



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:40 PM EDT

PDB ID : 1ORW
Title : Crystal Structure of Porcine Dipeptidyl Peptidase IV (CD26) in Complex with a Peptidomimetic Inhibitor
Authors : Engel, M.; Hoffmann, T.; Wagner, L.; Wermann, M.; Heiser, U.; Kiefersauer, R.; Huber, R.; Bode, W.; Demuth, H.U.; Brandstetter, H.
Deposited on : 2003-03-16
Resolution : 2.84 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:

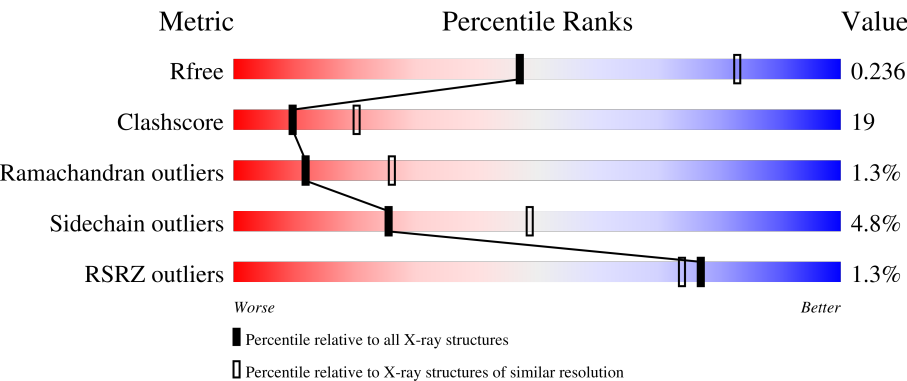
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.84 Å.

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



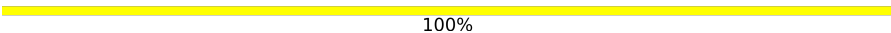
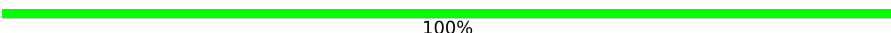
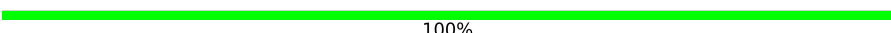
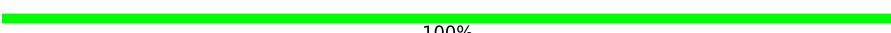
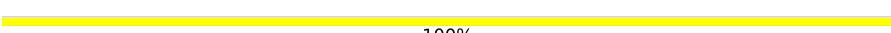
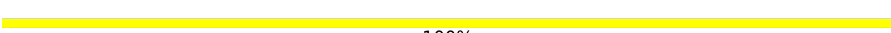

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	728	<div><div>2%</div><div>64%</div><div>33%</div><div>.</div></div>
1	B	728	<div><div>%</div><div>64%</div><div>34%</div><div>.</div></div>
1	C	728	<div><div>2%</div><div>56%</div><div>41%</div><div>..</div></div>
1	D	728	<div><div>%</div><div>60%</div><div>37%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	F	2	 100%
2	H	2	 100%
2	I	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
3	G	3	 33% 67%
3	J	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	767(A)	-	-	-	X
4	NAG	D	767(A)	-	-	-	X
6	PHI	C	805	-	-	X	-
6	PHI	D	807	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25262 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 dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	71	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	62	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

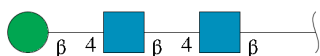
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	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			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

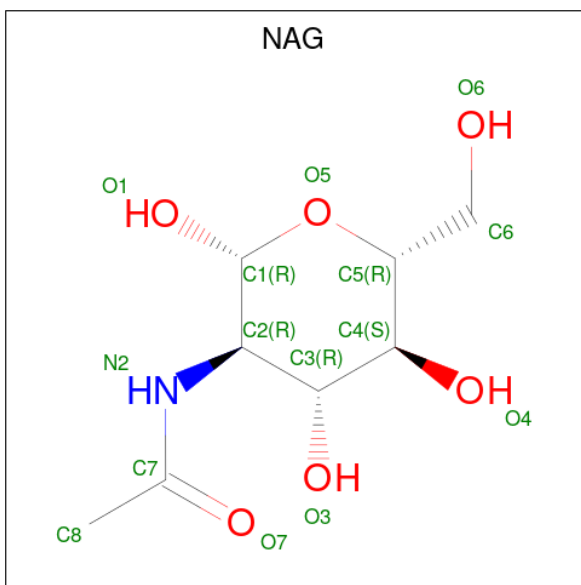
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



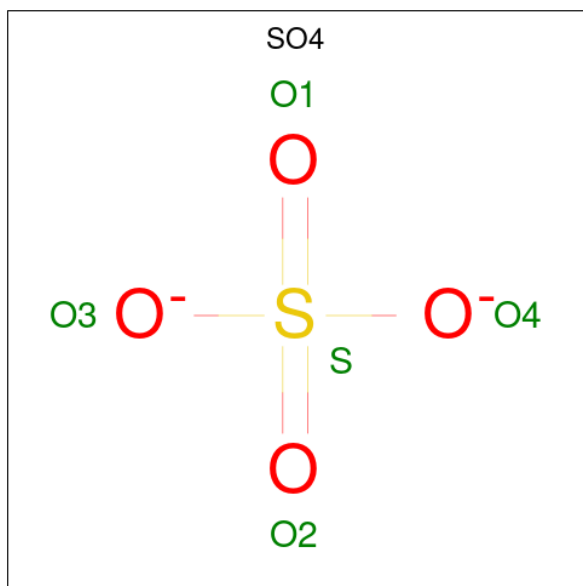
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	3	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



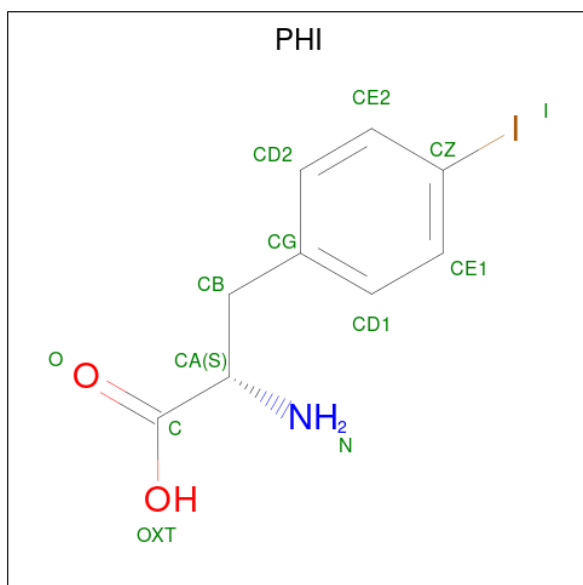
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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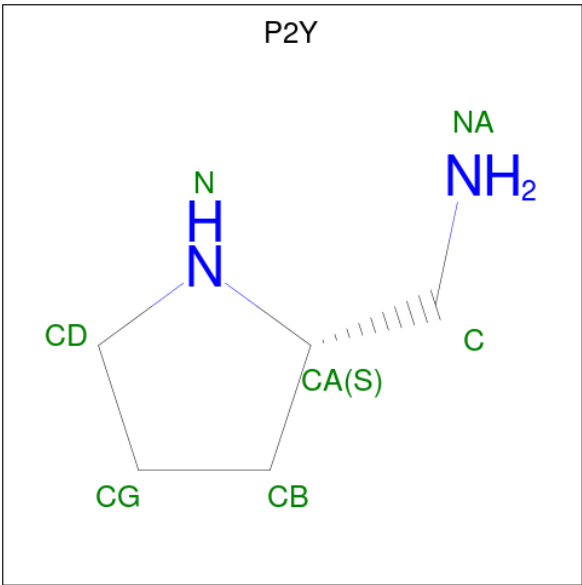
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is IODO-PHENYLALANINE (three-letter code: PHI) (formula: $C_9H_{10}INO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	I	N	O	0	0
			12	9	1	1	1		
6	B	1	Total	C	I	N	O	0	0
			12	9	1	1	1		
6	C	1	Total	C	I	N	O	0	0
			12	9	1	1	1		
6	D	1	Total	C	I	N	O	0	0
			12	9	1	1	1		

- Molecule 7 is (2S)-PYRROLIDIN-2-YLMETHYLAMINE (three-letter code: P2Y) (formula: $C_5H_{12}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			7	5	2		
7	B	1	Total	C	N	0	0
			7	5	2		
7	C	1	Total	C	N	0	0
			7	5	2		
7	D	1	Total	C	N	0	0
			7	5	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total	O	0	0
			206	206		
8	B	226	Total	O	0	0
			226	226		
8	C	213	Total	O	0	0
			213	213		
8	D	173	Total	O	0	0
			173	173		

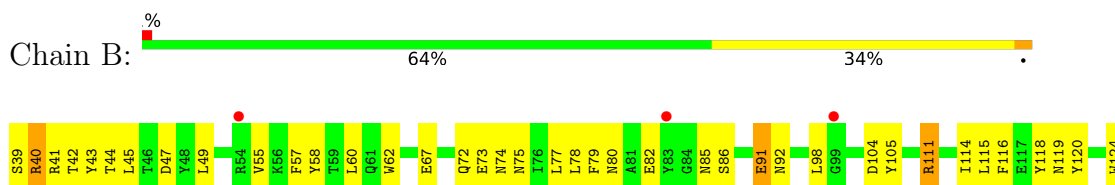
3 Residue-property plots

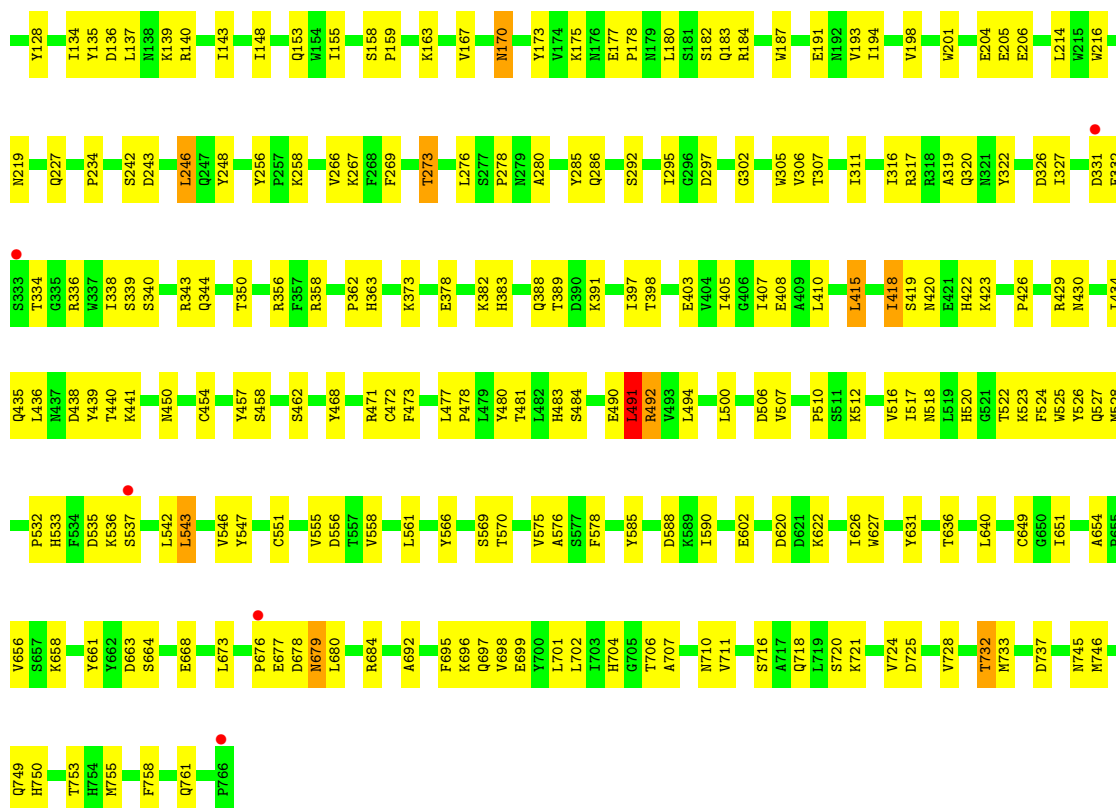
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

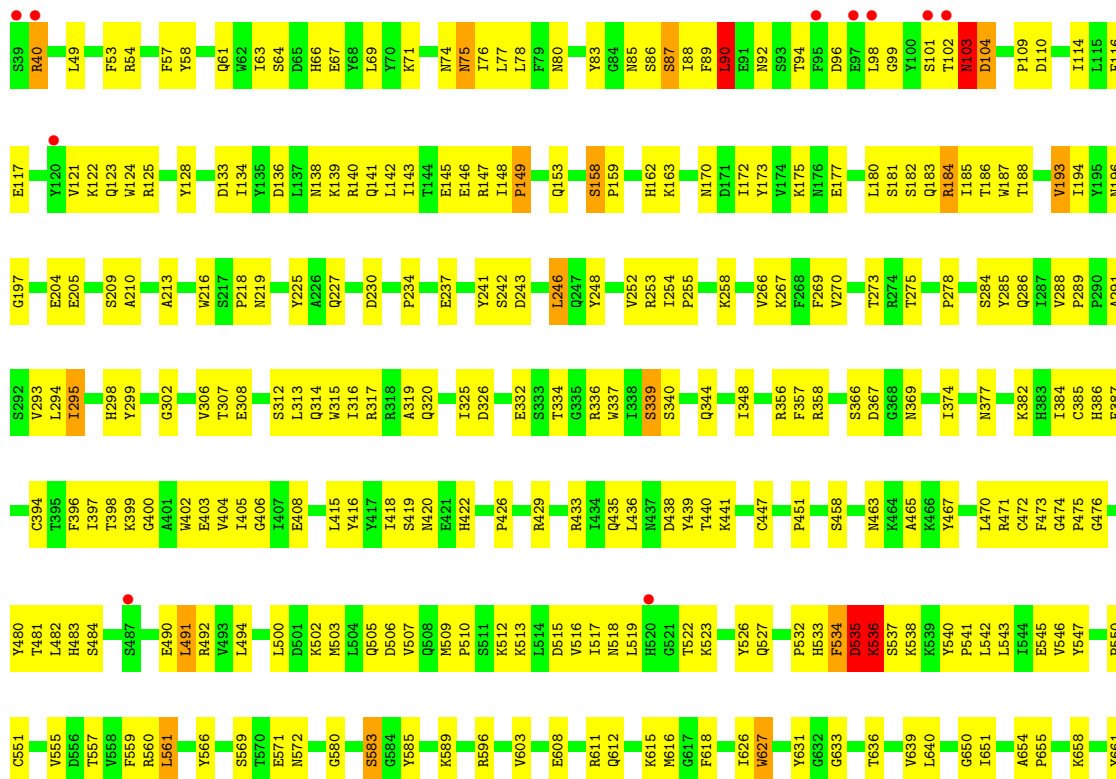


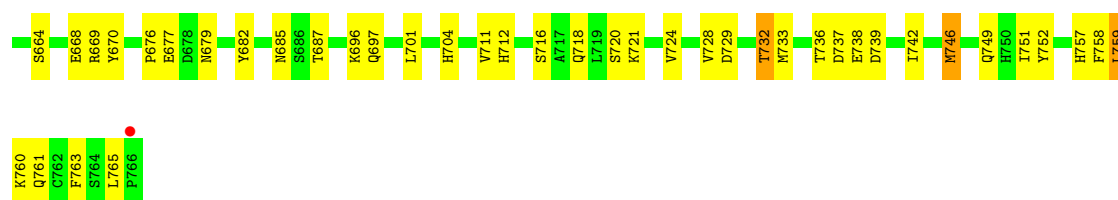
• Molecule 1: dipeptidyl peptidase IV



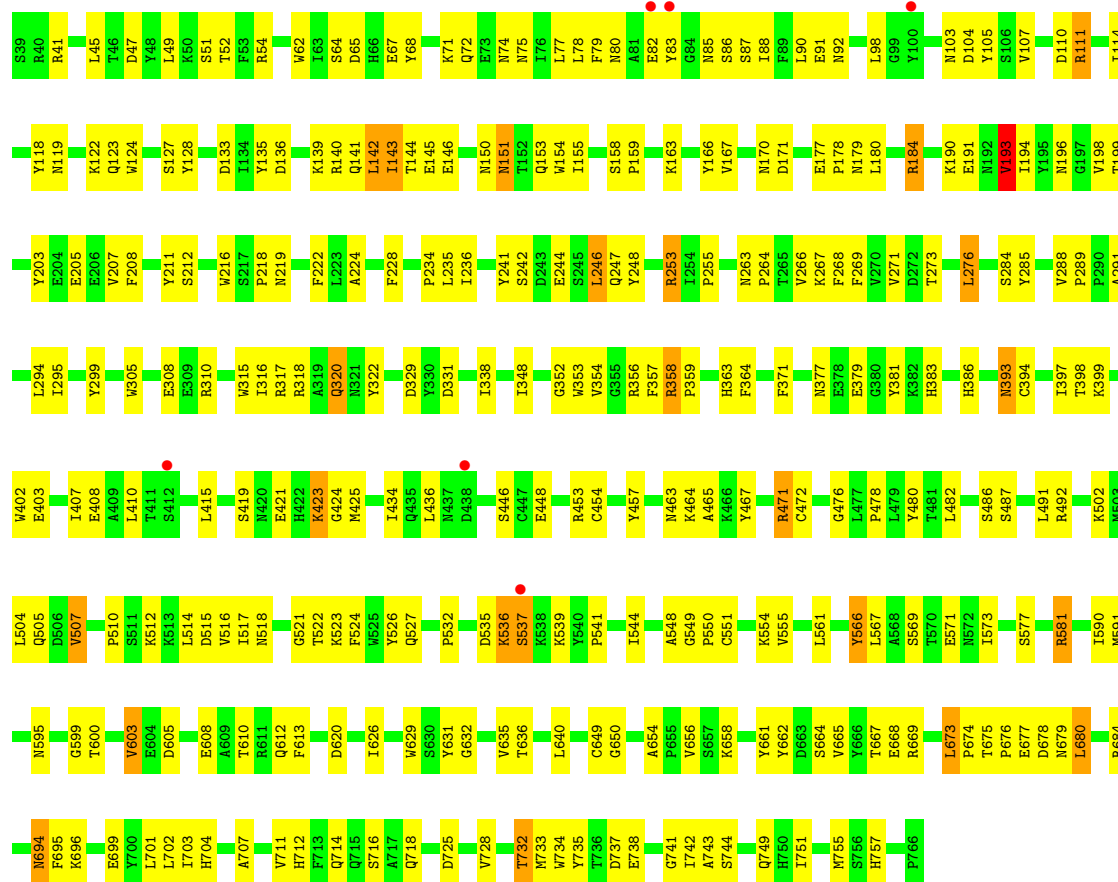


• Molecule 1: dipeptidyl peptidase IV





- Molecule 1: dipeptidyl peptidase IV



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



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



MAG1
MAG2

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

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

Chain K:  100%MAG1
MAG2

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

Chain L:  100%MAG1
MAG2

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

Chain M:  100%MAG1
MAG2

- Molecule 3: 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
EMAG

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

Chain J:

100%

MAG1
MAG2
EMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.97Å 117.71Å 133.56Å 112.65° 94.81° 91.17°	Depositor
Resolution (Å)	29.79 – 2.84 29.78 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.79-2.84) 97.7 (29.78-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.246 0.177 , 0.236	Depositor DCC
R_{free} test set	7805 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25262	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, PHI, P2Y, SO4

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	0.42	0/6141	0.67	1/8353 (0.0%)
1	B	0.42	0/6141	0.67	1/8353 (0.0%)
1	C	0.43	0/6141	0.70	2/8353 (0.0%)
1	D	0.39	0/6141	0.66	1/8353 (0.0%)
All	All	0.42	0/24564	0.68	5/33412 (0.0%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ASP	N-CA-C	-8.55	87.90	111.00
1	C	103	ASN	N-CA-C	7.38	130.91	111.00
1	B	656	VAL	N-CA-C	-5.32	96.65	111.00
1	A	656	VAL	N-CA-C	-5.18	97.01	111.00
1	D	656	VAL	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	468	TYR	Sidechain

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	5966	0	5662	207	0
1	B	5966	0	5662	212	0
1	C	5966	0	5661	264	0
1	D	5966	0	5662	247	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
3	G	39	0	34	1	0
3	J	39	0	34	2	0
4	A	56	0	52	1	0
4	B	56	0	52	5	0
4	C	70	0	65	2	0
4	D	28	0	26	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	12	0	9	3	0
6	B	12	0	9	4	0
6	C	12	0	9	7	0
6	D	12	0	9	7	0
7	A	7	0	9	2	0
7	B	7	0	9	3	0
7	C	7	0	9	1	0
7	D	7	0	9	2	0
8	A	206	0	0	10	0
8	B	226	0	0	14	0
8	C	213	0	0	18	0
8	D	173	0	0	5	0
All	All	25262	0	23157	910	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 19.

