Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 03:22 AM EDT

PDB ID	:	1Z8L
Title	:	Crystal structure of prostate-specific membrane antigen, a tumor marker and peptidase
Authors	:	Davis, M.I.; Bennett, M.J.; Thomas, L.M.; Bjorkman, P.J.
Deposited on	:	2005-03-30
Resolution	:	3.50 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:

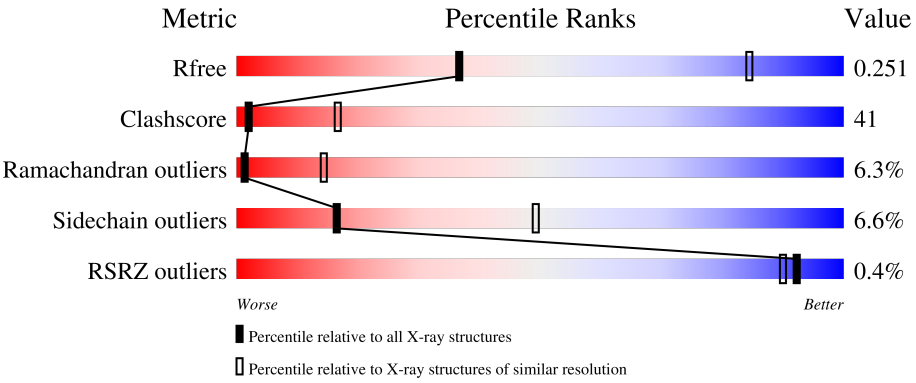
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	695	39% 52% 9%
1	B	695	40% 51% 9%
1	C	695	39% 52% 9%
1	D	695	39% 51% 9%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	100%
2	J	2	50% 50%
2	L	2	100%
2	O	2	50% 50%
2	Q	2	100%
2	T	2	50% 50%
2	V	2	100%
3	F	2	50% 50%
3	H	2	50% 50%
3	I	2	50% 50%
3	K	2	50% 50%
3	M	2	100%
3	N	2	50% 50%
3	P	2	50% 50%
3	R	2	50% 50%
3	S	2	100%
3	U	2	50% 50%
3	W	2	50% 50%
3	X	2	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
2	NAG	G	1	X	-	-	-
2	NAG	L	1	X	-	-	X
2	NAG	Q	1	X	-	-	X
2	NAG	V	1	X	-	-	X
3	NAG	H	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	4760	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22836 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 Glutamate carboxypeptidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	B	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	C	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	D	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			

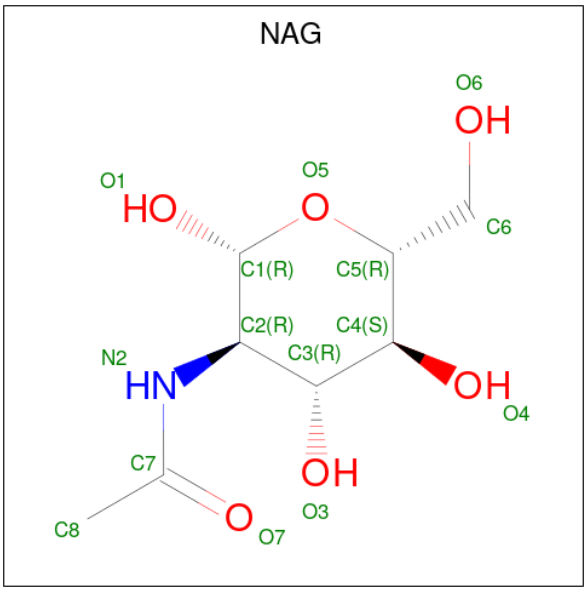
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	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	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	C	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0

- Molecule 6 is water.

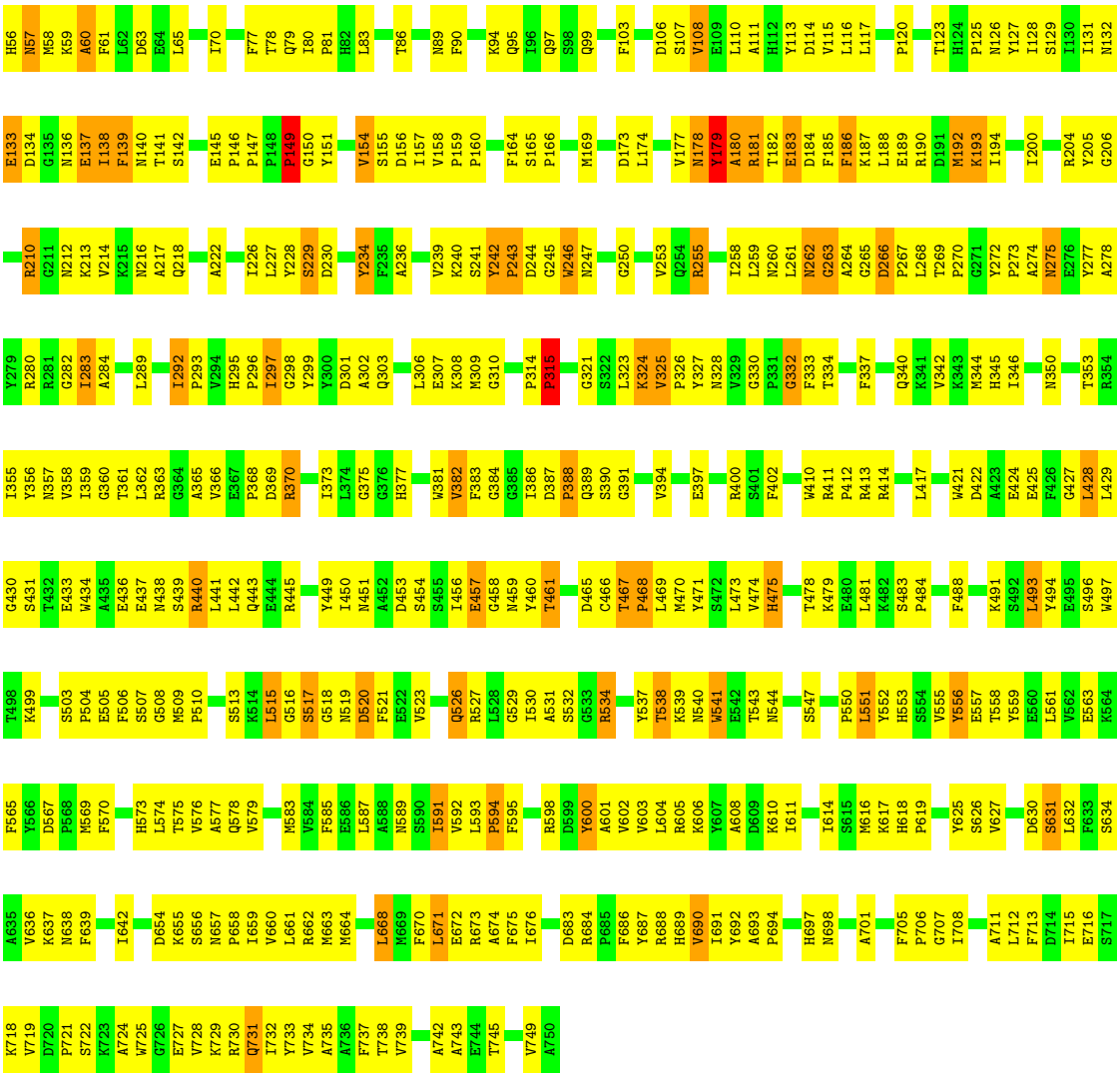
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total O 3 3	0	0
6	B	3	Total O 3 3	0	0
6	C	4	Total O 4 4	0	0
6	D	2	Total O 2 2	0	0

3 Residue-property plots (i)

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.

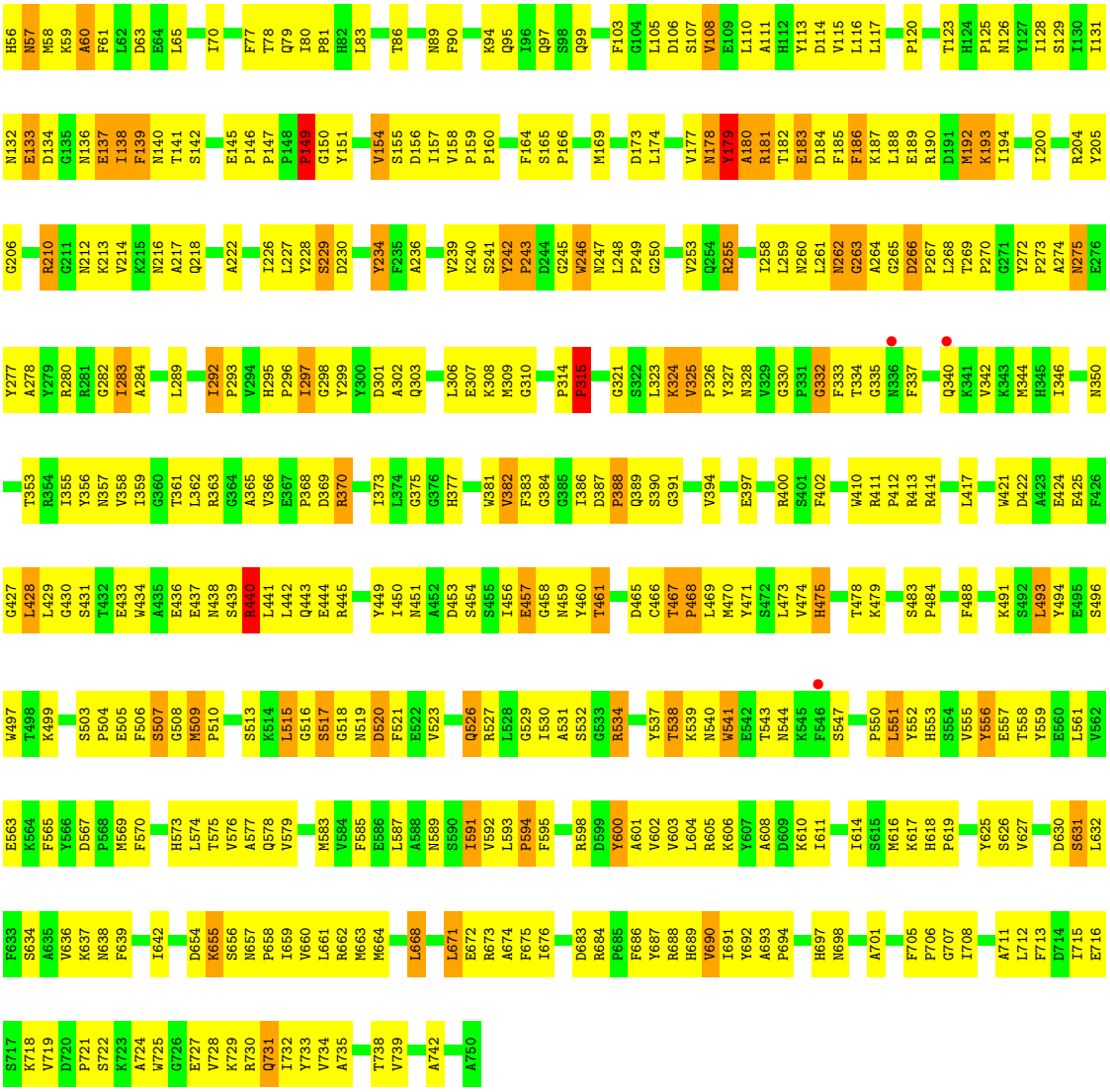
• Molecule 1: Glutamate carboxypeptidase II

Chain A:



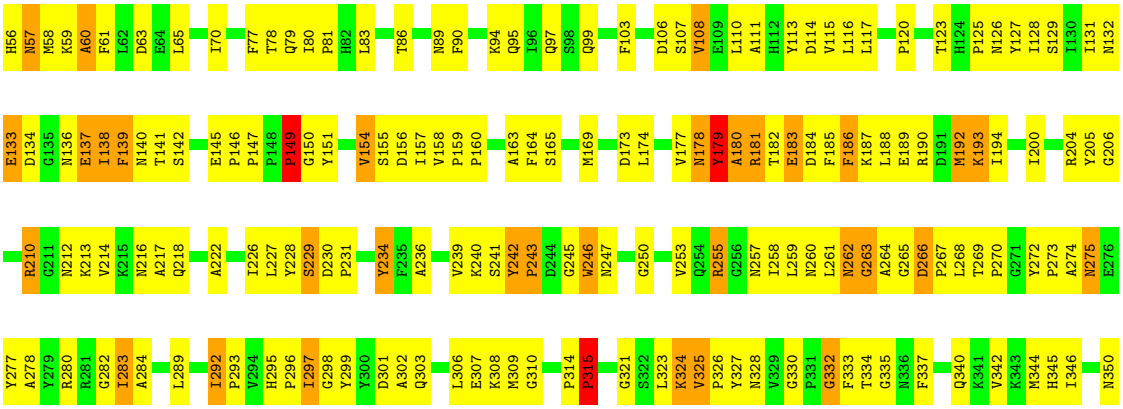
• Molecule 1: Glutamate carboxypeptidase II

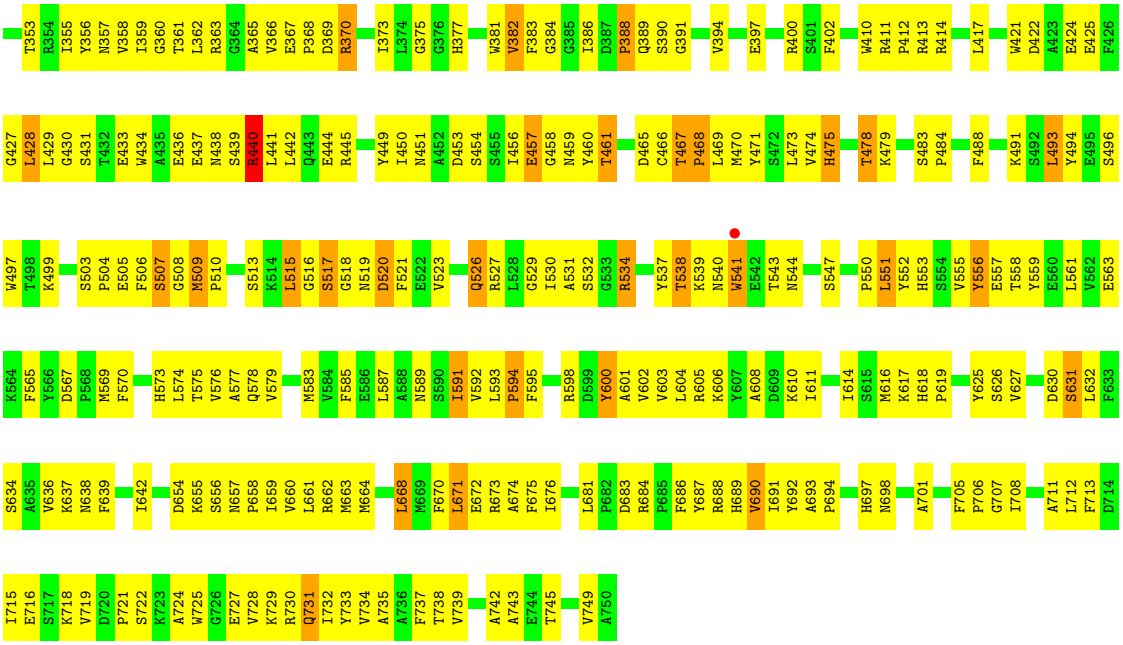
Chain B:



• Molecule 1: Glutamate carboxypeptidase II

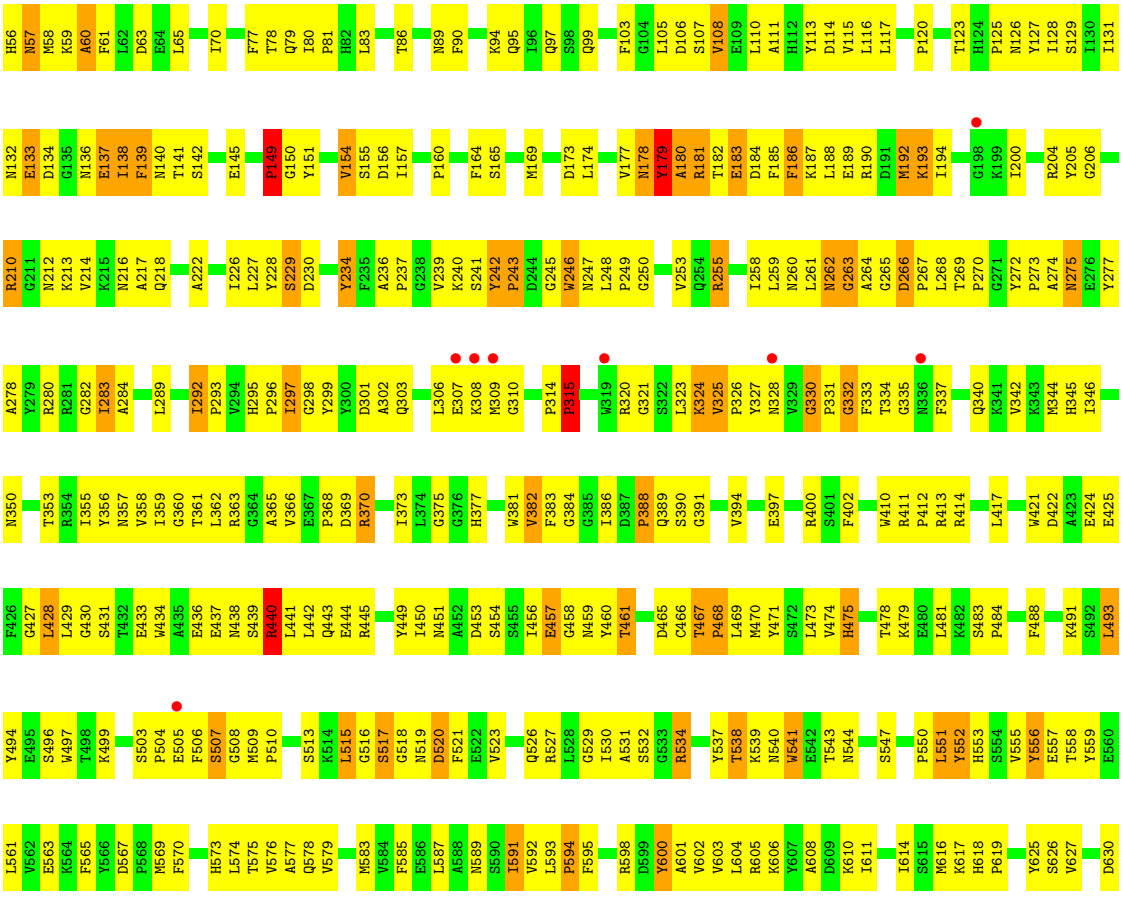
Chain C:

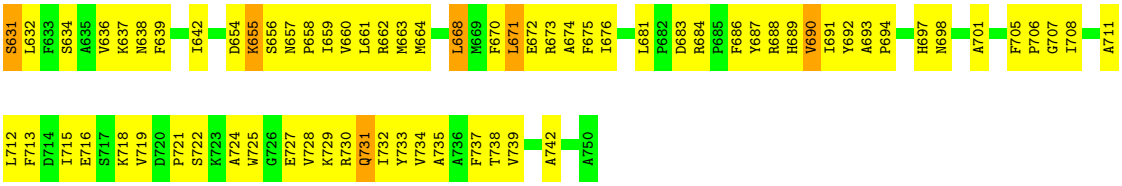




• Molecule 1: Glutamate carboxypeptidase II

Chain D:



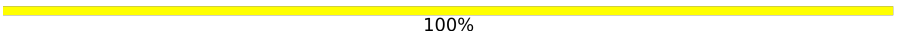


• Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain G:

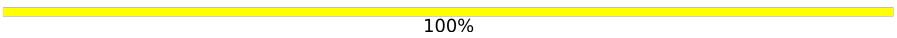


• Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain L:

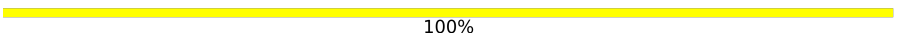


• Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain Q:

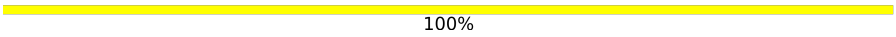


• Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

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

Chain V:



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

Chain F:

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

Chain H:

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

Chain I:

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

Chain K:

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

Chain M:

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

Chain N:

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

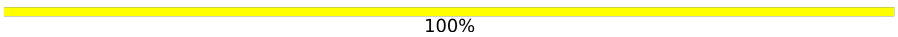
Chain P:

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

Chain R:

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

Chain S:



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

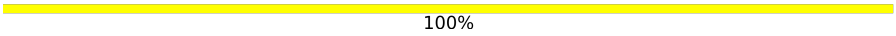
Chain U:

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

Chain W:

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

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.86Å 157.76Å 133.84Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 98.7 (30.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.284 0.258 , 0.251	Depositor DCC
R_{free} test set	3798 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	77.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	22836	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN, NDG

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	0/5693	0.69	0/7720
1	B	0.41	0/5693	0.69	0/7720
1	C	0.42	0/5693	0.69	0/7720
1	D	0.41	0/5693	0.69	0/7720
All	All	0.42	0/22772	0.69	0/30880

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5536	0	5373	458	11
1	B	5536	0	5373	467	9
1	C	5536	0	5373	468	14
1	D	5536	0	5373	468	16
2	E	28	0	24	2	0
2	G	28	0	24	1	1
2	J	28	0	24	2	0
2	L	28	0	24	1	0
2	O	28	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	28	0	24	1	0
2	T	28	0	24	1	0
2	V	28	0	24	1	0
3	F	28	0	25	1	0
3	H	28	0	25	5	0
3	I	28	0	25	0	0
3	K	28	0	25	1	0
3	M	28	0	25	5	1
3	N	28	0	25	0	0
3	P	28	0	25	1	0
3	R	28	0	25	5	0
3	S	28	0	25	0	0
3	U	28	0	25	1	0
3	W	28	0	25	5	0
3	X	28	0	25	0	0
4	A	28	0	26	5	0
4	B	28	0	26	6	0
4	C	28	0	26	5	0
4	D	28	0	26	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
All	All	22836	0	22088	1840	26

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 41.

