ILE:CD1	1:B:751:MET:HE3	2.43	0.47
1:A:138:TYR:CD1	1:A:161:ASN:HA	2.50	0.47
1:A:584:TRP:CD1	1:A:584:TRP:C	2.92	0.47
1:B:116:LEU:C	1:B:162:ILE:HD11	2.40	0.47
1:B:426:ILE:HD12	1:B:450:ARG:HG2	1.96	0.47
1:B:488:HIS:CB	1:B:504:HIS:O	2.63	0.47
1:B:571:PRO:HD3	1:B:652:TYR:CD2	2.50	0.47
1:B:585:ASP:HB2	1:B:596:VAL:HG11	1.97	0.47
1:B:605:GLY:HA2	1:B:612:LEU:HD13	1.97	0.47
1:A:301:GLY:HA3	1:A:302:PRO:HD3	1.80	0.47
1:A:431:TYR:CE1	1:A:457:THR:HG21	2.50	0.47
1:B:158:VAL:HG13	1:B:167:VAL:HG13	1.97	0.47
1:B:268:ARG:NH1	1:B:277:GLY:HA2	2.29	0.47
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.80	0.47
1:A:584:TRP:CH2	1:A:648:PHE:CZ	3.03	0.47
1:A:591:MET:O	1:A:592:ASP:CB	2.63	0.47
1:B:92:THR:O	1:B:108:ILE:HG12	2.15	0.47
1:B:410:SER:O	1:B:411:GLU:O	2.32	0.47
1:B:436:GLN:C	1:B:457:THR:HG22	2.39	0.47
1:B:751:MET:O	1:B:751:MET:HG2	2.14	0.47
1:A:738:LEU:HG	1:A:742:LEU:HD12	1.97	0.47
1:B:645:LEU:HD12	1:B:667:LEU:O	2.15	0.47
1:A:95:VAL:O	1:A:96:TYR:C	2.58	0.46
1:A:126:LYS:HE3	1:A:126:LYS:HA	1.98	0.46
1:B:130:HIS:ND1	1:B:130:HIS:C	2.73	0.46
1:B:431:TYR:CE1	1:B:457:THR:HG21	2.50	0.46
1:B:584:TRP:CD1	1:B:584:TRP:C	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:GLY:H	1:A:623:GLU:CD	2.22	0.46
1:A:740:LYS:HD2	1:B:270:THR:HG21	1.96	0.46
1:B:80:VAL:HG12	1:B:80:VAL:O	2.15	0.46
1:B:258:ASP:OD1	1:B:290:PRO:HB3	2.14	0.46
1:A:249:GLU:HG3	1:A:300:TYR:CE2	2.51	0.46
1:B:754:TYR:HB3	1:B:757:GLU:HG3	1.98	0.46
1:A:286:GLY:HA2	1:A:694:MET:HE1	1.98	0.46
1:A:292:ILE:HD11	1:A:321:ILE:CG1	2.45	0.46
1:A:470:PHE:HE2	1:A:511:LYS:HG3	1.80	0.46
1:A:158:VAL:HG13	1:A:167:VAL:HG13	1.98	0.46
1:A:450:ARG:H	1:A:477:TYR:HA	1.80	0.46
1:B:566:ILE:C	1:B:567:MET:HE3	2.40	0.46
1:B:617:ARG:NH2	1:B:699:GLU:OE2	2.48	0.46
1:B:640:ILE:HD13	1:B:640:ILE:O	2.15	0.46
1:A:80:VAL:HG12	1:A:80:VAL:O	2.14	0.46
1:A:142:ALA:HB2	1:A:157:TYR:CE2	2.51	0.46
1:A:328:SER:OG	1:A:330:THR:HG23	2.15	0.46
1:A:541:ASP:HB3	1:A:542:ASP:H	1.38	0.46
1:A:73:ASP:OD2	1:A:528:LYS:NZ	2.49	0.46
1:A:195:ILE:CD1	1:A:226:ILE:HG23	2.40	0.46
1:A:602:ARG:HA	1:A:611:ILE:HG23	1.98	0.46
1:A:409:LYS:CG	1:A:410:SER:N	2.67	0.46
1:A:436:GLN:HG2	1:A:458:GLU:HB2	1.97	0.46
1:A:753:VAL:HG11	1:B:753:VAL:CG1	2.41	0.46
1:B:609:LEU:HD13	1:B:613:GLN:NE2	2.31	0.46
1:B:126:LYS:HE3	1:B:126:LYS:HA	1.98	0.46
1:B:644:ARG:NH1	1:B:781:LEU:O	2.49	0.46
1:A:273:LEU:HD23	1:B:682:LEU:HD23	1.97	0.46
1:A:719:ILE:O	1:A:750:THR:HG23	2.16	0.46
1:B:409:LYS:O	1:B:410:SER:C	2.58	0.46
1:B:436:GLN:HG2	1:B:458:GLU:HB2	1.97	0.46
1:A:268:ARG:HH12	1:A:277:GLY:HA2	1.81	0.45
1:A:301:GLY:O	1:A:303:THR:HG23	2.16	0.45
1:A:328:SER:HG	1:A:331:LYS:N	2.13	0.45
1:A:460:LEU:HD23	1:A:462:ASN:N	2.26	0.45
1:B:714:LEU:HD12	1:B:747:VAL:HG11	1.97	0.45
3:G:1:NAG:O3	3:G:2:NAG:N2	2.49	0.45
1:A:545:LEU:HB3	1:A:600:ASP:O	2.17	0.45
1:A:644:ARG:NH1	1:A:781:LEU:O	2.49	0.45
1:B:378:SER:C	1:B:380:ASP:H	2.23	0.45
1:A:172:PRO:HG2	1:A:175:VAL:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:C	1:A:201:TYR:HD1	2.25	0.45
1:A:497:ARG:HD3	1:A:498:VAL:O	2.16	0.45
1:A:548:GLN:HB2	1:A:576:VAL:HG22	1.99	0.45
1:A:564:LEU:HD22	1:A:588:LEU:HD12	1.99	0.45
1:B:82:HIS:HB3	1:B:516:GLU:OE2	2.16	0.45
1:B:172:PRO:HG2	1:B:175:VAL:CB	2.46	0.45
1:B:591:MET:O	1:B:592:ASP:CB	2.61	0.45
1:A:147:GLN:HA	1:A:147:GLN:OE1	2.17	0.45
1:A:411:GLU:O	1:A:412:GLN:O	2.34	0.45
1:A:82:HIS:HB3	1:A:516:GLU:OE2	2.15	0.45
1:A:130:HIS:ND1	1:A:130:HIS:C	2.74	0.45
1:A:569:GLU:O	1:A:652:TYR:HB3	2.17	0.45
1:B:268:ARG:O	1:B:275:PRO:HB2	2.16	0.45
1:B:545:LEU:HB3	1:B:600:ASP:O	2.17	0.45
1:B:548:GLN:HB2	1:B:576:VAL:HG22	1.99	0.45
3:G:1:NAG:H4	3:G:2:NAG:N2	2.31	0.45
1:A:92:THR:O	1:A:108:ILE:HG12	2.17	0.45
1:A:221:ILE:HG22	1:A:222:ILE:HG13	1.98	0.45
1:A:291:THR:C	1:A:292:ILE:HG22	2.42	0.45
1:B:403:MET:CG	1:B:418:LEU:HD11	2.46	0.45
1:B:471:MET:O	1:B:472:LYS:HB2	2.17	0.45
1:B:691:TYR:N	1:B:691:TYR:CD1	2.85	0.45
1:A:157:TYR:CE2	1:A:183:ALA:HB3	2.52	0.45
1:A:193:ILE:HG12	1:A:244:TRP:HZ2	1.81	0.45
1:A:327:VAL:HG23	1:A:328:SER:H	1.81	0.45
1:A:645:LEU:HD12	1:A:667:LEU:O	2.17	0.45
1:B:541:ASP:HB3	1:B:542:ASP:H	1.37	0.45
1:A:143:TYR:O	1:A:144:ASP:HB2	2.17	0.45
1:A:161:ASN:ND2	1:A:164:THR:HG23	2.32	0.45
1:A:268:ARG:O	1:A:275:PRO:HB2	2.17	0.45
1:A:637:LEU:HD13	1:A:639:TYR:CZ	2.52	0.45
1:A:691:TYR:N	1:A:691:TYR:CD1	2.85	0.45
1:A:754:TYR:HB3	1:A:757:GLU:HG3	1.97	0.45
1:B:397:GLU:C	1:B:398:PHE:CD1	2.95	0.45
1:A:264:MET:HG2	1:A:731:HIS:CD2	2.52	0.45
1:B:564:LEU:HD22	1:B:588:LEU:HD12	1.99	0.45
1:A:664:ASP:C	1:A:665:GLU:HG2	2.42	0.44
1:A:762:SER:O	1:A:766:LYS:HB2	2.16	0.44
1:B:147:GLN:OE1	1:B:147:GLN:HA	2.17	0.44
1:B:401:ILE:HD11	1:B:440:PHE:HD2	1.80	0.44
1:B:510:ALA:C	1:B:512:TYR:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:HIS:HD1	1:A:118:GLU:HA	1.82	0.44