All (910) 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:D:358:ARG:NH2	6:D:807:PHI:I	2.51	1.13
1:B:358:ARG:NH2	6:B:803:PHI:I	2.57	1.08
1:A:358:ARG:NH2	6:A:801:PHI:I	2.60	1.05
1:B:358:ARG:NH1	6:B:803:PHI:I	2.65	0.99
1:C:535:ASP:C	1:C:536:LYS:HD3	1.83	0.99
1:C:358:ARG:NH2	6:C:805:PHI:I	2.69	0.95
1:B:358:ARG:CZ	6:B:803:PHI:I	2.84	0.95
1:D:358:ARG:CZ	6:D:807:PHI:I	2.84	0.94
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.51	0.92
1:D:75:ASN:ND2	1:D:92:ASN:H	1.69	0.90
1:A:40:ARG:HH11	1:A:40:ARG:HB2	1.35	0.90
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.53	0.90
1:C:77:LEU:HD23	1:C:88:ILE:HA	1.51	0.89
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.69	0.89
1:C:536:LYS:HG2	1:C:537:SER:H	1.39	0.86
1:A:75:ASN:HB3	1:A:92:ASN:N	1.91	0.86
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.41	0.83
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.60	0.83
1:A:492:ARG:HB3	1:A:492:ARG:NH2	1.92	0.82
1:A:540:TYR:HE2	1:A:572:ASN:HD22	1.28	0.82
1:B:184:ARG:NH1	1:B:187:TRP:HA	1.96	0.81
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.63	0.80
1:B:170:ASN:N	1:B:170:ASN:HD22	1.78	0.80
1:A:358:ARG:CZ	6:A:801:PHI:I	3.00	0.79
1:D:408:GLU:HG2	8:D:1031:HOH:O	1.83	0.79
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.66	0.79
1:D:291:ALA:O	1:D:295:ILE:HG13	1.81	0.79
1:D:654:ALA:HA	1:D:704:HIS:CD2	2.18	0.78
1:C:358:ARG:CZ	6:C:805:PHI:I	3.01	0.78
1:B:704:HIS:HD2	1:B:716:SER:OG	1.67	0.78
1:B:316:ILE:HD11	1:B:320:GLN:HA	1.64	0.78
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.64	0.78
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.64	0.77
1:D:75:ASN:HD22	1:D:92:ASN:H	1.34	0.76
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.67	0.75
1:D:472:CYS:O	1:D:478:PRO:HA	1.87	0.75
1:B:75:ASN:ND2	1:B:92:ASN:H	1.85	0.75
1:C:420:ASN:HD22	1:C:426:PRO:HA	1.52	0.75
1:C:40:ARG:HB2	1:C:506:ASP:O	1.88	0.73
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:VAL:HG13	1:B:524:PHE:O	1.89	0.73
1:C:183:GLN:OE1	1:C:278:PRO:HA	1.88	0.73
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.71	0.73
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.71	0.73
1:C:90:LEU:HD13	1:C:90:LEU:O	1.89	0.73
1:D:680:LEU:HD11	1:D:684:ARG:HE	1.53	0.73
1:C:513:LYS:HE2	1:C:515:ASP:HB2	1.72	0.72
1:C:704:HIS:HD2	1:C:716:SER:OG	1.72	0.72
1:C:75:ASN:ND2	1:C:92:ASN:HB2	2.06	0.71
1:B:184:ARG:HH12	1:B:187:TRP:HA	1.54	0.71
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.91	0.71
1:C:103:ASN:HA	1:C:117:GLU:O	1.90	0.70
1:D:694:ASN:N	1:D:694:ASN:HD22	1.88	0.70
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.56	0.70
1:C:733:MET:HA	1:D:732:THR:CG2	2.22	0.70
1:C:746:MET:HG3	1:D:725:ASP:OD1	1.91	0.70
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.21	0.70
1:C:367:ASP:OD2	1:C:369:ASN:HB2	1.92	0.70
1:C:357:PHE:CD1	6:C:805:PHI:HE2	2.26	0.69
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.23	0.69
1:A:74:ASN:O	1:A:95:PHE:HE2	1.75	0.69
1:D:177:GLU:HB2	1:D:180:LEU:HD23	1.74	0.69
1:D:193:VAL:HG22	1:D:194:ILE:HG12	1.75	0.69
1:B:408:GLU:HG2	8:B:921:HOH:O	1.90	0.69
1:D:317:ARG:HD2	1:D:322:TYR:HB3	1.75	0.69
1:B:378:GLU:CD	1:B:378:GLU:H	1.96	0.69
1:C:285:TYR:CE1	1:C:336:ARG:HB2	2.28	0.69
1:A:718:GLN:HE22	1:A:721:LYS:NZ	1.91	0.69
1:A:492:ARG:HH21	1:A:492:ARG:CB	2.05	0.68
1:D:190:LYS:HG2	1:D:193:VAL:CG1	2.23	0.68
1:C:253:ARG:HH21	1:D:253:ARG:HH22	1.41	0.68
1:B:332:GLU:HG3	8:B:986:HOH:O	1.94	0.68
1:B:356:ARG:HB3	1:B:551:CYS:SG	2.34	0.68
1:B:458:SER:OG	1:B:471:ARG:HB2	1.93	0.68
1:C:732:THR:O	1:D:732:THR:HG22	1.93	0.68
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.58	0.68
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.75	0.68
1:D:357:PHE:HB3	6:D:807:PHI:I	2.64	0.68
1:D:358:ARG:NE	6:D:807:PHI:I	2.97	0.67
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.10	0.67
1:A:502:LYS:O	1:A:505:GLN:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LYS:HG3	1:C:182:SER:HB3	1.75	0.67
1:B:334:THR:OG1	1:B:336:ARG:HG2	1.94	0.67
1:C:519:LEU:HD22	1:C:608:GLU:OE1	1.94	0.67
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.60	0.67
1:A:67:GLU:HB3	1:A:78:LEU:HD11	1.75	0.67
1:A:378:GLU:CD	1:A:378:GLU:H	1.97	0.67
1:C:704:HIS:HE1	1:C:711:VAL:O	1.77	0.67
1:C:184:ARG:HD3	1:C:186:THR:O	1.95	0.66
1:B:438:ASP:OD2	1:B:441:LYS:HE3	1.95	0.66
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.15	0.66
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.78	0.66
1:C:475:PRO:HD3	1:C:557:THR:HB	1.78	0.66
1:A:491:LEU:O	1:A:492:ARG:HB3	1.95	0.66
1:D:167:VAL:HG21	1:D:198:VAL:HG13	1.77	0.66
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.26	0.66
1:D:273:THR:HA	1:D:276:LEU:HD22	1.78	0.66
1:C:732:THR:HG22	1:D:732:THR:HG23	1.77	0.65
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.79	0.65
1:A:433:ARG:NH1	1:A:443:THR:HG21	2.11	0.65
1:C:720:SER:O	1:C:724:VAL:HG23	1.96	0.65
1:C:733:MET:HA	1:D:732:THR:HG21	1.79	0.65
1:D:67:GLU:CD	1:D:111:ARG:HH12	2.00	0.65
1:D:219:ASN:HB2	1:D:308:GLU:CD	2.17	0.65
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.96	0.65
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.78	0.65
1:B:167:VAL:HG21	1:B:198:VAL:HG13	1.79	0.65
1:A:103:ASN:O	1:A:104:ASP:HB2	1.97	0.64
1:D:453:ARG:HG3	1:D:476:GLY:HA3	1.80	0.64
1:D:532:PRO:HD3	1:D:569:SER:HA	1.79	0.64
1:A:93:SER:C	1:A:95:PHE:H	1.99	0.64
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.78	0.64
4:C:767(A):NAG:H61	8:C:1112:HOH:O	1.96	0.64
1:B:170:ASN:HD22	1:B:170:ASN:H	1.42	0.64
1:C:400:GLY:HA3	1:C:402:TRP:NE1	2.12	0.64
1:A:75:ASN:ND2	1:A:92:ASN:ND2	2.46	0.64
1:B:72:GLN:HG2	1:B:73:GLU:HG2	1.80	0.64
1:B:67:GLU:HB3	1:B:78:LEU:HD11	1.80	0.64
1:D:114:ILE:HG22	1:D:135:TYR:HB3	1.79	0.64
1:A:746:MET:HG3	1:B:725:ASP:HA	1.80	0.63
1:B:316:ILE:CD1	1:B:320:GLN:HA	2.28	0.63
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:O	1:D:151:ASN:HB2	1.96	0.63
1:C:357:PHE:HB3	6:C:805:PHI:I	2.69	0.63
1:B:410:LEU:HD13	1:B:415:LEU:CD2	2.28	0.63
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.97	0.63
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.97	0.62
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.13	0.62
1:C:358:ARG:NH1	6:C:805:PHI:I	3.03	0.62
1:B:177:GLU:HB2	1:B:180:LEU:HB2	1.81	0.62
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.97	0.62
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.29	0.62
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.35	0.62
1:B:41:ARG:O	1:B:507:VAL:HG23	1.99	0.62
1:C:136:ASP:O	1:C:140:ARG:HA	2.00	0.61
1:D:353:TRP:CZ2	1:D:591:MET:HE3	2.34	0.61
1:C:54:ARG:O	1:C:500:LEU:HD13	2.00	0.61
1:A:75:ASN:HD22	1:A:92:ASN:ND2	1.98	0.61
1:B:631:TYR:H	7:B:804:P2Y:HNA2	1.47	0.61
1:D:299:TYR:HB2	1:D:316:ILE:CG2	2.31	0.61
1:D:377:ASN:HD22	1:D:381:TYR:HB2	1.66	0.61
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.84	0.61
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.36	0.61
1:D:536:LYS:O	1:D:537:SER:CB	2.48	0.61
1:A:172:ILE:HB	1:A:185:ILE:HB	1.82	0.61
1:D:67:GLU:HB3	1:D:78:LEU:HD11	1.82	0.61
1:D:502:LYS:O	1:D:505:GLN:HG2	2.01	0.60
1:C:80:ASN:HB2	4:C:767(A):NAG:H82	1.81	0.60
1:A:75:ASN:ND2	1:A:92:ASN:HD22	2.00	0.60
1:A:377:ASN:HB3	1:A:379:GLU:H	1.66	0.60
1:C:288:VAL:HG11	1:C:294:LEU:HD11	1.82	0.60
1:B:651:ILE:HG21	1:B:755:MET:CE	2.31	0.60
1:B:746:MET:HG2	8:B:1062:HOH:O	2.02	0.60
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.84	0.59
1:A:317:ARG:HG2	8:A:974:HOH:O	2.02	0.59
1:C:658:LYS:HG3	1:C:687:THR:HG22	1.83	0.59
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.83	0.59
1:C:438:ASP:OD2	1:C:441:LYS:HG3	2.01	0.59
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.37	0.59
1:A:70:TYR:HB3	1:A:79:PHE:CE2	2.38	0.59
1:A:207:VAL:HG23	1:A:208:PHE:CD1	2.37	0.59
1:A:516:VAL:HG13	1:A:524:PHE:O	2.02	0.59
1:D:751:ILE:O	1:D:755:MET:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HD11	1:B:320:GLN:CA	2.33	0.59
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.17	0.59
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.38	0.59
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.33	0.59
1:A:75:ASN:HB3	1:A:92:ASN:H	1.67	0.59
1:B:420:ASN:HB2	1:B:426:PRO:HA	1.85	0.59
1:C:463:ASN:C	1:C:465:ALA:H	2.06	0.59
1:B:340:SER:O	1:B:344:GLN:HG3	2.03	0.59
1:C:580:GLY:O	1:C:583:SER:OG	2.21	0.59
1:D:205:GLU:OE2	6:D:807:PHI:N	2.36	0.59
1:A:58:TYR:CD2	1:A:494:LEU:HB3	2.36	0.59
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.38	0.59
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.38	0.59
1:C:253:ARG:NH2	1:D:253:ARG:NH2	2.45	0.58
1:D:242:SER:HB3	1:D:246:LEU:HD12	1.85	0.58
1:A:219:ASN:N	1:A:308:GLU:OE2	2.30	0.58
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.85	0.58
1:C:125:ARG:NH2	1:C:205:GLU:OE2	2.32	0.58
1:A:159:PRO:HB2	1:A:218:PRO:O	2.04	0.58
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.03	0.58
1:D:235:LEU:HD23	1:D:255:PRO:HA	1.84	0.58
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.39	0.58
1:D:133:ASP:HB3	1:D:142:LEU:HD21	1.86	0.58
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.85	0.58
1:D:536:LYS:O	1:D:537:SER:HB2	2.04	0.58
1:B:170:ASN:N	1:B:170:ASN:ND2	2.51	0.58
1:A:695:PHE:HB2	1:A:728:VAL:HG11	1.86	0.57
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.38	0.57
1:A:331:ASP:HB2	1:A:338:ILE:HD12	1.87	0.57
1:D:142:LEU:O	1:D:144:THR:HG23	2.04	0.57
1:B:704:HIS:CE1	1:B:711:VAL:O	2.57	0.57
1:C:291:ALA:O	1:C:295:ILE:HG13	2.05	0.57
1:C:313:LEU:N	1:C:313:LEU:HD12	2.19	0.57
1:C:543:LEU:HD22	1:C:759:LEU:HD11	1.85	0.57
1:A:658:LYS:HD3	1:A:661:TYR:CZ	2.40	0.57
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.39	0.57
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.70	0.57
1:D:357:PHE:CD1	6:D:807:PHI:HE2	2.40	0.57
1:B:191:GLU:O	1:B:193:VAL:HG23	2.05	0.56
1:B:673:LEU:HD12	1:B:673:LEU:N	2.19	0.56
1:C:306:VAL:HG12	1:C:307:THR:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:SER:HG	1:C:473:PHE:HE1	1.53	0.56
1:C:739:ASP:HB2	8:C:954:HOH:O	2.05	0.56
1:A:93:SER:C	1:A:95:PHE:N	2.57	0.56
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.35	0.56
1:B:704:HIS:HE1	1:B:711:VAL:O	1.88	0.56
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.41	0.56
1:D:522:THR:HB	1:D:524:PHE:CE1	2.39	0.56
1:D:526:TYR:HA	1:D:555:VAL:HG21	1.86	0.56
1:B:136:ASP:HB2	1:B:143:ILE:HD11	1.88	0.56
1:A:306:VAL:HB	1:A:310:ARG:HG2	1.87	0.56
1:A:597:ARG:O	1:A:597:ARG:HG3	2.05	0.56
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.40	0.56
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.86	0.56
1:C:484:SER:HB2	1:C:491:LEU:HD21	1.87	0.56
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.87	0.56
1:D:299:TYR:HB2	1:D:316:ILE:HG22	1.87	0.56
1:B:39:SER:OG	1:B:40:ARG:N	2.37	0.56
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.88	0.56
1:B:704:HIS:CD2	1:B:716:SER:OG	2.55	0.56
1:C:57:PHE:HA	1:C:480:TYR:CE1	2.40	0.56
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.88	0.56
1:C:146:GLU:OE1	1:C:181:SER:HA	2.06	0.56
1:D:83:TYR:HB3	1:D:85:ASN:OD1	2.04	0.56
1:D:410:LEU:HD13	1:D:415:LEU:HD12	1.87	0.56
1:A:92:ASN:C	1:A:94:THR:H	2.09	0.56
1:C:64:SER:HB2	8:C:1113:HOH:O	2.06	0.56
1:C:67:GLU:HB3	1:C:78:LEU:HD11	1.88	0.55
1:D:87:SER:HB3	4:D:767(A):NAG:O6	2.06	0.55
1:B:42:THR:HB	1:B:569:SER:OG	2.05	0.55
1:B:60:LEU:C	1:B:60:LEU:HD12	2.26	0.55
1:C:299:TYR:HB2	1:C:316:ILE:HG13	1.87	0.55
1:D:155:ILE:HG13	1:D:166:TYR:HB3	1.89	0.55
1:D:532:PRO:CD	1:D:569:SER:HA	2.36	0.55
1:A:527:GLN:HB3	1:A:555:VAL:HG13	1.87	0.55
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.42	0.55
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.42	0.55
1:B:73:GLU:O	1:B:74:ASN:HB2	2.06	0.55
1:D:154:TRP:CD2	1:D:212:SER:HB3	2.42	0.55
1:D:356:ARG:HB3	1:D:551:CYS:SG	2.47	0.55
1:C:763:PHE:HB3	1:C:765:LEU:HG	1.88	0.55
1:A:446:SER:HB2	1:A:457:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:HG22	2:F:1:NAG:HN2	1.72	0.54
1:C:273:THR:HB	8:C:1034:HOH:O	2.07	0.54
1:C:219:ASN:N	1:C:308:GLU:OE2	2.35	0.54
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.42	0.54
1:A:695:PHE:CB	1:A:728:VAL:HG11	2.38	0.54
1:C:491:LEU:H	1:C:491:LEU:CD2	2.20	0.54
1:C:502:LYS:O	1:C:505:GLN:HG2	2.08	0.54
1:B:280:ALA:HB2	1:D:285:TYR:HD1	1.72	0.54
1:C:340:SER:O	1:C:344:GLN:HG3	2.07	0.54
3:G:1:NAG:H62	3:G:2:NAG:H82	1.89	0.54
1:A:81:ALA:HA	1:A:482:LEU:HD21	1.90	0.54
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.90	0.54
1:A:675:THR:C	1:A:680:LEU:HB2	2.28	0.54
1:A:676:PRO:HD3	1:A:680:LEU:HD22	1.90	0.54
1:C:334:THR:OG1	1:C:336:ARG:HG2	2.08	0.54
1:D:658:LYS:HB3	1:D:661:TYR:CD2	2.42	0.54
1:B:454:CYS:HB3	1:B:457:TYR:CE1	2.43	0.54
1:C:138:ASN:O	1:C:140:ARG:HG3	2.08	0.54
1:C:536:LYS:HG2	1:C:537:SER:N	2.18	0.54
1:C:470:LEU:HD12	1:C:483:HIS:CE1	2.43	0.54
1:C:757:HIS:O	1:C:761:GLN:HG2	2.08	0.54
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.37	0.54
1:D:522:THR:HG22	1:D:523:LYS:N	2.22	0.54
1:C:242:SER:CB	1:C:246:LEU:HD12	2.35	0.54
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.43	0.54
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.73	0.54
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.89	0.54
1:C:535:ASP:O	1:C:536:LYS:HD3	2.08	0.54
1:D:179:ASN:C	1:D:180:LEU:HD22	2.28	0.54
1:A:67:GLU:CD	1:A:111:ARG:HH12	2.12	0.53
1:A:438:ASP:HB3	1:A:441:LYS:HD2	1.89	0.53
1:B:422:HIS:CD2	1:B:423:LYS:HD3	2.43	0.53
1:C:483:HIS:HA	1:C:491:LEU:HD23	1.90	0.53
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.09	0.53
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.22	0.53
1:C:219:ASN:H	1:C:308:GLU:CD	2.11	0.53
1:D:516:VAL:HG12	1:D:517:ILE:N	2.23	0.53
1:C:633:GLY:HA3	1:C:655:PRO:HB3	1.90	0.53
1:C:704:HIS:CE1	1:C:711:VAL:O	2.60	0.53
1:C:253:ARG:NH2	1:D:253:ARG:HH21	2.06	0.53
1:A:139:LYS:O	1:A:141:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ARG:HD2	8:C:1063:HOH:O	2.08	0.53
1:C:527:GLN:HB3	1:C:555:VAL:HG13	1.91	0.53
1:A:377:ASN:HB2	1:A:381:TYR:H	1.73	0.53
1:A:534:PHE:CZ	1:A:618:PHE:HB2	2.43	0.53
3:J:1:NAG:H62	3:J:2:NAG:HN2	1.73	0.53
1:A:620:ASP:O	1:A:622:LYS:N	2.42	0.53