All (1840) 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:140:ASN:HB2	4:A:1760:NAG:H62	1.33	1.10
1:C:140:ASN:HB2	4:C:3760:NAG:H62	1.33	1.10
1:D:128:ILE:HD13	1:D:226:ILE:HD12	1.33	1.08
1:C:128:ILE:HD13	1:C:226:ILE:HD12	1.33	1.07
1:A:128:ILE:HD13	1:A:226:ILE:HD12	1.33	1.07
1:B:128:ILE:HD13	1:B:226:ILE:HD12	1.33	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ASN:HB2	4:D:4760:NAG:H62	1.33	1.07
1:B:655:LYS:O	1:D:656:SER:HA	1.54	1.06
1:A:181:ARG:HB2	1:A:186:PHE:HD1	1.21	1.05
1:B:140:ASN:HB2	4:B:2760:NAG:H62	1.33	1.05
1:B:181:ARG:HB2	1:B:186:PHE:HD1	1.21	1.04
1:B:307:GLU:HA	1:B:325:VAL:HG21	1.40	1.03
1:D:307:GLU:HA	1:D:325:VAL:HG21	1.40	1.03
1:A:307:GLU:HA	1:A:325:VAL:HG21	1.40	1.02
1:C:307:GLU:HA	1:C:325:VAL:HG21	1.40	1.01
1:D:181:ARG:HB2	1:D:186:PHE:HD1	1.21	1.01
1:C:181:ARG:HB2	1:C:186:PHE:HD1	1.21	1.00
1:A:325:VAL:HG22	1:A:326:PRO:HD2	1.45	0.99
1:B:382:VAL:HG23	1:B:383:PHE:H	1.28	0.98
1:C:325:VAL:HG22	1:C:326:PRO:HD2	1.45	0.97
1:B:325:VAL:HG22	1:B:326:PRO:HD2	1.45	0.97
1:D:325:VAL:HG22	1:D:326:PRO:HD2	1.45	0.97
1:A:382:VAL:HG23	1:A:383:PHE:H	1.28	0.96
1:D:181:ARG:HB2	1:D:186:PHE:CD1	2.00	0.96
1:A:181:ARG:HB2	1:A:186:PHE:CD1	2.00	0.96
1:C:382:VAL:HG23	1:C:383:PHE:H	1.28	0.96
1:D:382:VAL:HG23	1:D:383:PHE:H	1.28	0.96
1:C:181:ARG:HB2	1:C:186:PHE:CD1	2.00	0.96
1:B:181:ARG:HB2	1:B:186:PHE:CD1	2.00	0.95
1:A:663:MET:HG2	1:B:369:ASP:CG	1.86	0.95
1:D:181:ARG:C	1:D:183:GLU:H	1.71	0.92
1:D:240:LYS:HB2	1:D:245:GLY:HA2	1.53	0.90
1:A:181:ARG:HB3	1:A:216:ASN:HB3	1.53	0.90
1:A:240:LYS:HB2	1:A:245:GLY:HA2	1.53	0.90
1:B:240:LYS:HB2	1:B:245:GLY:HA2	1.53	0.90
1:B:115:VAL:HG11	1:B:429:LEU:HD13	1.55	0.89
1:B:116:LEU:HD11	1:B:350:ASN:HB3	1.54	0.89
1:A:116:LEU:HD11	1:A:350:ASN:HB3	1.54	0.89
1:B:654:ASP:HB2	1:D:591:ILE:HD11	1.53	0.89
1:D:181:ARG:HB3	1:D:216:ASN:HB3	1.53	0.89
1:A:181:ARG:C	1:A:183:GLU:H	1.71	0.88
1:C:181:ARG:C	1:C:183:GLU:H	1.71	0.88
1:D:116:LEU:HD11	1:D:350:ASN:HB3	1.54	0.88
1:C:181:ARG:HB3	1:C:216:ASN:HB3	1.52	0.88
1:D:115:VAL:HG11	1:D:429:LEU:HD13	1.55	0.88
1:B:181:ARG:C	1:B:183:GLU:H	1.71	0.88
1:C:240:LYS:HB2	1:C:245:GLY:HA2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:HB3	1:A:332:GLY:H	1.39	0.88
1:B:173:ASP:HB3	1:B:332:GLY:H	1.39	0.87
1:B:181:ARG:HB3	1:B:216:ASN:HB3	1.53	0.87
1:D:173:ASP:HB3	1:D:332:GLY:H	1.39	0.87
1:A:81:PRO:HA	1:A:382:VAL:O	1.75	0.87
1:B:246:TRP:HZ2	3:M:1:NAG:H82	1.39	0.86
1:C:115:VAL:HG11	1:C:429:LEU:HD13	1.55	0.86
1:D:246:TRP:HZ2	3:W:1:NAG:H82	1.39	0.86
1:D:81:PRO:HA	1:D:382:VAL:O	1.75	0.86
1:C:116:LEU:HD11	1:C:350:ASN:HB3	1.54	0.86
1:A:246:TRP:HZ2	3:H:1:NAG:H82	1.39	0.86
1:C:81:PRO:HA	1:C:382:VAL:O	1.75	0.85
1:B:81:PRO:HA	1:B:382:VAL:O	1.75	0.85
1:C:246:TRP:HZ2	3:R:1:NAG:H82	1.40	0.85
1:D:70:ILE:CD1	1:D:573:HIS:HB3	2.07	0.85
1:D:478:THR:HG23	1:D:494:TYR:HB2	1.58	0.85
1:B:70:ILE:CD1	1:B:573:HIS:HB3	2.07	0.85
1:A:115:VAL:HG11	1:A:429:LEU:HD13	1.55	0.85
1:A:70:ILE:CD1	1:A:573:HIS:HB3	2.07	0.85
1:A:478:THR:HG23	1:A:494:TYR:HB2	1.59	0.84
1:C:70:ILE:CD1	1:C:573:HIS:HB3	2.07	0.84
1:B:478:THR:HG23	1:B:494:TYR:HB2	1.59	0.84
1:C:173:ASP:HB3	1:C:332:GLY:H	1.39	0.84
1:C:478:THR:HG23	1:C:494:TYR:HB2	1.59	0.84
1:C:663:MET:HG2	1:D:369:ASP:CG	1.98	0.84
1:A:749:VAL:HG12	1:B:445:ARG:CZ	2.08	0.83
1:A:255:ARG:HD2	1:A:553:HIS:O	1.80	0.82
1:C:255:ARG:HD2	1:C:553:HIS:O	1.79	0.81
1:B:255:ARG:HD2	1:B:553:HIS:O	1.79	0.81
1:D:468:PRO:HA	1:D:471:TYR:CE1	2.16	0.81
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.16	0.80
1:A:382:VAL:HG23	1:A:383:PHE:N	1.96	0.80
1:D:255:ARG:HD2	1:D:553:HIS:O	1.79	0.80
1:D:690:VAL:HG21	1:D:738:THR:HG21	1.63	0.80
1:D:157:ILE:HD11	1:D:383:PHE:CZ	2.17	0.80
1:C:690:VAL:HG21	1:C:738:THR:HG21	1.63	0.80
1:B:468:PRO:HA	1:B:471:TYR:CE1	2.16	0.80
1:C:468:PRO:HA	1:C:471:TYR:CE1	2.16	0.80
1:D:241:SER:O	1:D:243:PRO:HD2	1.82	0.80
1:B:157:ILE:HD11	1:B:383:PHE:CZ	2.17	0.80
1:A:157:ILE:HD11	1:A:383:PHE:CZ	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:VAL:HG21	1:B:738:THR:HG21	1.63	0.79
1:C:241:SER:O	1:C:243:PRO:HD2	1.82	0.79
1:C:157:ILE:HD11	1:C:383:PHE:CZ	2.17	0.79
1:C:382:VAL:HG23	1:C:383:PHE:N	1.97	0.79
1:D:366:VAL:C	1:D:368:PRO:HD3	2.03	0.79
1:C:77:PHE:HB3	1:C:389:GLN:HG3	1.65	0.79
1:B:241:SER:O	1:B:243:PRO:HD2	1.82	0.79
1:C:366:VAL:C	1:C:368:PRO:HD3	2.03	0.79
1:D:719:VAL:O	1:D:721:PRO:HD3	1.84	0.78
1:A:241:SER:O	1:A:243:PRO:HD2	1.82	0.78
1:A:366:VAL:C	1:A:368:PRO:HD3	2.03	0.78
1:B:382:VAL:HG23	1:B:383:PHE:N	1.96	0.78
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.66	0.78
1:B:366:VAL:C	1:B:368:PRO:HD3	2.03	0.78
1:D:228:TYR:HB2	1:D:297:ILE:HG22	1.66	0.78
1:D:382:VAL:HG23	1:D:383:PHE:N	1.96	0.78
1:B:719:VAL:O	1:B:721:PRO:HD3	1.84	0.78
1:C:228:TYR:HB2	1:C:297:ILE:HG22	1.66	0.78
1:B:551:LEU:HD22	1:B:556:TYR:HB2	1.66	0.78
1:A:690:VAL:HG21	1:A:738:THR:HG21	1.64	0.77
1:A:719:VAL:O	1:A:721:PRO:HD3	1.84	0.77
1:C:719:VAL:O	1:C:721:PRO:HD3	1.84	0.77
1:B:174:LEU:HD11	1:B:342:VAL:HG13	1.66	0.77
1:A:228:TYR:HB2	1:A:297:ILE:HG22	1.66	0.77
1:B:228:TYR:HB2	1:B:297:ILE:HG22	1.66	0.77
1:C:174:LEU:HD11	1:C:342:VAL:HG13	1.66	0.77
1:D:77:PHE:HB3	1:D:389:GLN:HG3	1.65	0.77
1:D:551:LEU:HD22	1:D:556:TYR:HB2	1.66	0.77
1:A:77:PHE:HB3	1:A:389:GLN:HG3	1.65	0.77
1:D:174:LEU:HD11	1:D:342:VAL:HG13	1.66	0.77
1:C:240:LYS:H	1:C:240:LYS:HD2	1.50	0.77
1:C:551:LEU:HD22	1:C:556:TYR:HB2	1.66	0.77
1:B:240:LYS:H	1:B:240:LYS:HD2	1.50	0.77
1:C:70:ILE:HD13	1:C:573:HIS:HB3	1.67	0.77
1:C:732:ILE:HD12	1:C:733:TYR:N	2.01	0.76
1:D:240:LYS:H	1:D:240:LYS:HD2	1.50	0.76
1:A:174:LEU:HD11	1:A:342:VAL:HG13	1.66	0.76
1:B:70:ILE:HD13	1:B:573:HIS:HB3	1.67	0.76
1:B:732:ILE:HD12	1:B:733:TYR:N	2.01	0.76
1:B:77:PHE:HB3	1:B:389:GLN:HG3	1.65	0.76
1:A:674:ALA:O	1:B:440:ARG:NH1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ILE:HD13	1:D:573:HIS:HB3	1.67	0.75
1:A:70:ILE:HD13	1:A:573:HIS:HB3	1.67	0.75
1:A:421:TRP:CE3	1:A:431:SER:HA	2.21	0.75
1:B:421:TRP:CE3	1:B:431:SER:HA	2.21	0.75
1:D:503:SER:HB2	1:D:510:PRO:O	1.87	0.75
1:D:632:LEU:O	1:D:636:VAL:HG23	1.87	0.75
1:A:515:LEU:HD21	1:A:534:ARG:HG2	1.68	0.75
1:B:515:LEU:HD21	1:B:534:ARG:HG2	1.68	0.75
1:A:732:ILE:HD12	1:A:733:TYR:N	2.01	0.74
1:C:515:LEU:HD21	1:C:534:ARG:HG2	1.68	0.74
1:D:421:TRP:CE3	1:D:431:SER:HA	2.21	0.74
1:C:421:TRP:CE3	1:C:431:SER:HA	2.21	0.74
1:A:698:ASN:HD22	1:A:701:ALA:HB3	1.53	0.74
1:C:503:SER:HB2	1:C:510:PRO:O	1.87	0.74
1:A:632:LEU:O	1:A:636:VAL:HG23	1.87	0.74
1:A:240:LYS:H	1:A:240:LYS:HD2	1.50	0.74
1:B:503:SER:HB2	1:B:510:PRO:O	1.87	0.73
1:B:632:LEU:O	1:B:636:VAL:HG23	1.87	0.73
1:D:698:ASN:HD22	1:D:701:ALA:HB3	1.53	0.73
1:D:732:ILE:HD12	1:D:733:TYR:N	2.01	0.73
1:B:654:ASP:CB	1:D:591:ILE:HD11	2.17	0.73
1:D:515:LEU:HD21	1:D:534:ARG:HG2	1.68	0.73
1:B:465:ASP:OD1	1:B:513:SER:HB2	1.88	0.73
1:B:698:ASN:HD22	1:B:701:ALA:HB3	1.53	0.73
1:D:181:ARG:HB3	1:D:216:ASN:CB	2.19	0.73
1:A:465:ASP:OD1	1:A:513:SER:HB2	1.88	0.73
1:C:465:ASP:OD1	1:C:513:SER:HB2	1.88	0.73
1:A:503:SER:HB2	1:A:510:PRO:O	1.87	0.73
1:C:632:LEU:O	1:C:636:VAL:HG23	1.87	0.73
1:C:698:ASN:HD22	1:C:701:ALA:HB3	1.53	0.72
1:A:181:ARG:HB3	1:A:216:ASN:CB	2.19	0.72
1:D:181:ARG:C	1:D:183:GLU:N	2.43	0.72
1:A:730:ARG:O	1:A:733:TYR:HB3	1.90	0.72
1:D:465:ASP:OD1	1:D:513:SER:HB2	1.88	0.72
1:B:394:VAL:HG13	1:B:577:ALA:HB2	1.72	0.72
1:D:730:ARG:O	1:D:733:TYR:HB3	1.90	0.72
1:B:373:ILE:HD12	1:B:417:LEU:HB2	1.72	0.72
1:B:293:PRO:HB2	1:B:346:ILE:HD12	1.72	0.72
1:B:181:ARG:HB3	1:B:216:ASN:CB	2.19	0.71
1:B:730:ARG:O	1:B:733:TYR:HB3	1.90	0.71
1:D:77:PHE:CB	1:D:389:GLN:HG3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:CB	1:A:216:ASN:HB3	2.21	0.71
1:C:181:ARG:HB3	1:C:216:ASN:CB	2.19	0.71
1:C:293:PRO:HB2	1:C:346:ILE:HD12	1.72	0.71
1:C:394:VAL:HG13	1:C:577:ALA:HB2	1.72	0.71
1:B:145:GLU:OE1	1:B:555:VAL:HG23	1.90	0.71
1:A:77:PHE:CB	1:A:389:GLN:HG3	2.20	0.71
1:A:394:VAL:HG13	1:A:577:ALA:HB2	1.72	0.71
1:C:730:ARG:O	1:C:733:TYR:HB3	1.90	0.71
1:A:145:GLU:CD	1:A:555:VAL:HG23	2.11	0.71
1:C:145:GLU:OE1	1:C:555:VAL:HG23	1.90	0.71
1:C:373:ILE:HD12	1:C:417:LEU:HB2	1.72	0.71
1:A:145:GLU:OE1	1:A:555:VAL:HG23	1.90	0.71
1:C:145:GLU:CD	1:C:555:VAL:HG23	2.11	0.71
1:D:181:ARG:HG2	1:D:183:GLU:HA	1.73	0.71
1:D:145:GLU:OE1	1:D:555:VAL:HG23	1.90	0.71
1:D:181:ARG:CB	1:D:216:ASN:HB3	2.21	0.71
1:D:293:PRO:HB2	1:D:346:ILE:HD12	1.72	0.71
1:B:113:TYR:HB3	1:B:274:ALA:HB3	1.73	0.71
1:B:145:GLU:CD	1:B:555:VAL:HG23	2.11	0.71
1:C:113:TYR:HB3	1:C:274:ALA:HB3	1.73	0.71
1:B:735:ALA:O	1:B:739:VAL:HG23	1.91	0.70
1:C:181:ARG:CB	1:C:216:ASN:HB3	2.21	0.70
1:A:113:TYR:HB3	1:A:274:ALA:HB3	1.73	0.70
1:A:181:ARG:HG2	1:A:183:GLU:HA	1.73	0.70
1:B:174:LEU:HD12	1:B:174:LEU:N	2.06	0.70
1:D:394:VAL:HG13	1:D:577:ALA:HB2	1.72	0.70
1:B:77:PHE:CB	1:B:389:GLN:HG3	2.20	0.70
1:B:90:PHE:CZ	1:B:94:LYS:HE3	2.27	0.70
1:A:174:LEU:HD12	1:A:174:LEU:N	2.06	0.70
1:A:735:ALA:O	1:A:739:VAL:HG23	1.91	0.70
1:C:174:LEU:N	1:C:174:LEU:HD12	2.07	0.70
1:A:659:ILE:H	1:A:659:ILE:HD12	1.57	0.70
1:B:181:ARG:HG3	1:B:186:PHE:HB2	1.74	0.70
1:D:181:ARG:HG3	1:D:186:PHE:HB2	1.74	0.70
1:C:77:PHE:CB	1:C:389:GLN:HG3	2.20	0.70
1:D:90:PHE:CZ	1:D:94:LYS:HE3	2.27	0.70
1:A:181:ARG:HG3	1:A:186:PHE:HB2	1.74	0.70
1:B:659:ILE:H	1:B:659:ILE:HD12	1.56	0.70
1:C:659:ILE:HD12	1:C:659:ILE:H	1.57	0.70
1:C:735:ALA:O	1:C:739:VAL:HG23	1.91	0.70
1:A:90:PHE:CZ	1:A:94:LYS:HE3	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ARG:HG3	1:C:186:PHE:HB2	1.74	0.70
1:D:735:ALA:O	1:D:739:VAL:HG23	1.91	0.70
1:D:174:LEU:HD12	1:D:174:LEU:N	2.06	0.69
1:D:659:ILE:H	1:D:659:ILE:HD12	1.56	0.69
1:A:293:PRO:HB2	1:A:346:ILE:HD12	1.72	0.69
1:A:373:ILE:HD12	1:A:417:LEU:HB2	1.72	0.69
1:D:70:ILE:HD11	1:D:573:HIS:HB3	1.74	0.69
1:A:70:ILE:HD11	1:A:573:HIS:HB3	1.74	0.69
1:C:90:PHE:CZ	1:C:94:LYS:HE3	2.27	0.69
1:C:181:ARG:C	1:C:183:GLU:N	2.42	0.69
1:D:373:ILE:HD12	1:D:417:LEU:HB2	1.72	0.69
1:A:187:LYS:HE3	1:A:190:ARG:HH22	1.58	0.69
1:B:187:LYS:HE3	1:B:190:ARG:HH22	1.58	0.69
1:D:145:GLU:CD	1:D:555:VAL:HG23	2.11	0.69
1:D:113:TYR:HB3	1:D:274:ALA:HB3	1.73	0.69
1:B:656:SER:HA	1:D:655:LYS:O	1.93	0.69
1:A:541:TRP:HA	1:A:541:TRP:CE3	2.28	0.69
1:B:181:ARG:HG2	1:B:183:GLU:HA	1.73	0.69
1:B:181:ARG:CB	1:B:216:ASN:HB3	2.21	0.68
1:C:70:ILE:HD11	1:C:573:HIS:HB3	1.74	0.68
1:C:261:LEU:O	1:C:262:ASN:C	2.32	0.68
1:D:261:LEU:O	1:D:262:ASN:C	2.32	0.68
1:A:261:LEU:O	1:A:262:ASN:C	2.31	0.68
1:A:504:PRO:O	1:A:505:GLU:HB3	1.93	0.68
1:B:550:PRO:O	1:B:551:LEU:HB2	1.94	0.68
1:C:181:ARG:HG2	1:C:183:GLU:HA	1.73	0.68
1:D:187:LYS:HE3	1:D:190:ARG:HH22	1.58	0.68
1:A:377:HIS:NE2	1:A:453:ASP:OD1	2.27	0.68
1:B:591:ILE:HD11	1:D:654:ASP:HB2	1.74	0.68
1:D:689:HIS:HB3	1:D:692:TYR:O	1.94	0.68
1:B:504:PRO:O	1:B:505:GLU:HB3	1.93	0.68
1:C:504:PRO:O	1:C:505:GLU:HB3	1.93	0.68
1:D:377:HIS:NE2	1:D:453:ASP:OD1	2.27	0.68
1:A:550:PRO:O	1:A:551:LEU:HB2	1.93	0.68
1:B:214:VAL:O	1:B:217:ALA:HB3	1.94	0.68
1:C:115:VAL:CG1	1:C:429:LEU:HD13	2.24	0.68
1:C:214:VAL:O	1:C:217:ALA:HB3	1.94	0.68
1:C:550:PRO:O	1:C:551:LEU:HB2	1.93	0.68
1:B:261:LEU:O	1:B:262:ASN:C	2.32	0.68
1:C:377:HIS:NE2	1:C:453:ASP:OD1	2.27	0.68
1:C:541:TRP:HA	1:C:541:TRP:CE3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HD11	1:B:573:HIS:HB3	1.75	0.68
1:B:541:TRP:HA	1:B:541:TRP:CE3	2.28	0.68
1:A:214:VAL:O	1:A:217:ALA:HB3	1.94	0.67
1:B:610:LYS:O	1:B:614:ILE:HG12	1.94	0.67
1:C:325:VAL:CG2	1:C:326:PRO:HD2	2.22	0.67
1:C:610:LYS:O	1:C:614:ILE:HG12	1.94	0.67
1:B:689:HIS:HB3	1:B:692:TYR:O	1.94	0.67
1:B:377:HIS:NE2	1:B:453:ASP:OD1	2.27	0.67
1:D:120:PRO:HB3	1:D:126:ASN:HD21	1.59	0.67
1:D:325:VAL:CG2	1:D:326:PRO:HD2	2.22	0.67
1:C:187:LYS:HE3	1:C:190:ARG:HH22	1.58	0.67
1:A:689:HIS:HB3	1:A:692:TYR:O	1.94	0.67
1:D:115:VAL:CG1	1:D:429:LEU:HD13	2.24	0.67
1:D:610:LYS:O	1:D:614:ILE:HG12	1.94	0.67
1:C:228:TYR:CB	1:C:297:ILE:HG22	2.24	0.67
1:C:689:HIS:HB3	1:C:692:TYR:O	1.94	0.67
1:D:541:TRP:HA	1:D:541:TRP:CE3	2.28	0.67
1:D:541:TRP:HA	1:D:541:TRP:HE3	1.60	0.67
1:A:610:LYS:O	1:A:614:ILE:HG12	1.94	0.67
1:C:120:PRO:HB3	1:C:126:ASN:HD21	1.59	0.67
1:D:79:GLN:O	1:D:80:ILE:HD13	1.95	0.67
1:D:214:VAL:O	1:D:217:ALA:HB3	1.94	0.67
1:A:140:ASN:CB	4:A:1760:NAG:H62	2.20	0.67
1:B:303:GLN:HE21	1:B:324:LYS:HB2	1.60	0.67
1:A:120:PRO:HB3	1:A:126:ASN:HD21	1.59	0.67
1:A:228:TYR:CB	1:A:297:ILE:HG22	2.24	0.67
1:C:79:GLN:O	1:C:80:ILE:HD13	1.95	0.67
1:D:504:PRO:O	1:D:505:GLU:HB3	1.93	0.67
1:A:78:THR:HG21	1:A:559:TYR:H	1.60	0.66
1:A:181:ARG:C	1:A:183:GLU:N	2.43	0.66
1:D:550:PRO:O	1:D:551:LEU:HB2	1.94	0.66
1:A:141:THR:CG2	1:A:142:SER:N	2.58	0.66
1:B:115:VAL:CG1	1:B:429:LEU:HD13	2.24	0.66
1:B:228:TYR:CB	1:B:297:ILE:HG22	2.24	0.66
1:A:123:THR:O	1:A:125:PRO:HD3	1.96	0.66
1:B:141:THR:CG2	1:B:142:SER:N	2.58	0.66
1:D:141:THR:CG2	1:D:142:SER:N	2.58	0.66
1:B:79:GLN:O	1:B:80:ILE:HD13	1.95	0.66
1:C:123:THR:O	1:C:125:PRO:HD3	1.96	0.66
1:C:239:VAL:HB	1:C:247:ASN:HD22	1.61	0.66
1:A:733:TYR:CE1	1:B:278:ALA:HA	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD11	1:B:342:VAL:CG1	2.26	0.66
1:C:141:THR:CG2	1:C:142:SER:N	2.58	0.66
1:C:337:PHE:HD2	1:C:340:GLN:HE21	1.43	0.66
1:D:337:PHE:HD2	1:D:340:GLN:HE21	1.43	0.66
1:A:218:GLN:HG2	1:A:292:ILE:HD12	1.76	0.66
1:B:123:THR:O	1:B:125:PRO:HD3	1.96	0.66
1:B:239:VAL:HB	1:B:247:ASN:HD22	1.61	0.66
1:B:246:TRP:CZ2	3:M:1:NAG:H82	2.28	0.66
1:A:173:ASP:HB3	1:A:332:GLY:N	2.10	0.66
1:A:263:GLY:CA	1:A:686:PHE:HB2	2.26	0.66
1:B:541:TRP:HA	1:B:541:TRP:HE3	1.60	0.66
1:C:78:THR:HG21	1:C:559:TYR:H	1.60	0.66
1:C:218:GLN:HG2	1:C:292:ILE:HD12	1.76	0.66
1:C:303:GLN:HE21	1:C:324:LYS:HB2	1.60	0.66
1:D:218:GLN:HG2	1:D:292:ILE:HD12	1.76	0.66
1:D:263:GLY:CA	1:D:686:PHE:HB2	2.26	0.66
1:C:174:LEU:HD11	1:C:342:VAL:CG1	2.26	0.66
1:C:460:TYR:O	1:C:461:THR:HG22	1.96	0.66
1:D:303:GLN:HE21	1:D:324:LYS:HB2	1.60	0.66
1:A:79:GLN:O	1:A:80:ILE:HD13	1.95	0.66
1:B:120:PRO:HB3	1:B:126:ASN:HD21	1.59	0.66
1:B:218:GLN:HG2	1:B:292:ILE:HD12	1.76	0.66
1:B:78:THR:HG21	1:B:559:TYR:H	1.60	0.66
1:C:263:GLY:CA	1:C:686:PHE:HB2	2.26	0.66
1:C:541:TRP:HA	1:C:541:TRP:HE3	1.60	0.66
1:D:174:LEU:HD11	1:D:342:VAL:CG1	2.26	0.66
1:D:228:TYR:CB	1:D:297:ILE:HG22	2.24	0.66
1:A:239:VAL:HB	1:A:247:ASN:HD22	1.61	0.65
1:A:325:VAL:CG2	1:A:326:PRO:HD2	2.22	0.65
1:D:543:THR:HG22	1:D:544:ASN:ND2	2.12	0.65
1:B:264:ALA:HB3	1:B:527:ARG:HH11	1.61	0.65
1:D:78:THR:HG21	1:D:559:TYR:H	1.61	0.65
1:D:373:ILE:HB	1:D:449:TYR:HD1	1.62	0.65
1:A:187:LYS:HG2	1:A:190:ARG:NH2	2.12	0.65
1:A:460:TYR:O	1:A:461:THR:HG22	1.96	0.65
1:D:123:THR:O	1:D:125:PRO:HD3	1.96	0.65
1:A:174:LEU:HD11	1:A:342:VAL:CG1	2.26	0.65
1:B:173:ASP:HB3	1:B:332:GLY:N	2.10	0.65
1:B:187:LYS:HG2	1:B:190:ARG:NH2	2.12	0.65
1:B:373:ILE:HB	1:B:449:TYR:HD1	1.62	0.65
1:C:174:LEU:HD21	1:C:342:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:GLY:O	1:C:389:GLN:HB2	1.97	0.65
1:B:325:VAL:CG2	1:B:326:PRO:HD2	2.22	0.65
1:A:264:ALA:HB3	1:A:527:ARG:HH11	1.61	0.65
1:B:337:PHE:HD2	1:B:340:GLN:HE21	1.44	0.65
1:D:174:LEU:HD21	1:D:342:VAL:HG11	1.79	0.65
1:D:187:LYS:HG2	1:D:190:ARG:NH2	2.12	0.65
1:D:239:VAL:HB	1:D:247:ASN:HD22	1.61	0.65
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.62	0.65
1:A:373:ILE:HB	1:A:449:TYR:HD1	1.62	0.65
1:B:658:PRO:HG2	1:B:659:ILE:HD12	1.79	0.65
1:B:707:GLY:HA3	1:B:731:GLN:HG2	1.78	0.65
1:D:264:ALA:HB3	1:D:527:ARG:HH11	1.61	0.65
1:D:293:PRO:CB	1:D:346:ILE:HD12	2.27	0.65
1:A:115:VAL:CG1	1:A:429:LEU:HD13	2.24	0.65
1:B:181:ARG:C	1:B:183:GLU:N	2.43	0.65
1:B:263:GLY:CA	1:B:686:PHE:HB2	2.26	0.65
1:C:173:ASP:HB3	1:C:332:GLY:N	2.10	0.65
1:A:384:GLY:O	1:A:389:GLN:HB2	1.97	0.64
1:A:707:GLY:HA3	1:A:731:GLN:HG2	1.78	0.64
1:C:674:ALA:O	1:D:440:ARG:NH1	2.30	0.64
1:C:707:GLY:CA	1:C:731:GLN:HG2	2.28	0.64
1:A:337:PHE:HD2	1:A:340:GLN:HE21	1.44	0.64
1:A:541:TRP:HA	1:A:541:TRP:HE3	1.60	0.64
1:A:707:GLY:CA	1:A:731:GLN:HG2	2.28	0.64
1:B:174:LEU:HD21	1:B:342:VAL:HG11	1.79	0.64
1:B:543:THR:HG22	1:B:544:ASN:ND2	2.12	0.64
1:D:658:PRO:HG2	1:D:659:ILE:HD12	1.79	0.64
1:D:707:GLY:HA3	1:D:731:GLN:HG2	1.78	0.64
1:A:543:THR:HG22	1:A:544:ASN:ND2	2.12	0.64
1:B:65:LEU:O	1:B:574:LEU:HD11	1.98	0.64
1:B:266:ASP:OD2	1:B:269:THR:HG23	1.98	0.64
1:B:460:TYR:O	1:B:461:THR:HG22	1.96	0.64
1:C:266:ASP:OD2	1:C:269:THR:HG23	1.98	0.64
1:C:373:ILE:HB	1:C:449:TYR:HD1	1.62	0.64
1:A:65:LEU:O	1:A:574:LEU:HD11	1.98	0.64
1:A:303:GLN:HE21	1:A:324:LYS:HB2	1.60	0.64
1:C:293:PRO:CB	1:C:346:ILE:HD12	2.27	0.64
1:D:240:LYS:HD2	1:D:240:LYS:N	2.13	0.64
1:A:174:LEU:HD21	1:A:342:VAL:HG11	1.79	0.64
1:A:263:GLY:HA3	1:A:686:PHE:HB2	1.79	0.64
1:A:658:PRO:HG2	1:A:659:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:GLY:O	1:B:389:GLN:HB2	1.97	0.64
1:B:707:GLY:CA	1:B:731:GLN:HG2	2.28	0.64
1:D:141:THR:HG22	1:D:142:SER:N	2.13	0.64
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.62	0.64
1:A:293:PRO:CB	1:A:346:ILE:HD12	2.27	0.64
1:C:187:LYS:HG2	1:C:190:ARG:NH2	2.12	0.64
1:C:543:THR:HG22	1:C:544:ASN:ND2	2.12	0.64
1:C:658:PRO:HG2	1:C:659:ILE:HD12	1.79	0.64
1:D:384:GLY:O	1:D:389:GLN:HB2	1.97	0.64
1:B:141:THR:HG22	1:B:142:SER:N	2.13	0.64
1:B:293:PRO:CB	1:B:346:ILE:HD12	2.27	0.64
1:B:382:VAL:CG2	1:B:383:PHE:H	2.08	0.64
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.62	0.64
1:D:460:TYR:O	1:D:461:THR:HG22	1.96	0.64
1:B:228:TYR:CE1	1:B:230:ASP:HB2	2.33	0.64
1:A:266:ASP:OD2	1:A:269:THR:HG23	1.98	0.63
1:B:263:GLY:HA3	1:B:686:PHE:HB2	1.79	0.63
1:C:707:GLY:HA3	1:C:731:GLN:HG2	1.78	0.63
1:D:140:ASN:CB	4:D:4760:NAG:H62	2.20	0.63
1:A:128:ILE:HD13	1:A:226:ILE:CD1	2.21	0.63
1:C:263:GLY:HA3	1:C:686:PHE:HB2	1.79	0.63
1:D:266:ASP:OD2	1:D:269:THR:HG23	1.98	0.63
1:A:246:TRP:CZ2	3:H:1:NAG:H82	2.28	0.63
1:B:140:ASN:CB	4:B:2760:NAG:H62	2.20	0.63
1:C:65:LEU:O	1:C:574:LEU:HD11	1.98	0.63
1:C:705:PHE:N	1:C:706:PRO:HD3	2.14	0.63
1:D:263:GLY:HA3	1:D:686:PHE:HB2	1.79	0.63
1:D:707:GLY:CA	1:D:731:GLN:HG2	2.28	0.63
1:A:382:VAL:CG2	1:A:383:PHE:H	2.08	0.63
1:C:128:ILE:HD13	1:C:226:ILE:CD1	2.21	0.63
1:C:205:TYR:HE2	1:C:227:LEU:HD13	1.64	0.63
1:C:264:ALA:HB3	1:C:527:ARG:HH11	1.61	0.63
1:A:141:THR:HG22	1:A:142:SER:N	2.13	0.63
1:A:377:HIS:CE1	1:A:388:PRO:HB3	2.34	0.63
1:D:205:TYR:HE2	1:D:227:LEU:HD13	1.64	0.63
1:A:181:ARG:CG	1:A:186:PHE:HB2	2.29	0.63
1:A:205:TYR:HE2	1:A:227:LEU:HD13	1.64	0.63
1:B:181:ARG:CG	1:B:186:PHE:HB2	2.29	0.63
1:C:377:HIS:CE1	1:C:388:PRO:HB3	2.34	0.63
1:D:228:TYR:CE1	1:D:230:ASP:HB2	2.34	0.63
1:D:377:HIS:CE1	1:D:388:PRO:HB3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:HD2	1:C:240:LYS:N	2.13	0.63
1:D:705:PHE:N	1:D:706:PRO:HD3	2.14	0.63
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.62	0.63
1:C:141:THR:HG22	1:C:142:SER:N	2.13	0.63
1:C:246:TRP:CZ2	3:R:1:NAG:H82	2.29	0.63
1:D:65:LEU:O	1:D:574:LEU:HD11	1.98	0.63
1:D:173:ASP:HB3	1:D:332:GLY:N	2.10	0.63
1:C:123:THR:C	1:C:125:PRO:HD3	2.20	0.62
1:C:567:ASP:OD2	1:C:570:PHE:HA	1.99	0.62
1:D:77:PHE:HB3	1:D:389:GLN:CG	2.29	0.62
1:A:567:ASP:OD2	1:A:570:PHE:HA	1.99	0.62
1:C:228:TYR:CE1	1:C:230:ASP:HB2	2.33	0.62
1:D:246:TRP:CZ2	3:W:1:NAG:H82	2.28	0.62
1:A:228:TYR:CE1	1:A:230:ASP:HB2	2.33	0.62
1:C:77:PHE:HB3	1:C:389:GLN:CG	2.29	0.62
1:B:705:PHE:N	1:B:706:PRO:HD3	2.14	0.62
1:C:712:LEU:HD23	1:C:728:VAL:HG21	1.81	0.62
1:D:712:LEU:HD23	1:D:728:VAL:HG21	1.81	0.62
1:A:123:THR:C	1:A:125:PRO:HD3	2.19	0.62
1:A:240:LYS:HD2	1:A:240:LYS:N	2.13	0.62
1:B:123:THR:C	1:B:125:PRO:HD3	2.19	0.62
1:B:567:ASP:OD2	1:B:570:PHE:HA	1.99	0.62
1:A:705:PHE:N	1:A:706:PRO:HD3	2.14	0.62
1:B:182:THR:O	1:B:183:GLU:HB2	2.00	0.62
1:C:140:ASN:CB	4:C:3760:NAG:H62	2.20	0.62
1:C:369:ASP:CG	1:D:663:MET:HG2	2.20	0.62
1:A:246:TRP:HE1	3:H:1:NAG:C7	2.13	0.62
1:B:245:GLY:O	1:B:246:TRP:CB	2.47	0.62
1:C:181:ARG:CG	1:C:186:PHE:HB2	2.29	0.62
1:C:673:ARG:HA	1:C:676:ILE:HD13	1.82	0.62
1:B:205:TYR:HE2	1:B:227:LEU:HD13	1.64	0.62
1:C:137:GLU:HB3	4:C:3760:NAG:O3	2.00	0.62
1:C:241:SER:C	1:C:245:GLY:HA3	2.20	0.62
1:C:468:PRO:HA	1:C:471:TYR:CD1	2.35	0.62
1:D:181:ARG:CG	1:D:186:PHE:HB2	2.29	0.62
1:D:567:ASP:OD2	1:D:570:PHE:HA	1.99	0.62
1:A:356:TYR:O	1:A:422:ASP:HB2	2.00	0.62
1:B:241:SER:C	1:B:245:GLY:HA3	2.20	0.62
1:D:120:PRO:HB3	1:D:126:ASN:ND2	2.15	0.62
1:D:123:THR:C	1:D:125:PRO:HD3	2.20	0.62
1:D:246:TRP:HE1	3:W:1:NAG:C7	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:HB3	1:A:126:ASN:ND2	2.15	0.62
1:B:377:HIS:CE1	1:B:388:PRO:HB3	2.34	0.62
1:A:137:GLU:HB3	4:A:1760:NAG:O3	2.00	0.61
1:A:245:GLY:O	1:A:246:TRP:CB	2.47	0.61
1:C:242:TYR:O	1:C:243:PRO:C	2.38	0.61
1:D:242:TYR:O	1:D:243:PRO:C	2.38	0.61
1:B:246:TRP:HE1	3:M:1:NAG:C7	2.13	0.61
1:B:366:VAL:O	1:B:368:PRO:HD3	2.00	0.61
1:C:120:PRO:HB3	1:C:126:ASN:ND2	2.15	0.61
1:B:120:PRO:HB3	1:B:126:ASN:ND2	2.15	0.61
1:B:712:LEU:HD23	1:B:728:VAL:HG21	1.81	0.61
1:C:246:TRP:HE1	3:R:1:NAG:C7	2.13	0.61
1:C:483:SER:HB2	1:C:493:LEU:HA	1.82	0.61
1:A:468:PRO:HA	1:A:471:TYR:CD1	2.35	0.61
1:B:240:LYS:HD2	1:B:240:LYS:N	2.13	0.61
1:D:245:GLY:O	1:D:246:TRP:CB	2.48	0.61
1:C:245:GLY:O	1:C:246:TRP:CB	2.47	0.61
1:D:241:SER:C	1:D:245:GLY:HA3	2.20	0.61
1:A:77:PHE:HB3	1:A:389:GLN:CG	2.29	0.61
1:C:356:TYR:O	1:C:422:ASP:HB2	2.00	0.61
1:D:182:THR:O	1:D:183:GLU:HB2	2.00	0.61
1:A:242:TYR:O	1:A:243:PRO:C	2.38	0.61
1:A:366:VAL:O	1:A:368:PRO:HD3	2.00	0.61
1:A:673:ARG:HA	1:A:676:ILE:HD13	1.82	0.61
1:D:137:GLU:HB3	4:D:4760:NAG:O3	2.00	0.61
1:A:402:PHE:HE2	1:A:585:PHE:HD1	1.49	0.61
1:B:242:TYR:O	1:B:243:PRO:C	2.38	0.61
1:B:356:TYR:O	1:B:422:ASP:HB2	2.00	0.61
1:B:402:PHE:HE2	1:B:585:PHE:HD1	1.49	0.61
1:D:128:ILE:HD13	1:D:226:ILE:CD1	2.21	0.61
1:A:241:SER:C	1:A:245:GLY:HA3	2.20	0.61
1:B:673:ARG:HA	1:B:676:ILE:HD13	1.82	0.61
1:D:483:SER:HB2	1:D:493:LEU:HA	1.82	0.61
1:D:673:ARG:HA	1:D:676:ILE:HD13	1.82	0.61
1:B:137:GLU:HB3	4:B:2760:NAG:O3	2.00	0.60
1:A:712:LEU:HD23	1:A:728:VAL:HG21	1.81	0.60
1:B:483:SER:HB2	1:B:493:LEU:HA	1.82	0.60
1:D:303:GLN:NE2	1:D:324:LYS:HB2	2.16	0.60
1:C:303:GLN:NE2	1:C:324:LYS:HB2	2.16	0.60
1:D:468:PRO:HA	1:D:471:TYR:CD1	2.35	0.60
1:A:483:SER:HB2	1:A:493:LEU:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:TYR:O	1:D:422:ASP:HB2	2.00	0.60
1:A:303:GLN:NE2	1:A:324:LYS:HB2	2.16	0.60
1:C:182:THR:O	1:C:183:GLU:HB2	2.00	0.60
1:D:366:VAL:O	1:D:368:PRO:HD3	2.00	0.60
1:B:303:GLN:NE2	1:B:324:LYS:HB2	2.16	0.60
1:C:357:ASN:OD1	1:C:421:TRP:HA	2.02	0.60
1:A:357:ASN:OD1	1:A:421:TRP:HA	2.02	0.60
1:B:468:PRO:HA	1:B:471:TYR:CD1	2.35	0.60
1:D:242:TYR:N	1:D:245:GLY:HA3	2.17	0.60
1:D:357:ASN:OD1	1:D:421:TRP:HA	2.02	0.60
1:A:182:THR:O	1:A:183:GLU:HB2	2.00	0.60
1:A:242:TYR:N	1:A:245:GLY:HA3	2.17	0.60
1:A:517:SER:HB3	1:A:694:PRO:HG3	1.84	0.60
1:D:638:ASN:O	1:D:642:ILE:HG12	2.01	0.60
1:B:77:PHE:HB3	1:B:389:GLN:CG	2.29	0.60
1:B:517:SER:HB3	1:B:694:PRO:HG3	1.84	0.60
1:C:638:ASN:O	1:C:642:ILE:HG12	2.01	0.60
1:B:357:ASN:OD1	1:B:421:TRP:HA	2.02	0.59
1:D:402:PHE:HE2	1:D:585:PHE:HD1	1.49	0.59
1:A:598:ARG:O	1:A:602:VAL:HG23	2.03	0.59
1:B:370:ARG:HB2	1:B:414:ARG:HG2	1.85	0.59
1:C:503:SER:HB2	1:C:510:PRO:C	2.23	0.59
1:C:517:SER:HB3	1:C:694:PRO:HG3	1.84	0.59
1:C:663:MET:HG2	1:D:369:ASP:OD1	2.02	0.59
1:D:517:SER:HB3	1:D:694:PRO:HG3	1.84	0.59
1:A:459:ASN:ND2	3:H:1:NAG:C7	2.66	0.59
1:B:242:TYR:N	1:B:245:GLY:HA3	2.17	0.59
1:B:598:ARG:O	1:B:602:VAL:HG23	2.03	0.59
1:C:242:TYR:N	1:C:245:GLY:HA3	2.17	0.59
1:C:598:ARG:O	1:C:602:VAL:HG23	2.03	0.59
1:A:683:ASP:C	1:A:684:ARG:HG3	2.23	0.59
1:B:638:ASN:O	1:B:642:ILE:HG12	2.01	0.59
1:C:272:TYR:CE2	1:D:734:VAL:HG13	2.37	0.59
1:C:366:VAL:O	1:C:368:PRO:HD3	2.00	0.59
1:D:459:ASN:ND2	3:W:1:NAG:C7	2.66	0.59
1:D:503:SER:HB2	1:D:510:PRO:C	2.22	0.59
1:A:638:ASN:O	1:A:642:ILE:HG12	2.01	0.59
1:A:210:ARG:O	1:A:213:LYS:HB2	2.03	0.59
1:B:459:ASN:ND2	3:M:1:NAG:C7	2.66	0.59
1:C:377:HIS:NE2	1:C:388:PRO:HB3	2.18	0.59
1:A:503:SER:HB2	1:A:510:PRO:C	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:VAL:CG2	1:D:383:PHE:H	2.08	0.59
1:A:574:LEU:O	1:A:578:GLN:HG3	2.03	0.59
1:B:210:ARG:O	1:B:213:LYS:HB2	2.03	0.59
1:B:683:ASP:C	1:B:684:ARG:HG3	2.23	0.59
1:D:377:HIS:NE2	1:D:388:PRO:HB3	2.18	0.59
1:A:264:ALA:HB3	1:A:527:ARG:NH1	2.18	0.59
1:B:574:LEU:O	1:B:578:GLN:HG3	2.03	0.58
1:C:402:PHE:HE2	1:C:585:PHE:HD1	1.49	0.58
1:C:683:ASP:C	1:C:684:ARG:HG3	2.23	0.58
1:D:598:ARG:O	1:D:602:VAL:HG23	2.03	0.58
1:A:377:HIS:NE2	1:A:388:PRO:HB3	2.18	0.58
1:B:503:SER:HB2	1:B:510:PRO:C	2.23	0.58
1:C:155:SER:O	1:C:156:ASP:HB2	2.03	0.58
1:C:210:ARG:O	1:C:213:LYS:HB2	2.03	0.58
1:C:264:ALA:HB3	1:C:527:ARG:NH1	2.18	0.58
1:D:683:ASP:C	1:D:684:ARG:HG3	2.23	0.58
1:A:242:TYR:C	1:A:245:GLY:H	2.07	0.58
1:A:370:ARG:HB2	1:A:414:ARG:HG2	1.85	0.58
1:B:128:ILE:CD1	1:B:226:ILE:HD12	2.23	0.58
1:B:377:HIS:NE2	1:B:388:PRO:HB3	2.18	0.58
1:C:368:PRO:HD2	1:D:663:MET:SD	2.43	0.58
1:C:382:VAL:CG2	1:C:383:PHE:H	2.08	0.58
1:D:155:SER:O	1:D:156:ASP:HB2	2.03	0.58
1:D:264:ALA:HB3	1:D:527:ARG:NH1	2.18	0.58
1:B:269:THR:O	1:B:269:THR:OG1	2.20	0.58
1:B:707:GLY:C	1:B:731:GLN:HG2	2.24	0.58
1:A:192:MET:HE1	1:A:315:PRO:HG3	1.86	0.58
1:A:269:THR:O	1:A:269:THR:OG1	2.20	0.58
1:C:268:LEU:C	1:C:270:PRO:HD3	2.24	0.58
1:D:210:ARG:O	1:D:213:LYS:HB2	2.03	0.58
1:D:574:LEU:O	1:D:578:GLN:HG3	2.03	0.58
1:C:459:ASN:ND2	3:R:1:NAG:C7	2.66	0.58
1:C:574:LEU:O	1:C:578:GLN:HG3	2.03	0.58
1:A:707:GLY:C	1:A:731:GLN:HG2	2.24	0.58
1:B:117:LEU:HD12	1:B:353:THR:HB	1.86	0.58
1:D:707:GLY:C	1:D:731:GLN:HG2	2.24	0.58
1:C:117:LEU:HD12	1:C:353:THR:HB	1.86	0.58
1:D:268:LEU:C	1:D:270:PRO:HD3	2.24	0.58
1:A:187:LYS:HG2	1:A:187:LYS:O	2.04	0.57
1:B:83:LEU:HB3	1:B:86:THR:CG2	2.34	0.57
1:B:242:TYR:C	1:B:245:GLY:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLU:HG2	1:C:438:ASN:ND2	2.19	0.57
1:C:187:LYS:HG2	1:C:187:LYS:O	2.04	0.57
1:C:370:ARG:HB2	1:C:414:ARG:HG2	1.85	0.57
1:D:437:GLU:HG2	1:D:438:ASN:ND2	2.19	0.57
1:A:155:SER:O	1:A:156:ASP:HB2	2.03	0.57
1:C:478:THR:HG23	1:C:494:TYR:CB	2.33	0.57
1:D:117:LEU:HD12	1:D:353:THR:HB	1.86	0.57
1:D:370:ARG:HB2	1:D:414:ARG:HG2	1.85	0.57
1:A:117:LEU:HD12	1:A:353:THR:HB	1.86	0.57
1:A:268:LEU:C	1:A:270:PRO:HD3	2.24	0.57
1:C:169:MET:HA	1:C:344:MET:O	2.05	0.57
1:C:242:TYR:C	1:C:245:GLY:H	2.07	0.57
1:D:242:TYR:C	1:D:245:GLY:H	2.07	0.57
1:D:550:PRO:O	1:D:551:LEU:CB	2.53	0.57
1:B:187:LYS:HG2	1:B:187:LYS:O	2.04	0.57
1:B:246:TRP:HB2	1:B:565:PHE:CD2	2.40	0.57
1:B:310:GLY:HA3	1:B:334:THR:HG23	1.87	0.57
1:B:437:GLU:HG2	1:B:438:ASN:ND2	2.19	0.57
1:C:83:LEU:HB3	1:C:86:THR:CG2	2.34	0.57
1:C:475:HIS:O	1:C:478:THR:HG22	2.05	0.57
1:C:749:VAL:HG12	1:D:445:ARG:CZ	2.34	0.57
1:D:187:LYS:HG2	1:D:187:LYS:O	2.04	0.57
1:A:242:TYR:CD2	1:A:556:TYR:HD2	2.22	0.57
1:B:169:MET:HA	1:B:344:MET:O	2.05	0.57
1:B:192:MET:CE	1:B:315:PRO:HG3	2.35	0.57
1:B:264:ALA:HB3	1:B:527:ARG:NH1	2.18	0.57
1:B:268:LEU:C	1:B:270:PRO:HD3	2.24	0.57