1:A:450:ARG:HD2	1:A:477:TYR:CZ	2.52	0.44
1:A:460:LEU:H	1:A:460:LEU:CD1	2.16	0.44
1:A:498:VAL:CG1	1:A:521:LEU:HD22	2.47	0.44
1:A:666:LYS:HD2	1:A:717:GLU:HG3	2.00	0.44
1:A:126:LYS:O	1:A:126:LYS:HG3	2.17	0.44
1:A:584:TRP:CD1	1:A:585:ASP:N	2.86	0.44
1:A:617:ARG:NH2	1:A:699:GLU:OE2	2.50	0.44
1:A:709:HIS:O	1:A:710:ASN:HB2	2.17	0.44
1:B:193:ILE:HD11	1:B:242:HIS:NE2	2.32	0.44
1:B:488:HIS:HB3	1:B:505:SER:CA	2.29	0.44
1:B:624:VAL:HG21	1:B:659:MET:HB2	1.99	0.44
1:A:193:ILE:HD11	1:A:242:HIS:NE2	2.32	0.44
1:A:241:ALA:HB1	1:A:254:LEU:HB2	1.98	0.44
1:A:609:LEU:HD13	1:A:613:GLN:NE2	2.33	0.44
1:A:666:LYS:HE2	1:A:716:GLU:HG2	2.00	0.44
1:A:714:LEU:HD12	1:A:747:VAL:HG11	1.99	0.44
1:A:739:ILE:O	1:A:743:ILE:HG13	2.17	0.44
1:B:204:PRO:HG2	1:B:208:SER:HB2	2.00	0.44
1:B:301:GLY:O	1:B:303:THR:HG23	2.17	0.44
1:B:498:VAL:CG1	1:B:521:LEU:HD22	2.47	0.44
1:B:565:LEU:HD22	1:B:567:MET:CE	2.48	0.44
1:A:506:THR:O	1:A:509:PRO:HD3	2.18	0.44
1:B:497:ARG:HD3	1:B:498:VAL:O	2.17	0.44
1:B:648:PHE:CD1	1:B:649:GLY:N	2.85	0.44
1:B:662:LYS:HB3	1:B:712:HIS:CE1	2.47	0.44
1:B:666:LYS:HE2	1:B:716:GLU:HG2	1.99	0.44
1:B:695:PRO:CA	1:B:702:TYR:CD2	2.97	0.44
1:A:620:GLY:N	1:A:623:GLU:OE1	2.42	0.44
1:B:366:THR:OG1	1:B:367:TRP:N	2.50	0.44
1:B:450:ARG:HD2	1:B:477:TYR:CZ	2.53	0.44
1:B:551:LEU:HA	1:B:552:PRO:HD3	1.89	0.44
1:B:411:GLU:C	1:B:412:GLN:O	2.59	0.44
1:A:159:ILE:HD13	1:A:206:ILE:HD11	1.98	0.44
1:A:172:PRO:HA	1:A:194:TYR:OH	2.17	0.44
1:B:183:ALA:O	1:B:193:ILE:O	2.36	0.44
1:B:291:THR:C	1:B:292:ILE:HG22	2.43	0.44
1:A:87:ARG:HB3	1:A:95:VAL:HG12	2.00	0.44
1:A:648:PHE:CD1	1:A:649:GLY:N	2.86	0.44
1:B:190:GLN:HG3	1:B:205:ASP:HA	2.00	0.44
1:B:243:TRP:HH2	1:B:254:LEU:HG	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LYS:CE	1:B:716:GLU:HG2	2.48	0.44
1:B:138:TYR:CD1	1:B:161:ASN:HA	2.53	0.43
1:B:286:GLY:HA2	1:B:694:MET:HE1	2.00	0.43
1:B:292:ILE:O	1:B:292:ILE:HD13	2.17	0.43
1:B:394:GLY:O	1:B:395:ARG:HB2	2.17	0.43
1:B:268:ARG:HH12	1:B:277:GLY:HA2	1.82	0.43
1:B:396:GLY:HA3	1:B:610:LYS:HB2	2.00	0.43
1:B:532:LYS:HA	1:B:533:PRO:HD3	1.55	0.43
1:B:681:LYS:HB2	1:B:681:LYS:HE3	1.70	0.43
1:B:157:TYR:CE2	1:B:183:ALA:HB3	2.53	0.43
1:B:221:ILE:HG22	1:B:222:ILE:HG13	2.00	0.43
1:B:411:GLU:C	1:B:412:GLN:CG	2.90	0.43
1:B:126:LYS:O	1:B:126:LYS:HG3	2.17	0.43
1:B:165:ARG:O	1:B:166:GLU:C	2.61	0.43
1:B:172:PRO:HA	1:B:194:TYR:OH	2.17	0.43
1:B:193:ILE:HG12	1:B:244:TRP:HZ2	1.83	0.43
1:B:715:LYS:C	1:B:717:GLU:H	2.23	0.43
1:A:584:TRP:CG	1:A:585:ASP:N	2.86	0.43
1:B:200:ILE:C	1:B:201:TYR:HD1	2.25	0.43
1:B:366:THR:OG1	1:B:613:GLN:OE1	2.30	0.43
1:A:183:ALA:O	1:A:193:ILE:O	2.36	0.43
1:A:311:PRO:HG2	1:A:314:PHE:HB2	2.00	0.43
1:B:95:VAL:O	1:B:96:TYR:C	2.60	0.43
1:A:148:ILE:HB	1:A:152:SER:HB3	2.00	0.43
1:A:289:ASN:HD22	1:A:289:ASN:HA	1.57	0.43
1:A:532:LYS:HA	1:A:533:PRO:HD3	1.57	0.43
1:A:695:PRO:C	1:A:697:LYS:H	2.27	0.43
1:B:148:ILE:HG13	1:B:154:THR:CG2	2.47	0.43
1:B:194:TYR:CZ	1:B:201:TYR:HD2	2.37	0.43
1:B:460:LEU:H	1:B:460:LEU:CD1	2.16	0.43
1:B:545:LEU:HA	1:B:546:PRO:HD3	1.74	0.43
1:A:429:LEU:HD11	1:A:441:LEU:CD2	2.48	0.43
1:A:498:VAL:HA	1:A:499:PRO:HD3	1.92	0.43
1:A:510:ALA:C	1:A:512:TYR:N	2.77	0.43
1:A:624:VAL:HG21	1:A:659:MET:HB2	2.01	0.43
1:A:194:TYR:CZ	1:A:201:TYR:HD2	2.36	0.43
1:A:270:THR:HG23	1:B:740:LYS:HD2	1.98	0.43
1:A:764:LYS:CE	1:B:744:LYS:HD2	2.49	0.43
1:B:121:THR:HG23	1:B:141:LEU:HD12	2.00	0.43
1:B:292:ILE:HD11	1:B:321:ILE:CG1	2.48	0.43
1:B:328:SER:OG	1:B:330:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:HA	1:B:515:LEU:HD12	1.70	0.43
1:A:397:GLU:C	1:A:398:PHE:CD1	2.97	0.43
1:A:605:GLY:HA2	1:A:612:LEU:HD13	2.00	0.43
1:A:662:LYS:HB3	1:A:712:HIS:CE1	2.45	0.43
1:B:692:LEU:HD12	1:B:702:TYR:CE1	2.54	0.43
1:A:342:ASN:CA	1:A:368:LEU:HD23	2.49	0.42
1:A:740:LYS:HD2	1:B:270:THR:HG23	2.00	0.42
1:B:374:GLU:HA	1:B:375:PRO:HD2	1.90	0.42
1:B:650:LYS:HG2	1:B:651:GLY:N	2.34	0.42
1:B:670:CYS:HB2	1:B:718:ASN:HB3	2.01	0.42
1:A:83:ASP:HA	1:A:84:PRO:HD3	1.81	0.42
1:A:440:PHE:N	1:A:440:PHE:HD1	2.15	0.42
1:A:585:ASP:HB2	1:A:596:VAL:HG11	2.01	0.42
1:A:775:LYS:HB2	1:A:775:LYS:HE3	1.71	0.42
1:B:520:MET:HG2	1:B:521:LEU:H	1.84	0.42
1:B:569:GLU:O	1:B:652:TYR:HB3	2.19	0.42
1:A:222:ILE:HD11	2:C:1:NAG:HN2	1.84	0.42
1:B:255:MET:SD	1:B:255:MET:C	3.02	0.42
1:B:264:MET:HG2	1:B:731:HIS:CD2	2.54	0.42
1:A:266:ILE:HG23	1:A:726:ALA:HA	2.02	0.42
1:A:396:GLY:HA3	1:A:610:LYS:HB2	2.01	0.42
1:A:419:THR:HG22	1:A:463:ARG:HD3	2.01	0.42
1:A:666:LYS:CE	1:A:716:GLU:HG2	2.49	0.42
1:B:616:HIS:CD2	1:B:617:ARG:HD2	2.55	0.42
1:A:385:PHE:CG	1:A:438:ILE:HD12	2.53	0.42
1:B:79:PHE:CD1	1:B:79:PHE:N	2.87	0.42
1:B:87:ARG:HB3	1:B:95:VAL:HG12	2.01	0.42
1:A:511:LYS:O	1:A:511:LYS:HG2	2.20	0.42
1:B:74:LEU:HD12	1:B:74:LEU:N	2.34	0.42