1:B:331:ASP:HB2	1:B:338:ILE:CD1	2.38	0.53
1:B:362:PRO:HA	1:B:373:LYS:HB2	1.90	0.53
1:C:536:LYS:CG	1:C:537:SER:H	2.13	0.53
1:D:676:PRO:HG2	1:D:677:GLU:OE1	2.07	0.53
1:A:271:VAL:HG22	1:A:284:SER:HB3	1.89	0.53
1:B:484:SER:HB2	1:B:491:LEU:HD21	1.91	0.53
1:B:732:THR:HG23	1:B:733:MET:N	2.24	0.53
1:C:71:LYS:NZ	1:C:103:ASN:ND2	2.56	0.53
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.90	0.53
1:A:467:TYR:CD1	1:A:484:SER:HA	2.44	0.53
1:B:415:LEU:HB3	1:B:434:ILE:CG2	2.39	0.53
1:C:356:ARG:HD3	1:C:551:CYS:SG	2.49	0.53
1:D:51:SER:O	1:D:54:ARG:HD2	2.09	0.53
1:D:90:LEU:HD12	1:D:140:ARG:NH2	2.24	0.53
1:D:72:GLN:HE21	1:D:77:LEU:CD1	2.21	0.52
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.38	0.52
1:C:205:GLU:OE2	6:C:805:PHI:N	2.42	0.52
1:D:377:ASN:HB3	1:D:379:GLU:H	1.74	0.52
1:C:325:ILE:O	1:C:344:GLN:HA	2.09	0.52
1:A:300:LEU:HB2	1:A:315:TRP:CZ3	2.44	0.52
1:A:726:ALA:HB3	1:A:728:VAL:HG23	1.90	0.52
1:B:491:LEU:HB3	1:B:492:ARG:NH1	2.24	0.52
1:D:177:GLU:CB	1:D:180:LEU:HD23	2.38	0.52
1:A:47:ASP:HA	1:A:52:THR:HG23	1.91	0.52
1:A:496:ASP:OD2	1:A:498:SER:HB3	2.09	0.52
1:B:184:ARG:HD3	1:B:187:TRP:CD2	2.44	0.52
1:A:120:TYR:HE2	1:A:122:LYS:HB2	1.75	0.52
1:A:534:PHE:HZ	1:A:618:PHE:HB2	1.75	0.52
1:B:305:TRP:CZ2	1:B:311:ILE:HD12	2.45	0.52
1:C:733:MET:HA	1:D:732:THR:HG22	1.89	0.52
1:A:94:THR:HG22	1:A:94:THR:O	2.10	0.52
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.91	0.52
1:C:736:THR:O	1:C:737:ASP:HB2	2.10	0.52
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.92	0.52
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:HB	1:B:343:ARG:HB3	1.91	0.52
1:B:658:LYS:HB3	1:B:661:TYR:CD2	2.45	0.52
1:B:696:LYS:HB2	8:B:955:HOH:O	2.09	0.52
1:D:379:GLU:O	1:D:379:GLU:HG2	2.10	0.52
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.44	0.52
1:C:77:LEU:CD2	1:C:88:ILE:HG12	2.40	0.52
1:C:658:LYS:HG3	1:C:687:THR:CG2	2.40	0.52
1:A:281:SER:HB2	8:A:1044:HOH:O	2.10	0.52
1:D:118:TYR:O	1:D:119:ASN:HB2	2.09	0.52
1:B:397:ILE:HD12	1:B:434:ILE:HD13	1.91	0.51
1:D:88:ILE:HG21	1:D:91:GLU:HG3	1.92	0.51
1:D:354:VAL:CG1	1:D:359:PRO:HB3	2.40	0.51
1:A:205:GLU:OE2	6:A:801:PHI:HB3	2.10	0.51
1:B:631:TYR:N	7:B:804:P2Y:NA	2.52	0.51
1:C:177:GLU:HB2	1:C:180:LEU:HD23	1.92	0.51
1:D:75:ASN:HD22	1:D:92:ASN:N	2.04	0.51
1:B:41:ARG:NH1	1:B:47:ASP:OD1	2.43	0.51
1:B:148:ILE:HD13	1:B:155:ILE:HD12	1.92	0.51
1:C:219:ASN:ND2	8:C:908:HOH:O	2.40	0.51
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.92	0.51
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.93	0.51
1:B:651:ILE:HD11	1:B:758:PHE:HD2	1.76	0.51
1:C:534:PHE:O	1:C:535:ASP:C	2.49	0.51
1:D:47:ASP:HA	1:D:52:THR:HG23	1.93	0.51
1:B:706:THR:HB	8:B:1038:HOH:O	2.10	0.51
1:B:104:ASP:OD1	1:B:105:TYR:N	2.40	0.51
1:A:662:TYR:CE2	7:A:802:P2Y:HD2	2.46	0.51
1:B:175:LYS:HG2	1:B:182:SER:HB3	1.92	0.51
1:C:83:TYR:HB2	1:C:85:ASN:OD1	2.11	0.51
1:C:416:TYR:CE2	1:C:433:ARG:HD3	2.46	0.50
1:D:139:LYS:O	1:D:141:GLN:HG3	2.11	0.50
1:D:273:THR:CA	1:D:276:LEU:HD22	2.41	0.50
1:D:518:ASN:HA	1:D:522:THR:O	2.11	0.50
1:B:45:LEU:HD21	1:B:753:THR:HA	1.92	0.50
1:B:331:ASP:HB2	1:B:338:ILE:HD12	1.92	0.50
1:D:191:GLU:O	1:D:193:VAL:HG12	2.11	0.50
1:D:271:VAL:HG22	1:D:284:SER:HB3	1.93	0.50
1:D:289:PRO:HB3	1:D:315:TRP:CE2	2.46	0.50
1:A:188:THR:HG21	8:A:1031:HOH:O	2.10	0.50
1:C:158:SER:OG	1:C:163:LYS:HB2	2.11	0.50
1:C:258:LYS:HD2	1:D:247:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.55	0.50
1:B:214:LEU:HD12	1:B:214:LEU:O	2.12	0.50
1:B:602:GLU:N	1:B:602:GLU:OE2	2.45	0.50
1:D:386:HIS:O	1:D:394:CYS:HB2	2.11	0.50
1:B:67:GLU:CD	1:B:111:ARG:HH12	2.15	0.50
1:D:662:TYR:CE2	7:D:808:P2Y:HD2	2.47	0.50
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.12	0.50
1:B:458:SER:HG	1:B:473:PHE:HE1	1.57	0.50
1:B:516:VAL:HG12	1:B:517:ILE:N	2.26	0.50
1:C:317:ARG:HG2	8:C:990:HOH:O	2.09	0.50
1:C:386:HIS:O	1:C:394:CYS:HB2	2.10	0.50
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.11	0.50
1:C:721:LYS:HB3	8:C:947:HOH:O	2.11	0.50
1:C:270:VAL:HG11	1:C:337:TRP:CE2	2.46	0.50
1:C:463:ASN:C	1:C:465:ALA:N	2.65	0.50
1:D:317:ARG:HB3	8:D:1008:HOH:O	2.12	0.50
1:D:539:LYS:HB3	1:D:620:ASP:HB2	1.93	0.50
1:A:42:THR:HB	1:A:569:SER:OG	2.12	0.50
1:C:148:ILE:HG23	1:C:149:PRO:HD2	1.94	0.50
1:C:512:LYS:HE3	1:C:527:GLN:NE2	2.27	0.50
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.93	0.50
1:B:285:TYR:CE1	1:B:336:ARG:HB2	2.47	0.50
1:D:554:LYS:HB3	1:D:577:SER:HB3	1.93	0.50
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.94	0.49
1:A:732:THR:OG1	1:B:733:MET:HA	2.12	0.49
1:B:405:ILE:HG13	1:B:429:ARG:HD2	1.92	0.49
1:C:540:TYR:HE2	1:C:572:ASN:HD22	1.61	0.49
1:D:199:THR:CG2	1:D:208:PHE:HD2	2.25	0.49
1:A:741:GLY:O	1:A:742:ILE:C	2.50	0.49
1:B:383:HIS:HB3	1:B:398:THR:OG1	2.12	0.49
1:D:139:LYS:HG3	1:D:141:GLN:HG3	1.94	0.49
1:A:591:MET:HE3	1:A:592:HIS:CD2	2.47	0.49
1:B:472:CYS:O	1:B:478:PRO:HA	2.12	0.49
1:B:547:TYR:OH	7:B:804:P2Y:NA	2.45	0.49
1:C:285:TYR:CE1	1:C:336:ARG:CB	2.95	0.49
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.47	0.49
1:D:403:GLU:O	1:D:419:SER:HB2	2.13	0.49
1:A:184:ARG:HD3	1:A:187:TRP:CZ3	2.48	0.49
1:B:512:LYS:HE3	1:B:527:GLN:NE2	2.28	0.49
1:C:288:VAL:CG1	1:C:294:LEU:HD11	2.41	0.49
1:D:310:ARG:NE	1:D:329:ASP:OD1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:741:GLY:O	1:D:742:ILE:C	2.51	0.49
1:B:422:HIS:NE2	1:B:423:LYS:HD3	2.27	0.49
1:D:150:ASN:O	1:D:151:ASN:CB	2.61	0.49
1:D:471:ARG:HH11	1:D:471:ARG:HG2	1.78	0.49
1:A:74:ASN:HB3	1:A:92:ASN:HB2	1.94	0.49
1:A:322:TYR:OH	1:A:346:ILE:HD13	2.11	0.49
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.95	0.49
1:D:704:HIS:HE1	1:D:711:VAL:O	1.96	0.49
1:B:175:LYS:CG	1:B:182:SER:HB3	2.42	0.49
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.93	0.49
1:D:110:ASP:C	1:D:110:ASP:OD1	2.51	0.49
1:D:158:SER:OG	1:D:163:LYS:HB2	2.12	0.49
1:A:418:ILE:HD12	8:A:1059:HOH:O	2.12	0.49
1:C:332:GLU:HG3	8:C:986:HOH:O	2.11	0.49
1:D:491:LEU:O	1:D:492:ARG:HB3	2.13	0.49
1:B:269:PHE:CE2	1:B:286:GLN:HG3	2.47	0.49
1:B:278:PRO:HG2	4:B:772(A):NAG:C8	2.43	0.49
1:D:377:ASN:HB2	1:D:381:TYR:H	1.78	0.49
1:B:526:TYR:HB3	1:B:578:PHE:HD1	1.78	0.49
1:C:738:GLU:HB3	1:C:742:ILE:HA	1.94	0.49
1:C:751:ILE:HG23	1:C:752:TYR:N	2.27	0.49
1:A:377:ASN:ND2	1:A:383:HIS:CD2	2.81	0.48
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.13	0.48
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.94	0.48
1:C:535:ASP:CA	1:C:536:LYS:HD3	2.42	0.48
1:D:354:VAL:HG12	1:D:359:PRO:HB3	1.94	0.48
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.94	0.48
1:C:484:SER:CB	1:C:491:LEU:HD21	2.43	0.48
1:C:732:THR:HG22	1:D:732:THR:CG2	2.43	0.48
1:A:453:ARG:HG3	1:A:476:GLY:HA3	1.94	0.48
1:C:481:THR:OG1	1:C:483:HIS:CE1	2.57	0.48
1:C:661:TYR:OH	1:C:718:GLN:HG3	2.12	0.48
1:D:127:SER:HB3	1:D:211:TYR:CD1	2.47	0.48
1:D:241:TYR:O	1:D:242:SER:HB3	2.13	0.48
1:D:244:GLU:HG2	8:D:921:HOH:O	2.13	0.48
1:D:550:PRO:O	1:D:551:CYS:HB3	2.14	0.48
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.11	0.48
1:D:512:LYS:HE3	1:D:527:GLN:CD	2.34	0.48
1:C:491:LEU:O	1:C:492:ARG:HB3	2.13	0.48
1:C:551:CYS:HB3	8:C:907:HOH:O	2.13	0.48
1:D:471:ARG:HD3	1:D:471:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PRO:HG2	4:B:772(A):NAG:H82	1.95	0.48
1:B:306:VAL:HG12	1:B:307:THR:HG23	1.96	0.48
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.48	0.48
1:D:377:ASN:HD21	1:D:383:HIS:CD2	2.32	0.48
1:B:326:ASP:OD1	1:B:339:SER:OG	2.32	0.48
1:B:350:THR:HG22	4:B:773(A):NAG:H81	1.94	0.48
1:D:167:VAL:HA	1:D:171:ASP:O	2.14	0.48
1:D:640:LEU:HD11	1:D:650:GLY:CA	2.42	0.48
1:B:543:LEU:HD13	1:B:575:VAL:HG13	1.96	0.48
1:C:615:LYS:HG2	1:C:616:MET:N	2.29	0.48
1:B:266:VAL:HG22	1:B:267:LYS:N	2.29	0.48
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.53	0.48
1:C:712:HIS:HB3	8:C:968:HOH:O	2.13	0.48
1:D:675:THR:C	1:D:680:LEU:HB2	2.33	0.48
1:A:122:LYS:HG2	1:A:123:GLN:N	2.28	0.48
1:A:219:ASN:H	1:A:308:GLU:CD	2.15	0.48
1:B:382:LYS:NZ	1:B:588:ASP:OD1	2.47	0.48
1:D:393:ASN:H	1:D:393:ASN:HD22	1.62	0.48
1:A:314:GLN:NE2	1:A:359:PRO:HB2	2.29	0.47
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.34	0.47
1:B:695:PHE:HB3	1:B:728:VAL:HG11	1.96	0.47
1:C:124:TRP:HB2	1:C:204:GLU:OE2	2.14	0.47
1:C:387:PHE:CD2	1:C:394:CYS:HB3	2.49	0.47
1:A:418:ILE:CD1	1:A:458:SER:HA	2.44	0.47
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.96	0.47
1:C:109:PRO:HG3	1:C:159:PRO:O	2.13	0.47
1:D:518:ASN:HD21	1:D:521:GLY:HA2	1.79	0.47
1:C:61:GLN:O	1:C:63:ILE:HG23	2.14	0.47
1:C:63:ILE:O	1:C:63:ILE:HG13	2.14	0.47
1:D:310:ARG:HH21	1:D:329:ASP:CG	2.17	0.47
1:D:502:LYS:HD2	1:D:505:GLN:OE1	2.13	0.47
1:A:92:ASN:O	1:A:94:THR:N	2.45	0.47
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.96	0.47
1:C:405:ILE:HG13	1:C:429:ARG:CD	2.44	0.47
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.30	0.47
1:D:471:ARG:HG2	1:D:471:ARG:NH1	2.29	0.47
1:B:158:SER:OG	1:B:163:LYS:HB2	2.15	0.47
1:C:463:ASN:N	1:C:463:ASN:HD22	2.13	0.47
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.96	0.47
1:A:40:ARG:HB2	1:A:40:ARG:NH1	2.16	0.47
1:B:697:GLN:HG3	8:B:955:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PHE:O	1:C:90:LEU:HB3	2.14	0.47
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.50	0.47
1:D:71:LYS:HA	1:D:75:ASN:O	2.14	0.47
1:D:104:ASP:OD1	1:D:105:TYR:N	2.48	0.47
1:A:112:GLN:O	1:A:137:LEU:HB2	2.15	0.47
1:A:154:TRP:CD2	1:A:212:SER:HB2	2.49	0.47
1:A:363:HIS:CE1	1:A:407:ILE:HB	2.50	0.47
1:A:378:GLU:CD	1:A:378:GLU:N	2.66	0.47
1:B:75:ASN:HD22	1:B:92:ASN:H	1.57	0.47
1:C:128:TYR:CD1	1:C:128:TYR:C	2.88	0.47
1:C:314:GLN:HE21	1:C:325:ILE:HD11	1.79	0.47
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.50	0.47
1:C:763:PHE:CB	1:C:765:LEU:HG	2.45	0.47
1:D:664:SER:O	1:D:668:GLU:HB2	2.15	0.47
1:D:694:ASN:N	1:D:694:ASN:ND2	2.56	0.47
1:A:175:LYS:NZ	1:A:178:PRO:O	2.43	0.47
1:A:739:ASP:HB2	8:A:1078:HOH:O	2.14	0.47
1:B:273:THR:HA	1:B:276:LEU:HG	1.96	0.47
1:C:123:GLN:HG2	1:C:124:TRP:CD2	2.50	0.47
1:C:248:TYR:CE2	1:D:234:PRO:HB2	2.50	0.47
1:D:82:GLU:H	1:D:491:LEU:HD13	1.80	0.47
1:D:680:LEU:O	1:D:684:ARG:HG2	2.15	0.47
1:D:718:GLN:HE21	1:D:718:GLN:CA	2.21	0.47
1:A:516:VAL:HG12	1:A:517:ILE:N	2.30	0.47
1:C:408:GLU:HG2	8:C:943:HOH:O	2.14	0.47
1:D:464:LYS:O	1:D:465:ALA:HB3	2.14	0.47
1:D:738:GLU:HB3	1:D:742:ILE:HA	1.97	0.47
1:A:334:THR:O	1:C:275:THR:HA	2.15	0.47
1:C:86:SER:O	1:C:87:SER:HB3	2.15	0.47
1:C:241:TYR:N	1:C:241:TYR:CD1	2.83	0.47
1:C:603:VAL:HG13	1:C:639:VAL:HG23	1.97	0.47
1:C:732:THR:HG23	1:C:733:MET:N	2.29	0.47
1:A:457:TYR:HA	1:A:471:ARG:O	2.14	0.46
1:B:297:ASP:HA	8:B:1026:HOH:O	2.15	0.46
1:B:317:ARG:HB3	8:B:1023:HOH:O	2.14	0.46
1:C:589:LYS:HB3	8:C:1032:HOH:O	2.15	0.46
1:A:430:ASN:HB2	8:A:990:HOH:O	2.14	0.46
1:B:410:LEU:HD13	1:B:415:LEU:HD22	1.97	0.46
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.97	0.46
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.49	0.46
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:TYR:HB3	1:A:667:THR:OG1	2.15	0.46
1:B:118:TYR:CE2	1:B:119:ASN:ND2	2.84	0.46
1:C:170:ASN:N	1:C:170:ASN:HD22	2.13	0.46
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.31	0.46
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.97	0.46
1:D:105:TYR:CD1	1:D:105:TYR:C	2.88	0.46
1:D:180:LEU:HD22	1:D:180:LEU:N	2.30	0.46
1:D:224:ALA:HA	1:D:269:PHE:O	2.14	0.46
1:D:600:THR:O	1:D:603:VAL:HG13	2.15	0.46
1:A:109:PRO:HG2	1:A:161:GLY:O	2.15	0.46
1:A:438:ASP:OD1	1:A:440:THR:HB	2.15	0.46
1:B:75:ASN:HD22	1:B:91:GLU:HA	1.80	0.46
1:D:331:ASP:HB2	1:D:338:ILE:HD12	1.98	0.46
1:D:393:ASN:H	1:D:393:ASN:ND2	2.13	0.46
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.97	0.46
1:A:489:LYS:N	8:A:962:HOH:O	2.47	0.46
1:B:58:TYR:CD2	1:B:494:LEU:HB3	2.51	0.46
1:B:327:ILE:HD13	1:B:389:THR:HG23	1.98	0.46
1:C:438:ASP:C	1:C:440:THR:H	2.17	0.46
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.98	0.46
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.97	0.46
1:A:143:ILE:N	1:A:143:ILE:HD12	2.31	0.46
1:B:205:GLU:OE2	6:B:803:PHI:N	2.49	0.46
1:B:319:ALA:O	1:B:320:GLN:HB2	2.15	0.46
1:D:566:TYR:CE2	1:D:567:LEU:HD23	2.51	0.46
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.51	0.46
1:A:458:SER:OG	1:A:471:ARG:HD3	2.16	0.46
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.16	0.46
1:C:175:LYS:NZ	1:C:180:LEU:O	2.49	0.46
1:D:480:TYR:N	1:D:480:TYR:CD1	2.83	0.46
1:A:472:CYS:O	1:A:478:PRO:HA	2.15	0.45
1:B:98:LEU:HD11	1:B:116:PHE:CD1	2.50	0.45
1:B:105:TYR:HA	1:B:115:LEU:O	2.15	0.45
1:B:680:LEU:HD11	1:B:684:ARG:HE	1.81	0.45
1:C:559:PHE:CZ	1:C:561:LEU:HD13	2.52	0.45
1:D:80:ASN:OD1	1:D:83:TYR:HD2	1.98	0.45
1:D:454:CYS:HB3	1:D:457:TYR:CZ	2.51	0.45
1:A:420:ASN:ND2	1:A:426:PRO:HA	2.31	0.45
1:A:718:GLN:HE22	1:A:721:LYS:HZ2	1.61	0.45
1:C:535:ASP:O	1:C:536:LYS:HB3	2.16	0.45
1:D:218:PRO:HD3	1:D:305:TRP:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ASP:O	1:A:592:HIS:HB2	2.16	0.45
1:A:704:HIS:HD2	1:A:716:SER:OG	1.99	0.45
1:A:718:GLN:HE21	1:A:718:GLN:CA	2.21	0.45
1:B:79:PHE:CD1	1:B:86:SER:HB2	2.50	0.45
1:C:71:LYS:HD2	1:C:103:ASN:ND2	2.32	0.45
1:D:62:TRP:CE3	1:D:68:TYR:HB3	2.52	0.45
1:D:541:PRO:HG2	1:D:573:ILE:HG23	1.97	0.45
1:A:39:SER:O	1:A:40:ARG:NH1	2.49	0.45
1:C:612:GLN:O	1:C:615:LYS:HG2	2.16	0.45
1:C:697:GLN:HE21	1:C:697:GLN:HA	1.81	0.45
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.82	0.45
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.98	0.45
1:B:184:ARG:HD3	1:B:187:TRP:CE2	2.52	0.45
1:B:492:ARG:HD2	8:B:911:HOH:O	2.16	0.45
1:C:467:TYR:HD1	1:C:484:SER:HA	1.82	0.45
1:D:128:TYR:CD1	1:D:128:TYR:C	2.90	0.45
1:D:486:SER:OG	1:D:487:SER:N	2.50	0.45
1:A:268:PHE:CE2	1:A:313:LEU:HD21	2.51	0.45
1:C:204:GLU:HA	1:C:210:ALA:O	2.17	0.45
1:D:90:LEU:HD12	1:D:140:ARG:HH22	1.82	0.45
1:A:155:ILE:HG13	1:A:166:TYR:HB3	1.99	0.45
1:A:482:LEU:O	1:A:490:GLU:O	2.35	0.45
1:B:516:VAL:HG22	1:B:525:TRP:CD2	2.51	0.45
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.45
1:D:512:LYS:HE2	1:D:514:LEU:HD11	1.99	0.45
1:D:673:LEU:HD12	1:D:673:LEU:HA	1.84	0.45
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.16	0.45