1:C:242:TYR:CD2	1:C:556:TYR:HD2	2.23	0.57
1:C:707:GLY:C	1:C:731:GLN:HG2	2.24	0.57
1:D:269:THR:O	1:D:269:THR:OG1	2.20	0.57
1:C:181:ARG:HD3	1:C:216:ASN:ND2	2.20	0.57
1:C:246:TRP:HB2	1:C:565:PHE:CD2	2.39	0.57
1:C:269:THR:OG1	1:C:269:THR:O	2.20	0.57
1:D:242:TYR:CD2	1:D:556:TYR:HD2	2.23	0.57
1:D:478:THR:HG23	1:D:494:TYR:CB	2.33	0.57
1:A:192:MET:CE	1:A:315:PRO:HG3	2.35	0.57
1:A:437:GLU:HG2	1:A:438:ASN:ND2	2.19	0.57
1:A:550:PRO:O	1:A:551:LEU:CB	2.53	0.57
1:B:242:TYR:CD2	1:B:556:TYR:HD2	2.22	0.57
1:A:131:ILE:O	1:A:340:GLN:HA	2.05	0.57
1:A:169:MET:HA	1:A:344:MET:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TRP:HB2	1:A:565:PHE:CD2	2.40	0.57
1:C:128:ILE:CD1	1:C:226:ILE:HD12	2.23	0.57
1:C:131:ILE:O	1:C:340:GLN:HA	2.05	0.57
1:A:412:PRO:HB2	1:A:414:ARG:O	2.05	0.57
1:C:192:MET:CE	1:C:315:PRO:HG3	2.35	0.57
1:D:83:LEU:HB3	1:D:86:THR:CG2	2.34	0.57
1:B:155:SER:O	1:B:156:ASP:HB2	2.03	0.56
1:D:131:ILE:O	1:D:340:GLN:HA	2.05	0.56
1:B:475:HIS:O	1:B:478:THR:HG22	2.05	0.56
1:D:181:ARG:HD3	1:D:216:ASN:ND2	2.20	0.56
1:D:412:PRO:HB2	1:D:414:ARG:O	2.05	0.56
1:A:373:ILE:CD1	1:A:417:LEU:HB2	2.36	0.56
1:A:478:THR:HG23	1:A:494:TYR:CB	2.33	0.56
1:B:478:THR:HG23	1:B:494:TYR:CB	2.33	0.56
1:D:169:MET:HA	1:D:344:MET:O	2.05	0.56
1:D:246:TRP:HB2	1:D:565:PHE:CD2	2.39	0.56
1:D:683:ASP:O	1:D:684:ARG:HG3	2.06	0.56
1:B:266:ASP:HA	1:B:429:LEU:HD22	1.88	0.56
1:D:192:MET:CE	1:D:315:PRO:HG3	2.35	0.56
1:A:460:TYR:CD2	1:A:540:ASN:HA	2.41	0.56
1:A:683:ASP:O	1:A:684:ARG:HG3	2.06	0.56
1:B:550:PRO:O	1:B:551:LEU:CB	2.53	0.56
1:C:465:ASP:O	1:C:466:CYS:HB3	2.06	0.56
1:C:683:ASP:O	1:C:684:ARG:HG3	2.06	0.56
1:D:310:GLY:HA3	1:D:334:THR:HG23	1.87	0.56
1:B:412:PRO:HB2	1:B:414:ARG:O	2.05	0.56
1:C:460:TYR:CD2	1:C:540:ASN:HA	2.41	0.56
1:D:229:SER:HB3	1:D:234:TYR:HE1	1.71	0.56
1:D:363:ARG:HB3	1:D:411:ARG:HH21	1.71	0.56
1:C:550:PRO:O	1:C:551:LEU:CB	2.53	0.56
1:C:670:PHE:CE2	1:D:444:GLU:OE1	2.59	0.56
1:D:465:ASP:O	1:D:466:CYS:HB3	2.06	0.56
1:A:242:TYR:O	1:A:245:GLY:N	2.39	0.56
1:A:363:ARG:HB3	1:A:411:ARG:HH21	1.71	0.56
1:A:672:GLU:OE1	1:A:689:HIS:HE1	1.89	0.56
1:B:131:ILE:O	1:B:340:GLN:HA	2.05	0.56
1:B:460:TYR:CD2	1:B:540:ASN:HA	2.41	0.56
1:C:412:PRO:HB2	1:C:414:ARG:O	2.05	0.56
1:C:529:GLY:HA3	1:C:676:ILE:HD11	1.88	0.56
1:A:310:GLY:HA3	1:A:334:THR:HG23	1.87	0.56
1:A:475:HIS:O	1:A:478:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:HD3	1:B:216:ASN:ND2	2.20	0.56
1:B:683:ASP:O	1:B:684:ARG:HG3	2.06	0.56
1:D:83:LEU:HB3	1:D:86:THR:HG21	1.88	0.56
1:D:475:HIS:O	1:D:478:THR:HG22	2.05	0.56
1:A:83:LEU:HB3	1:A:86:THR:CG2	2.34	0.56
1:B:465:ASP:O	1:B:466:CYS:HB3	2.06	0.56
1:D:460:TYR:CD2	1:D:540:ASN:HA	2.41	0.56
1:A:83:LEU:HB3	1:A:86:THR:HG21	1.88	0.55
1:B:229:SER:HB3	1:B:234:TYR:HE1	1.71	0.55
1:C:83:LEU:HB3	1:C:86:THR:HG21	1.88	0.55
1:D:529:GLY:HA3	1:D:676:ILE:HD11	1.88	0.55
1:A:181:ARG:HD3	1:A:216:ASN:ND2	2.20	0.55
1:B:708:ILE:HG13	1:B:731:GLN:HB3	1.89	0.55
1:C:242:TYR:O	1:C:245:GLY:N	2.39	0.55
1:C:310:GLY:HA3	1:C:334:THR:HG23	1.87	0.55
1:A:465:ASP:O	1:A:466:CYS:HB3	2.06	0.55
1:B:373:ILE:CD1	1:B:417:LEU:HB2	2.36	0.55
1:B:672:GLU:OE1	1:B:689:HIS:HE1	1.89	0.55
1:A:229:SER:HB3	1:A:234:TYR:HE1	1.71	0.55
1:A:266:ASP:HA	1:A:429:LEU:HD22	1.88	0.55
1:A:558:THR:O	1:A:561:LEU:HB3	2.07	0.55
1:B:363:ARG:HB3	1:B:411:ARG:HH21	1.71	0.55
1:B:558:THR:O	1:B:561:LEU:HB3	2.07	0.55
1:C:132:ASN:HB3	1:C:340:GLN:OE1	2.07	0.55
1:D:627:VAL:HG21	1:D:725:TRP:CE3	2.42	0.55
1:A:449:TYR:CE2	1:A:521:PHE:HA	2.42	0.55
1:A:737:PHE:CE1	1:B:273:PRO:HG2	2.42	0.55
1:B:128:ILE:HD13	1:B:226:ILE:CD1	2.21	0.55
1:B:529:GLY:HA3	1:B:676:ILE:HD11	1.88	0.55
1:C:672:GLU:OE1	1:C:689:HIS:HE1	1.89	0.55
1:A:497:TRP:CE2	1:A:510:PRO:HB3	2.42	0.55
1:B:497:TRP:CE2	1:B:510:PRO:HB3	2.42	0.55
1:C:78:THR:HG21	1:C:559:TYR:N	2.22	0.55
1:C:708:ILE:HG13	1:C:731:GLN:HB3	1.89	0.55
1:D:373:ILE:CD1	1:D:417:LEU:HB2	2.35	0.55
1:D:558:THR:O	1:D:561:LEU:HB3	2.07	0.55
1:A:59:LYS:O	1:A:60:ALA:C	2.46	0.55
1:B:627:VAL:HG21	1:B:725:TRP:CE3	2.42	0.55
1:A:178:ASN:O	1:A:180:ALA:N	2.40	0.55
1:A:529:GLY:HA3	1:A:676:ILE:HD11	1.88	0.55
1:C:363:ARG:HB3	1:C:411:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:LEU:HD13	1:C:594:PRO:HB3	1.89	0.55
1:C:488:PHE:HB3	1:C:491:LYS:HB2	1.89	0.55
1:D:266:ASP:HA	1:D:429:LEU:HD22	1.88	0.55
1:B:178:ASN:O	1:B:180:ALA:N	2.40	0.54
1:C:229:SER:HB3	1:C:234:TYR:HE1	1.71	0.54
1:A:657:ASN:OD1	1:A:660:VAL:HG23	2.07	0.54
1:B:449:TYR:CE2	1:B:521:PHE:HA	2.42	0.54
1:D:242:TYR:O	1:D:245:GLY:N	2.39	0.54
1:D:473:LEU:HD13	1:D:594:PRO:HB3	1.89	0.54
1:D:488:PHE:HB3	1:D:491:LYS:HB2	1.89	0.54
1:D:672:GLU:OE1	1:D:689:HIS:HE1	1.89	0.54
1:A:132:ASN:HB3	1:A:340:GLN:OE1	2.07	0.54
1:B:59:LYS:O	1:B:60:ALA:C	2.46	0.54
1:B:656:SER:O	1:D:656:SER:O	2.24	0.54
1:C:497:TRP:CE2	1:C:510:PRO:HB3	2.42	0.54
1:C:558:THR:O	1:C:561:LEU:HB3	2.07	0.54
1:D:192:MET:O	1:D:194:ILE:HG12	2.07	0.54
1:D:497:TRP:CE2	1:D:510:PRO:HB3	2.42	0.54
1:B:83:LEU:HB3	1:B:86:THR:HG21	1.88	0.54
1:B:181:ARG:HG2	1:B:183:GLU:CA	2.38	0.54
1:C:59:LYS:O	1:C:60:ALA:C	2.46	0.54
1:C:181:ARG:HG2	1:C:183:GLU:CA	2.38	0.54
1:A:78:THR:HG21	1:A:559:TYR:N	2.22	0.54
1:B:428:LEU:HD21	1:B:518:GLY:O	2.08	0.54
1:B:488:PHE:HB3	1:B:491:LYS:HB2	1.89	0.54
1:B:657:ASN:OD1	1:B:660:VAL:HG23	2.07	0.54
1:C:178:ASN:O	1:C:180:ALA:N	2.41	0.54
1:C:373:ILE:CD1	1:C:417:LEU:HB2	2.35	0.54
1:C:428:LEU:HD21	1:C:518:GLY:O	2.08	0.54
1:C:627:VAL:HG21	1:C:725:TRP:CE3	2.42	0.54
1:D:132:ASN:HB3	1:D:340:GLN:OE1	2.07	0.54
1:D:178:ASN:O	1:D:180:ALA:N	2.40	0.54
1:D:449:TYR:CE2	1:D:521:PHE:HA	2.42	0.54
1:A:192:MET:O	1:A:194:ILE:HG12	2.07	0.54
1:A:627:VAL:HG21	1:A:725:TRP:CE3	2.42	0.54
1:B:192:MET:O	1:B:194:ILE:HG12	2.07	0.54
1:B:402:PHE:CE2	1:B:585:PHE:HD1	2.26	0.54
1:C:192:MET:O	1:C:194:ILE:HG12	2.07	0.54
1:D:428:LEU:HD21	1:D:518:GLY:O	2.08	0.54
1:B:242:TYR:O	1:B:245:GLY:N	2.39	0.54
1:C:266:ASP:HA	1:C:429:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:ASN:OD1	1:D:660:VAL:HG23	2.07	0.54
1:C:449:TYR:CE2	1:C:521:PHE:HA	2.42	0.54
1:D:179:TYR:HA	1:D:204:ARG:O	2.08	0.54
1:D:708:ILE:HG13	1:D:731:GLN:HB3	1.89	0.54
1:B:107:SER:HB2	1:B:361:THR:HB	1.90	0.54
1:B:614:ILE:O	1:B:617:LYS:HB2	2.08	0.54
1:C:178:ASN:HB3	1:C:185:PHE:CD1	2.43	0.54
1:A:261:LEU:O	1:A:263:GLY:N	2.41	0.54
1:A:663:MET:HG2	1:B:369:ASP:OD2	2.08	0.54
1:B:78:THR:HG21	1:B:559:TYR:N	2.22	0.54
1:B:132:ASN:HB3	1:B:340:GLN:OE1	2.07	0.54
1:B:529:GLY:HA3	1:B:676:ILE:CD1	2.38	0.54
1:D:337:PHE:HB3	1:D:340:GLN:HG3	1.90	0.54
1:D:614:ILE:O	1:D:617:LYS:HB2	2.08	0.54
1:A:428:LEU:HD21	1:A:518:GLY:O	2.08	0.53
1:A:614:ILE:O	1:A:617:LYS:HB2	2.08	0.53
1:A:715:ILE:HD13	1:A:725:TRP:CE2	2.44	0.53
1:B:473:LEU:HD13	1:B:594:PRO:HB3	1.89	0.53
1:D:78:THR:HG21	1:D:559:TYR:N	2.22	0.53
1:A:473:LEU:HD13	1:A:594:PRO:HB3	1.89	0.53
1:A:610:LYS:CD	1:A:614:ILE:HD11	2.38	0.53
1:B:178:ASN:HB3	1:B:185:PHE:CD1	2.43	0.53
1:B:261:LEU:O	1:B:263:GLY:N	2.41	0.53
1:C:377:HIS:CD2	1:C:453:ASP:OD1	2.61	0.53
1:D:181:ARG:HG2	1:D:183:GLU:CA	2.38	0.53
1:D:323:LEU:HB2	1:D:327:TYR:OH	2.08	0.53
1:A:174:LEU:HD11	1:A:342:VAL:HG22	1.91	0.53
1:A:488:PHE:HB3	1:A:491:LYS:HB2	1.89	0.53
1:B:192:MET:HE1	1:B:315:PRO:HG3	1.90	0.53
1:B:625:TYR:CE2	1:B:722:SER:HA	2.44	0.53
1:C:261:LEU:O	1:C:263:GLY:N	2.41	0.53
1:C:273:PRO:HG2	1:D:737:PHE:CE1	2.43	0.53
1:D:261:LEU:O	1:D:263:GLY:N	2.41	0.53
1:D:625:TYR:CE2	1:D:722:SER:HA	2.44	0.53
1:B:323:LEU:HB2	1:B:327:TYR:OH	2.08	0.53
1:B:337:PHE:HB3	1:B:340:GLN:HG3	1.90	0.53
1:C:529:GLY:HA3	1:C:676:ILE:CD1	2.38	0.53
1:D:174:LEU:HD11	1:D:342:VAL:HG22	1.91	0.53
1:A:323:LEU:HB2	1:A:327:TYR:OH	2.08	0.53
1:A:337:PHE:HB3	1:A:340:GLN:HG3	1.90	0.53
1:A:529:GLY:HA3	1:A:676:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:TYR:CE2	1:A:722:SER:HA	2.44	0.53
1:A:708:ILE:HG13	1:A:731:GLN:HB3	1.89	0.53
1:B:610:LYS:CD	1:B:614:ILE:HD11	2.39	0.53
1:C:192:MET:HE1	1:C:315:PRO:HG3	1.89	0.53
1:C:610:LYS:CD	1:C:614:ILE:HD11	2.39	0.53
1:D:715:ILE:HD13	1:D:725:TRP:CE2	2.43	0.53
1:A:160:PRO:HB3	1:A:253:VAL:HG11	1.91	0.53
1:B:160:PRO:HB3	1:B:253:VAL:HG11	1.91	0.53
1:B:179:TYR:HA	1:B:204:ARG:O	2.08	0.53
1:C:179:TYR:HA	1:C:204:ARG:O	2.08	0.53
1:C:323:LEU:HB2	1:C:327:TYR:OH	2.08	0.53
1:C:337:PHE:HB3	1:C:340:GLN:HG3	1.90	0.53
1:D:178:ASN:HB3	1:D:185:PHE:CD1	2.43	0.53
1:D:377:HIS:CD2	1:D:453:ASP:OD1	2.61	0.53
1:D:402:PHE:CE2	1:D:585:PHE:HD1	2.26	0.53
1:A:107:SER:HB2	1:A:361:THR:HB	1.90	0.53
1:A:377:HIS:CD2	1:A:453:ASP:OD1	2.61	0.53
1:C:402:PHE:CE2	1:C:585:PHE:HD1	2.26	0.53
1:C:625:TYR:CE2	1:C:722:SER:HA	2.44	0.53
1:C:657:ASN:OD1	1:C:660:VAL:HG23	2.07	0.53
1:D:59:LYS:O	1:D:60:ALA:C	2.46	0.53
1:D:529:GLY:HA3	1:D:676:ILE:CD1	2.38	0.53
1:C:715:ILE:HD13	1:C:725:TRP:CE2	2.43	0.53
1:D:107:SER:HB2	1:D:361:THR:HB	1.90	0.53
1:A:402:PHE:CE2	1:A:585:PHE:HD1	2.26	0.53
1:B:377:HIS:CD2	1:B:453:ASP:OD1	2.61	0.53
1:C:614:ILE:O	1:C:617:LYS:HB2	2.08	0.53
1:A:178:ASN:HB3	1:A:185:PHE:CD1	2.43	0.53
1:A:690:VAL:CG2	1:A:738:THR:HG21	2.38	0.53
1:B:715:ILE:HD13	1:B:725:TRP:CE2	2.44	0.53
1:C:107:SER:HB2	1:C:361:THR:HB	1.90	0.53
1:A:179:TYR:HA	1:A:204:ARG:O	2.08	0.52
1:B:314:PRO:HG3	1:B:328:ASN:HA	1.91	0.52
1:C:174:LEU:HD11	1:C:342:VAL:HG22	1.91	0.52
1:C:239:VAL:HG12	1:C:240:LYS:N	2.25	0.52
1:A:368:PRO:HD2	1:B:663:MET:SD	2.49	0.52
1:B:465:ASP:HB2	1:B:534:ARG:HG3	1.91	0.52
1:A:181:ARG:HG2	1:A:183:GLU:CA	2.38	0.52
1:A:465:ASP:HB2	1:A:534:ARG:HG3	1.92	0.52
1:B:174:LEU:HD11	1:B:342:VAL:HG22	1.91	0.52
1:A:314:PRO:HG3	1:A:328:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:HB3	1:C:253:VAL:HG11	1.91	0.52
1:D:110:LEU:CD2	1:D:358:VAL:HG22	2.40	0.52
1:A:543:THR:C	1:A:544:ASN:HD22	2.13	0.52
1:B:110:LEU:CD2	1:B:358:VAL:HG22	2.40	0.52
1:B:269:THR:OG1	1:B:433:GLU:OE2	2.27	0.52
1:C:369:ASP:OD1	1:D:663:MET:HG2	2.08	0.52
1:C:465:ASP:HB2	1:C:534:ARG:HG3	1.91	0.52
1:D:239:VAL:HG12	1:D:240:LYS:N	2.24	0.52
1:B:616:MET:O	1:B:619:PRO:HD3	2.10	0.52
1:C:246:TRP:HD1	1:C:565:PHE:HB3	1.75	0.52
1:C:275:ASN:HD22	1:C:277:TYR:H	1.58	0.52
1:A:616:MET:O	1:A:619:PRO:HD3	2.10	0.52
1:D:275:ASN:HD22	1:D:277:TYR:H	1.58	0.52
1:D:610:LYS:CD	1:D:614:ILE:HD11	2.39	0.52
1:D:616:MET:O	1:D:619:PRO:HD3	2.10	0.52
1:C:239:VAL:HG11	1:C:246:TRP:HB3	1.92	0.51
1:C:269:THR:OG1	1:C:433:GLU:OE2	2.27	0.51
1:A:110:LEU:CD2	1:A:358:VAL:HG22	2.40	0.51
1:A:239:VAL:HG11	1:A:246:TRP:HB3	1.92	0.51
1:A:273:PRO:HA	1:A:433:GLU:OE1	2.10	0.51
1:B:424:GLU:HA	1:B:428:LEU:HA	1.92	0.51
1:C:314:PRO:HG3	1:C:328:ASN:HA	1.91	0.51
1:C:529:GLY:CA	1:C:676:ILE:HD11	2.41	0.51
1:C:737:PHE:CE1	1:D:273:PRO:HG2	2.45	0.51
1:D:186:PHE:C	1:D:188:LEU:H	2.13	0.51
1:D:246:TRP:HD1	1:D:565:PHE:HB3	1.75	0.51
1:A:246:TRP:HD1	1:A:565:PHE:HB3	1.75	0.51
1:D:465:ASP:HB2	1:D:534:ARG:HG3	1.91	0.51
1:A:269:THR:OG1	1:A:433:GLU:OE2	2.27	0.51
1:B:239:VAL:HG12	1:B:240:LYS:N	2.25	0.51
1:C:110:LEU:CD2	1:C:358:VAL:HG22	2.40	0.51
1:C:424:GLU:HA	1:C:428:LEU:HA	1.92	0.51
1:A:272:TYR:O	1:A:436:GLU:OE1	2.28	0.51
1:B:273:PRO:HA	1:B:433:GLU:OE1	2.10	0.51
1:C:178:ASN:HD21	1:C:204:ARG:HH21	1.59	0.51
1:C:273:PRO:HA	1:C:433:GLU:OE1	2.10	0.51
1:D:160:PRO:HB3	1:D:253:VAL:HG11	1.91	0.51
1:D:239:VAL:HG11	1:D:246:TRP:HB3	1.92	0.51
1:D:273:PRO:HA	1:D:433:GLU:OE1	2.10	0.51
1:A:239:VAL:HG12	1:A:240:LYS:N	2.25	0.51
1:B:246:TRP:HD1	1:B:565:PHE:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:TYR:O	1:B:436:GLU:OE1	2.28	0.51
1:C:543:THR:C	1:C:544:ASN:HD22	2.13	0.51
1:C:616:MET:O	1:C:619:PRO:HD3	2.10	0.51
1:D:424:GLU:HA	1:D:428:LEU:HA	1.92	0.51
1:A:128:ILE:HG22	1:A:129:SER:H	1.76	0.51
1:A:145:GLU:HG3	1:A:160:PRO:HG2	1.93	0.51
1:A:529:GLY:CA	1:A:676:ILE:HD11	2.41	0.51
1:B:128:ILE:HG22	1:B:129:SER:H	1.76	0.51
1:C:145:GLU:HB2	1:C:555:VAL:HG21	1.93	0.51
1:D:269:THR:OG1	1:D:433:GLU:OE2	2.27	0.51
1:D:314:PRO:HG3	1:D:328:ASN:HA	1.91	0.51
1:D:543:THR:C	1:D:544:ASN:HD22	2.13	0.51
1:A:128:ILE:HG22	1:A:129:SER:N	2.26	0.51
1:B:275:ASN:HD22	1:B:277:TYR:N	2.09	0.51
1:D:178:ASN:HD21	1:D:204:ARG:HH21	1.59	0.51
1:D:275:ASN:HD22	1:D:277:TYR:N	2.09	0.51
1:B:690:VAL:CG2	1:B:738:THR:HG21	2.38	0.51
1:D:145:GLU:HG3	1:D:160:PRO:HG2	1.93	0.51
1:D:266:ASP:OD1	1:D:267:PRO:HD2	2.11	0.51
1:A:266:ASP:OD1	1:A:267:PRO:HD2	2.11	0.51
1:B:402:PHE:HE2	1:B:585:PHE:CD1	2.29	0.51
1:D:241:SER:O	1:D:243:PRO:CD	2.58	0.51
1:B:543:THR:C	1:B:544:ASN:HD22	2.13	0.50
1:B:626:SER:O	1:B:729:LYS:HD2	2.11	0.50
1:B:715:ILE:HD13	1:B:725:TRP:CZ2	2.46	0.50
1:C:186:PHE:C	1:C:188:LEU:H	2.13	0.50
1:D:242:TYR:HB3	1:D:243:PRO:HD3	1.93	0.50
1:A:626:SER:O	1:A:729:LYS:HD2	2.11	0.50
1:B:145:GLU:HG3	1:B:160:PRO:HG2	1.93	0.50
1:B:239:VAL:HG11	1:B:246:TRP:HB3	1.92	0.50
1:D:272:TYR:O	1:D:436:GLU:OE1	2.28	0.50
1:A:242:TYR:HB3	1:A:243:PRO:HD3	1.94	0.50
1:A:303:GLN:O	1:A:307:GLU:N	2.44	0.50
1:A:424:GLU:HA	1:A:428:LEU:HA	1.92	0.50
1:C:128:ILE:HG22	1:C:129:SER:H	1.76	0.50
1:D:715:ILE:HD13	1:D:725:TRP:CZ2	2.46	0.50
1:B:186:PHE:C	1:B:188:LEU:H	2.13	0.50
1:B:242:TYR:HB3	1:B:243:PRO:HD3	1.94	0.50
1:B:676:ILE:HG23	1:B:688:ARG:HB2	1.94	0.50
1:C:210:ARG:HA	1:C:213:LYS:HG3	1.93	0.50
1:C:310:GLY:H	1:C:333:PHE:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ILE:HG22	1:D:129:SER:N	2.26	0.50
1:D:128:ILE:HG22	1:D:129:SER:H	1.76	0.50
1:D:529:GLY:CA	1:D:676:ILE:HD11	2.41	0.50
1:A:178:ASN:HD21	1:A:204:ARG:HH21	1.59	0.50
1:A:186:PHE:C	1:A:188:LEU:H	2.13	0.50
1:B:497:TRP:CD2	1:B:510:PRO:HB3	2.47	0.50
1:C:128:ILE:HG22	1:C:129:SER:N	2.26	0.50
1:C:272:TYR:O	1:C:436:GLU:OE1	2.28	0.50
1:D:136:ASN:O	1:D:138:ILE:N	2.45	0.50
1:D:210:ARG:HA	1:D:213:LYS:HG3	1.94	0.50
1:D:626:SER:O	1:D:729:LYS:HD2	2.11	0.50
1:A:145:GLU:HB2	1:A:555:VAL:HG21	1.93	0.50
1:A:268:LEU:O	1:A:270:PRO:HD3	2.12	0.50
1:A:275:ASN:HD22	1:A:277:TYR:H	1.58	0.50
1:A:497:TRP:CD2	1:A:510:PRO:HB3	2.47	0.50
1:B:275:ASN:HD22	1:B:277:TYR:H	1.58	0.50
1:B:470:MET:HE1	1:B:587:LEU:HD11	1.94	0.50
1:C:136:ASN:O	1:C:138:ILE:N	2.45	0.50
1:D:145:GLU:HB2	1:D:555:VAL:HG21	1.93	0.50
1:A:297:ILE:HG23	1:A:298:GLY:O	2.12	0.50
1:A:715:ILE:HD13	1:A:725:TRP:CZ2	2.46	0.50
1:B:268:LEU:O	1:B:270:PRO:HD3	2.12	0.50
1:B:529:GLY:CA	1:B:676:ILE:HD11	2.41	0.50
1:C:180:ALA:HB3	1:C:213:LYS:HG2	1.94	0.50
1:C:268:LEU:O	1:C:270:PRO:HD3	2.12	0.50
1:D:128:ILE:CD1	1:D:226:ILE:HD12	2.23	0.50
1:D:192:MET:HE3	1:D:315:PRO:HG3	1.92	0.50
1:D:297:ILE:HG23	1:D:298:GLY:O	2.12	0.50
1:A:242:TYR:HA	1:A:246:TRP:H	1.77	0.50
1:A:676:ILE:HG23	1:A:688:ARG:HB2	1.94	0.50
1:D:325:VAL:HG22	1:D:326:PRO:CD	2.32	0.50
1:D:483:SER:OG	1:D:496:SER:HB2	2.12	0.50
1:A:310:GLY:H	1:A:333:PHE:HA	1.77	0.50
1:A:402:PHE:HE2	1:A:585:PHE:CD1	2.29	0.50
1:B:128:ILE:HG22	1:B:129:SER:N	2.26	0.50
1:B:145:GLU:HB2	1:B:555:VAL:HG21	1.93	0.50
1:C:145:GLU:HG3	1:C:160:PRO:HG2	1.93	0.50
1:C:734:VAL:HG13	1:D:272:TYR:CE2	2.45	0.50
1:D:303:GLN:O	1:D:307:GLU:N	2.44	0.50
1:D:310:GLY:H	1:D:333:PHE:HA	1.77	0.50
1:D:579:VAL:O	1:D:583:MET:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:ILE:HG23	1:D:688:ARG:HB2	1.94	0.50
1:A:483:SER:OG	1:A:496:SER:HB2	2.12	0.49
1:B:180:ALA:HB3	1:B:213:LYS:HG2	1.94	0.49
1:B:297:ILE:CG2	1:B:302:ALA:HB2	2.42	0.49
1:A:275:ASN:HD22	1:A:277:TYR:N	2.09	0.49
1:A:297:ILE:CG2	1:A:302:ALA:HB2	2.42	0.49
1:B:483:SER:OG	1:B:496:SER:HB2	2.12	0.49
1:C:323:LEU:C	1:C:325:VAL:H	2.16	0.49
1:D:323:LEU:C	1:D:325:VAL:H	2.16	0.49
1:B:241:SER:O	1:B:243:PRO:CD	2.57	0.49
1:C:297:ILE:HG23	1:C:298:GLY:O	2.12	0.49
1:C:497:TRP:CD2	1:C:510:PRO:HB3	2.47	0.49
1:C:626:SER:O	1:C:729:LYS:HD2	2.11	0.49
1:A:141:THR:CG2	1:A:142:SER:H	2.25	0.49
1:B:178:ASN:HD21	1:B:204:ARG:HH21	1.59	0.49
1:B:242:TYR:HA	1:B:246:TRP:H	1.77	0.49
1:C:242:TYR:HB3	1:C:243:PRO:HD3	1.94	0.49
1:C:266:ASP:OD1	1:C:267:PRO:HD2	2.11	0.49
1:C:375:GLY:O	1:C:451:ASN:HA	2.13	0.49
1:C:483:SER:OG	1:C:496:SER:HB2	2.12	0.49
1:C:676:ILE:HG23	1:C:688:ARG:HB2	1.94	0.49
1:C:690:VAL:CG2	1:C:738:THR:HG21	2.38	0.49
1:C:715:ILE:HD13	1:C:725:TRP:CZ2	2.46	0.49
1:D:242:TYR:HA	1:D:246:TRP:H	1.77	0.49
1:D:297:ILE:CG2	1:D:302:ALA:HB2	2.42	0.49
1:D:375:GLY:O	1:D:451:ASN:HA	2.13	0.49
1:D:497:TRP:CD2	1:D:510:PRO:HB3	2.47	0.49
1:B:654:ASP:HB2	1:D:591:ILE:CD1	2.34	0.49
1:C:402:PHE:HE2	1:C:585:PHE:CD1	2.29	0.49
1:D:131:ILE:HG22	1:D:132:ASN:N	2.28	0.49
1:D:268:LEU:O	1:D:270:PRO:HD3	2.12	0.49
1:A:131:ILE:HG22	1:A:132:ASN:N	2.28	0.49
1:A:180:ALA:HB3	1:A:213:LYS:HG2	1.94	0.49
1:A:579:VAL:O	1:A:583:MET:HG2	2.12	0.49
1:B:310:GLY:H	1:B:333:PHE:HA	1.77	0.49
1:C:241:SER:O	1:C:243:PRO:CD	2.58	0.49
1:C:297:ILE:CG2	1:C:302:ALA:HB2	2.42	0.49
1:A:375:GLY:O	1:A:451:ASN:HA	2.12	0.49
1:C:275:ASN:HD22	1:C:277:TYR:N	2.09	0.49
1:C:733:TYR:CE1	1:D:278:ALA:HA	2.47	0.49
1:D:603:VAL:HG23	1:D:604:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:O	1:A:138:ILE:N	2.45	0.49
1:A:674:ALA:HB1	1:A:742:ALA:HA	1.95	0.49
1:B:136:ASN:O	1:B:138:ILE:N	2.45	0.49
1:B:297:ILE:HG23	1:B:298:GLY:O	2.12	0.49
1:B:579:VAL:O	1:B:583:MET:HG2	2.12	0.49
1:C:141:THR:CG2	1:C:142:SER:H	2.26	0.49
1:D:58:MET:HA	1:D:585:PHE:CE2	2.48	0.49
1:D:103:PHE:CD1	1:D:400:ARG:HG2	2.48	0.49
1:D:141:THR:CG2	1:D:142:SER:H	2.25	0.49
1:D:402:PHE:HE2	1:D:585:PHE:CD1	2.29	0.49
1:A:210:ARG:HA	1:A:213:LYS:HG3	1.94	0.49
1:B:103:PHE:CD1	1:B:400:ARG:HG2	2.48	0.49
1:B:206:GLY:H	1:B:213:LYS:NZ	2.11	0.49
1:B:266:ASP:OD1	1:B:267:PRO:HD2	2.11	0.49
1:C:579:VAL:O	1:C:583:MET:HG2	2.12	0.49
1:C:603:VAL:HG23	1:C:604:LEU:N	2.28	0.49
1:D:174:LEU:N	1:D:174:LEU:CD1	2.75	0.49
1:A:206:GLY:H	1:A:213:LYS:NZ	2.11	0.49
1:A:236:ALA:HB3	1:A:246:TRP:HZ3	1.78	0.49
1:A:598:ARG:O	1:A:601:ALA:HB3	2.13	0.49
1:C:440:ARG:NH1	1:D:674:ALA:O	2.45	0.49
1:D:359:ILE:CD1	1:D:434:TRP:NE1	2.76	0.49
1:A:128:ILE:CD1	1:A:226:ILE:HD12	2.23	0.48
1:A:602:VAL:HG12	1:A:606:LYS:HE3	1.95	0.48
1:B:323:LEU:C	1:B:325:VAL:H	2.16	0.48
1:B:359:ILE:CD1	1:B:434:TRP:NE1	2.76	0.48
1:B:603:VAL:HG23	1:B:604:LEU:N	2.28	0.48
1:B:674:ALA:HB1	1:B:742:ALA:HA	1.95	0.48
1:C:206:GLY:H	1:C:213:LYS:NZ	2.11	0.48
1:C:598:ARG:O	1:C:601:ALA:HB3	2.13	0.48
1:D:180:ALA:HB3	1:D:213:LYS:HG2	1.94	0.48
1:D:602:VAL:HG12	1:D:606:LYS:HE3	1.95	0.48
1:A:174:LEU:N	1:A:174:LEU:CD1	2.75	0.48
1:B:598:ARG:O	1:B:601:ALA:HB3	2.13	0.48
1:C:245:GLY:O	1:C:246:TRP:HB2	2.13	0.48
1:A:603:VAL:HG23	1:A:604:LEU:N	2.28	0.48
1:B:210:ARG:HA	1:B:213:LYS:HG3	1.94	0.48
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.29	0.48
1:D:598:ARG:O	1:D:601:ALA:HB3	2.13	0.48
1:D:676:ILE:HD12	1:D:676:ILE:N	2.28	0.48
1:A:174:LEU:HA	1:A:200:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:CD2	1:A:289:LEU:HD23	2.44	0.48
1:A:670:PHE:CE2	1:B:444:GLU:OE1	2.66	0.48
1:B:58:MET:HA	1:B:585:PHE:CE2	2.48	0.48
1:B:449:TYR:O	1:B:532:SER:CB	2.62	0.48
1:C:600:TYR:O	1:C:604:LEU:HG	2.14	0.48
1:D:206:GLY:H	1:D:213:LYS:NZ	2.11	0.48
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.29	0.48
1:D:630:ASP:O	1:D:634:SER:N	2.44	0.48
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.29	0.48
1:A:359:ILE:CD1	1:A:434:TRP:NE1	2.76	0.48
1:A:600:TYR:O	1:A:604:LEU:HG	2.14	0.48
1:A:631:SER:O	1:A:634:SER:HB3	2.14	0.48
1:B:422:ASP:O	1:B:430:GLY:HA3	2.13	0.48
1:B:600:TYR:O	1:B:604:LEU:HG	2.14	0.48
1:B:631:SER:O	1:B:634:SER:HB3	2.14	0.48
1:B:676:ILE:N	1:B:676:ILE:HD12	2.28	0.48
1:B:692:TYR:O	1:B:693:ALA:HB2	2.14	0.48
1:C:174:LEU:HA	1:C:200:ILE:O	2.14	0.48
1:C:449:TYR:O	1:C:532:SER:CB	2.62	0.48
1:C:676:ILE:HD12	1:C:676:ILE:N	2.28	0.48
1:D:236:ALA:HB3	1:D:246:TRP:HZ3	1.78	0.48
1:D:245:GLY:O	1:D:246:TRP:HB2	2.13	0.48
1:A:103:PHE:CD1	1:A:400:ARG:HG2	2.48	0.48
1:B:184:ASP:O	1:B:187:LYS:N	2.47	0.48
1:B:375:GLY:O	1:B:451:ASN:HA	2.13	0.48
1:B:732:ILE:CD1	1:B:733:TYR:N	2.75	0.48
1:C:131:ILE:HG22	1:C:132:ASN:N	2.28	0.48
1:C:631:SER:O	1:C:634:SER:HB3	2.14	0.48
1:A:323:LEU:C	1:A:325:VAL:H	2.16	0.48
1:A:595:PHE:HB2	1:A:668:LEU:HG	1.96	0.48
1:A:676:ILE:HD12	1:A:676:ILE:N	2.29	0.48
1:A:692:TYR:O	1:A:693:ALA:HB2	2.14	0.48
1:B:131:ILE:HG22	1:B:132:ASN:N	2.28	0.48
1:B:141:THR:CG2	1:B:142:SER:H	2.25	0.48
1:C:174:LEU:N	1:C:174:LEU:CD1	2.75	0.48
1:C:184:ASP:O	1:C:187:LYS:N	2.47	0.48
1:C:630:ASP:O	1:C:634:SER:N	2.44	0.48
1:C:692:TYR:O	1:C:693:ALA:HB2	2.14	0.48
1:D:600:TYR:O	1:D:604:LEU:HG	2.14	0.48
1:A:689:HIS:HD2	1:A:691:ILE:H	1.62	0.48
1:D:174:LEU:HA	1:D:200:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ALA:CB	1:D:246:TRP:HZ3	2.27	0.48
1:D:422:ASP:O	1:D:430:GLY:HA3	2.13	0.48
1:D:692:TYR:O	1:D:693:ALA:HB2	2.14	0.48
3:U:1:NAG:H62	3:U:2:NAG:C7	2.44	0.48
1:A:140:ASN:HB2	4:A:1760:NAG:C6	2.24	0.48
1:A:179:TYR:N	1:A:179:TYR:CD1	2.82	0.48
1:A:268:LEU:HD13	1:A:280:ARG:HB3	1.96	0.48
1:A:705:PHE:HB3	1:A:708:ILE:CD1	2.44	0.48
1:C:58:MET:HA	1:C:585:PHE:CE2	2.48	0.48
1:C:174:LEU:HD11	1:C:342:VAL:CG2	2.44	0.48
1:C:303:GLN:O	1:C:307:GLU:N	2.44	0.48
1:C:359:ILE:CD1	1:C:434:TRP:NE1	2.76	0.48
1:C:422:ASP:O	1:C:430:GLY:HA3	2.13	0.48
1:C:705:PHE:HB3	1:C:708:ILE:CD1	2.44	0.48
1:D:259:LEU:CD2	1:D:289:LEU:HD23	2.44	0.48
3:K:1:NAG:H62	3:K:2:NAG:C7	2.44	0.48
1:B:236:ALA:HB3	1:B:246:TRP:HZ3	1.78	0.48
1:B:303:GLN:O	1:B:307:GLU:N	2.44	0.48
1:B:689:HIS:HD2	1:B:691:ILE:H	1.62	0.48
1:B:705:PHE:HB3	1:B:708:ILE:CD1	2.44	0.48
1:C:242:TYR:HA	1:C:246:TRP:H	1.77	0.48
1:C:323:LEU:O	1:C:325:VAL:N	2.43	0.48
3:F:1:NAG:H62	3:F:2:NAG:C7	2.44	0.48
1:A:95:GLN:HG2	1:A:99:GLN:OE1	2.14	0.47
1:A:240:LYS:CB	1:A:245:GLY:HA2	2.37	0.47
1:A:422:ASP:O	1:A:430:GLY:HA3	2.13	0.47
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.28	0.47
1:C:179:TYR:CD1	1:C:179:TYR:N	2.82	0.47
1:D:95:GLN:HG2	1:D:99:GLN:OE1	2.14	0.47
1:D:595:PHE:HB2	1:D:668:LEU:HG	1.96	0.47
3:P:1:NAG:H62	3:P:2:NAG:C7	2.44	0.47
1:A:442:LEU:HB3	1:A:530:ILE:HD11	1.96	0.47
1:A:670:PHE:CE2	1:B:444:GLU:CD	2.87	0.47
1:B:602:VAL:HG12	1:B:606:LYS:HE3	1.95	0.47
1:C:236:ALA:CB	1:C:246:TRP:HZ3	2.27	0.47
1:D:184:ASP:O	1:D:187:LYS:N	2.47	0.47
1:D:268:LEU:HD13	1:D:280:ARG:HB3	1.96	0.47
1:D:690:VAL:CG2	1:D:738:THR:HG21	2.38	0.47
1:A:58:MET:HA	1:A:585:PHE:CE2	2.48	0.47
1:A:184:ASP:O	1:A:187:LYS:N	2.47	0.47
1:A:727:GLU:O	1:A:730:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:LEU:HB3	1:B:530:ILE:HD11	1.96	0.47
1:C:103:PHE:CD1	1:C:400:ARG:HG2	2.48	0.47
1:C:236:ALA:HB3	1:C:246:TRP:HZ3	1.78	0.47
1:A:391:GLY:HA3	1:A:453:ASP:O	2.15	0.47
1:B:95:GLN:HG2	1:B:99:GLN:OE1	2.14	0.47
1:B:174:LEU:HA	1:B:200:ILE:O	2.13	0.47
1:C:442:LEU:HB3	1:C:530:ILE:HD11	1.96	0.47
1:C:444:GLU:OE1	1:D:670:PHE:CE2	2.67	0.47
1:C:729:LYS:O	1:C:732:ILE:HG13	2.15	0.47
1:C:732:ILE:CD1	1:C:733:TYR:N	2.75	0.47
1:D:591:ILE:HG22	1:D:592:VAL:N	2.29	0.47
1:A:236:ALA:CB	1:A:246:TRP:HZ3	2.27	0.47
1:A:449:TYR:O	1:A:532:SER:CB	2.62	0.47
1:B:174:LEU:HD11	1:B:342:VAL:CG2	2.44	0.47
1:B:179:TYR:N	1:B:179:TYR:CD1	2.82	0.47
1:B:259:LEU:CD2	1:B:289:LEU:HD23	2.44	0.47
1:B:268:LEU:HD13	1:B:280:ARG:HB3	1.96	0.47
1:B:470:MET:CE	1:B:587:LEU:HD11	2.45	0.47
1:B:595:PHE:HB2	1:B:668:LEU:HG	1.96	0.47
1:B:727:GLU:O	1:B:730:ARG:HB3	2.15	0.47
1:C:674:ALA:HB1	1:C:742:ALA:HA	1.95	0.47
1:C:705:PHE:N	1:C:706:PRO:CD	2.78	0.47
1:D:174:LEU:HD11	1:D:342:VAL:CG2	2.44	0.47
1:D:250:GLY:HA2	1:D:299:TYR:CZ	2.50	0.47
1:D:421:TRP:HH2	1:D:434:TRP:CE3	2.33	0.47
1:D:631:SER:O	1:D:634:SER:HB3	2.14	0.47
1:A:245:GLY:O	1:A:246:TRP:HB2	2.13	0.47
1:A:705:PHE:N	1:A:706:PRO:CD	2.78	0.47
1:B:245:GLY:O	1:B:246:TRP:HB2	2.13	0.47
1:A:174:LEU:HD11	1:A:342:VAL:CG2	2.44	0.47
1:A:428:LEU:HD23	1:A:520:ASP:HA	1.97	0.47
1:A:591:ILE:HG22	1:A:592:VAL:N	2.29	0.47
1:A:729:LYS:O	1:A:732:ILE:HG13	2.15	0.47
1:B:236:ALA:CB	1:B:246:TRP:HZ3	2.27	0.47
1:C:259:LEU:CD2	1:C:289:LEU:HD23	2.44	0.47
1:C:268:LEU:HD13	1:C:280:ARG:HB3	1.96	0.47
1:C:468:PRO:HG2	1:C:603:VAL:HG21	1.97	0.47
1:C:470:MET:CE	1:C:587:LEU:HD11	2.45	0.47
1:C:595:PHE:HB2	1:C:668:LEU:HG	1.96	0.47
1:C:602:VAL:HG12	1:C:606:LYS:HE3	1.95	0.47
1:C:727:GLU:O	1:C:730:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:GLY:HA3	1:D:453:ASP:O	2.15	0.47
1:D:674:ALA:HB1	1:D:742:ALA:HA	1.95	0.47
1:D:705:PHE:HB3	1:D:708:ILE:CD1	2.44	0.47
1:A:241:SER:O	1:A:243:PRO:CD	2.57	0.47
1:A:272:TYR:CE2	1:B:734:VAL:HG13	2.49	0.47
1:B:174:LEU:N	1:B:174:LEU:CD1	2.75	0.47
1:B:250:GLY:HA2	1:B:299:TYR:CZ	2.50	0.47
1:C:133:GLU:O	1:C:134:ASP:HB2	2.15	0.47
1:D:470:MET:CE	1:D:587:LEU:HD11	2.45	0.47
1:A:250:GLY:HA2	1:A:299:TYR:CZ	2.50	0.47
1:A:538:THR:HG23	1:A:539:LYS:N	2.30	0.47
1:A:638:ASN:O	1:A:639:PHE:C	2.53	0.47
1:B:391:GLY:HA3	1:B:453:ASP:O	2.15	0.47
1:C:421:TRP:HH2	1:C:434:TRP:CE3	2.33	0.47
1:D:481:LEU:HA	1:D:481:LEU:HD23	1.70	0.47
1:D:729:LYS:O	1:D:732:ILE:HG13	2.15	0.47
1:A:661:LEU:O	1:A:664:MET:HB2	2.15	0.47
1:B:661:LEU:O	1:B:664:MET:HB2	2.15	0.47
1:D:449:TYR:O	1:D:532:SER:CB	2.62	0.47
1:D:521:PHE:CD1	1:D:521:PHE:C	2.88	0.46
1:D:591:ILE:HG22	1:D:592:VAL:HG23	1.97	0.46
1:B:591:ILE:HG22	1:B:592:VAL:N	2.29	0.46
1:C:95:GLN:HG2	1:C:99:GLN:OE1	2.14	0.46
1:C:140:ASN:HB2	4:C:3760:NAG:C6	2.24	0.46
1:C:250:GLY:HA2	1:C:299:TYR:CZ	2.50	0.46
1:C:521:PHE:CD1	1:C:521:PHE:C	2.88	0.46
1:D:355:ILE:HB	1:D:422:ASP:OD2	2.15	0.46
1:D:442:LEU:HB3	1:D:530:ILE:HD11	1.96	0.46
1:D:727:GLU:O	1:D:730:ARG:HB3	2.15	0.46
1:A:470:MET:CE	1:A:587:LEU:HD11	2.45	0.46
1:B:521:PHE:CD1	1:B:521:PHE:C	2.88	0.46
1:B:676:ILE:HG23	1:B:688:ARG:CB	2.45	0.46
1:B:690:VAL:HG21	1:B:738:THR:CG2	2.41	0.46
1:C:149:PRO:O	1:C:151:TYR:N	2.49	0.46
1:C:470:MET:HE1	1:C:587:LEU:HD11	1.97	0.46
1:D:456:ILE:O	1:D:457:GLU:HG3	2.15	0.46
1:D:515:LEU:HB3	1:D:516:GLY:H	1.49	0.46
1:D:661:LEU:O	1:D:664:MET:HB2	2.15	0.46
1:D:689:HIS:HD2	1:D:691:ILE:H	1.62	0.46
1:A:369:ASP:OD2	1:A:662:ARG:NH2	2.44	0.46
1:A:521:PHE:C	1:A:521:PHE:CD1	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:HD11	1:A:735:ALA:CB	2.46	0.46
1:B:133:GLU:O	1:B:134:ASP:HB2	2.15	0.46
1:B:145:GLU:OE1	1:B:160:PRO:HG3	2.16	0.46
1:B:323:LEU:O	1:B:325:VAL:N	2.43	0.46
1:B:456:ILE:O	1:B:457:GLU:HG3	2.15	0.46
1:B:468:PRO:HG2	1:B:603:VAL:HG21	1.97	0.46
1:B:593:LEU:HA	1:B:594:PRO:HD3	1.64	0.46
1:B:708:ILE:HD11	1:B:735:ALA:CB	2.46	0.46
1:C:145:GLU:OE1	1:C:160:PRO:HG3	2.16	0.46
1:C:428:LEU:HD23	1:C:520:ASP:HA	1.97	0.46
1:C:608:ALA:O	1:C:611:ILE:HG22	2.16	0.46
1:D:179:TYR:N	1:D:179:TYR:CD1	2.82	0.46
1:A:421:TRP:HH2	1:A:434:TRP:CE3	2.33	0.46
1:A:468:PRO:HG2	1:A:603:VAL:HG21	1.97	0.46
1:A:574:LEU:O	1:A:577:ALA:HB3	2.16	0.46
1:A:676:ILE:HG23	1:A:688:ARG:CB	2.45	0.46
1:A:732:ILE:CD1	1:A:733:TYR:N	2.75	0.46
1:B:421:TRP:HH2	1:B:434:TRP:CE3	2.33	0.46
1:C:483:SER:OG	1:C:496:SER:CB	2.64	0.46
1:C:538:THR:HG23	1:C:539:LYS:N	2.30	0.46
1:C:689:HIS:HD2	1:C:691:ILE:H	1.62	0.46
1:D:676:ILE:HG23	1:D:688:ARG:CB	2.45	0.46
1:A:483:SER:OG	1:A:496:SER:CB	2.64	0.46
1:A:654:ASP:C	1:A:656:SER:H	2.19	0.46
1:B:89:ASN:ND2	1:B:422:ASP:OD1	2.49	0.46
1:C:391:GLY:HA3	1:C:453:ASP:O	2.15	0.46