1:A:650:LYS:HG2	1:A:651:GLY:N	2.34	0.42
1:A:782:LYS:HB2	1:A:782:LYS:HE3	1.22	0.42
1:B:715:LYS:C	1:B:717:GLU:N	2.77	0.42
1:B:727:ASP:OD1	1:B:759:HIS:HB2	2.19	0.42
1:A:116:LEU:HB3	1:A:162:ILE:HD11	2.02	0.42
1:A:148:ILE:HG22	1:A:149:PHE:N	2.35	0.42
1:A:650:LYS:CG	1:A:651:GLY:N	2.83	0.42
1:B:315:LYS:O	1:B:316:SER:OG	2.32	0.42
1:A:720:LEU:HA	1:A:750:THR:O	2.19	0.42
1:A:765:SER:O	1:A:766:LYS:C	2.63	0.42
1:B:419:THR:HG22	1:B:463:ARG:HD3	2.02	0.42
1:B:584:TRP:CD1	1:B:585:ASP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:HB	1:A:447:PRO:HA	2.02	0.42
1:B:116:LEU:HB3	1:B:162:ILE:HD11	2.02	0.42
1:B:222:ILE:HD11	4:F:1:NAG:HN2	1.85	0.42
1:B:666:LYS:HD2	1:B:717:GLU:HG3	2.02	0.42
1:A:91:ASP:O	1:A:108:ILE:HD11	2.19	0.41
1:A:369:SER:O	1:A:370:GLN:C	2.62	0.41
1:B:298:ASN:OD1	1:B:303:THR:HA	2.20	0.41
1:B:301:GLY:HA3	1:B:302:PRO:HD3	1.78	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.78	0.41
1:A:87:ARG:HH22	1:A:132:VAL:H	1.68	0.41
1:A:498:VAL:HG13	1:A:521:LEU:HD22	2.03	0.41
1:A:575:LEU:HA	1:A:575:LEU:HD23	1.82	0.41
1:B:241:ALA:HB1	1:B:254:LEU:HB2	2.02	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.79	0.41
1:B:306:LEU:N	1:B:306:LEU:HD12	2.35	0.41
1:B:619:LEU:HB2	1:B:692:LEU:HD21	2.02	0.41
1:B:712:HIS:N	1:B:712:HIS:ND1	2.68	0.41
1:A:448:ARG:NH1	1:A:448:ARG:CG	2.82	0.41
1:A:692:LEU:HD12	1:A:702:TYR:CE1	2.55	0.41
1:A:765:SER:HA	1:B:743:ILE:HG21	2.01	0.41
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.93	0.41
1:B:327:VAL:HG23	1:B:328:SER:H	1.84	0.41
1:A:269:PHE:CD1	1:B:732:PHE:HD2	2.39	0.41
1:A:515:LEU:HA	1:A:515:LEU:HD12	1.72	0.41
1:B:93:ASP:HA	1:B:106:LEU:O	2.20	0.41
1:B:287:GLN:HE21	1:B:287:GLN:CA	2.28	0.41
1:B:559:ASN:OD1	1:B:559:ASN:N	2.52	0.41
1:B:601:GLY:O	1:B:604:SER:HB3	2.19	0.41
1:B:644:ARG:HB3	1:B:781:LEU:HD22	2.03	0.41
1:B:675:ALA:HA	1:B:723:HIS:CE1	2.55	0.41
1:A:460:LEU:O	1:A:461:LEU:HB2	2.21	0.41
1:A:476:THR:H	1:A:496:PRO:HD3	1.85	0.41
1:A:726:ALA:HB3	1:A:757:GLU:O	2.21	0.41
1:B:81:LEU:HA	1:B:521:LEU:HD13	2.01	0.41
1:B:148:ILE:HG22	1:B:149:PHE:N	2.35	0.41
1:A:74:LEU:N	1:A:74:LEU:HD12	2.34	0.41
1:A:204:PRO:HG2	1:A:208:SER:HB2	2.03	0.41
1:B:137:LYS:HB2	1:B:137:LYS:HE3	1.92	0.41
1:B:344:SER:C	1:B:345:ILE:HD12	2.46	0.41
1:B:584:TRP:CG	1:B:585:ASP:N	2.88	0.41
1:B:761:VAL:CG1	1:B:765:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:H	1:A:240:ILE:HG12	1.60	0.41
1:A:416:ARG:HH11	1:A:461:LEU:CD2	2.31	0.41
1:A:436:GLN:O	1:A:456:SER:HA	2.20	0.41
1:A:620:GLY:O	1:A:624:VAL:HB	2.19	0.41
1:B:782:LYS:HE3	1:B:782:LYS:HB2	1.08	0.41
1:A:190:GLN:HG3	1:A:205:ASP:HA	2.02	0.41
1:A:459:GLY:O	1:A:461:LEU:HD12	2.21	0.41
1:B:148:ILE:HB	1:B:152:SER:HB3	2.03	0.41
1:B:336:TRP:HE1	1:B:347:THR:HB	1.85	0.41
1:B:416:ARG:HH11	1:B:461:LEU:CD2	2.31	0.41
1:B:621:SER:O	1:B:625:LYS:HG3	2.21	0.41
1:B:666:LYS:HB3	1:B:666:LYS:HZ2	1.86	0.41
1:A:93:ASP:CG	1:A:105:LYS:HE3	2.46	0.41
1:A:137:LYS:HB2	1:A:137:LYS:HE3	1.92	0.41
1:A:261:VAL:HG11	1:A:283:PRO:HD3	2.03	0.41
1:A:294:LEU:CD2	1:A:308:LEU:HB2	2.50	0.41
1:A:306:LEU:HD12	1:A:306:LEU:N	2.36	0.41
1:A:644:ARG:HB3	1:A:781:LEU:HD22	2.03	0.41
1:B:73:ASP:O	1:B:76:ARG:HB2	2.21	0.41
1:B:91:ASP:O	1:B:108:ILE:HD11	2.21	0.41
1:B:231:TYR:CZ	1:B:292:ILE:HG21	2.55	0.41
1:B:411:GLU:O	1:B:412:GLN:CG	2.68	0.41
1:B:708:LEU:HD23	1:B:708:LEU:HA	1.87	0.41
1:A:92:THR:HG22	1:A:109:GLU:HG3	2.03	0.41
1:A:148:ILE:HG13	1:A:154:THR:CG2	2.46	0.41
1:A:344:SER:C	1:A:345:ILE:HD12	2.46	0.41
1:B:83:ASP:HA	1:B:84:PRO:HD3	1.80	0.41
1:B:200:ILE:O	1:B:201:TYR:HD1	2.04	0.41
1:B:326:TRP:HA	1:B:332:THR:HG22	2.03	0.41
1:B:369:SER:O	1:B:370:GLN:C	2.64	0.41
1:B:384:PHE:HD2	1:B:406:ILE:HG13	1.86	0.41
1:B:506:THR:O	1:B:509:PRO:HD3	2.21	0.41
1:B:650:LYS:CG	1:B:651:GLY:N	2.84	0.41
1:B:765:SER:O	1:B:768:HIS:N	2.54	0.41
1:A:394:GLY:O	1:A:395:ARG:HB2	2.20	0.40
1:A:652:TYR:HA	1:A:677:ILE:HG23	2.03	0.40
1:B:261:VAL:HG11	1:B:283:PRO:HD3	2.03	0.40
1:A:93:ASP:HA	1:A:106:LEU:O	2.21	0.40
1:A:571:PRO:HD3	1:A:652:TYR:CD2	2.57	0.40
1:B:459:GLY:O	1:B:461:LEU:HD12	2.20	0.40
1:B:664:ASP:C	1:B:665:GLU:HG2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:THR:HG23	1:B:737:GLU:OE2	2.21	0.40
1:B:266:ILE:HG23	1:B:726:ALA:HA	2.03	0.40
1:B:765:SER:O	1:B:766:LYS:C	2.65	0.40
1:A:79:PHE:CD1	1:A:79:PHE:N	2.88	0.40
1:B:311:PRO:HG2	1:B:314:PHE:HB2	2.03	0.40
1:B:342:ASN:CA	1:B:368:LEU:HD23	2.50	0.40
1:B:436:GLN:O	1:B:456:SER:HA	2.21	0.40
1:A:73:ASP:O	1:A:76:ARG:HB2	2.21	0.40
1:A:231:TYR:HA	1:A:235:LEU:HB2	2.04	0.40
1:A:359:LYS:HG3	1:A:406:ILE:CD1	2.52	0.40
1:B:359:LYS:HG3	1:B:406:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	715/719 (99%)	632 (88%)	71 (10%)	12 (2%)	7	28
1	B	717/719 (100%)	635 (89%)	72 (10%)	10 (1%)	9	31
All	All	1432/1438 (100%)	1267 (88%)	143 (10%)	22 (2%)	8	30