1:B:242:SER:OG	1:B:243:ASP:N	2.49	0.45
1:B:258:LYS:HA	1:B:663:ASP:HA	1.99	0.45
1:C:661:TYR:CZ	1:C:718:GLN:HG3	2.51	0.45
1:D:72:GLN:HE21	1:D:77:LEU:HD12	1.81	0.45
1:A:433:ARG:HH11	1:A:443:THR:HG21	1.81	0.45
1:A:434:ILE:HA	1:A:442:VAL:HA	1.99	0.45
1:C:704:HIS:CD2	1:C:716:SER:OG	2.60	0.45
1:D:599:GLY:O	2:M:1:NAG:H83	2.16	0.45
1:B:302:GLY:HA3	8:B:1080:HOH:O	2.17	0.45
1:B:477:LEU:HD13	1:B:500:LEU:HD23	1.99	0.45
1:C:159:PRO:HB2	1:C:218:PRO:O	2.17	0.45
1:C:326:ASP:OD1	1:C:339:SER:OG	2.35	0.45
1:D:316:ILE:HD11	1:D:320:GLN:HB3	1.99	0.45
1:A:353:TRP:CZ2	1:A:591:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:LEU:N	1:C:491:LEU:HD22	2.31	0.44
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.47	0.44
1:D:704:HIS:CD2	1:D:716:SER:OG	2.69	0.44
1:B:148:ILE:HD13	1:B:155:ILE:CD1	2.47	0.44
1:B:418:ILE:HA	1:B:430:ASN:O	2.16	0.44
1:B:526:TYR:CD1	1:B:526:TYR:C	2.90	0.44
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.53	0.44
1:C:491:LEU:CD2	1:C:491:LEU:N	2.80	0.44
1:C:509:MET:HE3	1:C:510:PRO:HD2	1.99	0.44
1:D:658:LYS:HB3	1:D:661:TYR:CE2	2.53	0.44
1:A:433:ARG:NH2	8:A:992:HOH:O	2.35	0.44
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.99	0.44
1:B:673:LEU:N	1:B:673:LEU:CD1	2.79	0.44
1:D:352:GLY:HA2	1:D:595:ASN:OD1	2.16	0.44
1:D:581:ARG:HE	1:D:605:ASP:CG	2.20	0.44
1:A:87:SER:OG	4:A:767(A):NAG:H81	2.17	0.44
1:A:158:SER:HA	1:A:216:TRP:CD1	2.53	0.44
1:A:658:LYS:HB3	1:A:661:TYR:CD2	2.52	0.44
1:B:159:PRO:HD3	1:B:216:TRP:HB2	1.98	0.44
1:C:293:VAL:HG13	1:C:298:HIS:CB	2.47	0.44
1:C:302:GLY:HA3	8:C:1050:HOH:O	2.18	0.44
1:C:471:ARG:HG2	1:C:480:TYR:HD2	1.82	0.44
1:C:541:PRO:HB2	1:C:763:PHE:CE2	2.52	0.44
1:D:571:GLU:HA	1:D:571:GLU:OE1	2.18	0.44
6:D:807:PHI:HA	7:D:808:P2Y:HD3	1.82	0.44
1:A:40:ARG:HH11	1:A:40:ARG:CB	2.18	0.44
1:A:68:TYR:CE1	1:A:79:PHE:HB2	2.52	0.44
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.99	0.44
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.53	0.44
1:A:700:TYR:OH	1:A:702:LEU:HD13	2.18	0.44
1:B:718:GLN:HA	1:B:718:GLN:NE2	2.33	0.44
1:C:532:PRO:HD3	1:C:569:SER:HA	1.98	0.44
1:C:654:ALA:N	1:C:655:PRO:CD	2.81	0.44
1:A:47:ASP:HA	1:A:52:THR:CG2	2.48	0.44
1:A:266:VAL:HG22	1:A:267:LYS:N	2.33	0.44
1:C:114:ILE:HD13	1:C:116:PHE:CZ	2.52	0.44
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.98	0.44
1:A:70:TYR:HB3	1:A:79:PHE:HE2	1.81	0.44
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.17	0.44
1:B:128:TYR:CD1	1:B:128:TYR:C	2.90	0.44
1:B:326:ASP:CG	1:B:339:SER:HG	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:O	1:C:128:TYR:HB2	2.18	0.44
1:C:293:VAL:HG13	1:C:298:HIS:HB3	1.98	0.44
1:C:319:ALA:O	1:C:320:GLN:HB2	2.18	0.44
1:C:538:LYS:O	1:C:618:PHE:HA	2.17	0.44
1:C:697:GLN:HA	1:C:697:GLN:NE2	2.32	0.44
1:A:106:SER:HB3	1:A:115:LEU:HB2	1.99	0.44
1:A:433:ARG:O	1:A:442:VAL:HA	2.17	0.44
1:C:110:ASP:OD2	1:C:162:HIS:ND1	2.46	0.44
1:C:266:VAL:HG22	1:C:267:LYS:N	2.33	0.44
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.52	0.44
1:D:273:THR:O	1:D:276:LEU:HB2	2.17	0.44
1:A:527:GLN:O	1:A:576:ALA:HA	2.18	0.44
1:C:77:LEU:HD21	1:C:88:ILE:HG12	1.99	0.44
1:C:759:LEU:HD23	1:C:759:LEU:HA	1.78	0.44
1:D:629:TRP:O	1:D:632:GLY:N	2.51	0.44
1:A:192:ASN:HA	1:A:195:TYR:OH	2.18	0.43
1:A:356:ARG:HD3	1:A:551:CYS:SG	2.58	0.43
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.82	0.43
1:C:225:TYR:CE1	1:C:269:PHE:HB2	2.53	0.43
1:C:640:LEU:HD11	1:C:650:GLY:CA	2.41	0.43
1:B:556:ASP:CG	1:B:558:VAL:HG23	2.38	0.43
1:C:197:GLY:C	1:C:213:ALA:HB3	2.38	0.43
1:D:423:LYS:O	1:D:424:GLY:C	2.56	0.43
1:D:673:LEU:O	1:D:678:ASP:HB3	2.18	0.43
1:D:707:ALA:HB2	1:D:737:ASP:HA	2.01	0.43
1:A:318:ARG:O	1:A:320:GLN:HG3	2.17	0.43
1:A:405:ILE:HG13	1:A:429:ARG:HD2	2.00	0.43
1:A:519:LEU:HD22	1:A:608:GLU:OE2	2.17	0.43
1:B:140:ARG:HG2	1:B:140:ARG:HH11	1.83	0.43
1:B:651:ILE:HD11	1:B:758:PHE:CD2	2.54	0.43
1:C:77:LEU:HD23	1:C:88:ILE:CA	2.37	0.43
1:C:384:ILE:HG21	1:C:397:ILE:HD11	1.99	0.43
1:C:400:GLY:HA3	1:C:402:TRP:HE1	1.81	0.43
1:C:533:HIS:O	1:C:535:ASP:N	2.52	0.43
1:C:615:LYS:CG	1:C:616:MET:N	2.80	0.43
1:D:82:GLU:HA	1:D:491:LEU:HD22	2.01	0.43
1:D:662:TYR:HB3	1:D:667:THR:OG1	2.18	0.43
1:A:216:TRP:CZ3	1:A:273:THR:HG21	2.53	0.43
1:A:502:LYS:HD2	1:A:505:GLN:OE1	2.18	0.43
1:A:566:TYR:CE2	1:A:567:LEU:HD23	2.53	0.43
1:B:528:MET:HG2	1:B:576:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LYS:CG	1:C:182:SER:HB3	2.45	0.43
1:C:193:VAL:HG12	1:C:194:ILE:HG12	2.01	0.43
1:C:397:ILE:HG22	1:C:439:TYR:CE2	2.53	0.43
1:C:518:ASN:HA	1:C:522:THR:O	2.19	0.43
1:A:258:LYS:O	1:A:259:ALA:C	2.55	0.43
1:B:677:GLU:CD	1:B:677:GLU:H	2.22	0.43
1:B:720:SER:O	1:B:724:VAL:HG23	2.19	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.54	0.43
1:B:664:SER:O	1:B:668:GLU:HB2	2.18	0.43
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.33	0.43
1:D:133:ASP:HB3	1:D:142:LEU:CD2	2.48	0.43
1:B:49:LEU:HD22	1:B:749:GLN:HA	2.01	0.43
1:D:171:ASP:OD2	1:D:184:ARG:NH1	2.52	0.43
1:D:199:THR:HA	1:D:228:PHE:CE2	2.53	0.43
1:D:612:GLN:HE21	1:D:612:GLN:HB3	1.60	0.43
1:D:734:TRP:CD1	1:D:734:TRP:C	2.91	0.43
1:A:128:TYR:C	1:A:128:TYR:CD1	2.91	0.43
1:A:235:LEU:HD21	1:A:255:PRO:HG3	2.01	0.43
1:B:86:SER:C	4:B:767(A):NAG:H81	2.38	0.43
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.38	0.43
1:B:640:LEU:HB3	1:B:698:VAL:HG21	2.01	0.43
1:C:196:ASN:OD1	1:C:227:GLN:HG3	2.19	0.43
1:C:269:PHE:CE2	1:C:286:GLN:HB2	2.54	0.43
1:D:177:GLU:HA	1:D:178:PRO:HD3	1.89	0.43
1:D:190:LYS:HG2	1:D:193:VAL:HG13	1.96	0.43
1:D:535:ASP:O	1:D:536:LYS:C	2.57	0.43
1:A:230:ASP:O	1:A:232:GLU:N	2.52	0.43
1:A:453:ARG:CZ	1:A:479:LEU:HB2	2.49	0.43
1:B:490:GLU:O	1:B:491:LEU:C	2.57	0.43
1:C:312:SER:C	1:C:313:LEU:HD12	2.38	0.43
1:D:544:ILE:O	1:D:626:ILE:HA	2.19	0.43
1:D:674:PRO:O	1:D:680:LEU:HD13	2.19	0.43
1:B:39:SER:O	1:B:40:ARG:O	2.36	0.42
1:B:85:ASN:ND2	4:B:767(A):NAG:O7	2.52	0.42
1:C:519:LEU:HD22	1:C:608:GLU:CD	2.38	0.42
1:C:571:GLU:OE1	1:C:760:LYS:HE3	2.19	0.42
1:D:363:HIS:CD2	1:D:407:ILE:HB	2.53	0.42
1:A:74:ASN:O	1:A:95:PHE:CE2	2.63	0.42
1:A:134:ILE:HG21	1:A:178:PRO:HB3	2.00	0.42
1:B:678:ASP:HB3	1:B:679:ASN:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:ASP:OD2	1:D:757:HIS:HD2	2.01	0.42
6:C:805:PHI:HA	7:C:806:P2Y:HD3	1.90	0.42
1:D:153:GLN:HE22	1:D:170:ASN:HD21	1.63	0.42
1:D:163:LYS:HE2	8:D:1056:HOH:O	2.19	0.42
1:A:203:TYR:CD2	1:A:207:VAL:HG21	2.55	0.42
1:C:49:LEU:HB3	1:C:749:GLN:HG2	2.01	0.42
1:C:143:ILE:N	1:C:143:ILE:HD12	2.34	0.42
1:C:490:GLU:O	1:C:490:GLU:HG2	2.19	0.42
1:D:517:ILE:HG23	1:D:526:TYR:CE2	2.54	0.42
1:A:150:ASN:O	1:A:151:ASN:CB	2.67	0.42
1:B:473:PHE:HB3	1:B:558:VAL:HG13	2.00	0.42
1:B:546:VAL:HG11	1:B:626:ILE:HD11	2.02	0.42
1:C:133:ASP:HA	8:C:1042:HOH:O	2.20	0.42
1:C:313:LEU:N	1:C:313:LEU:CD1	2.82	0.42
1:C:374:ILE:CD1	1:C:406:GLY:HA2	2.50	0.42
1:C:517:ILE:HG23	1:C:526:TYR:CD2	2.54	0.42
1:C:560:ARG:HD2	8:C:914:HOH:O	2.19	0.42
1:D:123:GLN:HG2	1:D:124:TRP:CD2	2.54	0.42
1:D:219:ASN:HB2	1:D:308:GLU:CG	2.50	0.42
1:A:257:PRO:O	1:A:663:ASP:HA	2.19	0.42
1:A:620:ASP:OD1	1:A:620:ASP:C	2.58	0.42
1:B:80:ASN:OD1	1:B:82:GLU:HB2	2.20	0.42
1:B:227:GLN:O	1:B:266:VAL:HA	2.19	0.42
1:C:463:ASN:N	1:C:463:ASN:ND2	2.67	0.42
1:C:545:GLU:HG3	1:C:627:TRP:NE1	2.34	0.42
1:C:679:ASN:HD21	1:C:682:TYR:HB2	1.84	0.42
1:D:515:ASP:HB3	1:D:526:TYR:CZ	2.54	0.42
1:D:522:THR:CG2	1:D:523:LYS:N	2.82	0.42
1:D:703:ILE:HG12	1:D:733:MET:HB3	2.01	0.42
1:B:143:ILE:HD12	1:B:143:ILE:N	2.35	0.42
1:C:53:PHE:CZ	1:C:507:VAL:HG11	2.55	0.42
1:C:66:HIS:CD2	1:C:67:GLU:HG3	2.55	0.42
1:C:142:LEU:C	1:C:142:LEU:HD23	2.40	0.42
1:C:534:PHE:O	1:C:535:ASP:O	2.37	0.42
1:D:199:THR:CG2	1:D:208:PHE:CD2	3.03	0.42
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.34	0.42
1:D:549:GLY:HA2	1:D:631:TYR:CD1	2.54	0.42
1:A:435:GLN:OE1	1:A:437:ASN:OD1	2.38	0.42
1:A:532:PRO:O	1:A:533:HIS:C	2.58	0.42
1:B:120:TYR:CD2	1:B:120:TYR:C	2.92	0.42
1:C:435:GLN:HG2	8:C:1051:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:ND2	1:D:92:ASN:N	2.53	0.42
1:A:59:THR:O	1:A:70:TYR:HD1	2.03	0.42
1:A:161:GLY:HA3	8:A:1030:HOH:O	2.20	0.42
1:A:515:ASP:HB3	1:A:526:TYR:CE2	2.55	0.42
1:B:516:VAL:HG11	1:B:523:LYS:HB2	2.02	0.42
1:C:122:LYS:HG2	1:C:123:GLN:N	2.34	0.42
1:C:651:ILE:HD11	1:C:758:PHE:CD2	2.55	0.42
1:D:415:LEU:O	1:D:434:ILE:HG22	2.20	0.42
1:A:438:ASP:C	1:A:440:THR:H	2.23	0.42
1:A:452:GLU:HA	1:A:452:GLU:OE1	2.19	0.42
1:A:474:GLY:HA2	1:A:476:GLY:O	2.20	0.42
1:A:759:LEU:HD23	1:A:759:LEU:HA	1.86	0.42
1:B:41:ARG:HG2	1:B:42:THR:O	2.20	0.42
1:B:137:LEU:O	1:B:140:ARG:NH1	2.53	0.42
1:B:219:ASN:ND2	8:B:1066:HOH:O	2.47	0.42
1:B:518:ASN:HA	1:B:522:THR:O	2.20	0.42
1:D:317:ARG:O	1:D:318:ARG:C	2.57	0.42
1:D:695:PHE:HB3	1:D:728:VAL:HG11	2.02	0.42
1:A:74:ASN:HD22	1:A:74:ASN:HA	1.62	0.41
1:A:184:ARG:HD3	1:A:187:TRP:CE3	2.55	0.41
1:B:62:TRP:CG	1:B:462:SER:HA	2.55	0.41
1:C:209:SER:HA	8:C:1007:HOH:O	2.18	0.41
1:C:241:TYR:CE2	1:D:714:GLN:HA	2.54	0.41
1:C:356:ARG:HB3	1:C:551:CYS:SG	2.60	0.41
1:D:446:SER:HB2	1:D:457:TYR:CE1	2.54	0.41
1:B:193:VAL:HG12	1:B:194:ILE:HG12	2.01	0.41
1:B:206:GLU:HB3	8:B:1039:HOH:O	2.18	0.41
1:B:524:PHE:CE2	1:B:590:ILE:HD12	2.56	0.41
1:C:96:ASP:O	1:C:98:LEU:HG	2.19	0.41
1:D:423:LYS:O	1:D:425:MET:N	2.53	0.41
1:C:58:TYR:CD1	1:C:494:LEU:HD13	2.56	0.41
1:C:463:ASN:O	1:C:465:ALA:N	2.52	0.41
1:C:536:LYS:CG	1:C:537:SER:N	2.82	0.41
1:C:664:SER:O	1:C:668:GLU:HB2	2.19	0.41
1:D:266:VAL:HG22	1:D:267:LYS:N	2.36	0.41
1:A:439:TYR:N	1:A:439:TYR:CD1	2.87	0.41
1:A:535:ASP:OD2	1:A:535:ASP:C	2.57	0.41
1:A:732:THR:O	1:B:732:THR:HG22	2.20	0.41
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.20	0.41
1:B:692:ALA:O	1:B:728:VAL:HG21	2.21	0.41
1:C:63:ILE:HG21	1:C:69:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ASN:HD22	1:C:426:PRO:CA	2.26	0.41
1:D:512:LYS:HE3	1:D:527:GLN:NE2	2.35	0.41
3:J:2:NAG:H82	3:J:2:NAG:O3	2.20	0.41
1:B:327:ILE:CD1	1:B:389:THR:HG23	2.49	0.41
1:B:363:HIS:CD2	1:B:407:ILE:HB	2.55	0.41
1:C:172:ILE:HB	1:C:185:ILE:HB	2.02	0.41
1:C:237:GLU:HA	1:C:252:VAL:O	2.19	0.41
1:C:242:SER:OG	1:C:243:ASP:N	2.52	0.41
1:C:377:ASN:HA	1:C:396:PHE:CZ	2.55	0.41
1:C:422:HIS:CE1	1:C:447:CYS:HB3	2.56	0.41
1:C:474:GLY:HA2	1:C:476:GLY:O	2.21	0.41
1:C:550:PRO:HD2	1:C:631:TYR:CE2	2.55	0.41
1:D:45:LEU:O	1:D:49:LEU:HG	2.21	0.41
1:D:65:ASP:O	1:D:467:TYR:HD2	2.03	0.41
1:A:198:VAL:HA	1:A:211:TYR:O	2.21	0.41
1:A:429:ARG:HH11	1:A:429:ARG:HG3	1.85	0.41
1:D:47:ASP:HA	1:D:52:THR:CG2	2.51	0.41
1:D:64:SER:C	1:D:463:ASN:HB2	2.41	0.41
1:D:98:LEU:HD22	1:D:142:LEU:HD11	2.02	0.41
1:A:92:ASN:C	1:A:94:THR:N	2.73	0.41
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.81	0.41
1:B:44:THR:O	1:B:47:ASP:HB2	2.20	0.41
1:B:49:LEU:HB3	1:B:749:GLN:HG2	2.03	0.41
1:B:280:ALA:HB2	1:D:285:TYR:CD1	2.55	0.41
1:D:145:GLU:O	1:D:146:GLU:HB2	2.21	0.41
1:D:170:ASN:O	1:D:196:ASN:HB2	2.21	0.41
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.55	0.41
1:B:44:THR:HB	8:B:1059:HOH:O	2.21	0.41
1:D:143:ILE:HD13	1:D:178:PRO:HB2	2.02	0.41
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.51	0.41
1:A:664:SER:O	1:A:668:GLU:HB2	2.20	0.41
1:B:44:THR:OG1	1:B:47:ASP:OD2	2.37	0.41
1:B:57:PHE:HA	1:B:480:TYR:CE1	2.56	0.41
1:B:492:ARG:NE	8:B:911:HOH:O	2.53	0.41
1:B:527:GLN:HB3	1:B:555:VAL:HG13	2.03	0.41
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.01	0.41
1:C:101:SER:O	1:C:102:THR:CG2	2.69	0.41
1:C:102:THR:HB	1:C:103:ASN:H	1.51	0.41
1:C:551:CYS:SG	1:C:551:CYS:O	2.78	0.41
1:D:49:LEU:HB3	1:D:749:GLN:HG2	2.02	0.41
1:D:67:GLU:OE2	1:D:111:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:HE21	1:D:77:LEU:HD11	1.86	0.41
1:D:263:ASN:HB3	1:D:264:PRO:HD2	2.02	0.41
1:D:320:GLN:N	8:D:918:HOH:O	2.54	0.41
1:D:712:HIS:CD2	1:D:712:HIS:N	2.88	0.41
1:A:59:THR:O	1:A:70:TYR:CD1	2.74	0.41
1:A:268:PHE:CE1	1:A:303:VAL:HG21	2.56	0.41
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.42	0.41
1:D:222:PHE:HE2	1:D:308:GLU:O	2.03	0.41
1:A:534:PHE:CE1	1:A:540:TYR:CE1	3.08	0.40
1:C:658:LYS:HB3	1:C:661:TYR:CD2	2.55	0.40
1:D:743:ALA:O	1:D:744:SER:C	2.58	0.40
1:A:151:ASN:ND2	8:A:1011:HOH:O	2.54	0.40
1:A:505:GLN:HE21	1:A:505:GLN:HB3	1.66	0.40
1:B:55:VAL:HG22	1:B:500:LEU:HD22	2.03	0.40
1:B:532:PRO:O	1:B:533:HIS:C	2.60	0.40
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.56	0.40
1:C:546:VAL:HG22	1:C:547:TYR:N	2.36	0.40
1:D:122:LYS:HA	1:D:128:TYR:CB	2.51	0.40
1:D:524:PHE:CE2	1:D:590:ILE:HD12	2.57	0.40
1:D:610:THR:HA	1:D:613:PHE:HD2	1.87	0.40
1:D:675:THR:HB	1:D:676:PRO:HD2	2.03	0.40
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.56	0.40
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.50	0.40
1:A:489:LYS:HG3	1:A:491:LEU:H	1.87	0.40
1:A:547:TYR:OH	7:A:802:P2Y:NA	2.54	0.40
1:B:43:TYR:O	1:B:570:THR:OG1	2.34	0.40
1:B:118:TYR:CD2	1:B:119:ASN:ND2	2.90	0.40
1:B:322:TYR:CD1	1:B:322:TYR:C	2.94	0.40
1:B:438:ASP:C	1:B:440:THR:H	2.25	0.40
1:B:620:ASP:OD1	1:B:622:LYS:HB2	2.21	0.40
1:C:382:LYS:H	1:C:403:GLU:HG2	1.86	0.40
1:C:535:ASP:O	1:C:536:LYS:CB	2.70	0.40
1:D:703:ILE:HG21	1:D:751:ILE:CD1	2.51	0.40
1:A:345:HIS:ND1	1:A:345:HIS:N	2.70	0.40
1:B:72:GLN:NE2	1:B:77:LEU:HD11	2.37	0.40
1:B:143:ILE:HG21	1:B:178:PRO:O	2.21	0.40
1:B:491:LEU:H	1:B:491:LEU:CD2	2.34	0.40
1:B:707:ALA:HB2	1:B:737:ASP:HA	2.02	0.40
1:C:254:ILE:HA	1:C:255:PRO:HD3	1.95	0.40
1:C:294:LEU:O	1:C:295:ILE:C	2.59	0.40
1:D:735:TYR:OH	1:D:751:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:CD1	1:A:141:GLN:O	2.75	0.40
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.04	0.40
1:B:201:TRP:CZ2	1:B:710:ASN:HA	2.56	0.40
1:B:405:ILE:HG12	1:B:419:SER:HA	2.04	0.40
1:B:491:LEU:H	1:B:491:LEU:HD23	1.87	0.40
1:B:746:MET:O	1:B:750:HIS:HB2	2.22	0.40
1:C:71:LYS:HD2	1:C:103:ASN:HD21	1.86	0.40
1:C:596:ARG:N	1:C:670:TYR:O	2.46	0.40
1:D:74:ASN:O	1:D:92:ASN:HB3	2.22	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	726/728 (100%)	656 (90%)	58 (8%)	12 (2%)	9	20
1	B	726/728 (100%)	670 (92%)	50 (7%)	6 (1%)	19	38
1	C	726/728 (100%)	652 (90%)	59 (8%)	15 (2%)	7	15
1	D	726/728 (100%)	656 (90%)	64 (9%)	6 (1%)	19	38
All	All	2904/2912 (100%)	2634 (91%)	231 (8%)	39 (1%)	12	26