1:C:661:LEU:O	1:C:664:MET:HB2	2.15	0.46
1:D:386:ILE:HA	1:D:390:SER:HB2	1.98	0.46
1:D:538:THR:HG23	1:D:539:LYS:N	2.30	0.46
1:D:658:PRO:O	1:D:661:LEU:HB3	2.16	0.46
1:B:428:LEU:HD23	1:B:520:ASP:HA	1.97	0.46
1:B:450:ILE:HD11	1:B:470:MET:HE1	1.97	0.46
1:B:538:THR:HG23	1:B:539:LYS:N	2.30	0.46
1:B:574:LEU:O	1:B:577:ALA:HB3	2.16	0.46
1:B:729:LYS:O	1:B:732:ILE:HG13	2.15	0.46
1:C:89:ASN:ND2	1:C:422:ASP:OD1	2.49	0.46
1:C:591:ILE:HG22	1:C:592:VAL:N	2.29	0.46
1:D:133:GLU:O	1:D:134:ASP:HB2	2.15	0.46
1:D:178:ASN:HD22	1:D:178:ASN:HA	1.52	0.46
1:D:654:ASP:C	1:D:656:SER:H	2.19	0.46
1:A:106:ASP:OD2	1:A:362:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:HA	1:A:296:PRO:HD3	1.66	0.46
1:B:591:ILE:HG22	1:B:592:VAL:HG23	1.97	0.46
1:C:355:ILE:HB	1:C:422:ASP:OD2	2.15	0.46
1:C:456:ILE:O	1:C:457:GLU:HG3	2.15	0.46
1:D:149:PRO:O	1:D:151:TYR:N	2.49	0.46
1:D:608:ALA:O	1:D:611:ILE:HG22	2.16	0.46
1:A:456:ILE:O	1:A:457:GLU:HG3	2.15	0.46
1:A:658:PRO:O	1:A:661:LEU:HB3	2.16	0.46
1:B:65:LEU:HD22	1:B:397:GLU:HG3	1.98	0.46
1:B:149:PRO:O	1:B:151:TYR:N	2.49	0.46
1:B:483:SER:OG	1:B:496:SER:CB	2.64	0.46
1:B:705:PHE:N	1:B:706:PRO:CD	2.78	0.46
1:D:65:LEU:HD22	1:D:397:GLU:HG3	1.98	0.46
1:D:145:GLU:OE1	1:D:160:PRO:HG3	2.16	0.46
1:D:468:PRO:HG2	1:D:603:VAL:HG21	1.97	0.46
1:A:146:PRO:HA	1:A:147:PRO:HD2	1.82	0.46
1:A:355:ILE:HB	1:A:422:ASP:OD2	2.16	0.46
1:A:386:ILE:HA	1:A:390:SER:HB2	1.98	0.46
1:B:214:VAL:HG21	1:B:258:ILE:HG21	1.98	0.46
1:B:658:PRO:O	1:B:661:LEU:HB3	2.16	0.46
1:C:386:ILE:HA	1:C:390:SER:HB2	1.98	0.46
1:C:708:ILE:HD11	1:C:735:ALA:CB	2.46	0.46
1:D:106:ASP:OD2	1:D:362:LEU:HD12	2.16	0.46
1:A:89:ASN:ND2	1:A:422:ASP:OD1	2.49	0.45
1:A:149:PRO:O	1:A:151:TYR:N	2.49	0.45
1:A:214:VAL:HG21	1:A:258:ILE:HG21	1.98	0.45
1:B:325:VAL:HG22	1:B:326:PRO:CD	2.32	0.45
1:B:608:ALA:O	1:B:611:ILE:HG22	2.16	0.45
1:C:627:VAL:HG21	1:C:725:TRP:HE3	1.81	0.45
1:D:483:SER:OG	1:D:496:SER:CB	2.64	0.45
1:A:133:GLU:O	1:A:134:ASP:HB2	2.15	0.45
1:A:608:ALA:O	1:A:611:ILE:HG22	2.16	0.45
1:A:663:MET:HG2	1:B:369:ASP:OD1	2.12	0.45
1:B:308:LYS:HD3	1:B:337:PHE:CD2	2.52	0.45
1:C:65:LEU:HD22	1:C:397:GLU:HG3	1.98	0.45
1:C:574:LEU:O	1:C:577:ALA:HB3	2.16	0.45
1:D:140:ASN:HB2	4:D:4760:NAG:C6	2.24	0.45
1:A:591:ILE:HG22	1:A:592:VAL:HG23	1.98	0.45
1:A:630:ASP:O	1:A:634:SER:N	2.44	0.45
1:C:240:LYS:CB	1:C:245:GLY:HA2	2.37	0.45
1:D:89:ASN:ND2	1:D:422:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:O	1:A:469:LEU:N	2.49	0.45
1:A:479:LYS:HG2	1:A:494:TYR:CG	2.52	0.45
1:B:131:ILE:HD12	1:B:136:ASN:HA	1.99	0.45
1:B:467:THR:HG21	1:B:531:ALA:HB1	1.99	0.45
1:B:575:THR:O	1:B:576:VAL:C	2.54	0.45
1:B:708:ILE:HD11	1:B:735:ALA:HB2	1.99	0.45
1:C:177:VAL:O	1:C:178:ASN:C	2.55	0.45
1:C:593:LEU:HA	1:C:594:PRO:HD3	1.64	0.45
1:C:638:ASN:O	1:C:639:PHE:C	2.53	0.45
1:C:676:ILE:HG23	1:C:688:ARG:CB	2.45	0.45
1:C:708:ILE:HD11	1:C:735:ALA:HB2	1.99	0.45
1:D:214:VAL:HG21	1:D:258:ILE:HG21	1.98	0.45
1:D:240:LYS:H	1:D:240:LYS:CD	2.25	0.45
1:A:165:SER:OG	1:A:293:PRO:HA	2.17	0.45
1:B:240:LYS:CB	1:B:245:GLY:HA2	2.37	0.45
1:B:369:ASP:OD2	1:B:662:ARG:NH2	2.44	0.45
1:B:479:LYS:HG2	1:B:494:TYR:CG	2.52	0.45
1:B:610:LYS:HD2	1:B:614:ILE:HD11	1.98	0.45
1:C:308:LYS:HD3	1:C:337:PHE:CD2	2.52	0.45
1:D:441:LEU:O	1:D:445:ARG:N	2.50	0.45
1:D:732:ILE:CD1	1:D:733:TYR:N	2.75	0.45
1:A:131:ILE:HD12	1:A:136:ASN:HA	1.99	0.45
1:A:450:ILE:HD11	1:A:470:MET:HE1	1.99	0.45
1:A:610:LYS:HD2	1:A:614:ILE:HD11	1.98	0.45
1:B:177:VAL:O	1:B:178:ASN:C	2.55	0.45
1:B:355:ILE:HB	1:B:422:ASP:OD2	2.16	0.45
1:C:189:GLU:HB3	1:C:194:ILE:HB	1.98	0.45
1:C:214:VAL:HG21	1:C:258:ILE:HG21	1.98	0.45
1:C:658:PRO:O	1:C:661:LEU:HB3	2.16	0.45
1:D:574:LEU:O	1:D:577:ALA:HB3	2.16	0.45
1:D:638:ASN:O	1:D:639:PHE:C	2.53	0.45
1:A:145:GLU:OE1	1:A:160:PRO:HG3	2.16	0.45
1:A:308:LYS:HD3	1:A:337:PHE:CD2	2.52	0.45
1:A:441:LEU:O	1:A:445:ARG:N	2.50	0.45
1:A:690:VAL:HG21	1:A:738:THR:CG2	2.41	0.45
1:B:638:ASN:O	1:B:639:PHE:C	2.53	0.45
1:C:151:TYR:HB3	1:C:154:VAL:HG21	1.99	0.45
1:C:160:PRO:HB3	1:C:253:VAL:CG1	2.47	0.45
1:D:65:LEU:CD2	1:D:397:GLU:HG3	2.47	0.45
1:D:131:ILE:HD12	1:D:136:ASN:HA	1.99	0.45
1:D:467:THR:O	1:D:469:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:MET:O	1:D:570:PHE:HB2	2.16	0.45
1:A:65:LEU:HD22	1:A:397:GLU:HG3	1.98	0.45
1:A:151:TYR:HB3	1:A:154:VAL:HG21	1.99	0.45
1:A:538:THR:HG23	1:A:539:LYS:O	2.17	0.45
1:B:106:ASP:OD2	1:B:362:LEU:HD12	2.16	0.45
1:B:189:GLU:HB3	1:B:194:ILE:HB	1.98	0.45
1:B:240:LYS:H	1:B:240:LYS:CD	2.25	0.45
1:B:387:ASP:HA	1:B:388:PRO:HA	1.84	0.45
1:C:106:ASP:OD2	1:C:362:LEU:HD12	2.16	0.45
1:C:450:ILE:HD11	1:C:470:MET:HE1	1.98	0.45
1:C:467:THR:O	1:C:469:LEU:N	2.49	0.45
1:C:675:PHE:O	1:C:690:VAL:HG23	2.17	0.45
1:A:160:PRO:HB3	1:A:253:VAL:CG1	2.47	0.45
1:B:242:TYR:HD2	1:B:556:TYR:HD2	1.65	0.45
1:C:65:LEU:CD2	1:C:397:GLU:HG3	2.47	0.45
1:D:160:PRO:HB3	1:D:253:VAL:CG1	2.47	0.45
1:D:314:PRO:CG	1:D:327:TYR:O	2.65	0.45
1:D:575:THR:O	1:D:576:VAL:C	2.54	0.45
1:D:708:ILE:HD11	1:D:735:ALA:CB	2.46	0.45
1:A:189:GLU:HB3	1:A:194:ILE:HB	1.97	0.45
1:B:160:PRO:HB3	1:B:253:VAL:CG1	2.47	0.45
1:C:610:LYS:HD2	1:C:614:ILE:HD11	1.98	0.45
1:D:369:ASP:OD2	1:D:662:ARG:NH2	2.44	0.45
1:A:314:PRO:CG	1:A:327:TYR:O	2.65	0.44
1:B:107:SER:O	1:B:108:VAL:CG2	2.66	0.44
1:C:441:LEU:O	1:C:445:ARG:N	2.50	0.44
1:C:569:MET:O	1:C:570:PHE:HB2	2.16	0.44
1:D:182:THR:OG1	1:D:185:PHE:CE1	2.67	0.44
1:D:675:PHE:O	1:D:690:VAL:HG23	2.17	0.44
1:A:569:MET:O	1:A:570:PHE:HB2	2.16	0.44
1:B:182:THR:O	1:B:183:GLU:CB	2.65	0.44
1:B:212:ASN:O	1:B:213:LYS:C	2.56	0.44
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.82	0.44
1:B:386:ILE:HA	1:B:390:SER:HB2	1.98	0.44
1:C:107:SER:O	1:C:108:VAL:CG2	2.66	0.44
1:C:314:PRO:CG	1:C:327:TYR:O	2.65	0.44
1:C:591:ILE:HG22	1:C:592:VAL:HG23	1.97	0.44
1:C:654:ASP:C	1:C:656:SER:H	2.19	0.44
1:C:663:MET:SD	1:D:368:PRO:HD2	2.56	0.44
1:D:107:SER:O	1:D:108:VAL:CG2	2.66	0.44
1:D:428:LEU:HD23	1:D:520:ASP:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:LYS:HG2	1:D:494:TYR:CG	2.52	0.44
1:D:538:THR:HG23	1:D:539:LYS:O	2.17	0.44
1:A:78:THR:HG21	1:A:559:TYR:HB2	1.99	0.44
1:A:323:LEU:O	1:A:325:VAL:N	2.43	0.44
1:B:165:SER:OG	1:B:293:PRO:HA	2.17	0.44
1:C:292:ILE:HD13	1:C:292:ILE:H	1.83	0.44
1:C:575:THR:O	1:C:576:VAL:C	2.54	0.44
1:D:177:VAL:O	1:D:178:ASN:C	2.55	0.44
1:D:189:GLU:HB3	1:D:194:ILE:HB	1.98	0.44
1:D:272:TYR:HA	1:D:273:PRO:HD3	1.77	0.44
1:A:242:TYR:HD2	1:A:556:TYR:HD2	1.65	0.44
1:A:245:GLY:O	1:A:246:TRP:HB3	2.18	0.44
1:A:515:LEU:HB3	1:A:516:GLY:H	1.49	0.44
1:A:708:ILE:HD11	1:A:735:ALA:HB2	1.99	0.44
1:B:78:THR:HG21	1:B:559:TYR:HB2	1.99	0.44
1:B:569:MET:O	1:B:570:PHE:HB2	2.16	0.44
1:C:78:THR:HG21	1:C:559:TYR:HB2	1.99	0.44
1:D:151:TYR:HB3	1:D:154:VAL:HG21	1.99	0.44
1:D:165:SER:OG	1:D:293:PRO:HA	2.17	0.44
1:A:65:LEU:CD2	1:A:397:GLU:HG3	2.47	0.44
1:A:77:PHE:HB2	1:A:389:GLN:HG3	1.99	0.44
1:A:182:THR:O	1:A:183:GLU:CB	2.65	0.44
1:B:65:LEU:CD2	1:B:397:GLU:HG3	2.47	0.44
1:B:151:TYR:HB3	1:B:154:VAL:HG21	1.99	0.44
1:B:165:SER:HA	1:B:166:PRO:HD3	1.83	0.44
1:B:538:THR:HG23	1:B:539:LYS:O	2.17	0.44
1:C:725:TRP:O	1:C:729:LYS:HB2	2.18	0.44
1:D:78:THR:HG21	1:D:559:TYR:HB2	1.99	0.44
1:A:212:ASN:O	1:A:213:LYS:C	2.56	0.44
1:A:656:SER:HB3	1:C:591:ILE:HD12	2.00	0.44
1:B:245:GLY:O	1:B:246:TRP:HB3	2.18	0.44
1:B:314:PRO:CG	1:B:327:TYR:O	2.65	0.44
1:B:441:LEU:O	1:B:445:ARG:N	2.50	0.44
1:B:467:THR:O	1:B:469:LEU:N	2.49	0.44
1:B:654:ASP:C	1:B:656:SER:H	2.19	0.44
1:B:675:PHE:O	1:B:690:VAL:HG23	2.17	0.44
1:C:151:TYR:N	1:C:151:TYR:CD1	2.86	0.44
1:C:212:ASN:O	1:C:213:LYS:C	2.56	0.44
1:C:325:VAL:HG22	1:C:326:PRO:CD	2.32	0.44
1:C:538:THR:HG23	1:C:539:LYS:O	2.17	0.44
1:D:105:LEU:HD23	1:D:105:LEU:HA	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:ILE:HD11	1:D:470:MET:HE1	2.00	0.44
1:D:610:LYS:HD2	1:D:614:ILE:HD11	1.98	0.44
1:A:107:SER:O	1:A:108:VAL:CG2	2.66	0.44
1:A:212:ASN:O	1:A:216:ASN:N	2.44	0.44
1:A:306:LEU:O	1:A:309:MET:HB3	2.18	0.44
1:A:675:PHE:O	1:A:690:VAL:HG23	2.17	0.44
1:D:129:SER:O	1:D:342:VAL:HA	2.18	0.44
1:D:708:ILE:HD11	1:D:735:ALA:HB2	1.99	0.44
1:D:725:TRP:O	1:D:729:LYS:HB2	2.18	0.44
1:A:627:VAL:HG21	1:A:725:TRP:HE3	1.81	0.44
1:B:306:LEU:O	1:B:309:MET:HB3	2.18	0.44
1:C:369:ASP:OD2	1:C:662:ARG:NH2	2.44	0.44
1:C:467:THR:HG21	1:C:531:ALA:HB1	1.98	0.44
1:D:192:MET:O	1:D:193:LYS:C	2.56	0.44
1:A:458:GLY:HA2	3:H:1:NAG:H81	2.00	0.44
1:B:107:SER:O	1:B:108:VAL:HG23	2.18	0.44
1:C:131:ILE:HD12	1:C:136:ASN:HA	1.99	0.44
1:C:306:LEU:O	1:C:309:MET:HB3	2.18	0.44
4:C:3760:NAG:H83	4:C:3760:NAG:H3	2.00	0.44
1:D:467:THR:HG21	1:D:531:ALA:HB1	1.99	0.44
1:A:107:SER:O	1:A:108:VAL:HG23	2.18	0.43
1:A:129:SER:O	1:A:342:VAL:HA	2.18	0.43
1:A:467:THR:HG21	1:A:531:ALA:HB1	1.99	0.43
1:B:141:THR:HG23	1:B:142:SER:H	1.83	0.43
1:B:698:ASN:ND2	1:B:701:ALA:O	2.51	0.43
1:C:107:SER:O	1:C:108:VAL:HG23	2.18	0.43
1:C:240:LYS:H	1:C:240:LYS:CD	2.25	0.43
1:C:245:GLY:O	1:C:246:TRP:HB3	2.18	0.43
1:C:479:LYS:HG2	1:C:494:TYR:CG	2.52	0.43
1:C:593:LEU:C	1:C:595:PHE:H	2.22	0.43
1:C:698:ASN:ND2	1:C:701:ALA:O	2.51	0.43
1:D:206:GLY:H	1:D:213:LYS:HZ1	1.66	0.43
1:D:295:HIS:HA	1:D:296:PRO:HD3	1.66	0.43
1:B:151:TYR:N	1:B:151:TYR:CD1	2.86	0.43
1:C:165:SER:OG	1:C:293:PRO:HA	2.17	0.43
1:C:458:GLY:HA2	3:R:1:NAG:H81	2.00	0.43
1:D:141:THR:HG23	1:D:142:SER:H	1.83	0.43
1:D:306:LEU:O	1:D:309:MET:HB3	2.18	0.43
1:D:308:LYS:HD3	1:D:337:PHE:CD2	2.52	0.43
1:D:593:LEU:C	1:D:595:PHE:H	2.22	0.43
1:D:618:HIS:HE1	1:D:716:GLU:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HD13	1:A:292:ILE:H	1.83	0.43
1:A:386:ILE:HG22	1:A:454:SER:HB3	1.99	0.43
1:A:698:ASN:ND2	1:A:701:ALA:O	2.51	0.43
1:B:77:PHE:HB2	1:B:389:GLN:HG3	1.99	0.43
1:B:275:ASN:HD22	1:B:275:ASN:C	2.22	0.43
1:C:114:ASP:O	1:C:274:ALA:HB1	2.18	0.43
1:C:129:SER:O	1:C:342:VAL:HA	2.18	0.43
1:D:245:GLY:O	1:D:246:TRP:HB3	2.18	0.43
1:D:292:ILE:HD13	1:D:292:ILE:H	1.83	0.43
1:A:132:ASN:O	1:A:134:ASP:N	2.51	0.43
1:B:212:ASN:O	1:B:216:ASN:N	2.44	0.43
1:C:181:ARG:HD3	1:C:216:ASN:HD22	1.82	0.43
1:D:107:SER:O	1:D:108:VAL:HG23	2.18	0.43
1:D:250:GLY:HA2	1:D:299:TYR:CE1	2.54	0.43
1:D:449:TYR:HE2	1:D:521:PHE:HA	1.83	0.43
1:A:114:ASP:O	1:A:274:ALA:HB1	2.18	0.43
1:A:151:TYR:N	1:A:151:TYR:CD1	2.86	0.43
1:A:275:ASN:HD22	1:A:275:ASN:C	2.22	0.43
1:A:618:HIS:HE1	1:A:716:GLU:HG2	1.84	0.43
1:B:140:ASN:HB2	4:B:2760:NAG:C6	2.24	0.43
1:B:413:ARG:HG2	1:B:413:ARG:HH11	1.84	0.43
1:B:449:TYR:HE2	1:B:521:PHE:HA	1.83	0.43
1:C:575:THR:O	1:C:578:GLN:N	2.51	0.43
1:C:605:ARG:HG2	1:C:605:ARG:HH11	1.84	0.43
1:D:181:ARG:HD3	1:D:216:ASN:HD22	1.82	0.43
1:D:182:THR:O	1:D:183:GLU:CB	2.65	0.43
1:D:323:LEU:O	1:D:325:VAL:N	2.43	0.43
1:A:141:THR:HG23	1:A:142:SER:H	1.83	0.43
1:A:192:MET:O	1:A:193:LYS:C	2.57	0.43
1:B:59:LYS:O	1:B:61:PHE:N	2.51	0.43
1:B:240:LYS:C	1:B:245:GLY:HA2	2.39	0.43
1:B:382:VAL:CG2	1:B:383:PHE:N	2.68	0.43
1:B:618:HIS:HE1	1:B:716:GLU:HG2	1.84	0.43
1:C:132:ASN:O	1:C:134:ASP:N	2.51	0.43
1:C:146:PRO:HA	1:C:147:PRO:HD2	1.82	0.43
1:D:114:ASP:O	1:D:274:ALA:HB1	2.18	0.43
1:D:386:ILE:HG22	1:D:454:SER:HB3	1.99	0.43
1:D:427:GLY:C	1:D:429:LEU:H	2.22	0.43
1:D:443:GLN:O	1:D:673:ARG:NH1	2.46	0.43
1:D:605:ARG:HH11	1:D:605:ARG:HG2	1.84	0.43
1:B:129:SER:O	1:B:342:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LYS:O	1:C:61:PHE:N	2.51	0.43
1:C:192:MET:O	1:C:193:LYS:C	2.57	0.43
1:C:295:HIS:HA	1:C:296:PRO:HD3	1.66	0.43
1:D:151:TYR:N	1:D:151:TYR:CD1	2.86	0.43
1:D:575:THR:O	1:D:578:GLN:N	2.51	0.43
1:D:690:VAL:HG21	1:D:738:THR:CG2	2.41	0.43
1:D:698:ASN:ND2	1:D:701:ALA:O	2.51	0.43
1:A:56:HIS:O	1:A:57:ASN:CB	2.67	0.43
1:A:59:LYS:O	1:A:61:PHE:N	2.51	0.43
1:A:206:GLY:H	1:A:213:LYS:HZ1	1.66	0.43
1:A:575:THR:O	1:A:578:GLN:N	2.51	0.43
1:A:733:TYR:CD1	1:B:278:ALA:HA	2.54	0.43
1:B:593:LEU:C	1:B:595:PHE:H	2.22	0.43
1:B:630:ASP:O	1:B:634:SER:N	2.44	0.43
1:B:725:TRP:O	1:B:729:LYS:HB2	2.18	0.43
1:C:438:ASN:O	1:C:439:SER:C	2.57	0.43
1:A:240:LYS:C	1:A:245:GLY:HA2	2.39	0.43
1:A:250:GLY:HA2	1:A:299:TYR:CE1	2.54	0.43
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.19	0.43
1:A:725:TRP:O	1:A:729:LYS:HB2	2.18	0.43
1:B:114:ASP:O	1:B:274:ALA:HB1	2.18	0.43
1:B:292:ILE:H	1:B:292:ILE:HD13	1.83	0.43
1:B:438:ASN:O	1:B:439:SER:C	2.57	0.43
1:C:141:THR:HG23	1:C:142:SER:H	1.83	0.43
1:C:386:ILE:HG22	1:C:454:SER:HB3	1.99	0.43
1:C:506:PHE:O	1:C:508:GLY:N	2.52	0.43
1:D:229:SER:HB3	1:D:234:TYR:CE1	2.53	0.43
1:D:275:ASN:HD22	1:D:275:ASN:C	2.22	0.43
1:D:438:ASN:O	1:D:439:SER:C	2.57	0.43
2:L:1:NAG:O3	2:L:2:NDG:N2	2.52	0.43
1:A:178:ASN:O	1:A:179:TYR:C	2.58	0.43
1:A:718:LYS:HG2	1:A:724:ALA:HB2	2.01	0.43
4:A:1760:NAG:H3	4:A:1760:NAG:H83	2.00	0.43
1:B:192:MET:O	1:B:193:LYS:C	2.56	0.43
1:B:205:TYR:HA	1:B:213:LYS:HZ3	1.83	0.43
1:B:412:PRO:HA	1:B:589:ASN:OD1	2.19	0.43
1:B:458:GLY:HA2	3:M:1:NAG:H81	2.00	0.43
1:B:575:THR:O	1:B:578:GLN:N	2.51	0.43
4:B:2760:NAG:H83	4:B:2760:NAG:H3	2.00	0.43
1:C:618:HIS:HE1	1:C:716:GLU:HG2	1.84	0.43
1:D:412:PRO:HA	1:D:589:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.84	0.43
1:A:174:LEU:CD1	1:A:342:VAL:HG22	2.49	0.42
1:B:506:PHE:C	1:B:508:GLY:H	2.22	0.42
1:C:182:THR:O	1:C:182:THR:HG22	2.19	0.42
1:C:275:ASN:HD22	1:C:275:ASN:C	2.22	0.42
1:C:657:ASN:HA	1:C:658:PRO:HD2	1.88	0.42
1:D:59:LYS:O	1:D:61:PHE:N	2.51	0.42
1:D:192:MET:HE1	1:D:315:PRO:HG3	2.00	0.42
1:D:634:SER:O	1:D:637:LYS:N	2.52	0.42
1:A:158:VAL:HA	1:A:159:PRO:HD3	1.87	0.42
1:A:181:ARG:HD3	1:A:216:ASN:HD22	1.82	0.42
1:A:410:TRP:CH2	1:A:412:PRO:HG3	2.54	0.42
1:A:478:THR:OG1	1:A:493:LEU:HD13	2.19	0.42
1:A:575:THR:O	1:A:576:VAL:C	2.54	0.42
1:B:443:GLN:O	1:B:673:ARG:NH1	2.46	0.42
1:B:671:LEU:O	1:B:674:ALA:HB3	2.19	0.42
1:C:413:ARG:HG2	1:C:413:ARG:HH11	1.84	0.42
1:D:56:HIS:O	1:D:57:ASN:CB	2.67	0.42
1:D:182:THR:O	1:D:182:THR:HG22	2.19	0.42
1:D:253:VAL:HG11	1:D:296:PRO:HB2	2.01	0.42
1:D:506:PHE:O	1:D:508:GLY:N	2.52	0.42
4:D:4760:NAG:H3	4:D:4760:NAG:H83	2.00	0.42
1:A:387:ASP:HA	1:A:388:PRO:HA	1.84	0.42
1:B:178:ASN:O	1:B:179:TYR:C	2.58	0.42
1:B:192:MET:HE3	1:B:315:PRO:HG3	2.02	0.42
1:B:410:TRP:CH2	1:B:412:PRO:HG3	2.54	0.42
1:C:240:LYS:C	1:C:245:GLY:HA2	2.39	0.42
1:C:250:GLY:HA2	1:C:299:TYR:CE1	2.54	0.42
1:C:275:ASN:ND2	1:C:278:ALA:N	2.68	0.42
1:C:718:LYS:HG2	1:C:724:ALA:HB2	2.01	0.42
2:T:1:NAG:O3	2:T:2:NDG:C1	2.67	0.42
1:B:253:VAL:HG11	1:B:296:PRO:HB2	2.01	0.42
1:B:386:ILE:HG22	1:B:454:SER:HB3	1.99	0.42
1:B:605:ARG:HG2	1:B:605:ARG:HH11	1.84	0.42
1:B:634:SER:O	1:B:637:LYS:N	2.53	0.42
1:B:718:LYS:HG2	1:B:724:ALA:HB2	2.01	0.42
1:B:732:ILE:HD12	1:B:733:TYR:CA	2.50	0.42
1:C:77:PHE:HB2	1:C:389:GLN:HG3	1.98	0.42
1:C:111:ALA:HB3	1:C:357:ASN:HB2	2.01	0.42
1:C:515:LEU:HB3	1:C:516:GLY:H	1.49	0.42
1:A:321:GLY:N	1:A:327:TYR:CZ	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:LEU:C	1:A:595:PHE:H	2.22	0.42
1:A:634:SER:O	1:A:637:LYS:N	2.53	0.42
1:B:506:PHE:O	1:B:508:GLY:N	2.52	0.42
1:C:365:ALA:HB2	1:C:411:ARG:HB2	2.02	0.42
1:C:671:LEU:O	1:C:674:ALA:HB3	2.19	0.42
1:D:127:TYR:HH	1:D:345:HIS:CE1	2.37	0.42
1:D:240:LYS:CB	1:D:245:GLY:HA2	2.37	0.42
1:D:242:TYR:HD2	1:D:556:TYR:HD2	1.65	0.42
1:D:708:ILE:O	1:D:711:ALA:HB3	2.19	0.42
2:E:1:NAG:O3	2:E:2:NDG:C1	2.67	0.42
1:A:261:LEU:HD13	1:A:265:GLY:O	2.19	0.42
1:A:365:ALA:HB2	1:A:411:ARG:HB2	2.02	0.42
1:A:506:PHE:O	1:A:508:GLY:N	2.52	0.42
1:A:708:ILE:O	1:A:711:ALA:HB3	2.19	0.42
1:B:250:GLY:HA2	1:B:299:TYR:CE1	2.54	0.42
1:B:732:ILE:HD12	1:B:732:ILE:C	2.40	0.42
1:C:382:VAL:CG2	1:C:383:PHE:N	2.68	0.42
1:C:506:PHE:C	1:C:508:GLY:H	2.22	0.42
1:C:670:PHE:CE2	1:D:444:GLU:CD	2.93	0.42
1:D:544:ASN:HD22	1:D:544:ASN:N	2.17	0.42
1:D:671:LEU:O	1:D:674:ALA:HB3	2.19	0.42
1:D:718:LYS:HG2	1:D:724:ALA:HB2	2.01	0.42
2:J:1:NAG:O3	2:J:2:NDG:C1	2.67	0.42
1:A:177:VAL:O	1:A:178:ASN:C	2.55	0.42
1:A:427:GLY:C	1:A:429:LEU:H	2.22	0.42
1:B:83:LEU:O	1:B:86:THR:HG23	2.20	0.42
1:B:335:GLY:C	1:B:337:PHE:N	2.73	0.42
1:B:708:ILE:O	1:B:711:ALA:HB3	2.19	0.42
1:C:174:LEU:CD1	1:C:342:VAL:HG22	2.49	0.42
1:C:182:THR:O	1:C:183:GLU:CB	2.65	0.42
1:C:527:ARG:HD2	1:C:686:PHE:HB3	2.02	0.42
1:D:132:ASN:O	1:D:134:ASP:N	2.51	0.42
1:D:335:GLY:C	1:D:337:PHE:N	2.73	0.42
1:D:478:THR:OG1	1:D:493:LEU:HD13	2.20	0.42
2:G:1:NAG:O3	2:G:2:NDG:N2	2.52	0.42
1:A:182:THR:O	1:A:182:THR:HG22	2.19	0.42
1:A:275:ASN:ND2	1:A:278:ALA:N	2.68	0.42
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.84	0.42
1:B:97:GLN:HG3	1:B:108:VAL:HG12	2.02	0.42
1:B:137:GLU:O	1:B:139:PHE:N	2.53	0.42
1:B:381:TRP:NE1	1:B:425:GLU:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:HIS:O	1:C:57:ASN:CB	2.67	0.42
1:C:321:GLY:N	1:C:327:TYR:CZ	2.88	0.42
1:C:708:ILE:O	1:C:711:ALA:HB3	2.19	0.42
1:D:83:LEU:O	1:D:86:THR:HG23	2.20	0.42
1:D:178:ASN:O	1:D:179:TYR:C	2.58	0.42
1:D:239:VAL:HG12	1:D:240:LYS:H	1.85	0.42
1:A:282:GLY:O	1:A:283:ILE:C	2.58	0.42
1:A:381:TRP:NE1	1:A:425:GLU:HB3	2.35	0.42
1:B:181:ARG:HD3	1:B:216:ASN:HD22	1.82	0.42
1:B:248:LEU:HA	1:B:249:PRO:HD3	1.88	0.42
1:B:427:GLY:C	1:B:429:LEU:H	2.22	0.42
1:B:527:ARG:HD2	1:B:686:PHE:HB3	2.02	0.42
1:C:206:GLY:H	1:C:213:LYS:HZ1	1.66	0.42
1:C:229:SER:HB3	1:C:234:TYR:CE1	2.53	0.42
1:C:412:PRO:HA	1:C:589:ASN:OD1	2.19	0.42
1:C:449:TYR:HE2	1:C:521:PHE:HA	1.83	0.42
1:D:174:LEU:CD1	1:D:342:VAL:HG22	2.49	0.42
1:D:410:TRP:CH2	1:D:412:PRO:HG3	2.54	0.42
2:O:1:NAG:O3	2:O:2:NDG:C1	2.67	0.42
2:V:1:NAG:O3	2:V:2:NDG:N2	2.51	0.42
1:A:165:SER:HA	1:A:166:PRO:HD3	1.83	0.42
1:A:438:ASN:O	1:A:439:SER:C	2.56	0.42
1:A:449:TYR:HE2	1:A:521:PHE:HA	1.83	0.42
1:A:470:MET:HE1	1:A:587:LEU:HD11	2.01	0.42
1:A:732:ILE:HD12	1:A:733:TYR:CA	2.50	0.42
1:B:365:ALA:HB2	1:B:411:ARG:HB2	2.02	0.42
1:B:544:ASN:HD22	1:B:544:ASN:N	2.17	0.42
1:B:555:VAL:C	1:B:557:GLU:H	2.23	0.42
1:C:178:ASN:O	1:C:179:TYR:C	2.58	0.42
1:C:277:TYR:OH	1:D:737:PHE:HA	2.20	0.42
1:D:212:ASN:O	1:D:216:ASN:N	2.44	0.42
1:D:240:LYS:C	1:D:245:GLY:HA2	2.39	0.42
1:A:111:ALA:HB3	1:A:357:ASN:HB2	2.01	0.41
1:B:182:THR:O	1:B:182:THR:HG22	2.19	0.41
1:B:478:THR:OG1	1:B:493:LEU:HD13	2.19	0.41
1:C:106:ASP:CG	1:C:411:ARG:HH22	2.24	0.41
1:C:370:ARG:HG2	1:C:370:ARG:NH1	2.35	0.41
1:C:427:GLY:C	1:C:429:LEU:H	2.22	0.41
1:D:330:GLY:HA2	1:D:331:PRO:HD3	1.79	0.41
1:D:527:ARG:HD2	1:D:686:PHE:HB3	2.02	0.41
1:A:240:LYS:H	1:A:240:LYS:CD	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLY:O	1:A:284:ALA:N	2.53	0.41
1:B:56:HIS:O	1:B:57:ASN:CB	2.67	0.41
1:B:146:PRO:HA	1:B:147:PRO:HD2	1.82	0.41
1:B:174:LEU:CD1	1:B:342:VAL:HG22	2.49	0.41
1:B:507:SER:C	1:B:509:MET:H	2.24	0.41
1:C:335:GLY:C	1:C:337:PHE:N	2.73	0.41
1:C:634:SER:O	1:C:637:LYS:N	2.53	0.41
1:D:111:ALA:HB3	1:D:357:ASN:HB2	2.01	0.41
1:D:275:ASN:ND2	1:D:278:ALA:N	2.68	0.41
1:D:715:ILE:CD1	1:D:725:TRP:CE2	3.03	0.41
1:A:83:LEU:O	1:A:86:THR:HG23	2.20	0.41
1:A:506:PHE:C	1:A:508:GLY:H	2.22	0.41
1:A:544:ASN:HD22	1:A:544:ASN:N	2.17	0.41
1:A:555:VAL:C	1:A:557:GLU:H	2.23	0.41
1:A:605:ARG:HG2	1:A:605:ARG:HH11	1.84	0.41
1:A:671:LEU:O	1:A:674:ALA:HB3	2.19	0.41
1:A:715:ILE:CD1	1:A:725:TRP:CE2	3.03	0.41
1:A:732:ILE:HD12	1:A:732:ILE:C	2.40	0.41
1:B:242:TYR:CG	1:B:243:PRO:N	2.87	0.41
1:B:282:GLY:O	1:B:283:ILE:C	2.58	0.41
1:C:261:LEU:HD13	1:C:265:GLY:O	2.19	0.41
1:C:272:TYR:HA	1:C:273:PRO:HD3	1.77	0.41
1:C:410:TRP:CH2	1:C:412:PRO:HG3	2.54	0.41
1:D:212:ASN:O	1:D:213:LYS:C	2.56	0.41
1:D:248:LEU:HA	1:D:249:PRO:HD3	1.88	0.41
1:D:261:LEU:HD13	1:D:265:GLY:O	2.19	0.41
1:D:337:PHE:CB	1:D:340:GLN:HG3	2.50	0.41
1:D:365:ALA:HB2	1:D:411:ARG:HB2	2.02	0.41
1:D:627:VAL:HG21	1:D:725:TRP:HE3	1.81	0.41
1:A:137:GLU:O	1:A:139:PHE:N	2.53	0.41
1:B:106:ASP:CG	1:B:411:ARG:HH22	2.24	0.41
1:B:111:ALA:HB3	1:B:357:ASN:HB2	2.01	0.41
1:B:239:VAL:HG12	1:B:240:LYS:H	1.85	0.41
1:B:321:GLY:N	1:B:327:TYR:CZ	2.88	0.41
1:B:470:MET:O	1:B:474:VAL:HG23	2.21	0.41
1:D:282:GLY:O	1:D:284:ALA:N	2.53	0.41
1:D:321:GLY:N	1:D:327:TYR:CZ	2.88	0.41
1:D:458:GLY:HA2	3:W:1:NAG:H81	2.00	0.41
1:D:470:MET:O	1:D:474:VAL:HG23	2.21	0.41
2:J:1:NAG:HO3	2:J:2:NDG:C1	2.32	0.41
1:A:113:TYR:O	1:A:355:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HD12	1:A:297:ILE:HD13	2.02	0.41
1:A:734:VAL:HG13	1:B:272:TYR:CE2	2.55	0.41
1:B:282:GLY:O	1:B:284:ALA:N	2.53	0.41
1:B:488:PHE:HE2	1:B:499:LYS:HD2	1.85	0.41
1:B:627:VAL:HG21	1:B:725:TRP:HE3	1.81	0.41
1:C:83:LEU:O	1:C:86:THR:HG23	2.20	0.41
1:C:337:PHE:CB	1:C:340:GLN:HG3	2.50	0.41
1:C:478:THR:OG1	1:C:493:LEU:HD13	2.19	0.41
1:D:488:PHE:HE2	1:D:499:LYS:HD2	1.85	0.41
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.70	0.41
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.56	0.41
1:A:693:ALA:HB3	1:A:706:PRO:HG2	2.03	0.41
1:B:526:GLN:HE21	1:B:692:TYR:C	2.24	0.41
1:C:108:VAL:HG22	1:C:360:GLY:HA2	2.03	0.41
1:C:282:GLY:O	1:C:284:ALA:N	2.53	0.41
1:C:687:TYR:CZ	1:C:694:PRO:HG2	2.56	0.41
1:D:506:PHE:C	1:D:508:GLY:H	2.22	0.41
1:A:97:GLN:HG3	1:A:108:VAL:HG12	2.02	0.41
1:A:229:SER:HB3	1:A:234:TYR:CE1	2.53	0.41
1:A:253:VAL:HG11	1:A:296:PRO:HB2	2.01	0.41
1:A:370:ARG:NH1	1:A:370:ARG:HG2	2.35	0.41
1:A:470:MET:O	1:A:474:VAL:HG23	2.21	0.41
1:A:610:LYS:HD3	1:A:614:ILE:HD11	2.03	0.41
1:B:261:LEU:HD13	1:B:265:GLY:O	2.19	0.41
1:C:544:ASN:HD22	1:C:544:ASN:N	2.17	0.41
1:D:108:VAL:HG22	1:D:360:GLY:HA2	2.03	0.41
1:D:137:GLU:O	1:D:139:PHE:N	2.53	0.41
1:D:370:ARG:NH1	1:D:370:ARG:HG2	2.35	0.41
1:D:377:HIS:CE1	1:D:424:GLU:OE1	2.74	0.41
1:D:555:VAL:C	1:D:557:GLU:H	2.23	0.41
1:D:611:ILE:HA	1:D:614:ILE:HG12	2.03	0.41
1:A:239:VAL:HG12	1:A:240:LYS:H	1.85	0.41
1:A:427:GLY:C	1:A:429:LEU:N	2.74	0.41
1:B:275:ASN:ND2	1:B:278:ALA:N	2.68	0.41
1:B:377:HIS:CE1	1:B:424:GLU:OE1	2.74	0.41
1:C:127:TYR:HH	1:C:345:HIS:CE1	2.38	0.41
1:C:377:HIS:CE1	1:C:424:GLU:OE1	2.74	0.41
1:C:555:VAL:C	1:C:557:GLU:H	2.23	0.41
1:C:705:PHE:HB3	1:C:708:ILE:HD13	2.03	0.41
1:D:128:ILE:HD12	1:D:297:ILE:HD13	2.02	0.41
1:D:732:ILE:HD12	1:D:732:ILE:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CB	1:A:340:GLN:HG3	2.50	0.41
1:A:449:TYR:HE2	1:A:521:PHE:CA	2.34	0.41
1:A:488:PHE:HE2	1:A:499:LYS:HD2	1.85	0.41
1:A:527:ARG:HD2	1:A:686:PHE:HB3	2.02	0.41
1:B:128:ILE:HD12	1:B:297:ILE:HD13	2.02	0.41
1:B:687:TYR:CZ	1:B:694:PRO:HG2	2.56	0.41
1:B:705:PHE:HB3	1:B:708:ILE:HD13	2.03	0.41
1:C:137:GLU:O	1:C:139:PHE:N	2.53	0.41
1:C:192:MET:HE3	1:C:315:PRO:HG3	2.03	0.41
1:C:230:ASP:HA	1:C:231:PRO:HD3	1.91	0.41
1:C:253:VAL:HG11	1:C:296:PRO:HB2	2.01	0.41
1:C:275:ASN:C	1:C:275:ASN:ND2	2.74	0.41
1:C:381:TRP:NE1	1:C:425:GLU:HB3	2.35	0.41
1:C:470:MET:O	1:C:474:VAL:HG23	2.21	0.41
1:C:505:GLU:OE1	1:C:606:LYS:HE2	2.21	0.41
1:C:567:ASP:CG	1:C:570:PHE:HA	2.41	0.41
1:D:97:GLN:HG3	1:D:108:VAL:HG12	2.02	0.41
1:D:106:ASP:CG	1:D:411:ARG:HH22	2.24	0.41
1:D:282:GLY:O	1:D:283:ILE:C	2.58	0.41
1:D:681:LEU:HD23	1:D:681:LEU:HA	1.86	0.41
1:A:567:ASP:CG	1:A:570:PHE:HA	2.41	0.41
1:A:697:HIS:CG	1:A:713:PHE:CD2	3.09	0.41
1:A:705:PHE:HB3	1:A:708:ILE:HD13	2.03	0.41
1:B:164:PHE:CD1	1:B:259:LEU:HG	2.56	0.41
1:B:275:ASN:C	1:B:275:ASN:ND2	2.75	0.41
1:B:295:HIS:HA	1:B:296:PRO:HD3	1.66	0.41
1:B:370:ARG:NH1	1:B:370:ARG:HG2	2.35	0.41
1:B:516:GLY:O	1:B:517:SER:O	2.39	0.41
1:B:698:ASN:ND2	1:B:701:ALA:C	2.75	0.41
1:C:128:ILE:HD12	1:C:297:ILE:HD13	2.02	0.41
1:C:205:TYR:HA	1:C:213:LYS:HZ3	1.86	0.41
1:C:427:GLY:C	1:C:429:LEU:N	2.74	0.41
1:C:516:GLY:O	1:C:517:SER:O	2.39	0.41
1:C:611:ILE:HA	1:C:614:ILE:HG12	2.03	0.41
1:C:715:ILE:CD1	1:C:725:TRP:CE2	3.03	0.41
1:C:732:ILE:HD12	1:C:732:ILE:C	2.40	0.41
1:D:381:TRP:NE1	1:D:425:GLU:HB3	2.35	0.41
1:D:657:ASN:HA	1:D:658:PRO:HD2	1.88	0.41
1:D:687:TYR:CZ	1:D:694:PRO:HG2	2.56	0.41
1:D:732:ILE:HD12	1:D:733:TYR:CA	2.50	0.41
1:A:108:VAL:HG22	1:A:360:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:C	1:A:275:ASN:ND2	2.75	0.40
1:B:115:VAL:CG1	1:B:116:LEU:N	2.84	0.40
1:B:337:PHE:CB	1:B:340:GLN:HG3	2.50	0.40
1:C:164:PHE:CD1	1:C:259:LEU:HG	2.56	0.40
1:C:539:LYS:H	1:C:539:LYS:HG2	1.74	0.40
1:C:728:VAL:C	1:C:730:ARG:N	2.75	0.40
1:D:275:ASN:C	1:D:275:ASN:ND2	2.74	0.40
1:D:449:TYR:HE2	1:D:521:PHE:CA	2.34	0.40
1:D:698:ASN:ND2	1:D:701:ALA:C	2.74	0.40
1:A:362:LEU:HD12	1:A:362:LEU:HA	1.82	0.40
1:A:377:HIS:CE1	1:A:424:GLU:OE1	2.74	0.40
1:A:526:GLN:HE21	1:A:692:TYR:C	2.24	0.40
1:A:749:VAL:HG12	1:B:445:ARG:NH2	2.35	0.40
1:B:113:TYR:O	1:B:355:ILE:HG12	2.21	0.40
1:B:693:ALA:HB3	1:B:706:PRO:HG2	2.03	0.40
1:C:79:GLN:C	1:C:80:ILE:HD13	2.42	0.40
1:C:507:SER:C	1:C:509:MET:H	2.23	0.40
1:C:693:ALA:HB3	1:C:706:PRO:HG2	2.03	0.40
1:C:697:HIS:CG	1:C:713:PHE:CD2	3.09	0.40
1:C:732:ILE:HD12	1:C:733:TYR:CA	2.50	0.40
1:C:743:ALA:C	1:C:745:THR:N	2.75	0.40
1:D:427:GLY:C	1:D:429:LEU:N	2.74	0.40
1:D:728:VAL:C	1:D:730:ARG:N	2.75	0.40
2:Q:1:NAG:O3	2:Q:2:NDG:N2	2.52	0.40
1:A:127:TYR:HH	1:A:345:HIS:CE1	2.39	0.40
1:A:164:PHE:CD1	1:A:259:LEU:HG	2.56	0.40
1:A:382:VAL:CG2	1:A:383:PHE:N	2.68	0.40
1:A:443:GLN:O	1:A:673:ARG:NH1	2.46	0.40
1:A:662:ARG:O	1:A:663:MET:C	2.59	0.40
1:A:743:ALA:C	1:A:745:THR:N	2.75	0.40
1:B:79:GLN:C	1:B:80:ILE:HD13	2.42	0.40
1:B:697:HIS:CG	1:B:713:PHE:CD2	3.09	0.40
1:B:715:ILE:CD1	1:B:725:TRP:CE2	3.03	0.40
4:B:2759:NAG:O7	4:B:2759:NAG:O3	2.32	0.40
1:C:97:GLN:HG3	1:C:108:VAL:HG12	2.02	0.40
1:C:163:ALA:HB3	1:C:257:ASN:HA	2.04	0.40
1:C:367:GLU:N	1:C:368:PRO:HD3	2.37	0.40
1:C:449:TYR:HE2	1:C:521:PHE:CA	2.34	0.40
1:C:488:PHE:HE2	1:C:499:LYS:HD2	1.85	0.40
1:C:526:GLN:HE21	1:C:692:TYR:C	2.24	0.40
1:C:681:LEU:HD23	1:C:681:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLN:C	1:D:80:ILE:HD13	2.42	0.40
1:D:262:ASN:O	1:D:687:TYR:CZ	2.75	0.40
1:D:697:HIS:CG	1:D:713:PHE:CD2	3.09	0.40
2:E:1:NAG:HO3	2:E:2:NDG:C1	2.34	0.40
1:A:272:TYR:HA	1:A:273:PRO:HD3	1.77	0.40
1:A:427:GLY:O	1:A:429:LEU:N	2.55	0.40
1:B:83:LEU:HB3	1:B:86:THR:HG23	2.04	0.40
1:B:158:VAL:HA	1:B:159:PRO:HD3	1.86	0.40
1:B:611:ILE:HA	1:B:614:ILE:HG12	2.03	0.40
1:C:113:TYR:O	1:C:355:ILE:HG12	2.21	0.40
1:C:242:TYR:CG	1:C:243:PRO:N	2.87	0.40
1:C:282:GLY:O	1:C:283:ILE:C	2.58	0.40
1:D:113:TYR:O	1:D:355:ILE:HG12	2.21	0.40
1:D:164:PHE:CD1	1:D:259:LEU:HG	2.56	0.40
1:D:516:GLY:O	1:D:517:SER:O	2.39	0.40
1:A:106:ASP:CG	1:A:411:ARG:HH22	2.24	0.40
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.88	0.40
1:A:397:GLU:OE2	1:A:400:ARG:NH2	2.55	0.40
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.66	0.40
1:B:272:TYR:HA	1:B:273:PRO:HD3	1.77	0.40
1:B:427:GLY:O	1:B:429:LEU:N	2.55	0.40
1:B:515:LEU:HB3	1:B:516:GLY:H	1.49	0.40
1:B:551:LEU:HD13	1:B:561:LEU:CD2	2.52	0.40
1:B:676:ILE:HA	1:B:688:ARG:O	2.21	0.40
1:C:158:VAL:HA	1:C:159:PRO:HD3	1.87	0.40
1:C:239:VAL:HG12	1:C:240:LYS:H	1.85	0.40
1:C:690:VAL:HG21	1:C:738:THR:CG2	2.42	0.40
1:D:236:ALA:HA	1:D:237:PRO:HD3	1.92	0.40
1:D:552:TYR:O	1:D:557:GLU:OE1	2.40	0.40
1:D:567:ASP:CG	1:D:570:PHE:HA	2.41	0.40