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	413	ILE
1	A	663	SER
1	A	711	VAL
1	B	165	ARG
1	B	711	VAL
1	A	695	PRO

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Mol	Chain	Res	Type
1	A	766	LYS
1	B	411	GLU
1	B	663	SER
1	B	695	PRO
1	A	715	LYS
1	A	716	GLU
1	A	529	LYS
1	A	697	LYS
1	B	410	SER
1	B	412	GLN
1	B	529	LYS
1	A	80	VAL
1	B	80	VAL
1	A	530	ILE
1	B	530	ILE

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	645/650 (99%)	539 (84%)	106 (16%)	2	10
1	B	646/650 (99%)	540 (84%)	106 (16%)	2	10
All	All	1291/1300 (99%)	1079 (84%)	212 (16%)	2	10

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	91	ASP
1	A	95	VAL
1	A	99	GLU
1	A	100	ASN
1	A	113	THR
1	A	116	LEU
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	118	GLU
1	A	120	THR
1	A	121	THR
1	A	126	LYS
1	A	128	SER
1	A	129	ARG
1	A	140	LEU
1	A	148	ILE
1	A	152	SER
1	A	154	THR
1	A	158	VAL
1	A	164	THR
1	A	166	GLU
1	A	188	GLN
1	A	192	LEU
1	A	206	ILE
1	A	209	SER
1	A	211	LEU
1	A	226	ILE
1	A	240	ILE
1	A	249	GLU
1	A	284	LYS
1	A	289	ASN
1	A	291	THR
1	A	292	ILE
1	A	294	LEU
1	A	305	THR
1	A	306	LEU
1	A	313	SER
1	A	317	ARG
1	A	324	VAL
1	A	330	THR
1	A	339	ARG
1	A	347	THR
1	A	368	LEU
1	A	391	LYS
1	A	401	ILE
1	A	403	MET
1	A	406	ILE
1	A	407	GLN
1	A	412	GLN
1	A	414	THR

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Mol	Chain	Res	Type
1	A	435	THR
1	A	440	PHE
1	A	448	ARG
1	A	457	THR
1	A	460	LEU
1	A	462	ASN
1	A	487	GLN
1	A	488	HIS
1	A	491	LEU
1	A	497	ARG
1	A	503	LEU
1	A	512	TYR
1	A	514	ILE
1	A	519	SER
1	A	525	ILE
1	A	530	ILE
1	A	532	LYS
1	A	542	ASP
1	A	547	LEU
1	A	556	MET
1	A	559	ASN
1	A	560	GLN
1	A	565	LEU
1	A	567	MET
1	A	570	GLU
1	A	581	HIS
1	A	584	TRP
1	A	588	LEU
1	A	596	VAL
1	A	604	SER
1	A	607	GLN
1	A	617	ARG
1	A	618	ARG
1	A	623	GLU
1	A	635	LEU
1	A	640	ILE
1	A	646	SER
1	A	663	SER
1	A	665	GLU
1	A	666	LYS
1	A	669	LYS
1	A	677	ILE

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Mol	Chain	Res	Type
1	A	681	LYS
1	A	711	VAL
1	A	712	HIS
1	A	716	GLU
1	A	720	LEU
1	A	725	THR
1	A	728	THR
1	A	742	LEU
1	A	750	THR
1	A	753	VAL
1	A	761	VAL
1	A	763	GLU
1	A	769	LEU
1	A	782	LYS
1	B	83	ASP
1	B	91	ASP
1	B	95	VAL
1	B	99	GLU
1	B	100	ASN
1	B	113	THR
1	B	116	LEU
1	B	117	LEU
1	B	118	GLU
1	B	120	THR
1	B	121	THR
1	B	126	LYS
1	B	128	SER
1	B	129	ARG
1	B	130	HIS
1	B	148	ILE
1	B	152	SER
1	B	154	THR
1	B	158	VAL
1	B	164	THR
1	B	166	GLU
1	B	188	GLN
1	B	192	LEU
1	B	206	ILE
1	B	209	SER
1	B	211	LEU
1	B	226	ILE
1	B	240	ILE

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Mol	Chain	Res	Type
1	B	249	GLU
1	B	284	LYS
1	B	289	ASN
1	B	291	THR
1	B	292	ILE
1	B	294	LEU
1	B	305	THR
1	B	306	LEU
1	B	313	SER
1	B	317	ARG
1	B	322	THR
1	B	324	VAL
1	B	330	THR
1	B	339	ARG
1	B	347	THR
1	B	368	LEU
1	B	391	LYS
1	B	401	ILE
1	B	403	MET
1	B	406	ILE
1	B	407	GLN
1	B	411	GLU
1	B	414	THR
1	B	435	THR
1	B	440	PHE
1	B	448	ARG
1	B	457	THR
1	B	460	LEU
1	B	462	ASN
1	B	487	GLN
1	B	488	HIS
1	B	491	LEU
1	B	497	ARG
1	B	503	LEU
1	B	512	TYR
1	B	514	ILE
1	B	519	SER
1	B	525	ILE
1	B	530	ILE
1	B	532	LYS
1	B	542	ASP
1	B	547	LEU

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Mol	Chain	Res	Type
1	B	556	MET
1	B	559	ASN
1	B	560	GLN
1	B	565	LEU
1	B	567	MET
1	B	570	GLU
1	B	581	HIS
1	B	584	TRP
1	B	588	LEU
1	B	596	VAL
1	B	604	SER
1	B	607	GLN
1	B	617	ARG
1	B	618	ARG
1	B	623	GLU
1	B	635	LEU
1	B	640	ILE
1	B	646	SER
1	B	663	SER
1	B	665	GLU
1	B	666	LYS
1	B	677	ILE
1	B	681	LYS
1	B	712	HIS
1	B	716	GLU
1	B	720	LEU
1	B	725	THR
1	B	728	THR
1	B	742	LEU
1	B	750	THR
1	B	753	VAL
1	B	761	VAL
1	B	763	GLU
1	B	765	SER
1	B	769	LEU
1	B	782	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	HIS
1	A	372	ASN

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Mol	Chain	Res	Type
1	A	400	HIS
1	A	548	GLN
1	A	709	HIS
1	B	237	HIS
1	B	287	GLN
1	B	289	ASN
1	B	372	ASN
1	B	400	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	C	1	2,1	14,14,15	0.49	0	17,19,21	1.60	2 (11%)
2	NAG	C	2	2	14,14,15	0.63	0	17,19,21	1.51	3 (17%)
2	BMA	C	3	2	11,11,12	0.67	0	15,15,17	2.46	5 (33%)
2	MAN	C	4	2	11,11,12	0.47	0	15,15,17	1.56	3 (20%)
3	NAG	D	1	3,1	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.38	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	1.68	3 (17%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	0.74	0
4	NAG	F	1	4,1	14,14,15	0.75	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	0.74	0
4	BMA	F	3	4	11,11,12	0.54	0	15,15,17	1.29	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.65	0	17,19,21	1.58	3 (17%)
3	NAG	G	2	3	14,14,15	0.48	0	17,19,21	1.53	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	1/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	5/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	2.19	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	C1-C2-C3	-6.95	99.52	109.64
2	C	1	NAG	C2-N2-C7	-5.54	115.47	122.90
3	G	2	NAG	C1-O5-C5	5.38	119.40	112.19
3	E	1	NAG	O5-C1-C2	-5.25	103.17	111.29
3	D	2	NAG	C1-O5-C5	4.67	118.44	112.19
2	C	4	MAN	C1-O5-C5	4.15	117.74	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	C1-O5-C5	4.11	117.69	112.19
3	D	1	NAG	O5-C1-C2	-3.65	105.64	111.29
2	C	3	BMA	C3-C4-C5	3.65	116.84	110.23
2	C	2	NAG	C1-O5-C5	3.47	116.83	112.19
2	C	3	BMA	C1-O5-C5	3.08	116.32	112.19
3	G	1	NAG	O4-C4-C3	2.66	116.65	110.38
3	D	1	NAG	C1-O5-C5	2.59	115.66	112.19
3	G	1	NAG	C4-C3-C2	-2.51	107.34	111.02
2	C	3	BMA	O5-C5-C4	2.49	116.88	110.83
2	C	4	MAN	O5-C5-C6	2.26	112.06	107.66
2	C	2	NAG	C3-C4-C5	2.23	114.27	110.23
3	G	1	NAG	O5-C1-C2	-2.21	107.87	111.29
2	C	2	NAG	O4-C4-C5	-2.16	103.99	109.32
2	C	1	NAG	C1-O5-C5	2.16	115.09	112.19
3	E	1	NAG	C4-C3-C2	2.16	114.19	111.02
3	E	1	NAG	C3-C4-C5	2.14	114.11	110.23
4	F	1	NAG	C2-N2-C7	-2.06	120.14	122.90
2	C	4	MAN	C2-C3-C4	-2.03	107.29	110.86
2	C	3	BMA	O2-C2-C1	2.02	113.84	109.22