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	B	40	ARG
1	C	103	ASN
1	C	534	PHE
1	C	535	ASP
1	C	536	LYS

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Mol	Chain	Res	Type
1	A	97	GLU
1	A	231	THR
1	A	621	ASP
1	B	273	THR
1	B	491	LEU
1	C	40	ARG
1	C	74	ASN
1	C	104	ASP
1	D	537	SER
1	A	82	GLU
1	A	104	ASP
1	B	292	SER
1	B	439	TYR
1	C	87	SER
1	D	151	ASN
1	A	149	PRO
1	A	377	ASN
1	A	492	ARG
1	C	94	THR
1	C	451	PRO
1	A	102	THR
1	A	121	VAL
1	A	151	ASN
1	B	295	ILE
1	C	90	LEU
1	C	149	PRO
1	D	320	GLN
1	C	295	ILE
1	D	193	VAL
1	D	680	LEU
1	D	143	ILE
1	C	99	GLY
1	C	193	VAL

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	652/652 (100%)	620 (95%)	32 (5%)	25	47
1	B	652/652 (100%)	626 (96%)	26 (4%)	31	57
1	C	652/652 (100%)	618 (95%)	34 (5%)	23	44
1	D	652/652 (100%)	620 (95%)	32 (5%)	25	47
All	All	2608/2608 (100%)	2484 (95%)	124 (5%)	25	49

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	74	ASN
1	A	90	LEU
1	A	111	ARG
1	A	145	GLU
1	A	150	ASN
1	A	180	LEU
1	A	207	VAL
1	A	246	LEU
1	A	247	GLN
1	A	250	LYS
1	A	294	LEU
1	A	385	CYS
1	A	399	LYS
1	A	415	LEU
1	A	423	LYS
1	A	442	VAL
1	A	443	THR
1	A	471	ARG
1	A	472	CYS
1	A	491	LEU
1	A	492	ARG
1	A	520	HIS
1	A	542	LEU
1	A	543	LEU
1	A	561	LEU
1	A	566	TYR
1	A	679	ASN
1	A	683	TYR
1	A	701	LEU
1	A	718	GLN
1	A	761	GLN
1	B	91	GLU

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Mol	Chain	Res	Type
1	B	111	ARG
1	B	170	ASN
1	B	246	LEU
1	B	256	TYR
1	B	415	LEU
1	B	418	ILE
1	B	435	GLN
1	B	450	ASN
1	B	491	LEU
1	B	492	ARG
1	B	506	ASP
1	B	520	HIS
1	B	535	ASP
1	B	536	LYS
1	B	537	SER
1	B	542	LEU
1	B	543	LEU
1	B	561	LEU
1	B	566	TYR
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	732	THR
1	B	745	ASN
1	B	761	GLN
1	C	75	ASN
1	C	90	LEU
1	C	145	GLU
1	C	147	ARG
1	C	158	SER
1	C	184	ARG
1	C	188	THR
1	C	230	ASP
1	C	246	LEU
1	C	284	SER
1	C	339	SER
1	C	348	ILE
1	C	366	SER
1	C	385	CYS
1	C	399	LYS
1	C	418	ILE
1	C	419	SER

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Mol	Chain	Res	Type
1	C	472	CYS
1	C	482	LEU
1	C	491	LEU
1	C	503	MET
1	C	535	ASP
1	C	536	LYS
1	C	542	LEU
1	C	561	LEU
1	C	566	TYR
1	C	583	SER
1	C	611	ARG
1	C	627	TRP
1	C	685	ASN
1	C	701	LEU
1	C	732	THR
1	C	746	MET
1	C	759	LEU
1	D	41	ARG
1	D	103	ASN
1	D	107	VAL
1	D	111	ARG
1	D	142	LEU
1	D	184	ARG
1	D	193	VAL
1	D	246	LEU
1	D	253	ARG
1	D	276	LEU
1	D	294	LEU
1	D	348	ILE
1	D	358	ARG
1	D	393	ASN
1	D	399	LYS
1	D	423	LYS
1	D	448	GLU
1	D	471	ARG
1	D	482	LEU
1	D	507	VAL
1	D	536	LYS
1	D	561	LEU
1	D	566	TYR
1	D	581	ARG
1	D	603	VAL

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Mol	Chain	Res	Type
1	D	608	GLU
1	D	673	LEU
1	D	679	ASN
1	D	694	ASN
1	D	701	LEU
1	D	702	LEU
1	D	732	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	75	ASN
1	A	119	ASN
1	A	123	GLN
1	A	138	ASN
1	A	141	GLN
1	A	151	ASN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	183	GLN
1	A	192	ASN
1	A	247	GLN
1	A	314	GLN
1	A	377	ASN
1	A	435	GLN
1	A	463	ASN
1	A	469	GLN
1	A	483	HIS
1	A	505	GLN
1	A	572	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	697	GLN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	B	72	GLN
1	B	75	ASN

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	119	ASN
1	B	170	ASN
1	B	176	ASN
1	B	183	GLN
1	B	192	ASN
1	B	219	ASN
1	B	227	GLN
1	B	247	GLN
1	B	345	HIS
1	B	369	ASN
1	B	435	GLN
1	B	455	GLN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	572	ASN
1	B	586	GLN
1	B	595	ASN
1	B	606	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	749	GLN
1	B	761	GLN
1	C	72	GLN
1	C	75	ASN
1	C	103	ASN
1	C	141	GLN
1	C	170	ASN
1	C	176	ASN
1	C	192	ASN
1	C	227	GLN
1	C	247	GLN
1	C	314	GLN
1	C	369	ASN
1	C	430	ASN
1	C	435	GLN
1	C	463	ASN

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Mol	Chain	Res	Type
1	C	483	HIS
1	C	505	GLN
1	C	572	ASN
1	C	595	ASN
1	C	606	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	697	GLN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN
1	C	761	GLN
1	D	72	GLN
1	D	75	ASN
1	D	123	GLN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	227	GLN
1	D	247	GLN
1	D	377	ASN
1	D	393	ASN
1	D	463	ASN
1	D	483	HIS
1	D	572	ASN
1	D	606	GLN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	757	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 ⓘ

20 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	1,2	14,14,15	0.46	0	17,19,21	0.61	0
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	0.75	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.53	0	17,19,21	0.69	0
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	0.73	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.55	0	17,19,21	0.84	0
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	0.77	0
3	BMA	G	3	3	11,11,12	0.51	0	15,15,17	0.52	0
2	NAG	H	1	1,2	14,14,15	0.57	0	17,19,21	0.78	0
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	0.78	0
2	NAG	I	1	1,2	14,14,15	0.53	0	17,19,21	0.63	0
2	NAG	I	2	2	14,14,15	0.62	0	17,19,21	0.67	0
3	NAG	J	1	3,1	14,14,15	0.64	0	17,19,21	0.78	0
3	NAG	J	2	3	14,14,15	0.58	0	17,19,21	0.53	0
3	BMA	J	3	3	11,11,12	0.70	0	15,15,17	0.72	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.51	0	17,19,21	0.64	0
2	NAG	K	2	2	14,14,15	0.53	0	17,19,21	0.62	0
2	NAG	L	1	1,2	14,14,15	0.58	0	17,19,21	1.01	2 (11%)
2	NAG	L	2	2	14,14,15	0.62	0	17,19,21	0.79	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.55	0	17,19,21	0.72	0
2	NAG	M	2	2	14,14,15	0.56	0	17,19,21	1.33	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	NAG	C1-C2-N2	2.91	115.45	110.49
2	M	2	NAG	O5-C1-C2	-2.36	107.56	111.29
2	L	2	NAG	C2-N2-C7	-2.33	119.59	122.90
3	J	3	BMA	C1-C2-C3	2.31	112.50	109.67
2	L	1	NAG	C3-C4-C5	-2.26	106.20	110.24
2	E	2	NAG	C2-N2-C7	-2.20	119.77	122.90
2	M	2	NAG	C6-C5-C4	-2.14	108.00	113.00
2	L	1	NAG	C2-N2-C7	-2.11	119.90	122.90
2	F	2	NAG	C2-N2-C7	-2.07	119.96	122.90

There are no chirality outliers.

All (35) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 5 short contacts:

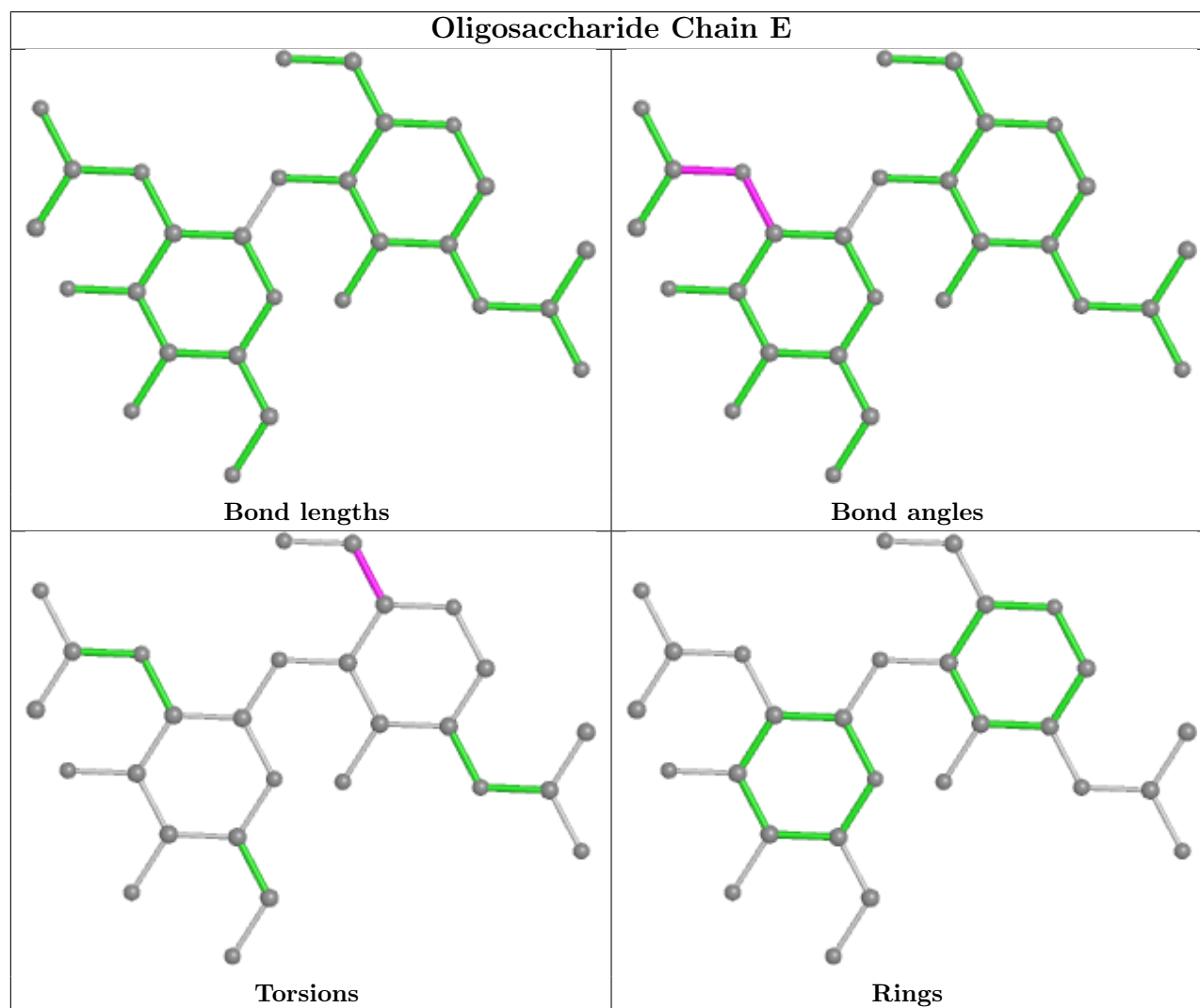
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
2	F	1	NAG	1	0
3	G	1	NAG	1	0

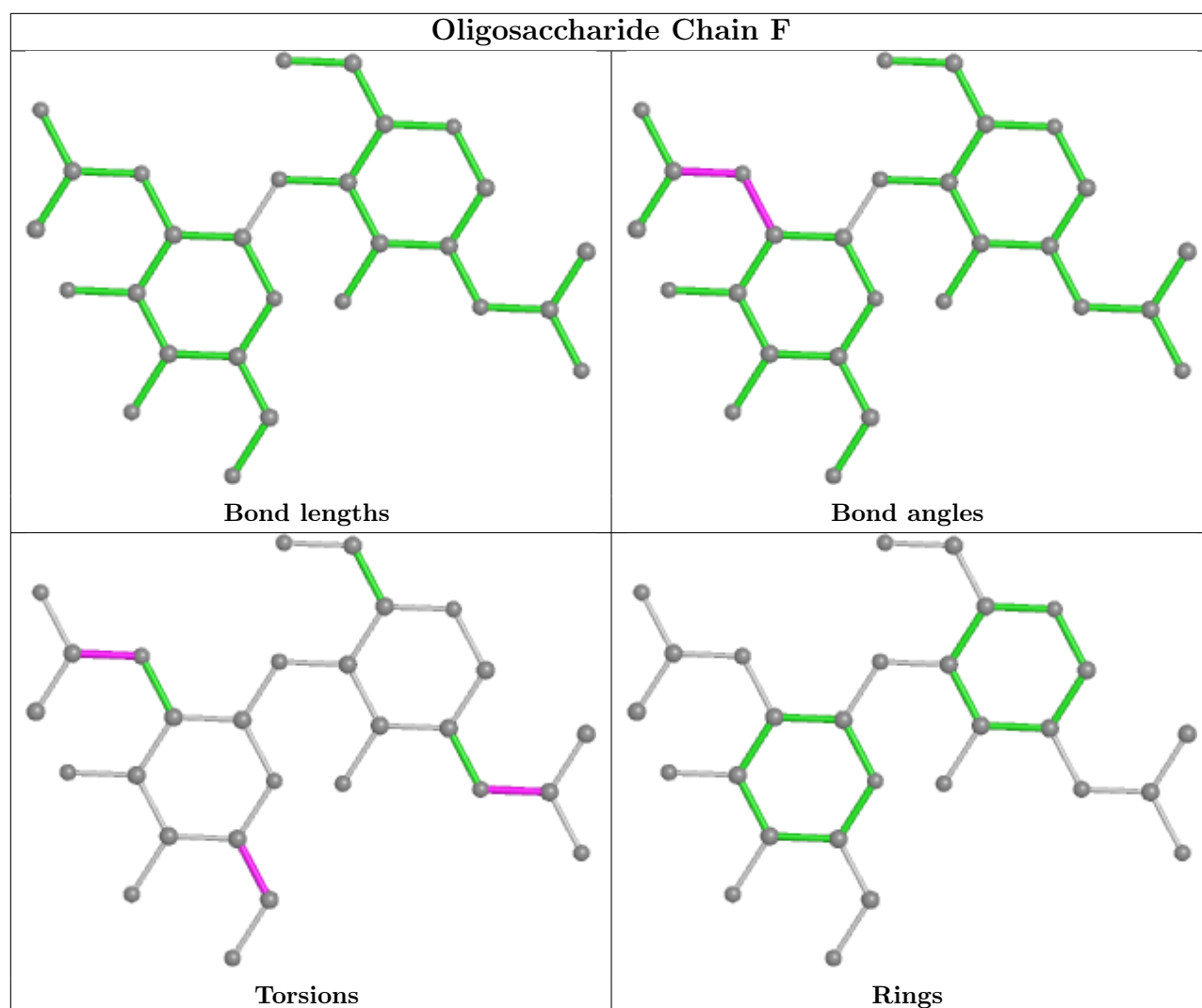
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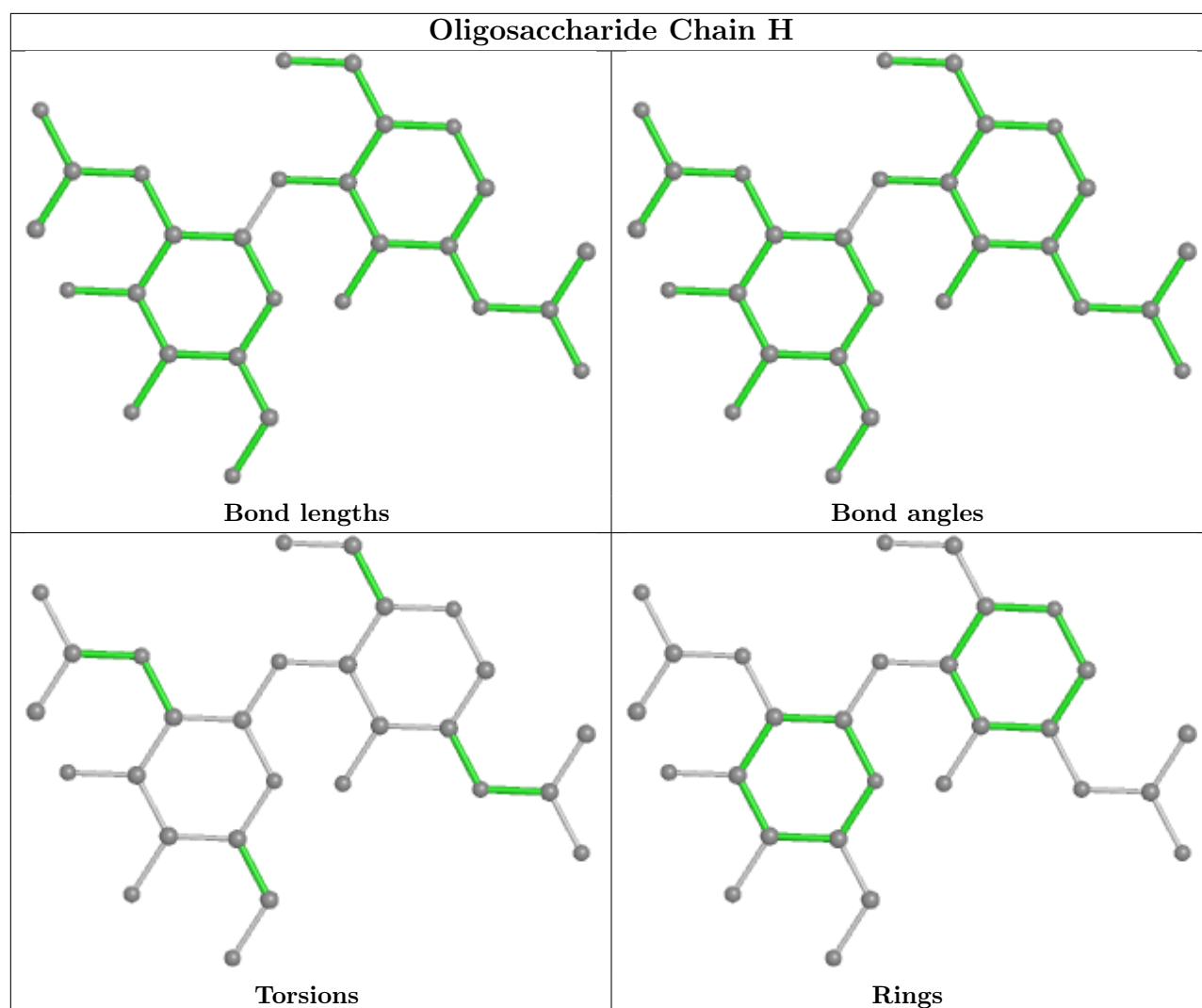
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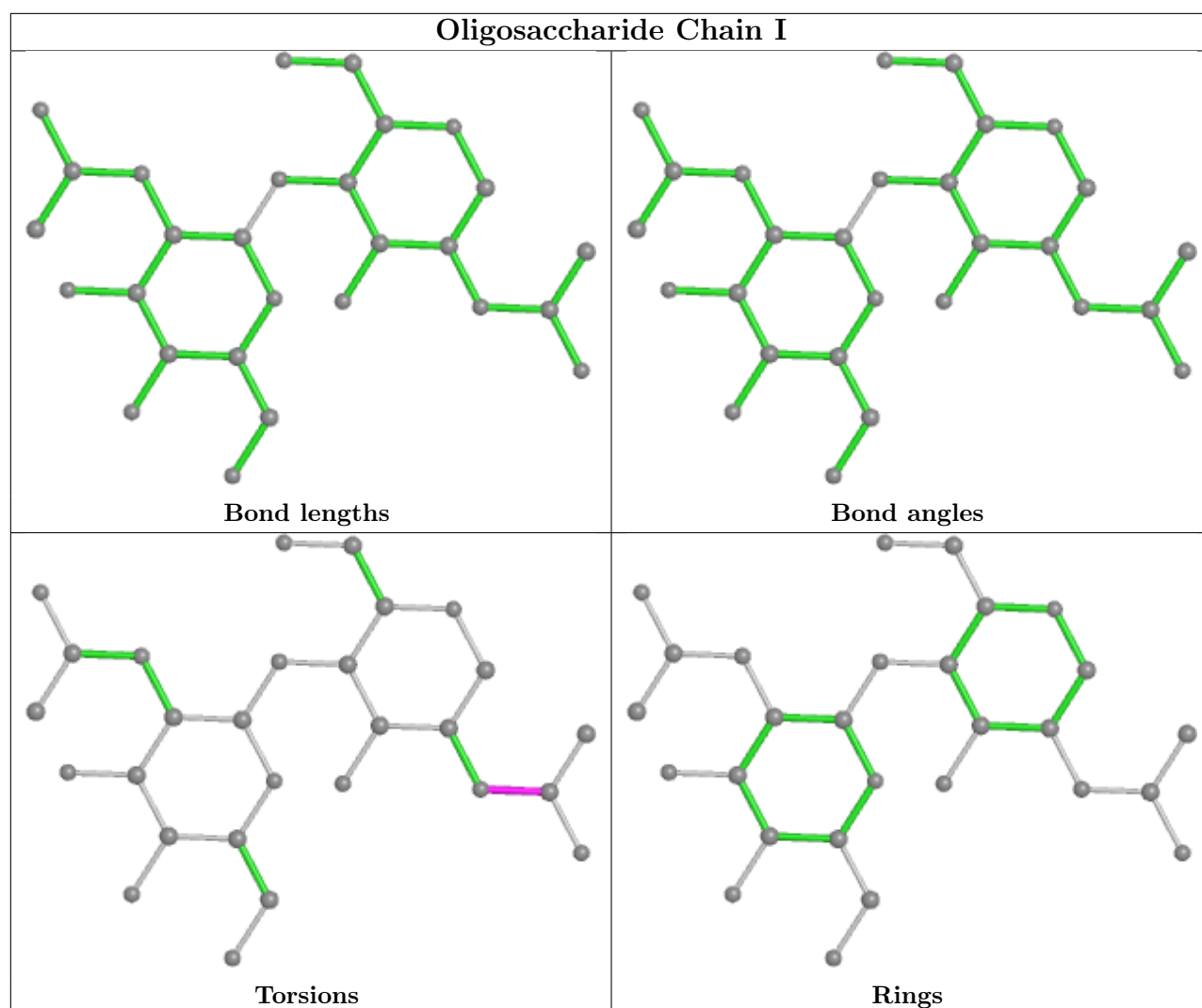
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	2	0
3	J	1	NAG	1	0
2	M	1	NAG	1	0