All (26) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:SER:OG	1:D:506:PHE:CE2[1_455]	0.99	1.21
1:C:507:SER:CB	1:D:506:PHE:CZ[1_455]	1.07	1.13
1:C:505:GLU:CA	1:D:507:SER:OG[1_455]	1.09	1.11
1:A:506:PHE:CZ	1:B:507:SER:OG[1_455]	1.18	1.02
1:C:505:GLU:N	1:D:507:SER:OG[1_455]	1.23	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:SER:OG	1:D:506:PHE:CZ[1_455]	1.37	0.83
1:A:506:PHE:CZ	1:B:507:SER:CB[1_455]	1.44	0.76
1:A:244:ASP:OD1	1:B:94:LYS:NZ[2_555]	1.49	0.71
2:G:2:NDG:C6	3:M:2:NAG:C8[2_655]	1.54	0.66
1:C:507:SER:CB	1:D:506:PHE:CE1[1_455]	1.55	0.65
1:A:508:GLY:CA	1:B:505:GLU:O[1_455]	1.63	0.57
1:C:505:GLU:O	1:D:508:GLY:N[1_455]	1.65	0.55
1:C:505:GLU:O	1:D:508:GLY:CA[1_455]	1.71	0.49
1:C:505:GLU:O	1:D:507:SER:C[1_455]	1.76	0.44
1:A:244:ASP:CG	1:B:94:LYS:NZ[2_555]	1.84	0.36
1:C:505:GLU:CB	1:D:507:SER:OG[1_455]	1.84	0.36
1:A:244:ASP:OD2	1:B:94:LYS:NZ[2_555]	1.85	0.35
1:A:506:PHE:CE2	1:B:507:SER:OG[1_455]	1.85	0.35
1:C:505:GLU:O	1:D:507:SER:O[1_455]	1.86	0.34
1:A:506:PHE:CE1	1:B:507:SER:CB[1_455]	1.90	0.30
1:C:507:SER:CB	1:D:506:PHE:CE2[1_455]	1.95	0.25
1:A:508:GLY:N	1:B:505:GLU:O[1_455]	1.98	0.22
1:C:505:GLU:CA	1:D:507:SER:CB[1_455]	1.98	0.22
1:A:334:THR:CG2	1:D:320:ARG:NH1[1_454]	1.99	0.21
1:C:507:SER:OG	1:D:506:PHE:CD2[1_455]	2.12	0.08
1:A:334:THR:CG2	1:D:320:ARG:CZ[1_454]	2.18	0.02