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C1-C2-N2-C7
2	C	3	BMA	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
2	C	4	MAN	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7

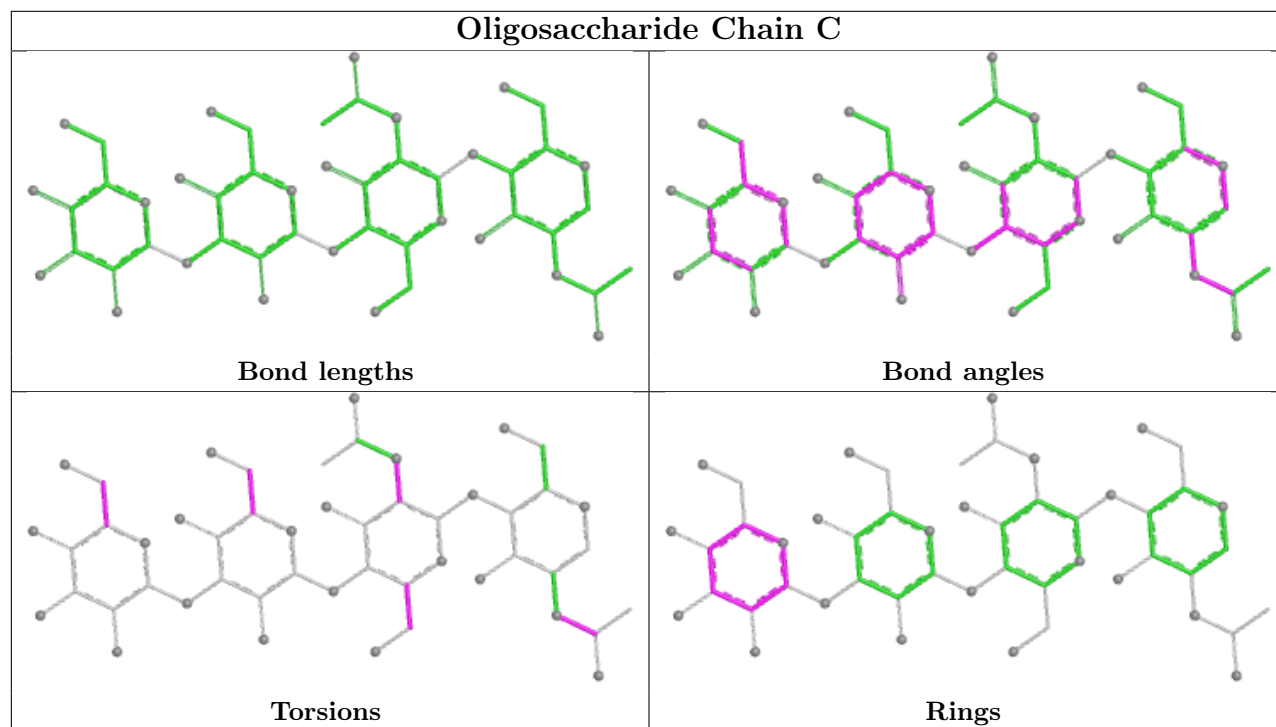
All (1) ring outliers are listed below:

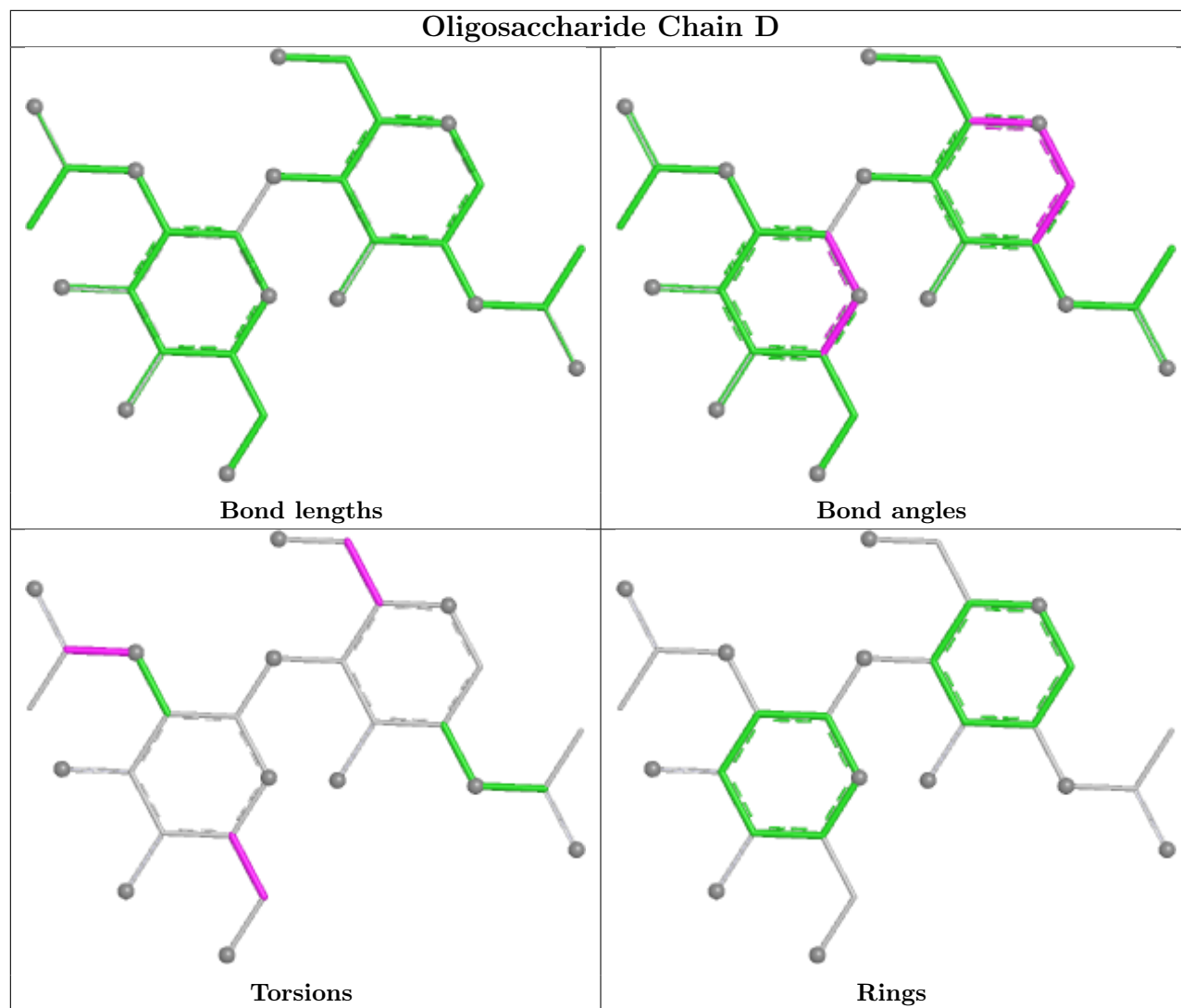
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C1-C2-C3-C4-C5-O5