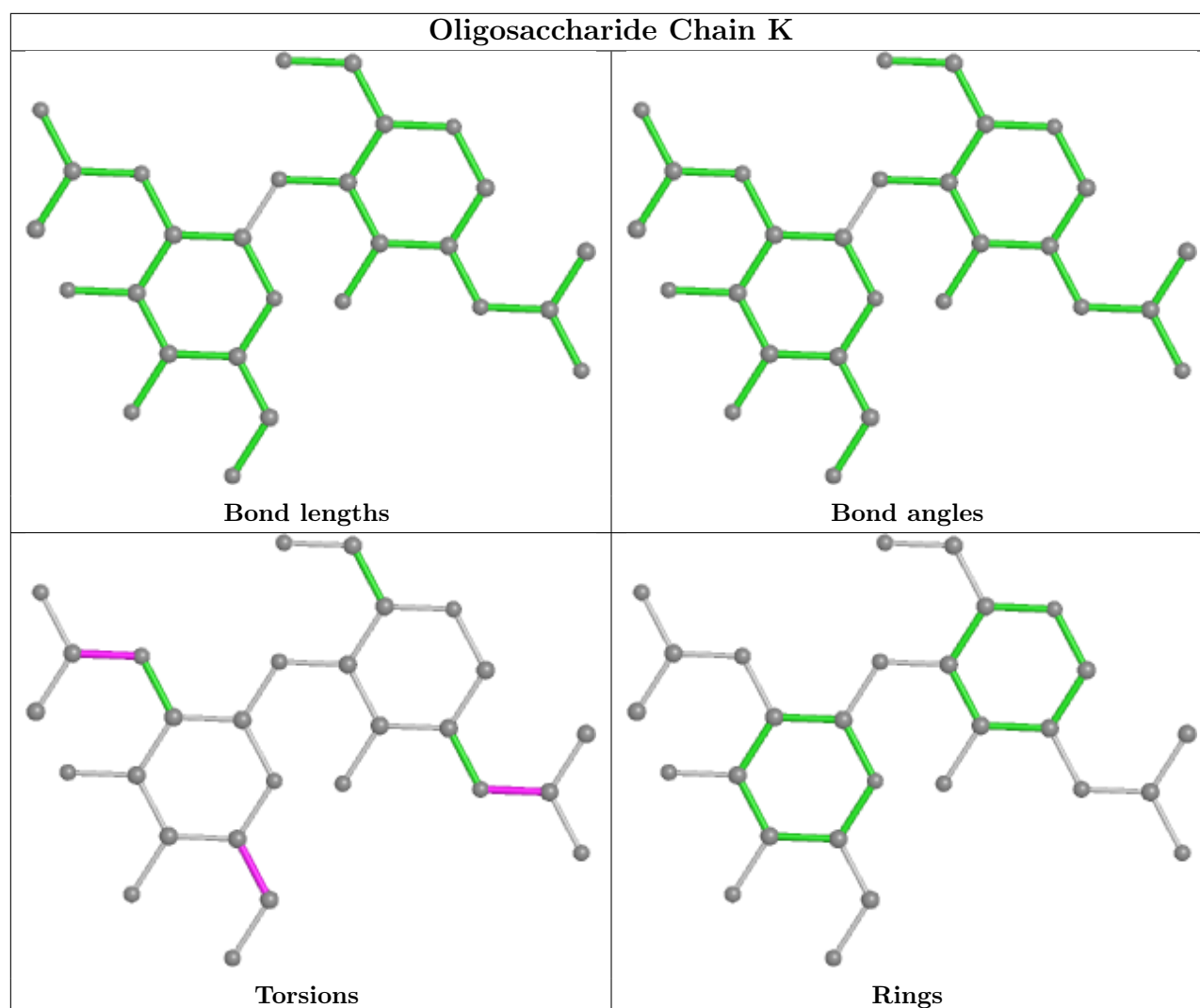
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

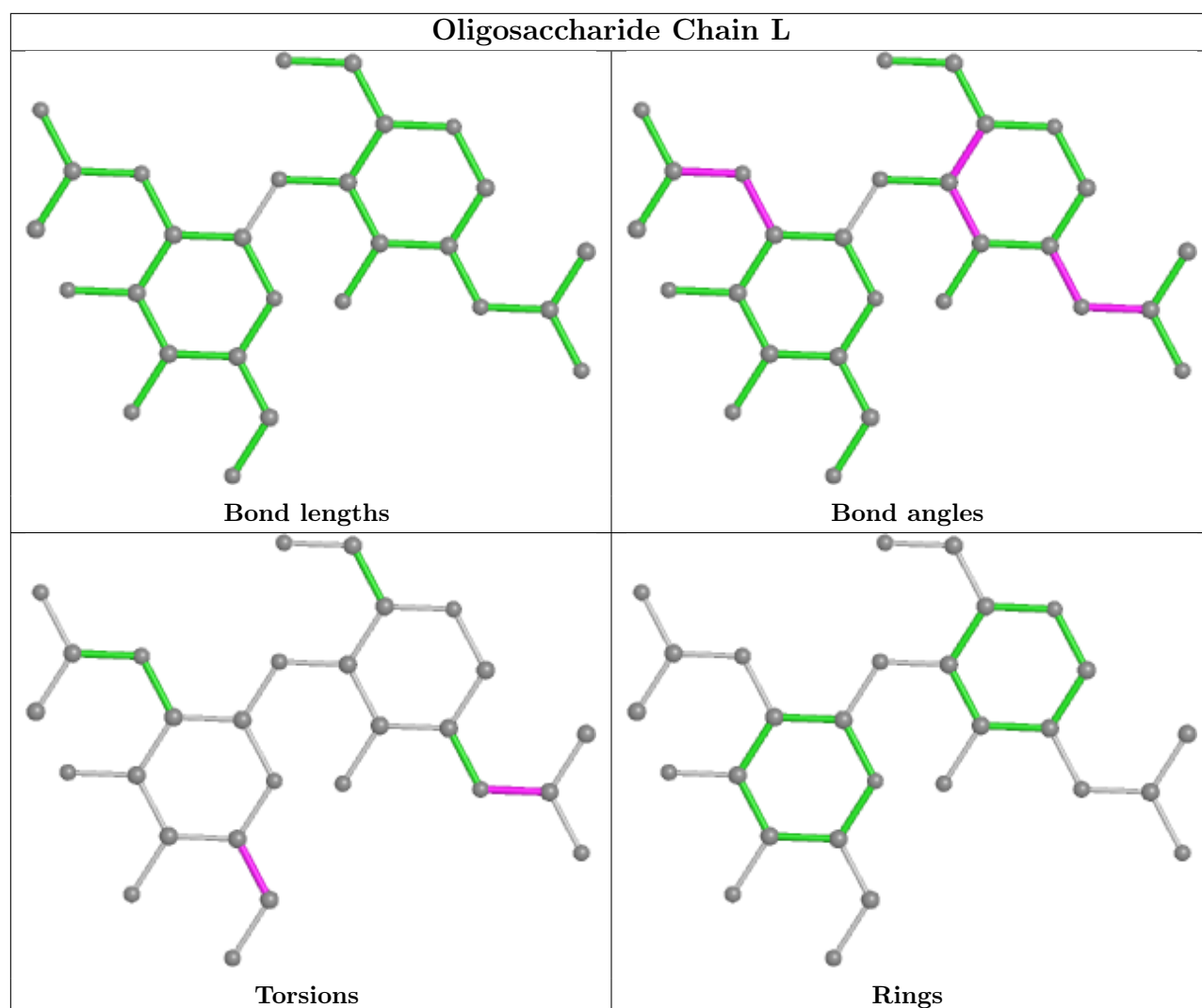


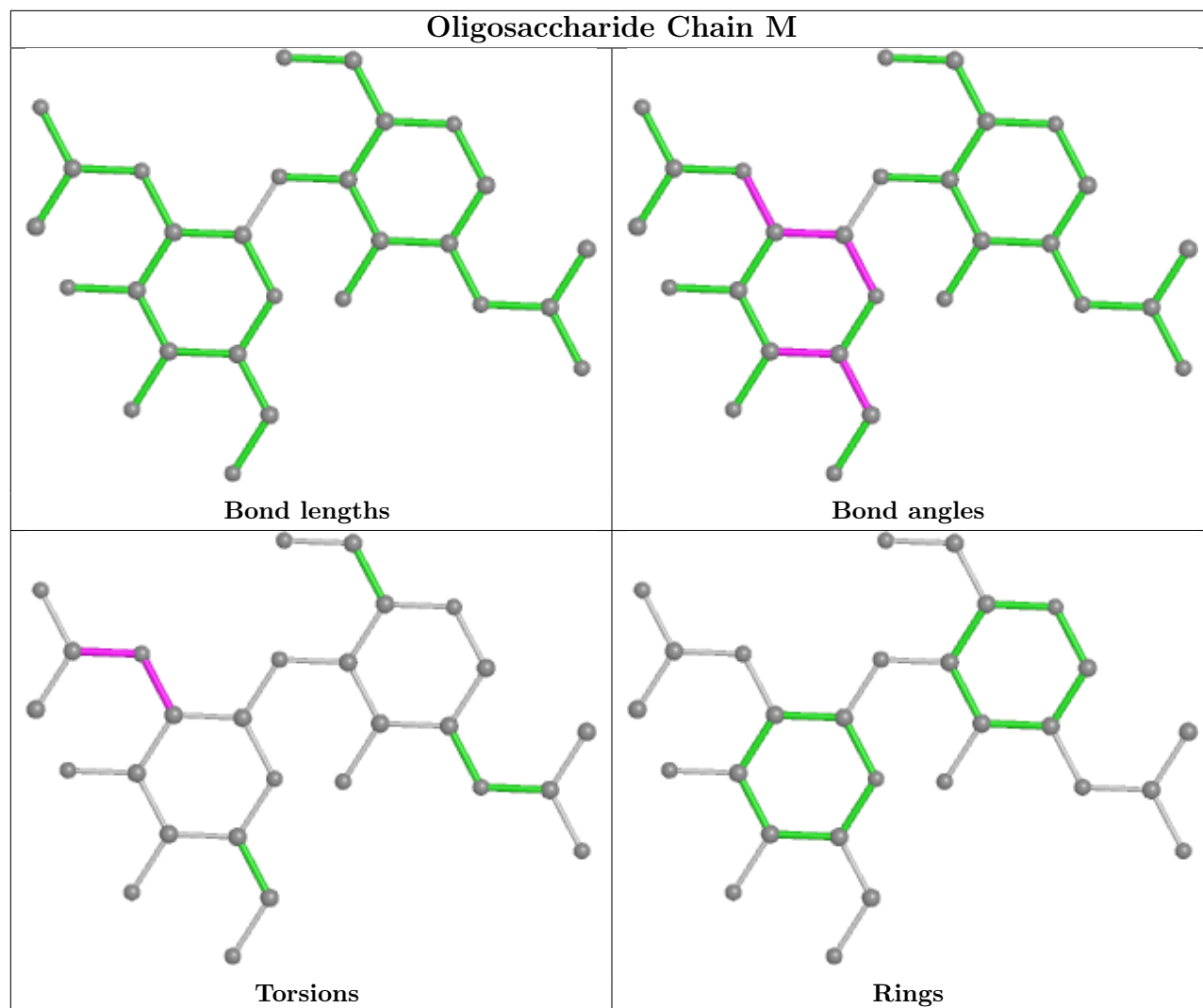


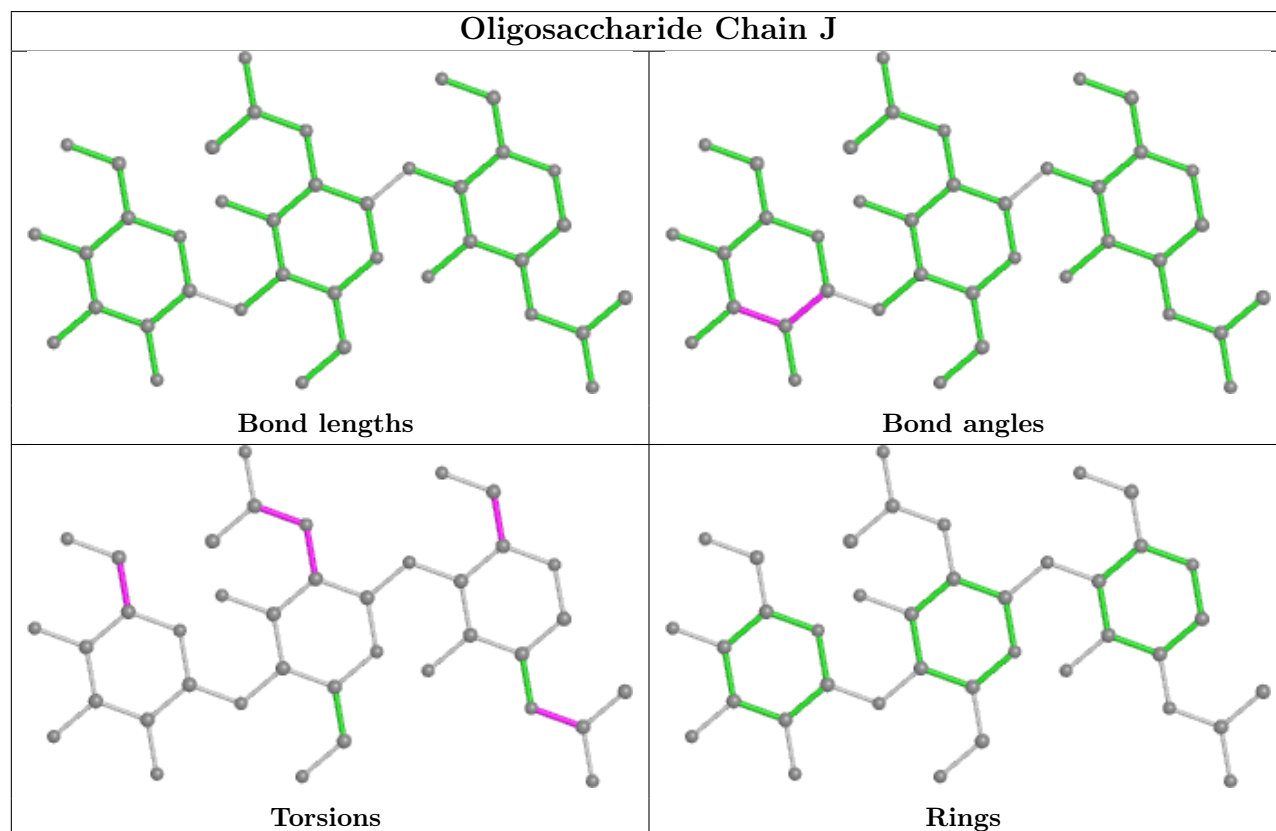
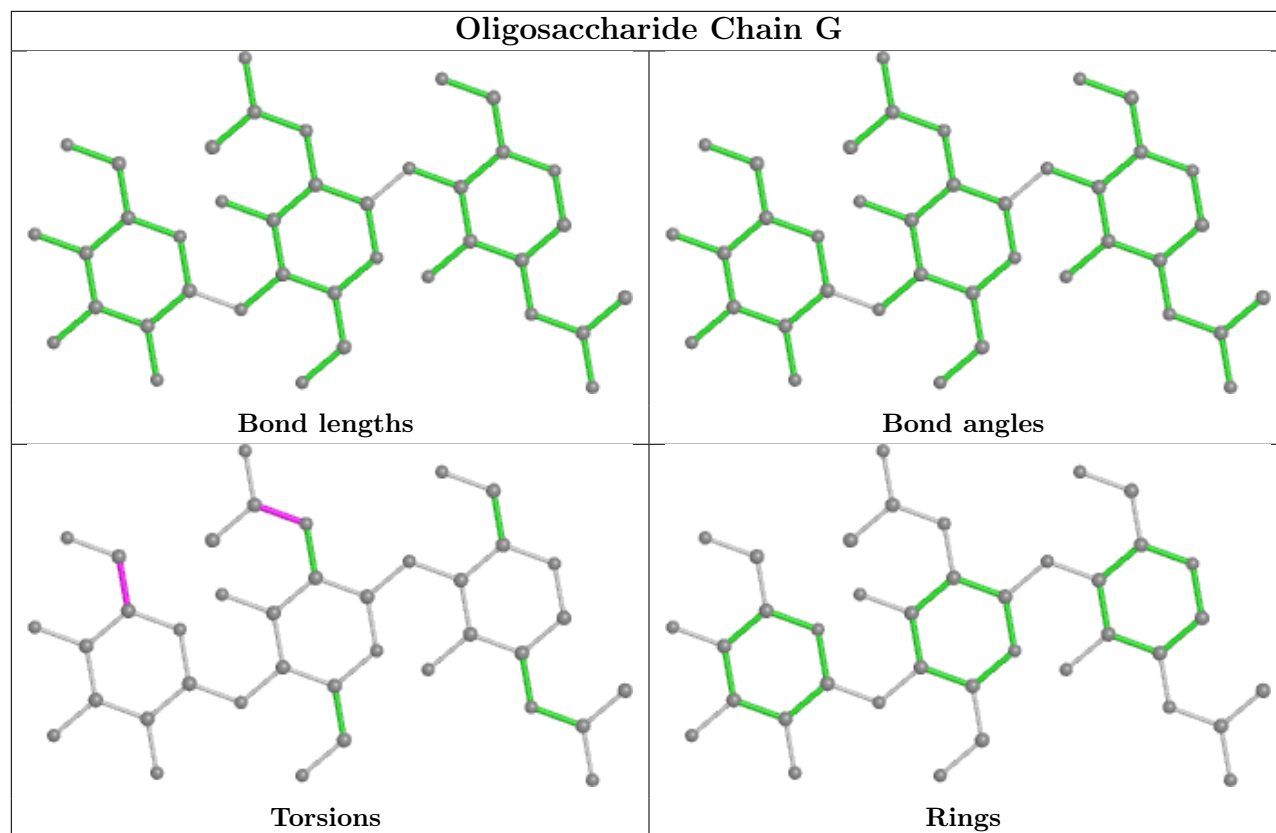