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	693/695 (100%)	534 (77%)	115 (17%)	44 (6%)	1	14
1	B	693/695 (100%)	533 (77%)	116 (17%)	44 (6%)	1	14
1	C	693/695 (100%)	533 (77%)	116 (17%)	44 (6%)	1	14
1	D	693/695 (100%)	532 (77%)	117 (17%)	44 (6%)	1	14
All	All	2772/2780 (100%)	2132 (77%)	464 (17%)	176 (6%)	1	14

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	138	ILE
1	A	149	PRO
1	A	179	TYR
1	A	183	GLU
1	A	222	ALA
1	A	242	TYR
1	A	262	ASN
1	A	283	ILE
1	A	315	PRO
1	A	330	GLY
1	A	517	SER
1	A	547	SER
1	A	552	TYR
1	B	137	GLU
1	B	138	ILE
1	B	149	PRO
1	B	179	TYR
1	B	183	GLU
1	B	222	ALA
1	B	242	TYR
1	B	262	ASN
1	B	283	ILE
1	B	315	PRO
1	B	330	GLY
1	B	517	SER
1	B	547	SER
1	B	552	TYR
1	C	137	GLU
1	C	138	ILE
1	C	149	PRO
1	C	179	TYR
1	C	183	GLU
1	C	222	ALA
1	C	242	TYR
1	C	262	ASN
1	C	283	ILE
1	C	315	PRO
1	C	330	GLY
1	C	517	SER
1	C	547	SER
1	C	552	TYR