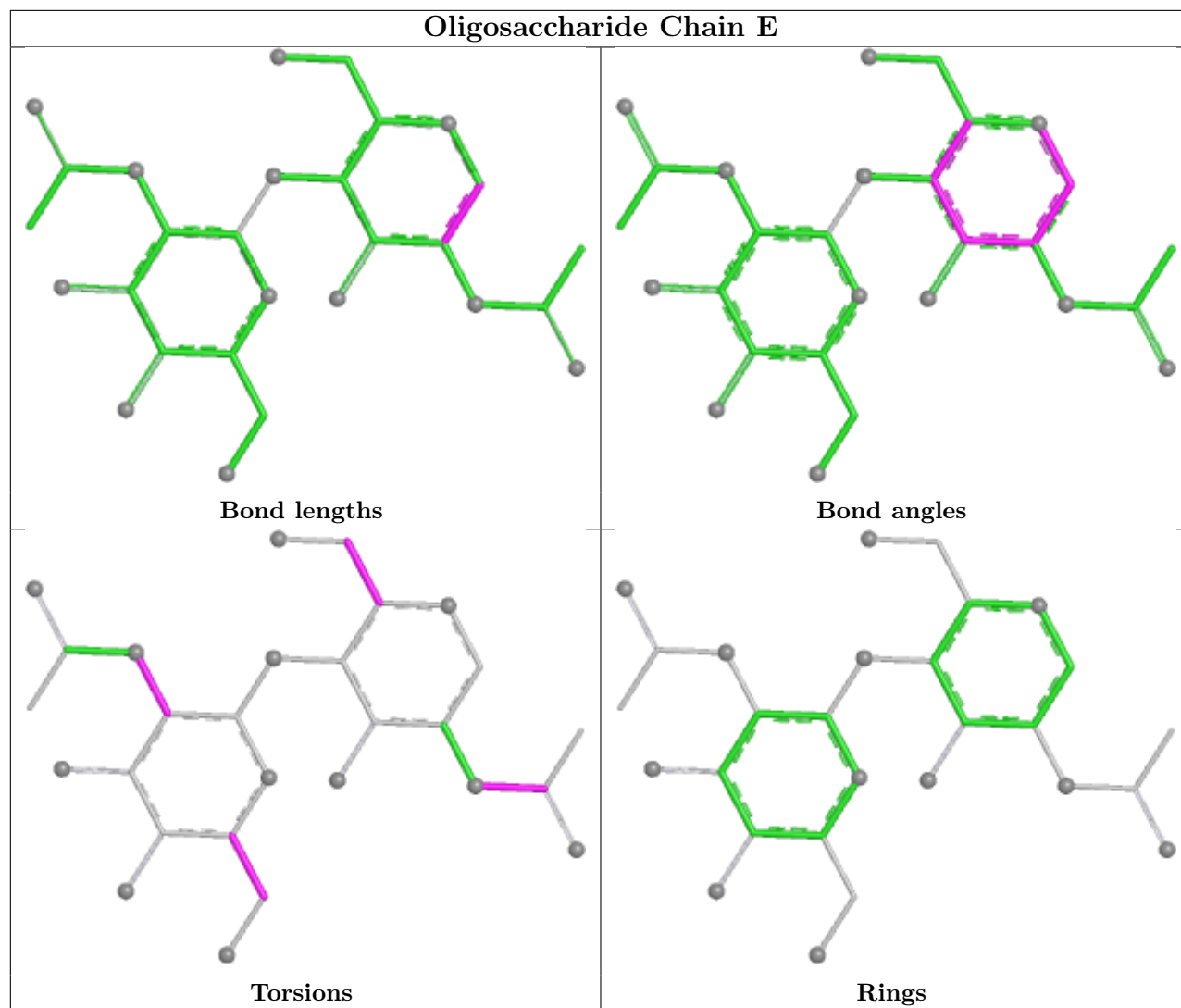
12 monomers are involved in 19 short contacts:

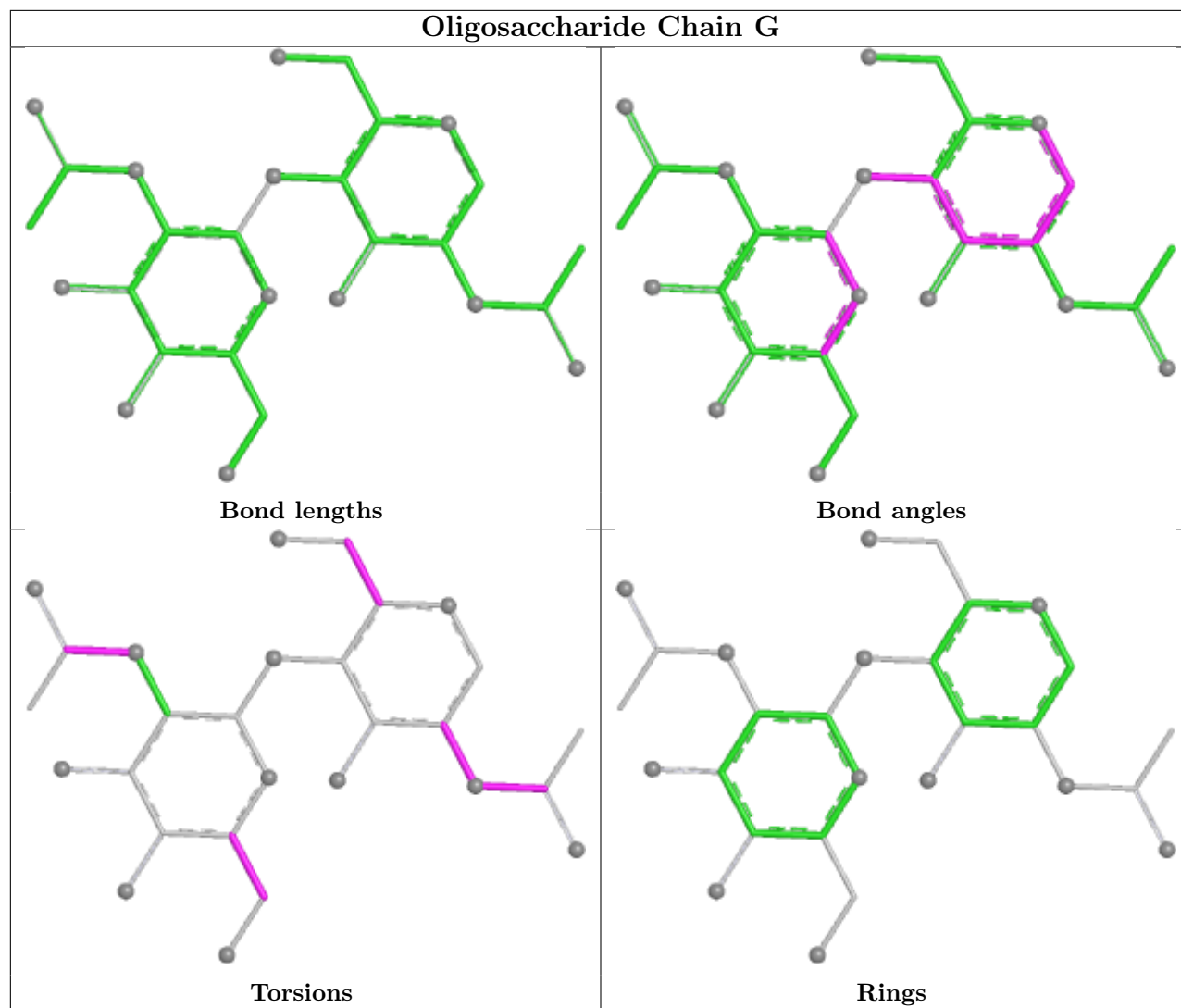
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	3	0
3	D	2	NAG	4	0
3	E	1	NAG	3	0
4	F	1	NAG	3	0
2	C	2	NAG	2	0
3	G	2	NAG	4	0
3	D	1	NAG	4	0
3	G	1	NAG	4	0
4	F	3	BMA	1	0
2	C	1	NAG	2	0
2	C	3	BMA	1	0
2	C	4	MAN	1	0