5.6 Ligand geometry

27 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
6	PHI	D	807	7	11,12,13	0.91	0	12,15,17	0.87	0
4	NAG	B	767(A)	1	14,14,15	0.54	0	17,19,21	0.73	1 (5%)
5	SO4	A	900	-	4,4,4	0.42	0	6,6,6	0.67	0
4	NAG	D	767(A)	1	14,14,15	0.59	0	17,19,21	0.68	0
4	NAG	C	768(A)	1	14,14,15	0.59	0	17,19,21	0.71	0
6	PHI	B	803	7	11,12,13	0.50	0	12,15,17	0.66	1 (8%)
4	NAG	C	769(A)	1	14,14,15	0.45	0	17,19,21	0.74	1 (5%)
4	NAG	C	771(A)	1	14,14,15	0.63	0	17,19,21	1.11	3 (17%)
4	NAG	A	772(A)	1	14,14,15	0.61	0	17,19,21	0.73	0
5	SO4	D	903	-	4,4,4	0.40	0	6,6,6	0.68	0
4	NAG	A	768(A)	1	14,14,15	0.60	0	17,19,21	0.79	1 (5%)
6	PHI	A	801	7	11,12,13	0.77	0	12,15,17	0.50	0
7	P2Y	C	806	1,6	5,7,7	1.45	1 (20%)	6,8,8	0.79	0
4	NAG	A	767(A)	1	14,14,15	0.57	0	17,19,21	0.65	0
5	SO4	B	901	-	4,4,4	0.39	0	6,6,6	0.67	0
4	NAG	A	771(A)	1	14,14,15	0.60	0	17,19,21	0.66	0
4	NAG	D	773(A)	1	14,14,15	0.64	0	17,19,21	0.76	0
4	NAG	C	767(A)	1	14,14,15	0.54	0	17,19,21	0.87	0
7	P2Y	A	802	1,6	5,7,7	1.45	1 (20%)	6,8,8	0.99	0
4	NAG	B	772(A)	1	14,14,15	0.63	0	17,19,21	0.77	0
5	SO4	C	902	-	4,4,4	0.34	0	6,6,6	0.64	0
7	P2Y	D	808	1,6	5,7,7	1.65	1 (20%)	6,8,8	0.87	0
7	P2Y	B	804	1,6	5,7,7	1.74	1 (20%)	6,8,8	0.71	0
4	NAG	B	773(A)	1	14,14,15	0.40	0	17,19,21	0.98	1 (5%)
4	NAG	C	770(A)	1	14,14,15	0.64	0	17,19,21	0.61	0
4	NAG	B	771(A)	1	14,14,15	0.48	0	17,19,21	0.71	0
6	PHI	C	805	7	11,12,13	0.77	0	12,15,17	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PHI	D	807	7	-	0/5/6/8	0/1/1/1
4	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	D	767(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	768(A)	1	-	3/6/23/26	0/1/1/1
6	PHI	B	803	7	-	0/5/6/8	0/1/1/1
4	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	C	771(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	772(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	768(A)	1	-	4/6/23/26	0/1/1/1
6	PHI	A	801	7	-	0/5/6/8	0/1/1/1
7	P2Y	C	806	1,6	-	2/2/9/9	0/1/1/1
4	NAG	A	767(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	A	771(A)	1	-	3/6/23/26	0/1/1/1
4	NAG	D	773(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	C	767(A)	1	-	2/6/23/26	0/1/1/1
7	P2Y	A	802	1,6	-	2/2/9/9	0/1/1/1
4	NAG	B	772(A)	1	-	4/6/23/26	0/1/1/1
7	P2Y	D	808	1,6	-	2/2/9/9	0/1/1/1
7	P2Y	B	804	1,6	-	0/2/9/9	0/1/1/1
4	NAG	B	773(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	770(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
6	PHI	C	805	7	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	804	P2Y	C-NA	-3.73	1.32	1.48
7	D	808	P2Y	C-NA	-3.44	1.34	1.48
7	A	802	P2Y	C-NA	-3.13	1.35	1.48
7	C	806	P2Y	C-NA	-2.93	1.36	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	773(A)	NAG	C2-N2-C7	-2.94	118.71	122.90
4	C	769(A)	NAG	C2-N2-C7	-2.17	119.81	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	768(A)	NAG	C2-N2-C7	-2.08	119.94	122.90
4	C	771(A)	NAG	C4-C3-C2	-2.07	107.99	111.02
6	B	803	PHI	CB-CA-C	-2.03	107.67	111.47
4	C	771(A)	NAG	C8-C7-N2	2.02	119.53	116.10
4	C	771(A)	NAG	C3-C4-C5	-2.01	106.64	110.24
4	B	767(A)	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	768(A)	NAG	C8-C7-N2-C2
4	A	768(A)	NAG	O7-C7-N2-C2
4	A	771(A)	NAG	C8-C7-N2-C2
4	A	771(A)	NAG	O7-C7-N2-C2
4	B	772(A)	NAG	C8-C7-N2-C2
4	B	772(A)	NAG	O7-C7-N2-C2
4	C	768(A)	NAG	C8-C7-N2-C2
4	C	768(A)	NAG	O7-C7-N2-C2
4	C	770(A)	NAG	O7-C7-N2-C2
4	D	767(A)	NAG	C8-C7-N2-C2
4	D	767(A)	NAG	O7-C7-N2-C2
4	D	773(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O7-C7-N2-C2
7	A	802	P2Y	NA-C-CA-N
7	C	806	P2Y	NA-C-CA-N
7	C	806	P2Y	NA-C-CA-CB
7	D	808	P2Y	NA-C-CA-N
7	D	808	P2Y	NA-C-CA-CB
4	C	770(A)	NAG	C8-C7-N2-C2
4	B	773(A)	NAG	O5-C5-C6-O6
4	C	770(A)	NAG	O5-C5-C6-O6
4	D	773(A)	NAG	O5-C5-C6-O6
4	A	772(A)	NAG	C4-C5-C6-O6
4	A	767(A)	NAG	C4-C5-C6-O6
4	A	772(A)	NAG	O5-C5-C6-O6
4	D	773(A)	NAG	C4-C5-C6-O6
4	C	771(A)	NAG	C8-C7-N2-C2
4	C	771(A)	NAG	O7-C7-N2-C2
4	B	773(A)	NAG	C4-C5-C6-O6
4	C	770(A)	NAG	C4-C5-C6-O6
4	B	772(A)	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	767(A)	NAG	O5-C5-C6-O6
4	A	768(A)	NAG	O5-C5-C6-O6
4	C	767(A)	NAG	C4-C5-C6-O6
4	B	772(A)	NAG	C4-C5-C6-O6
4	A	771(A)	NAG	O5-C5-C6-O6
4	C	767(A)	NAG	O5-C5-C6-O6
4	A	768(A)	NAG	C4-C5-C6-O6
4	A	767(A)	NAG	C8-C7-N2-C2
4	C	768(A)	NAG	C4-C5-C6-O6
7	A	802	P2Y	NA-C-CA-CB
4	A	767(A)	NAG	O7-C7-N2-C2

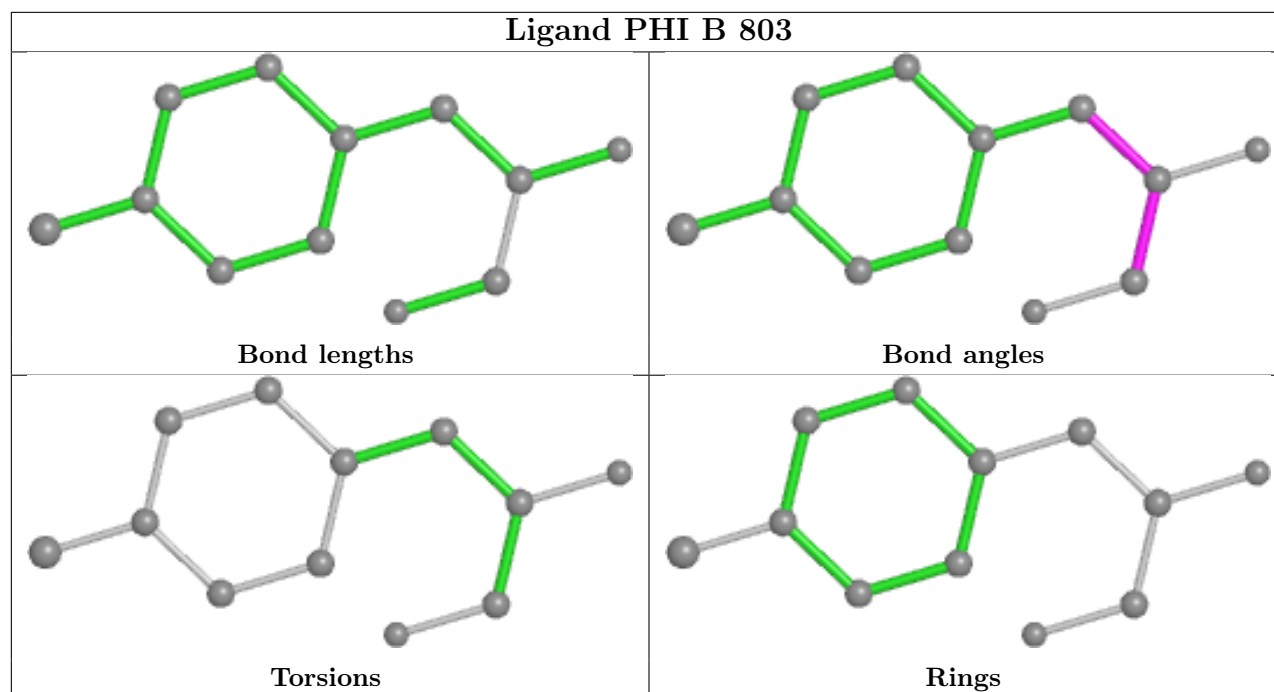
There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	807	PHI	7	0
4	B	767(A)	NAG	2	0
4	D	767(A)	NAG	1	0
6	B	803	PHI	4	0
6	A	801	PHI	3	0
7	C	806	P2Y	1	0
4	A	767(A)	NAG	1	0
4	C	767(A)	NAG	2	0
7	A	802	P2Y	2	0
4	B	772(A)	NAG	2	0
7	D	808	P2Y	2	0
7	B	804	P2Y	3	0
4	B	773(A)	NAG	1	0
6	C	805	PHI	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



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	724/728 (99%)	-0.39	13 (1%) 68 63	7, 27, 58, 95	11 (1%)
1	B	728/728 (100%)	-0.52	8 (1%) 80 78	6, 25, 51, 67	12 (1%)
1	C	726/728 (99%)	-0.42	11 (1%) 73 70	6, 25, 54, 102	12 (1%)
1	D	728/728 (100%)	-0.37	6 (0%) 86 85	8, 31, 57, 80	10 (1%)
All	All	2906/2912 (99%)	-0.42	38 (1%) 77 74	6, 27, 55, 102	45 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	SER	6.8
1	D	83	TYR	5.2
1	C	39	SER	5.0
1	C	97	GLU	4.3
1	A	39	SER	4.0
1	C	95	PHE	4.0
1	A	766	PRO	3.9
1	C	98	LEU	3.7
1	D	82	GLU	3.7
1	C	766	PRO	3.4
1	B	54	ARG	3.3
1	D	537	SER	3.2
1	A	505	GLN	3.1
1	C	101	SER	3.1
1	C	102	THR	3.0
1	C	40	ARG	2.8
1	A	96	ASP	2.7
1	A	102	THR	2.6
1	D	438	ASP	2.5
1	A	103	ASN	2.5
1	A	94	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	ARG	2.4
1	A	85	ASN	2.4
1	D	412	SER	2.3
1	A	83	TYR	2.3
1	C	120	TYR	2.3
1	B	537	SER	2.3
1	B	83	TYR	2.3
1	B	766	PRO	2.2
1	B	331	ASP	2.2
1	B	333	SER	2.1
1	C	520	HIS	2.1
1	B	99	GLY	2.1
1	A	86	SER	2.1
1	A	745	ASN	2.1
1	B	676	PRO	2.1
1	C	487	SER	2.1
1	D	100	TYR	2.1

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

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

6.3 Carbohydrates ⓘ

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

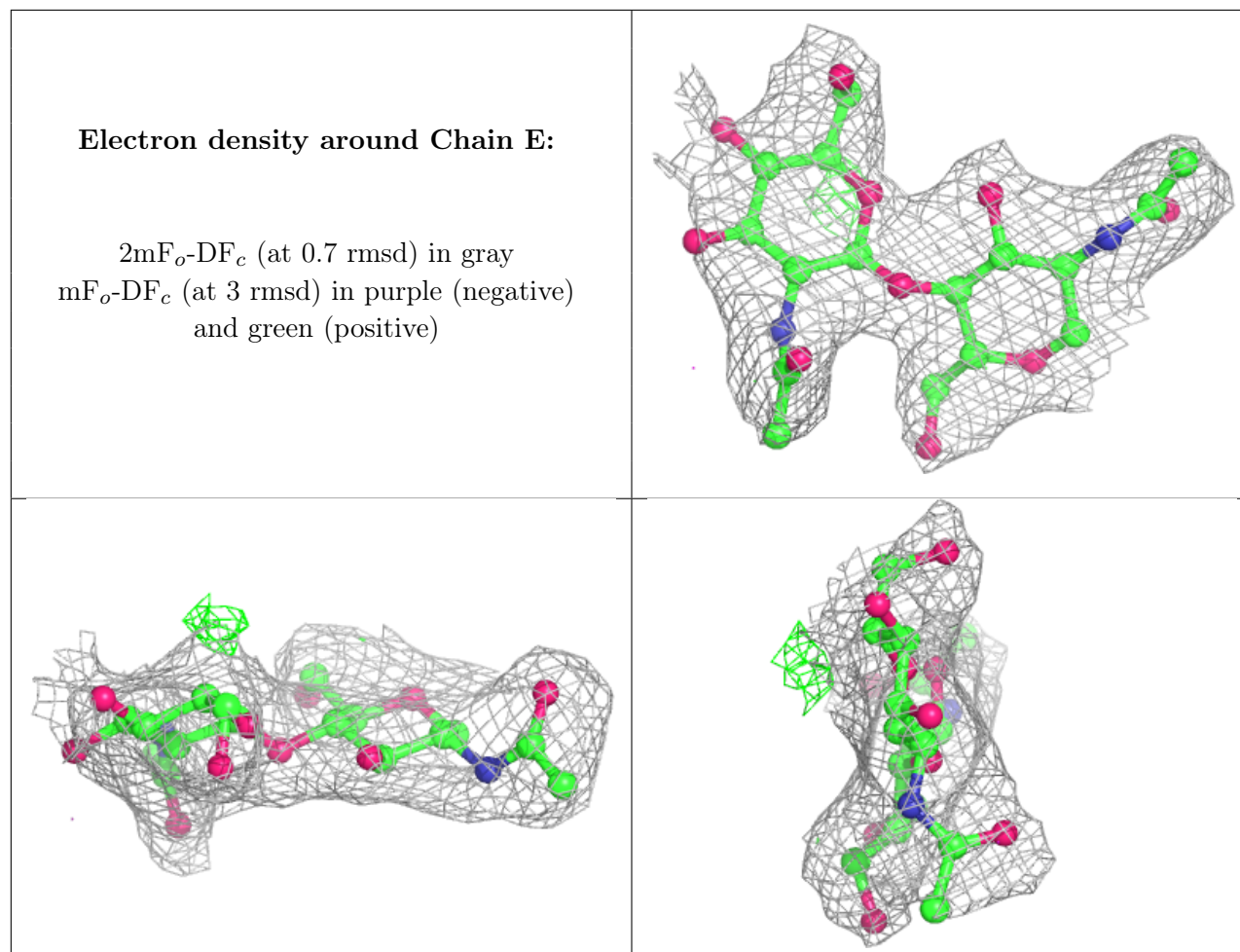
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	J	3	11/12	0.76	0.37	53,56,57,58	0
2	NAG	K	2	14/15	0.79	0.36	47,55,59,61	0
2	NAG	L	2	14/15	0.87	0.39	60,61,62,62	0
3	NAG	J	2	14/15	0.87	0.33	58,60,66,67	0
2	NAG	L	1	14/15	0.87	0.18	50,54,55,59	0
2	NAG	H	2	14/15	0.88	0.39	46,52,58,60	0
2	NAG	E	2	14/15	0.88	0.28	48,52,54,55	0
2	NAG	F	2	14/15	0.89	0.34	47,51,54,55	0
3	BMA	G	3	11/12	0.89	0.25	53,54,56,56	0
2	NAG	M	2	14/15	0.92	0.37	50,52,54,54	0
2	NAG	M	1	14/15	0.92	0.18	33,36,41,46	0

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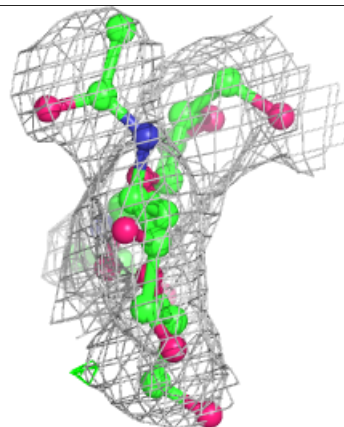
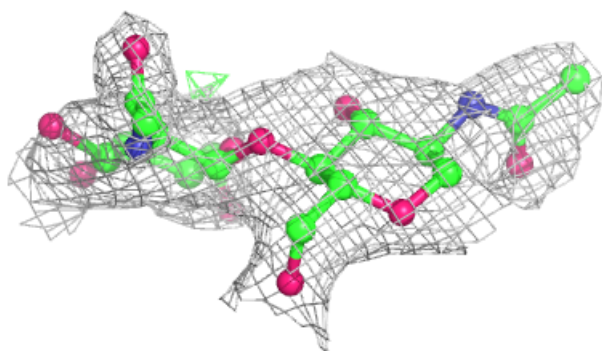
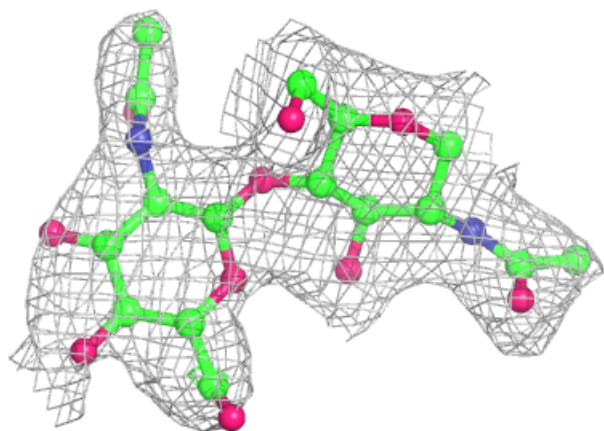
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	I	2	14/15	0.93	0.31	28,33,37,40	0
3	NAG	G	1	14/15	0.93	0.16	45,47,49,49	0
3	NAG	G	2	14/15	0.93	0.20	46,47,49,51	0
2	NAG	E	1	14/15	0.94	0.12	26,28,34,41	0
3	NAG	J	1	14/15	0.94	0.12	54,57,58,59	0
2	NAG	K	1	14/15	0.94	0.16	27,34,40,46	0
2	NAG	F	1	14/15	0.94	0.15	30,32,39,41	0
2	NAG	H	1	14/15	0.95	0.21	26,34,38,44	0
2	NAG	I	1	14/15	0.96	0.20	21,28,34,36	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.