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Mol	Chain	Res	Type
1	D	137	GLU
1	D	138	ILE
1	D	149	PRO
1	D	179	TYR
1	D	183	GLU
1	D	222	ALA
1	D	242	TYR
1	D	262	ASN
1	D	283	ILE
1	D	315	PRO
1	D	330	GLY
1	D	517	SER
1	D	547	SER
1	D	552	TYR
1	A	150	GLY
1	A	181	ARG
1	A	192	MET
1	A	193	LYS
1	A	210	ARG
1	A	246	TRP
1	A	263	GLY
1	A	332	GLY
1	A	440	ARG
1	A	507	SER
1	A	556	TYR
1	A	591	ILE
1	B	150	GLY
1	B	181	ARG
1	B	192	MET
1	B	193	LYS
1	B	210	ARG
1	B	246	TRP
1	B	263	GLY
1	B	332	GLY
1	B	440	ARG
1	B	507	SER
1	B	556	TYR
1	B	591	ILE
1	C	150	GLY
1	C	181	ARG
1	C	192	MET
1	C	193	LYS

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Mol	Chain	Res	Type
1	C	210	ARG
1	C	246	TRP
1	C	263	GLY
1	C	332	GLY
1	C	440	ARG
1	C	507	SER
1	C	556	TYR
1	C	591	ILE
1	D	150	GLY
1	D	181	ARG
1	D	192	MET
1	D	193	LYS
1	D	210	ARG
1	D	246	TRP
1	D	263	GLY
1	D	332	GLY
1	D	440	ARG
1	D	507	SER
1	D	556	TYR
1	D	591	ILE
1	A	57	ASN
1	A	324	LYS
1	A	382	VAL
1	A	520	ASP
1	B	57	ASN
1	B	324	LYS
1	B	382	VAL
1	B	520	ASP
1	B	551	LEU
1	C	57	ASN
1	C	324	LYS
1	C	382	VAL
1	C	520	ASP
1	C	551	LEU
1	D	57	ASN
1	D	324	LYS
1	D	382	VAL
1	D	520	ASP
1	D	551	LEU
1	A	133	GLU
1	A	180	ALA
1	A	428	LEU

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Mol	Chain	Res	Type
1	A	457	GLU
1	A	515	LEU
1	A	551	LEU
1	A	594	PRO
1	B	133	GLU
1	B	180	ALA
1	B	428	LEU
1	B	457	GLU
1	B	515	LEU
1	B	594	PRO
1	C	133	GLU
1	C	180	ALA
1	C	428	LEU
1	C	457	GLU
1	C	515	LEU
1	D	133	GLU
1	D	180	ALA
1	D	428	LEU
1	D	457	GLU
1	D	515	LEU
1	A	60	ALA
1	A	139	PHE
1	B	60	ALA
1	B	139	PHE
1	C	60	ALA
1	C	139	PHE
1	C	594	PRO
1	D	60	ALA
1	D	139	PHE
1	D	594	PRO
1	A	655	LYS
1	B	655	LYS
1	C	655	LYS
1	D	655	LYS
1	A	243	PRO
1	B	243	PRO
1	C	243	PRO
1	D	243	PRO
1	A	690	VAL
1	B	690	VAL
1	C	690	VAL
1	D	690	VAL

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Mol	Chain	Res	Type
1	A	108	VAL
1	A	468	PRO
1	B	108	VAL
1	B	468	PRO
1	C	108	VAL
1	C	468	PRO
1	D	108	VAL
1	D	468	PRO

5.3.2 Protein sidechains (i)

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	592/592 (100%)	553 (93%)	39 (7%)	16	49
1	B	592/592 (100%)	553 (93%)	39 (7%)	16	49
1	C	592/592 (100%)	552 (93%)	40 (7%)	16	48
1	D	592/592 (100%)	553 (93%)	39 (7%)	16	49
All	All	2368/2368 (100%)	2211 (93%)	157 (7%)	16	49

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	149	PRO
1	A	154	VAL
1	A	178	ASN
1	A	179	TYR
1	A	186	PHE
1	A	229	SER
1	A	234	TYR
1	A	255	ARG
1	A	260	ASN
1	A	266	ASP
1	A	275	ASN
1	A	292	ILE