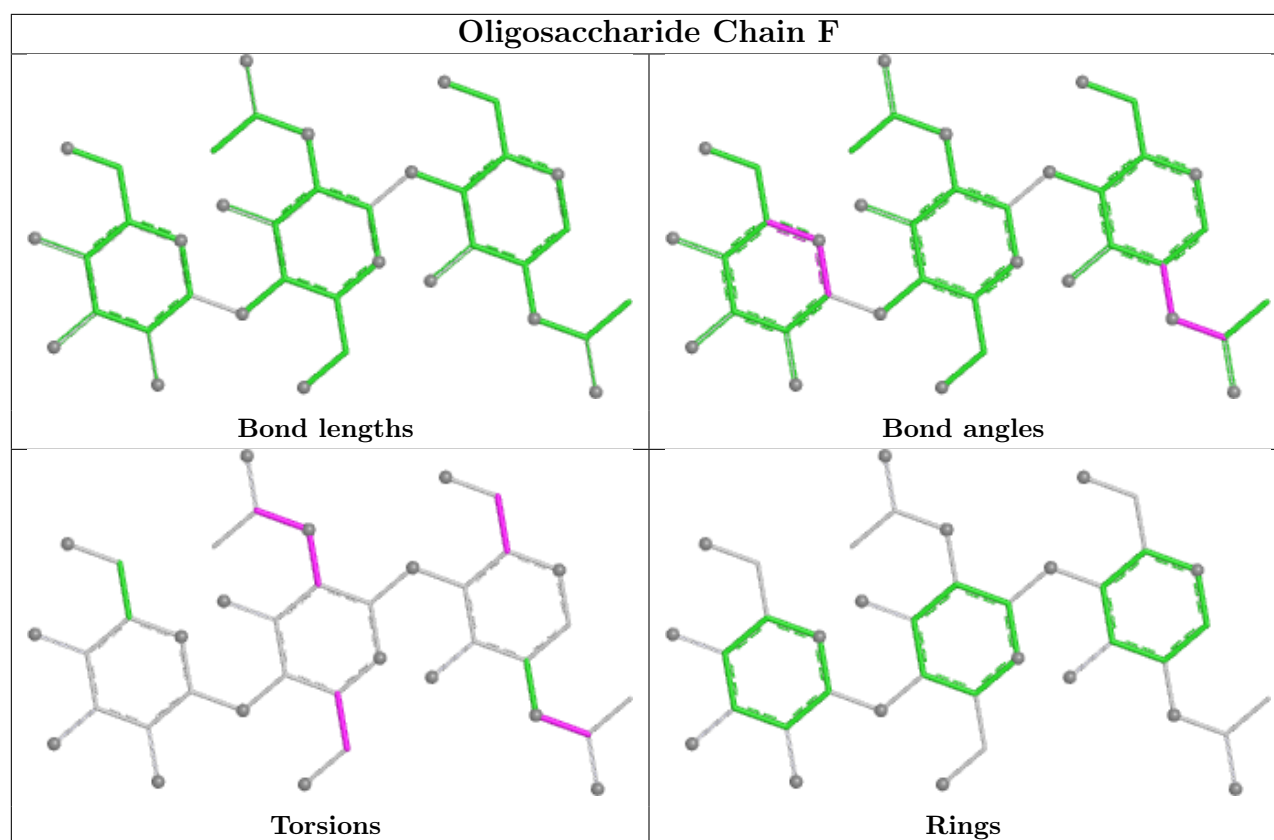
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	801	1	14,14,15	0.66	0	17,19,21	0.93	0
5	NAG	B	809	1	14,14,15	0.61	0	17,19,21	1.41	3 (17%)
5	NAG	B	801	1	14,14,15	0.44	0	17,19,21	1.84	2 (11%)
5	NAG	A	802	1	14,14,15	0.56	0	17,19,21	1.96	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	B	809	1	-	4/6/23/26	0/1/1/1
5	NAG	B	801	1	-	5/6/23/26	0/1/1/1
5	NAG	A	802	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	NAG	C1-O5-C5	6.27	120.59	112.19
5	A	802	NAG	O5-C1-C2	-5.89	102.17	111.29
5	A	802	NAG	C2-N2-C7	3.45	127.53	122.90
5	B	809	NAG	C6-C5-C4	-3.37	104.74	113.02
5	B	809	NAG	C1-O5-C5	2.90	116.07	112.19
5	A	802	NAG	O5-C5-C6	2.40	112.33	107.66
5	B	809	NAG	C3-C4-C5	2.34	114.47	110.23
5	B	801	NAG	C2-N2-C7	2.28	125.95	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	802	NAG	C3-C2-N2-C7
5	B	801	NAG	C3-C2-N2-C7
5	B	801	NAG	C8-C7-N2-C2
5	B	801	NAG	O7-C7-N2-C2
5	B	809	NAG	O5-C5-C6-O6
5	A	802	NAG	O5-C5-C6-O6
5	B	809	NAG	C4-C5-C6-O6
5	B	801	NAG	O5-C5-C6-O6
5	A	802	NAG	C8-C7-N2-C2
5	A	802	NAG	O7-C7-N2-C2
5	B	809	NAG	C8-C7-N2-C2
5	A	802	NAG	C4-C5-C6-O6
5	B	809	NAG	O7-C7-N2-C2
5	A	801	NAG	C8-C7-N2-C2
5	B	801	NAG	C4-C5-C6-O6
5	A	801	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	NAG	1	0
5	B	809	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	717/719 (99%)	0.02	10 (1%)	73 59	33, 68, 138, 251	19 (2%)
1	B	719/719 (100%)	-0.02	18 (2%)	58 43	32, 67, 129, 227	11 (1%)
All	All	1436/1438 (99%)	-0.00	28 (1%)	66 51	32, 68, 131, 251	30 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	THR	4.1
1	A	125	PHE	4.0
1	B	122	PHE	3.5
1	B	696	SER	3.2
1	B	554	ASP	3.0
1	B	406	ILE	3.0
1	B	125	PHE	2.9
1	B	184	ALA	2.8
1	B	512	TYR	2.7
1	A	121	THR	2.6
1	B	394	GLY	2.6
1	A	780	CYS	2.5
1	B	513	PHE	2.5
1	A	512	TYR	2.5
1	A	184	ALA	2.4
1	B	664	ASP	2.4
1	B	67	THR	2.4
1	B	700	SER	2.4
1	B	168	TRP	2.4
1	B	665	GLU	2.3
1	A	122	PHE	2.3
1	A	168	TRP	2.3
1	A	406	ILE	2.2
1	A	99	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	461	LEU	2.1
1	B	716	GLU	2.1
1	B	165	ARG	2.1
1	A	696	SER	2.0

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

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

6.3 Carbohydrates [i](#)

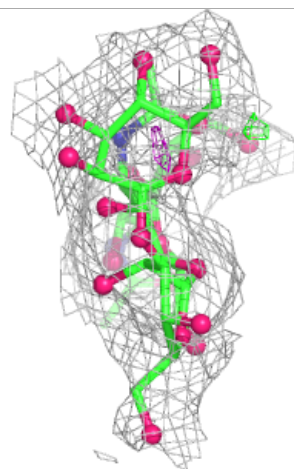
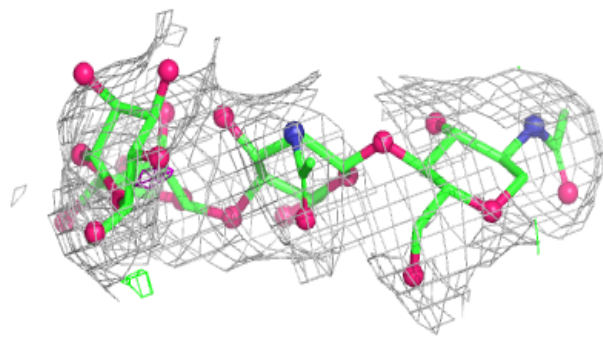
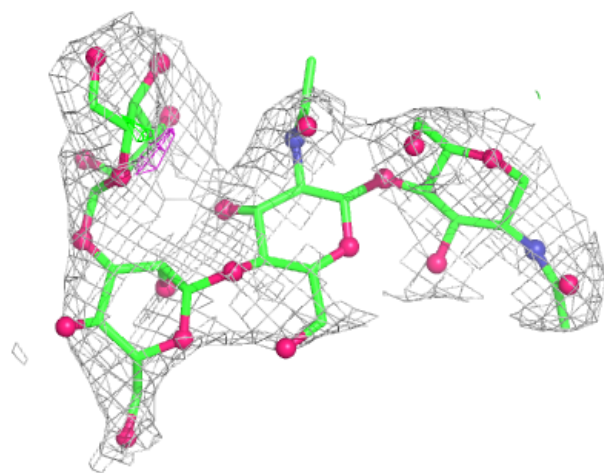
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	F	3	11/12	0.41	0.12	127,127,127,127	0
2	BMA	C	3	11/12	0.54	0.11	135,135,135,135	0
3	NAG	E	2	14/15	0.64	0.15	128,128,128,128	0
2	MAN	C	4	11/12	0.67	0.13	113,113,113,113	0
3	NAG	D	2	14/15	0.69	0.13	131,131,131,131	0
3	NAG	G	2	14/15	0.71	0.10	128,128,128,128	0
4	NAG	F	2	14/15	0.76	0.11	113,113,113,113	0
4	NAG	F	1	14/15	0.77	0.14	83,83,83,83	0
2	NAG	C	2	14/15	0.79	0.11	88,88,88,88	0
3	NAG	E	1	14/15	0.87	0.07	69,69,69,69	0
3	NAG	G	1	14/15	0.88	0.09	71,71,71,71	0
2	NAG	C	1	14/15	0.92	0.08	74,74,74,74	0
3	NAG	D	1	14/15	0.92	0.09	77,77,77,77	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.