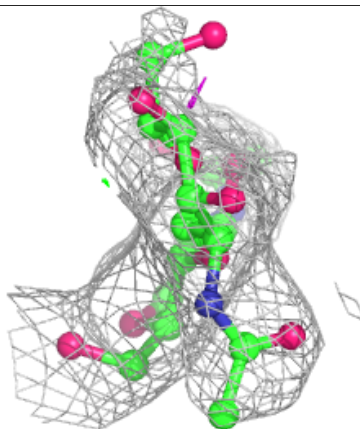
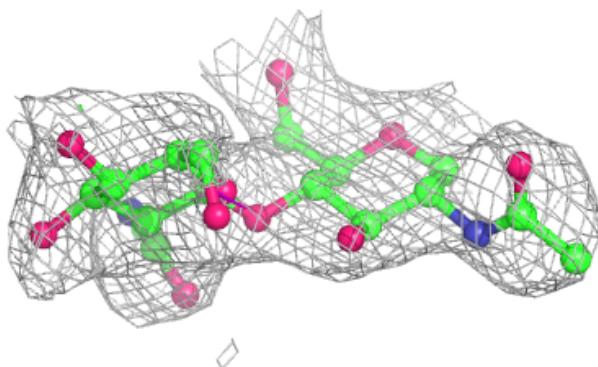
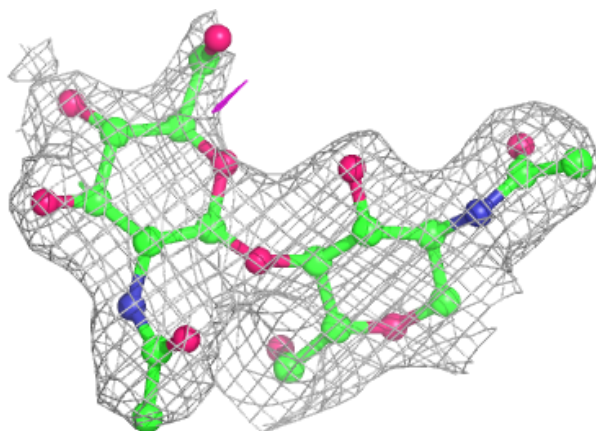
Electron density around Chain F:

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



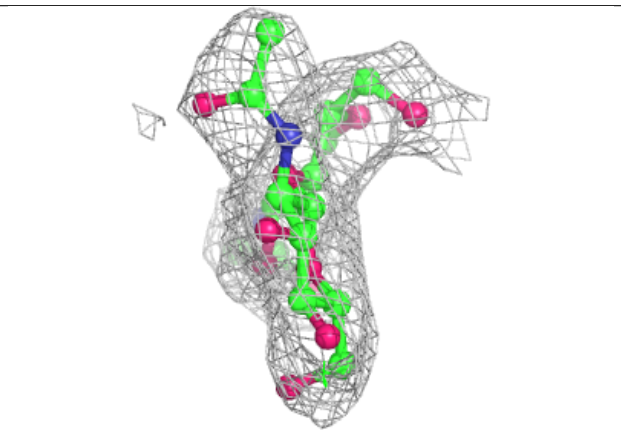
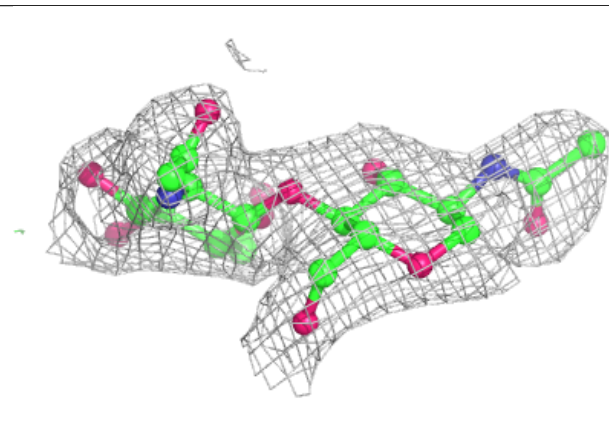
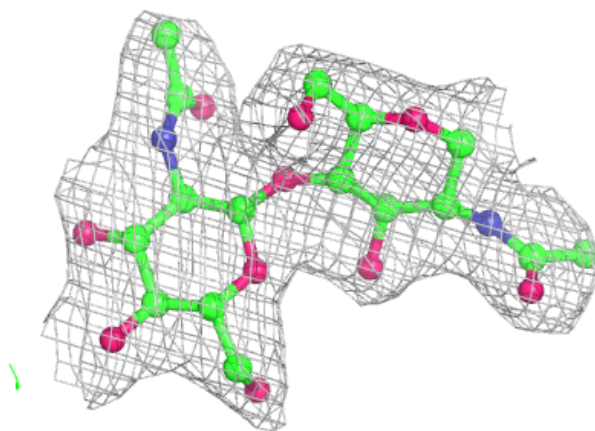
Electron density around Chain H:

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



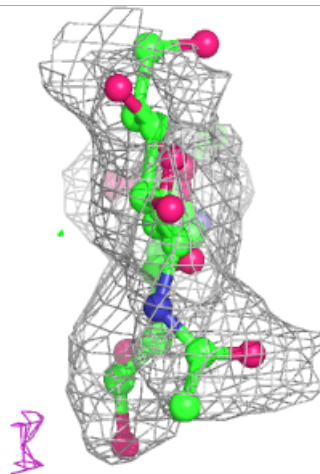
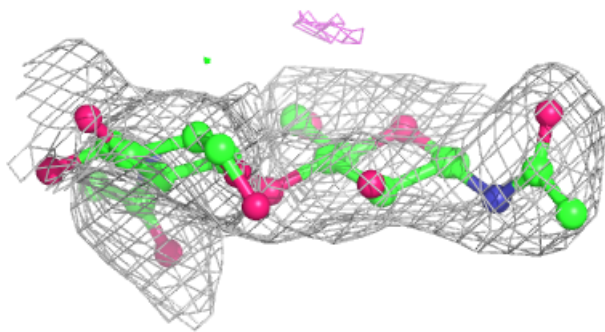
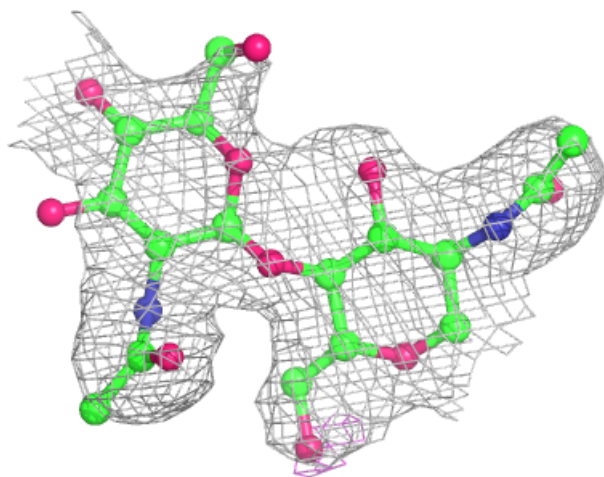
Electron density around Chain I:

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



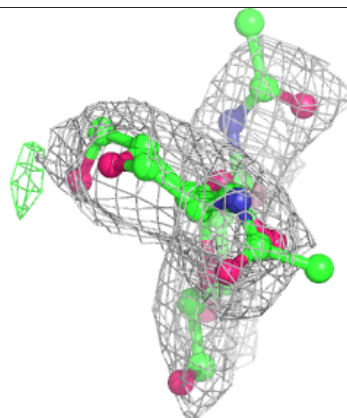
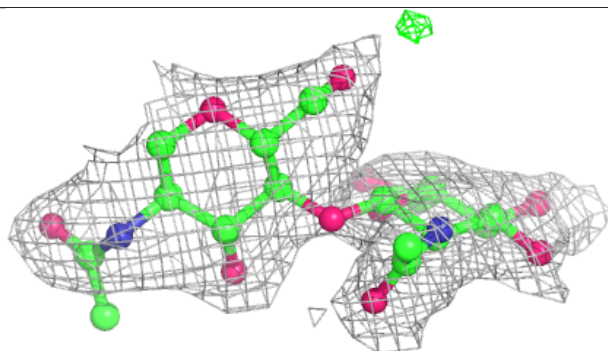
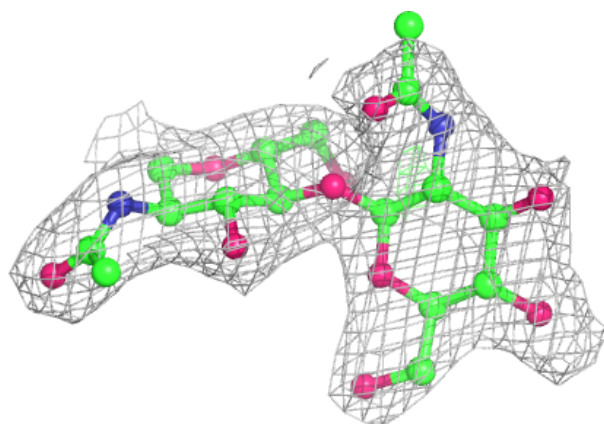
Electron density around Chain K:

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



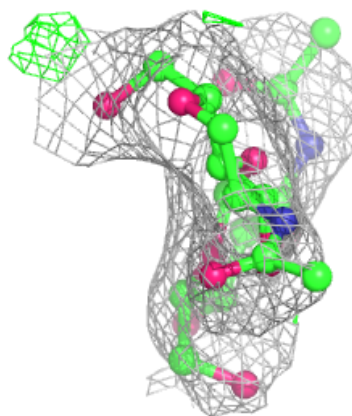
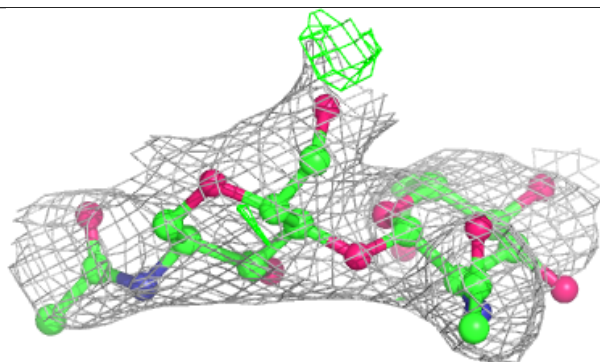
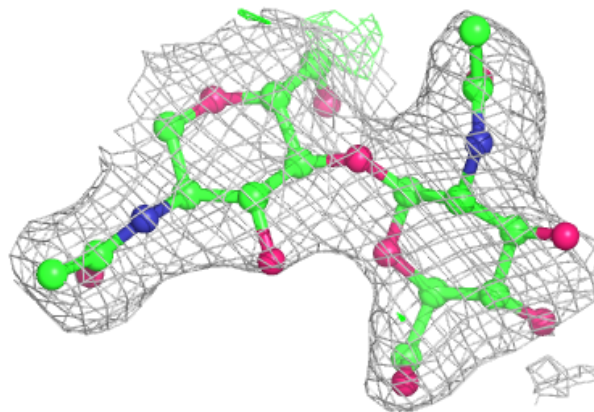
Electron density around Chain L:

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

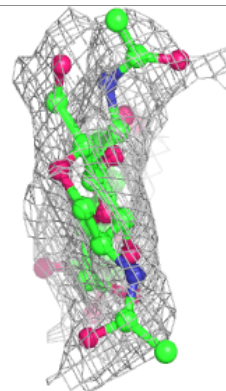
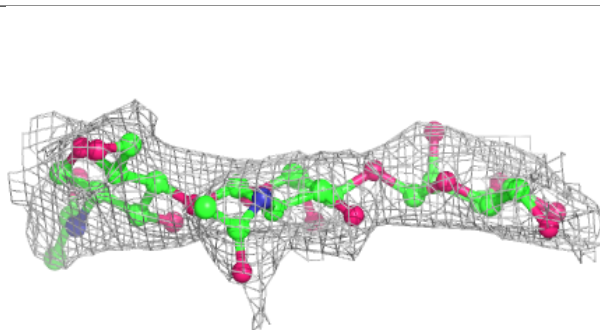
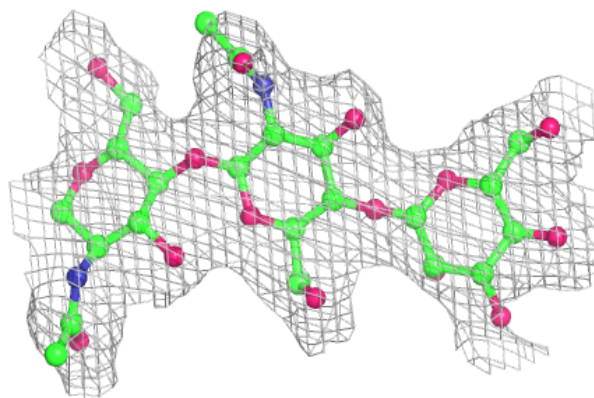


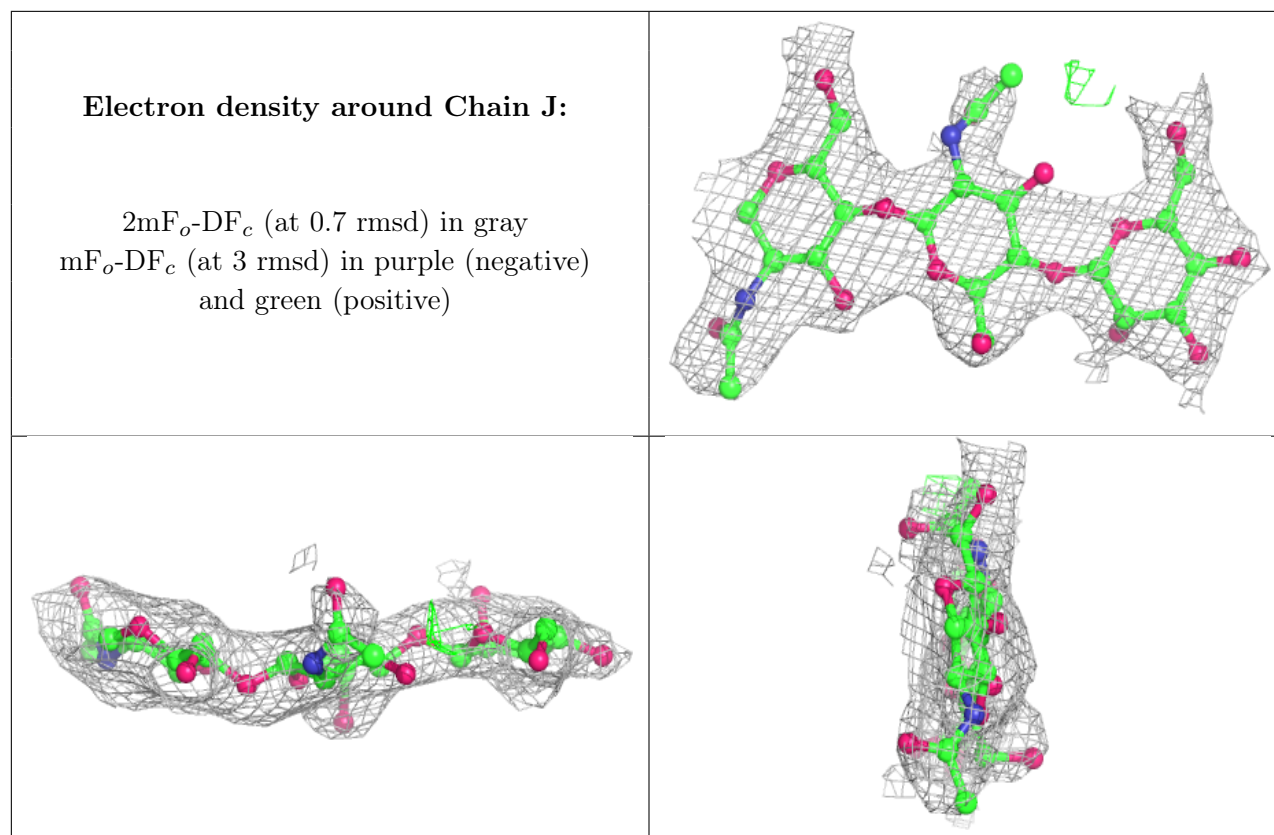
Electron density around Chain M:

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

**Electron density around Chain 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 ⓘ

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
4	NAG	D	767(A)	14/15	0.63	0.47	79,82,83,83	0
4	NAG	C	768(A)	14/15	0.70	0.34	78,84,87,87	0
4	NAG	A	767(A)	14/15	0.79	0.40	82,82,83,83	0
6	PHI	A	801	12/13	0.80	0.27	46,65,80,97	0
4	NAG	D	773(A)	14/15	0.82	0.21	46,49,54,55	0
4	NAG	B	767(A)	14/15	0.83	0.34	64,66,70,71	0
4	NAG	C	770(A)	14/15	0.85	0.25	35,38,42,43	0
4	NAG	B	772(A)	14/15	0.86	0.18	43,46,53,54	0
6	PHI	D	807	12/13	0.86	0.27	50,67,81,99	0
4	NAG	A	768(A)	14/15	0.87	0.21	65,66,68,68	0
4	NAG	C	767(A)	14/15	0.87	0.18	55,56,58,58	0
4	NAG	C	771(A)	14/15	0.88	0.18	35,38,43,43	0
6	PHI	C	805	12/13	0.90	0.22	44,59,72,89	0
6	PHI	B	803	12/13	0.90	0.20	42,59,72,88	0

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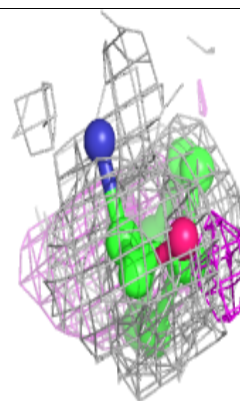
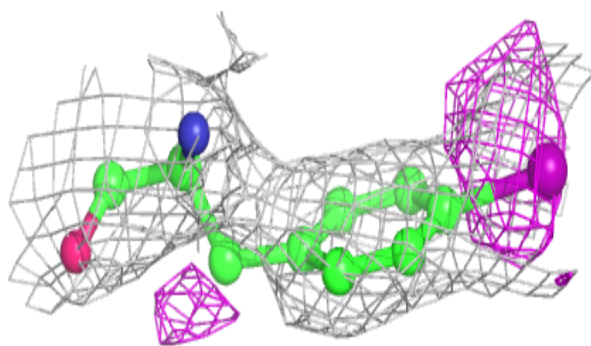
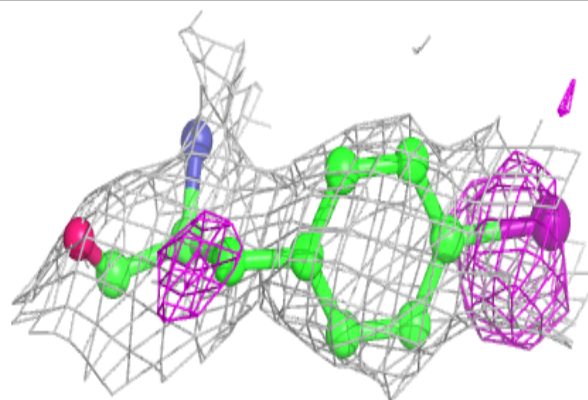
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	771(A)	14/15	0.92	0.19	38,39,40,42	3
4	NAG	A	772(A)	14/15	0.93	0.16	35,38,40,40	0
7	P2Y	B	804	7/7	0.93	0.18	36,37,37,38	0
4	NAG	C	769(A)	14/15	0.94	0.17	28,31,32,35	0
4	NAG	B	773(A)	14/15	0.94	0.16	37,40,44,45	0
7	P2Y	D	808	7/7	0.94	0.21	42,43,45,47	0
7	P2Y	C	806	7/7	0.95	0.18	33,35,38,40	0
4	NAG	B	771(A)	14/15	0.95	0.19	19,21,23,26	0
7	P2Y	A	802	7/7	0.97	0.18	35,39,41,42	0
5	SO4	A	900	5/5	0.97	0.12	50,50,51,52	0
5	SO4	C	902	5/5	0.98	0.13	35,37,37,39	0
5	SO4	D	903	5/5	0.98	0.11	47,48,48,49	0
5	SO4	B	901	5/5	0.99	0.11	42,43,43,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PHI B 803:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.