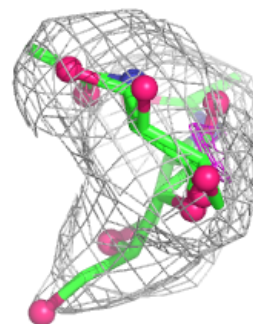
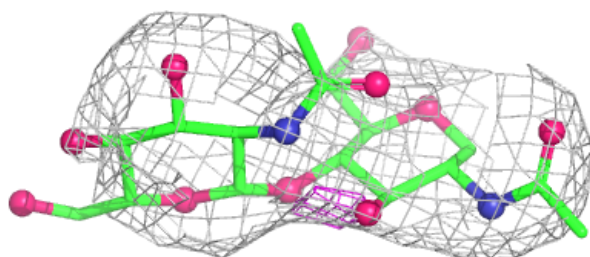
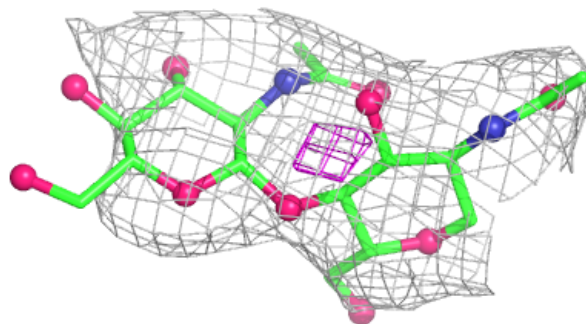
Electron density around Chain C:

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



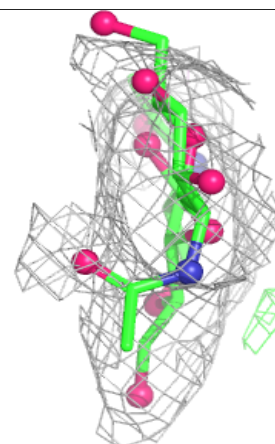
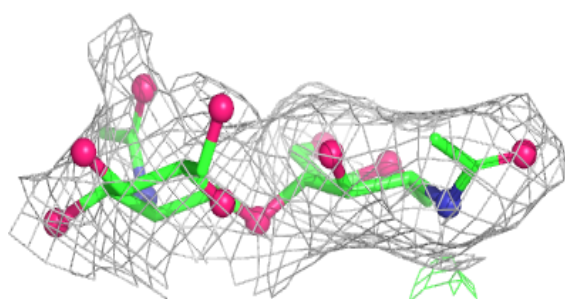
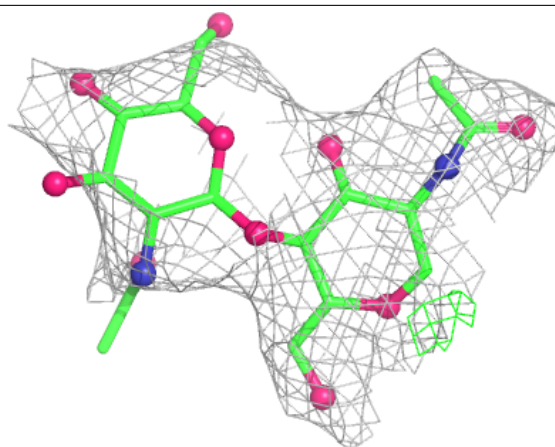
Electron density around Chain D:

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

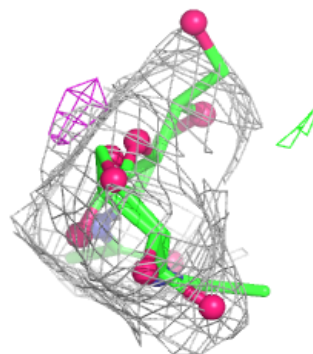
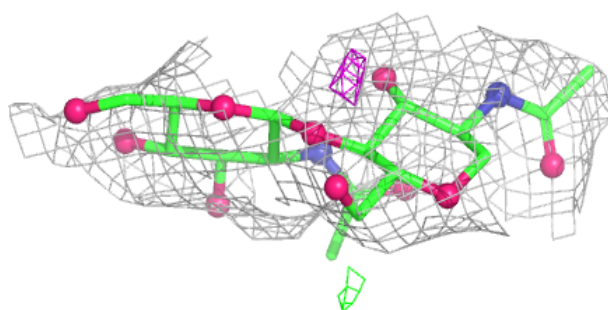
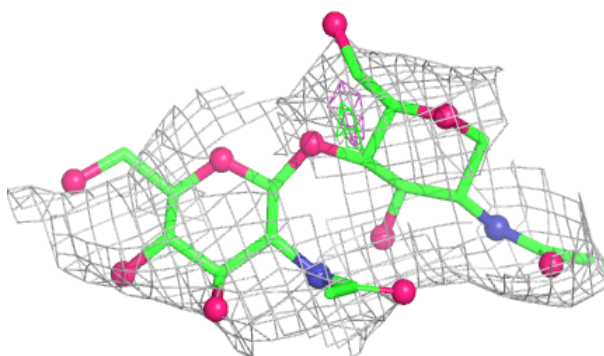


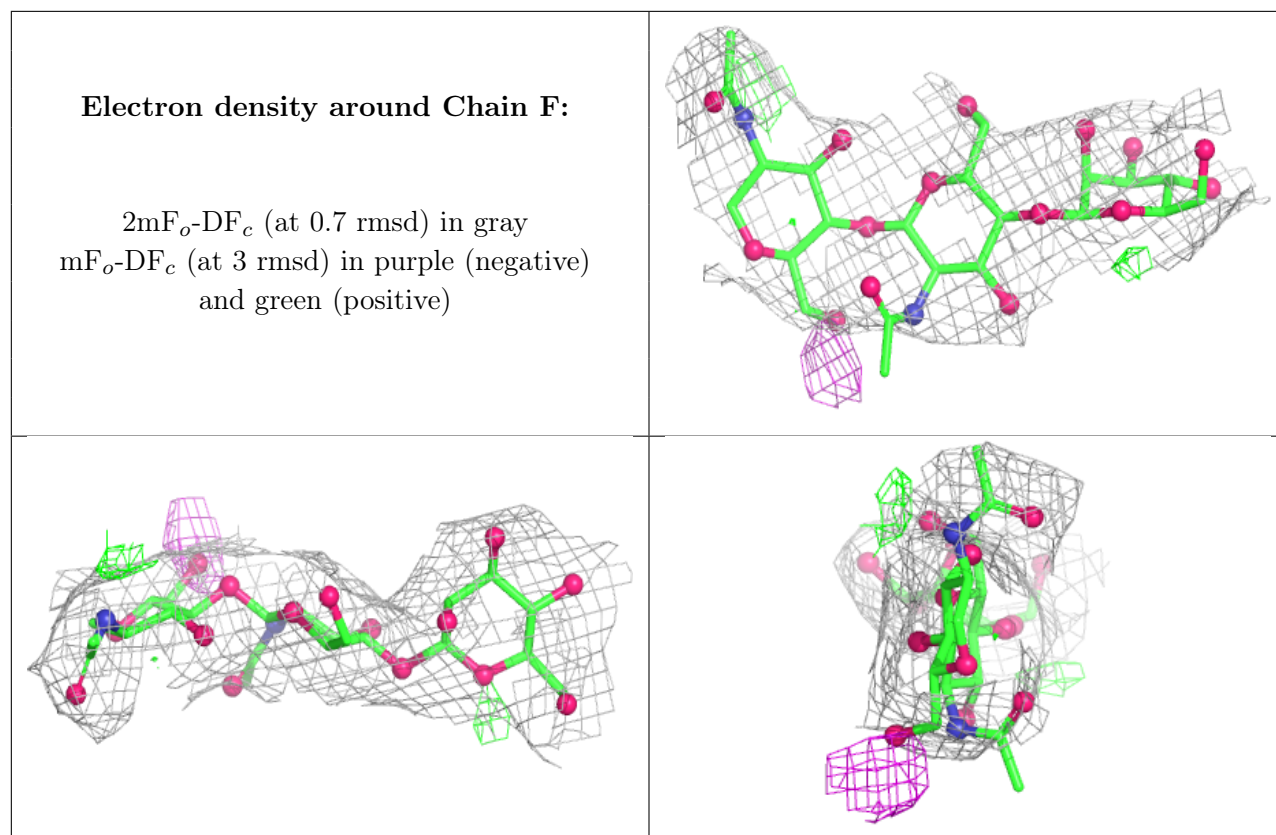
Electron density around Chain E:

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

**Electron density around Chain G:**

$2mF_o-DF_c$ (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
5	NAG	B	809	14/15	0.48	0.15	189,189,189,189	0
5	NAG	A	801	14/15	0.72	0.10	109,109,109,109	0
5	NAG	B	801	14/15	0.76	0.10	106,106,106,106	0
5	NAG	A	802	14/15	0.85	0.09	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.