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Mol	Chain	Res	Type
1	A	297	ILE
1	A	301	ASP
1	A	315	PRO
1	A	325	VAL
1	A	370	ARG
1	A	388	PRO
1	A	440	ARG
1	A	461	THR
1	A	467	THR
1	A	475	HIS
1	A	484	PRO
1	A	493	LEU
1	A	509	MET
1	A	519	ASN
1	A	523	VAL
1	A	526	GLN
1	A	534	ARG
1	A	537	TYR
1	A	538	THR
1	A	541	TRP
1	A	563	GLU
1	A	600	TYR
1	A	631	SER
1	A	668	LEU
1	A	671	LEU
1	A	731	GLN
1	B	63	ASP
1	B	149	PRO
1	B	154	VAL
1	B	178	ASN
1	B	179	TYR
1	B	186	PHE
1	B	229	SER
1	B	234	TYR
1	B	255	ARG
1	B	260	ASN
1	B	266	ASP
1	B	275	ASN
1	B	292	ILE
1	B	297	ILE
1	B	301	ASP
1	B	315	PRO

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Mol	Chain	Res	Type
1	B	325	VAL
1	B	370	ARG
1	B	388	PRO
1	B	440	ARG
1	B	461	THR
1	B	467	THR
1	B	475	HIS
1	B	484	PRO
1	B	493	LEU
1	B	509	MET
1	B	519	ASN
1	B	523	VAL
1	B	526	GLN
1	B	534	ARG
1	B	537	TYR
1	B	538	THR
1	B	541	TRP
1	B	563	GLU
1	B	600	TYR
1	B	631	SER
1	B	668	LEU
1	B	671	LEU
1	B	731	GLN
1	C	63	ASP
1	C	149	PRO
1	C	154	VAL
1	C	178	ASN
1	C	179	TYR
1	C	186	PHE
1	C	229	SER
1	C	234	TYR
1	C	255	ARG
1	C	260	ASN
1	C	266	ASP
1	C	275	ASN
1	C	292	ILE
1	C	297	ILE
1	C	301	ASP
1	C	315	PRO
1	C	325	VAL
1	C	370	ARG
1	C	388	PRO

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Mol	Chain	Res	Type
1	C	440	ARG
1	C	461	THR
1	C	467	THR
1	C	475	HIS
1	C	478	THR
1	C	484	PRO
1	C	493	LEU
1	C	509	MET
1	C	519	ASN
1	C	523	VAL
1	C	526	GLN
1	C	534	ARG
1	C	537	TYR
1	C	538	THR
1	C	541	TRP
1	C	563	GLU
1	C	600	TYR
1	C	631	SER
1	C	668	LEU
1	C	671	LEU
1	C	731	GLN
1	D	63	ASP
1	D	149	PRO
1	D	154	VAL
1	D	178	ASN
1	D	179	TYR
1	D	186	PHE
1	D	229	SER
1	D	234	TYR
1	D	255	ARG
1	D	260	ASN
1	D	266	ASP
1	D	275	ASN
1	D	292	ILE
1	D	297	ILE
1	D	301	ASP
1	D	315	PRO
1	D	325	VAL
1	D	370	ARG
1	D	388	PRO
1	D	440	ARG
1	D	461	THR

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Mol	Chain	Res	Type
1	D	467	THR
1	D	475	HIS
1	D	484	PRO
1	D	493	LEU
1	D	509	MET
1	D	519	ASN
1	D	523	VAL
1	D	526	GLN
1	D	534	ARG
1	D	537	TYR
1	D	538	THR
1	D	541	TRP
1	D	563	GLU
1	D	600	TYR
1	D	631	SER
1	D	668	LEU
1	D	671	LEU
1	D	731	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	97	GLN
1	A	112	HIS
1	A	178	ASN
1	A	216	ASN
1	A	275	ASN
1	A	303	GLN
1	A	347	HIS
1	A	438	ASN
1	A	544	ASN
1	A	618	HIS
1	A	689	HIS
1	A	697	HIS
1	A	731	GLN
1	B	82	HIS
1	B	97	GLN
1	B	112	HIS
1	B	178	ASN
1	B	216	ASN
1	B	275	ASN

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Mol	Chain	Res	Type
1	B	303	GLN
1	B	347	HIS
1	B	438	ASN
1	B	544	ASN
1	B	618	HIS
1	B	689	HIS
1	B	731	GLN
1	C	82	HIS
1	C	97	GLN
1	C	112	HIS
1	C	178	ASN
1	C	216	ASN
1	C	275	ASN
1	C	303	GLN
1	C	347	HIS
1	C	438	ASN
1	C	544	ASN
1	C	618	HIS
1	C	689	HIS
1	C	697	HIS
1	C	731	GLN
1	D	82	HIS
1	D	97	GLN
1	D	112	HIS
1	D	178	ASN
1	D	216	ASN
1	D	275	ASN
1	D	303	GLN
1	D	347	HIS
1	D	438	ASN
1	D	544	ASN
1	D	618	HIS
1	D	689	HIS
1	D	731	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

40 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	0.79	0	17,19,21	1.06	2 (11%)
2	NDG	E	2	2	14,14,15	0.72	0	17,19,21	0.66	0
3	NAG	F	1	1,3	14,14,15	0.71	0	17,19,21	0.77	0
3	NAG	F	2	3	14,14,15	0.77	0	17,19,21	0.81	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.65	0	17,19,21	0.93	0
2	NDG	G	2	2	14,14,15	0.66	0	17,19,21	0.60	0
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	0.92	1 (5%)
3	NAG	H	2	3	14,14,15	0.59	0	17,19,21	0.73	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.61	0	17,19,21	0.94	1 (5%)
3	NAG	I	2	3	14,14,15	0.51	0	17,19,21	0.66	0
2	NAG	J	1	1,2	14,14,15	0.79	0	17,19,21	1.07	2 (11%)
2	NDG	J	2	2	14,14,15	0.72	0	17,19,21	0.66	0
3	NAG	K	1	1,3	14,14,15	0.71	0	17,19,21	0.77	0
3	NAG	K	2	3	14,14,15	0.77	0	17,19,21	0.81	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.65	0	17,19,21	0.93	0
2	NDG	L	2	2	14,14,15	0.66	0	17,19,21	0.60	0
3	NAG	M	1	1,3	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
3	NAG	M	2	3	14,14,15	0.59	0	17,19,21	0.73	1 (5%)
3	NAG	N	1	1,3	14,14,15	0.61	0	17,19,21	0.94	1 (5%)
3	NAG	N	2	3	14,14,15	0.51	0	17,19,21	0.66	0
2	NAG	O	1	1,2	14,14,15	0.79	0	17,19,21	1.06	2 (11%)
2	NDG	O	2	2	14,14,15	0.74	0	17,19,21	0.65	0
3	NAG	P	1	1,3	14,14,15	0.71	0	17,19,21	0.76	0
3	NAG	P	2	3	14,14,15	0.78	0	17,19,21	0.81	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.65	0	17,19,21	0.93	0
2	NDG	Q	2	2	14,14,15	0.65	0	17,19,21	0.60	0
3	NAG	R	1	1,3	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
3	NAG	R	2	3	14,14,15	0.58	0	17,19,21	0.73	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.61	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	S	2	3	14,14,15	0.52	0	17,19,21	0.67	1 (5%)
2	NAG	T	1	1,2	14,14,15	0.79	0	17,19,21	1.06	2 (11%)
2	NDG	T	2	2	14,14,15	0.72	0	17,19,21	0.65	0
3	NAG	U	1	1,3	14,14,15	0.71	0	17,19,21	0.77	0
3	NAG	U	2	3	14,14,15	0.78	0	17,19,21	0.81	1 (5%)
2	NAG	V	1	1,2	14,14,15	0.66	0	17,19,21	0.93	0
2	NDG	V	2	2	14,14,15	0.67	0	17,19,21	0.60	0
3	NAG	W	1	1,3	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
3	NAG	W	2	3	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
3	NAG	X	1	1,3	14,14,15	0.61	0	17,19,21	0.94	1 (5%)
3	NAG	X	2	3	14,14,15	0.51	0	17,19,21	0.67	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	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NDG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	1/1/5/7	5/6/23/26	0/1/1/1
2	NDG	G	2	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	4/6/23/26	0/1/1/1
2	NDG	J	2	2	-	4/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	1/1/5/7	5/6/23/26	0/1/1/1
2	NDG	L	2	2	-	3/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	4/6/23/26	0/1/1/1
2	NDG	O	2	2	-	4/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	1/1/5/7	5/6/23/26	0/1/1/1
2	NDG	Q	2	2	-	3/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	4/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	4/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	4/6/23/26	0/1/1/1
2	NDG	T	2	2	-	4/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
2	NAG	V	1	1,2	1/1/5/7	5/6/23/26	0/1/1/1
2	NDG	V	2	2	-	3/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	W	2	3	-	4/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	X	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	NAG	C2-N2-C7	-3.05	118.56	122.90
3	S	1	NAG	C2-N2-C7	-3.05	118.56	122.90
3	N	1	NAG	C2-N2-C7	-3.04	118.57	122.90
3	X	1	NAG	C2-N2-C7	-3.03	118.59	122.90
2	J	1	NAG	C2-N2-C7	-2.49	119.35	122.90
2	T	1	NAG	C2-N2-C7	-2.47	119.38	122.90
2	E	1	NAG	C2-N2-C7	-2.47	119.39	122.90
2	O	1	NAG	C2-N2-C7	-2.47	119.39	122.90
2	J	1	NAG	C4-C3-C2	-2.45	107.42	111.02
2	O	1	NAG	C4-C3-C2	-2.45	107.43	111.02
2	E	1	NAG	C4-C3-C2	-2.45	107.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	1	NAG	C4-C3-C2	-2.44	107.44	111.02
3	W	2	NAG	C2-N2-C7	-2.17	119.82	122.90
3	R	2	NAG	C2-N2-C7	-2.16	119.83	122.90
3	U	2	NAG	C1-O5-C5	2.15	115.10	112.19
3	M	2	NAG	C2-N2-C7	-2.15	119.85	122.90
3	P	2	NAG	C1-O5-C5	2.13	115.07	112.19
3	H	2	NAG	C2-N2-C7	-2.12	119.89	122.90
3	K	2	NAG	C1-O5-C5	2.08	115.02	112.19
3	W	1	NAG	C4-C3-C2	-2.08	107.97	111.02
3	F	2	NAG	C1-O5-C5	2.08	115.01	112.19
3	M	1	NAG	C4-C3-C2	-2.08	107.97	111.02
3	H	1	NAG	C4-C3-C2	-2.07	107.98	111.02
3	R	1	NAG	C4-C3-C2	-2.06	108.00	111.02
3	S	2	NAG	C2-N2-C7	-2.04	120.00	122.90
3	X	2	NAG	C2-N2-C7	-2.02	120.02	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	L	1	NAG	C1
2	Q	1	NAG	C1
2	V	1	NAG	C1

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NDG	C8-C7-N2-C2
2	E	2	NDG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NDG	C8-C7-N2-C2
2	G	2	NDG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NDG	C8-C7-N2-C2
2	J	2	NDG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NDG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	L	2	NDG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	O	2	NDG	C8-C7-N2-C2
2	O	2	NDG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	Q	2	NDG	C8-C7-N2-C2
2	Q	2	NDG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	T	2	NDG	C8-C7-N2-C2
2	T	2	NDG	O7-C7-N2-C2
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	V	2	NDG	C8-C7-N2-C2
2	V	2	NDG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C3-C2-N2-C7
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	P	2	NAG	O7-C7-N2-C2
3	R	1	NAG	C3-C2-N2-C7
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2
3	R	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C3-C2-N2-C7
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	X	1	NAG	C8-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	F	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	U	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C1-C2-N2-C7
3	K	1	NAG	C1-C2-N2-C7
3	P	1	NAG	C1-C2-N2-C7
3	U	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	E	2	NDG	C1-C2-N2-C7
2	G	1	NAG	C1-C2-N2-C7
2	J	2	NDG	C1-C2-N2-C7
2	L	1	NAG	C1-C2-N2-C7
2	O	2	NDG	C1-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	T	2	NDG	C1-C2-N2-C7
2	V	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
2	L	2	NDG	C4-C5-C6-O6
2	Q	2	NDG	C4-C5-C6-O6
2	V	2	NDG	C4-C5-C6-O6
2	G	2	NDG	C4-C5-C6-O6
3	F	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
3	M	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	R	2	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	W	2	NAG	C3-C2-N2-C7
3	W	1	NAG	C1-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
2	Q	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	E	2	NDG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	J	2	NDG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	O	2	NDG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	T	2	NDG	C3-C2-N2-C7
2	V	1	NAG	C3-C2-N2-C7

There are no ring outliers.

29 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	T	2	NDG	1	0
3	F	1	NAG	1	0
3	P	2	NAG	1	0
2	Q	1	NAG	1	0
2	Q	2	NDG	1	0
2	O	2	NDG	1	0
2	L	1	NAG	1	0
2	L	2	NDG	1	0
3	F	2	NAG	1	0
2	E	2	NDG	2	0
3	U	1	NAG	1	0
2	T	1	NAG	1	0
3	H	1	NAG	5	0
3	M	1	NAG	5	0
3	K	2	NAG	1	0
2	J	2	NDG	2	0
3	K	1	NAG	1	0

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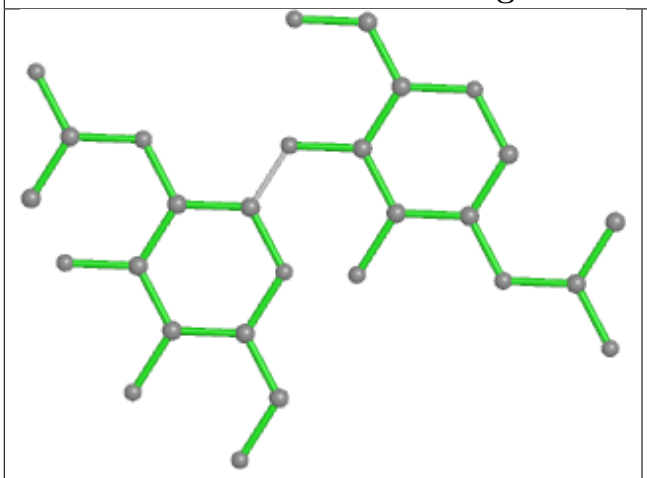
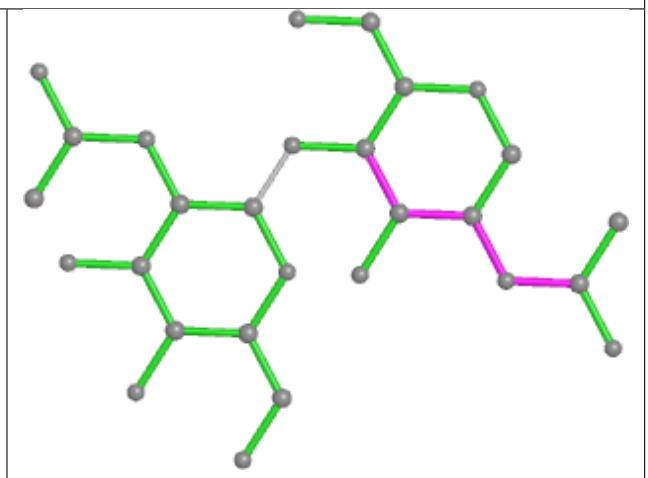
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	2	0
3	R	1	NAG	5	0
3	P	1	NAG	1	0
3	U	2	NAG	1	0
2	O	1	NAG	1	0
2	G	2	NDG	1	1
3	M	2	NAG	0	1
2	V	2	NDG	1	0
2	E	1	NAG	2	0
2	V	1	NAG	1	0
3	W	1	NAG	5	0

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

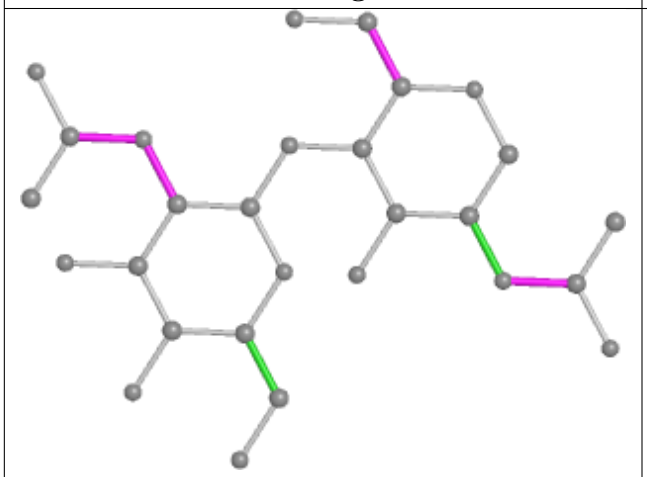
Oligosaccharide Chain E



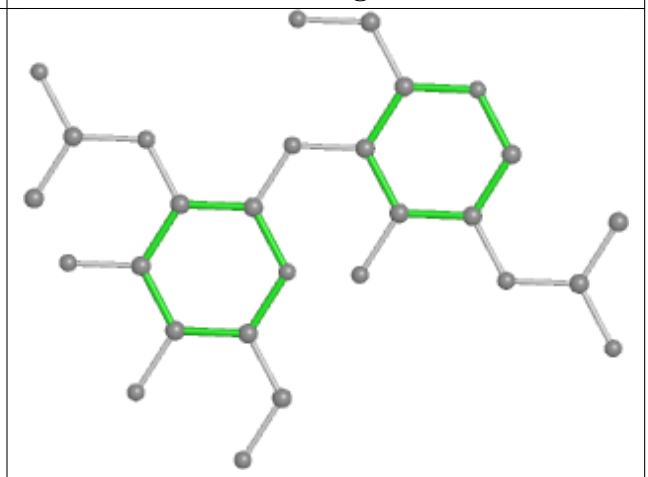
Bond lengths



Bond angles

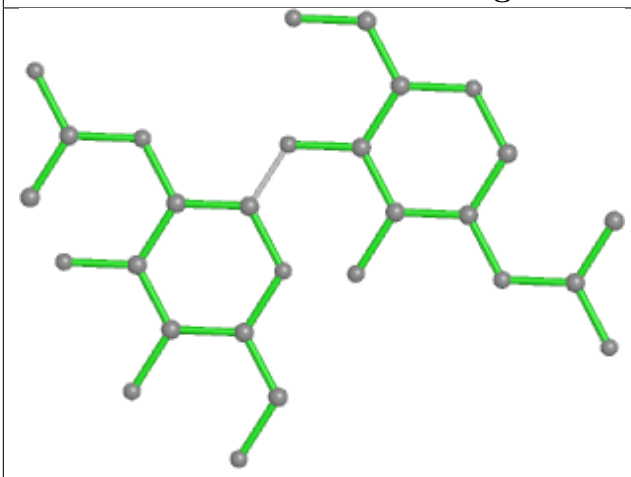


Torsions

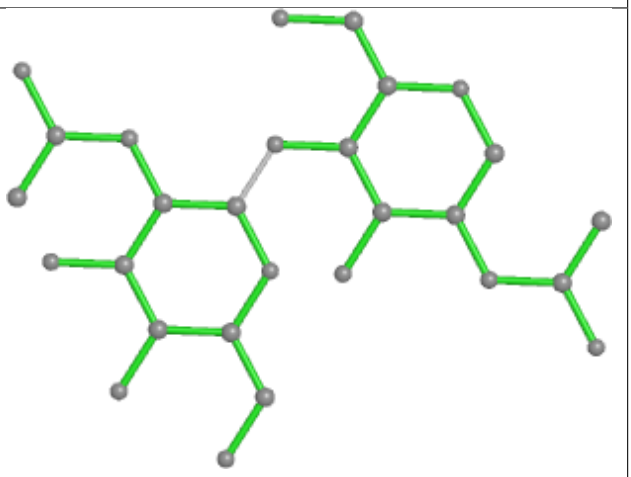


Rings

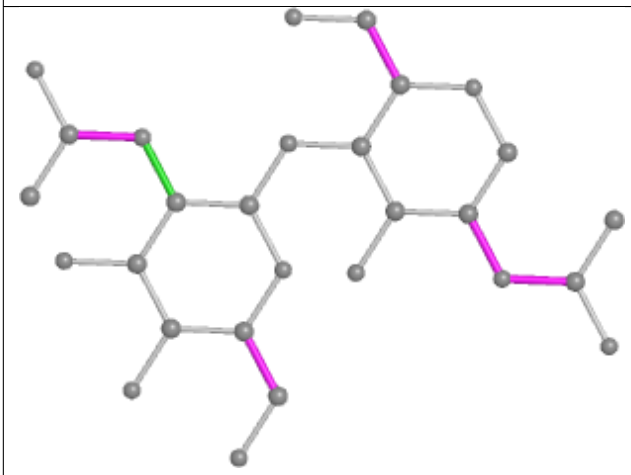
Oligosaccharide Chain G



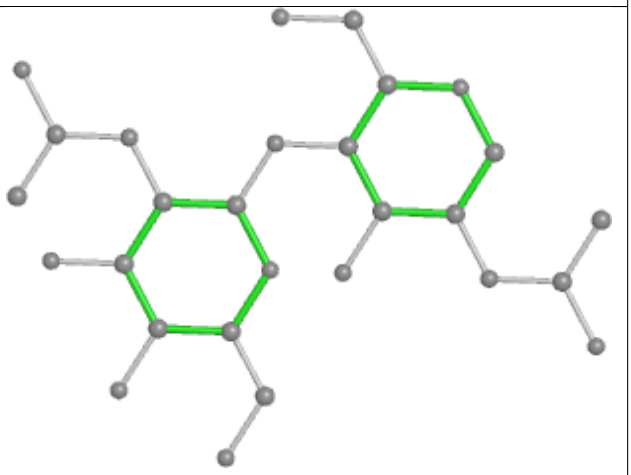
Bond lengths



Bond angles

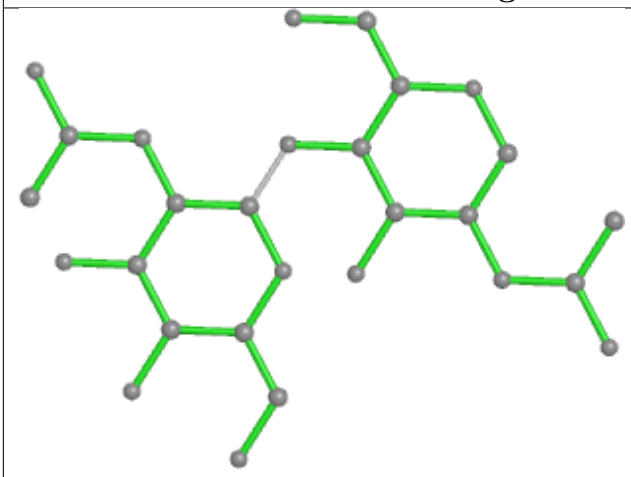


Torsions

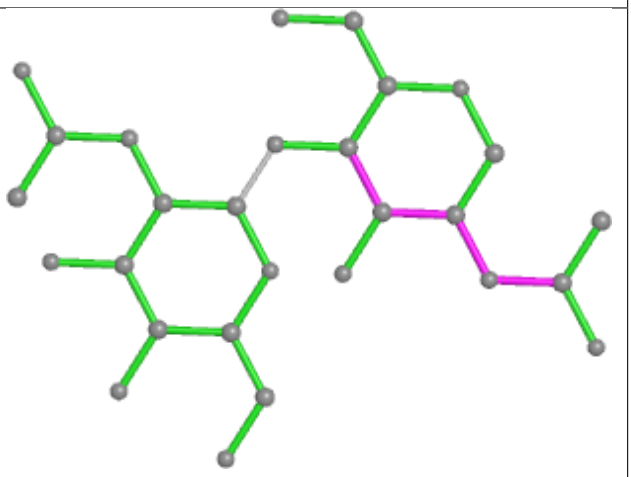


Rings

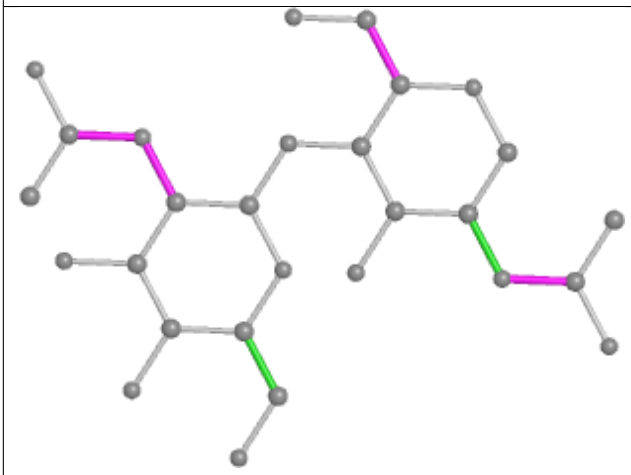
Oligosaccharide Chain J



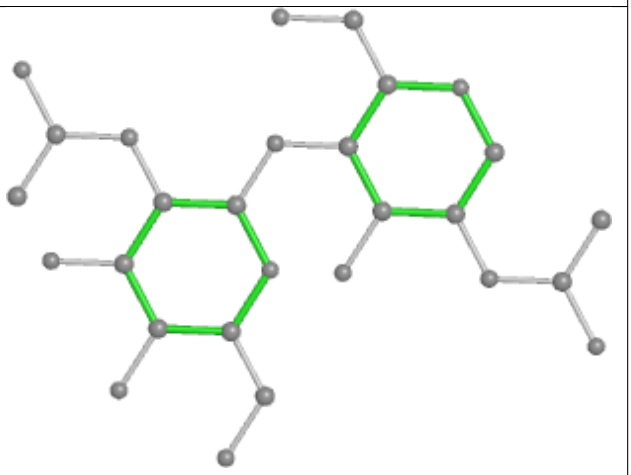
Bond lengths



Bond angles

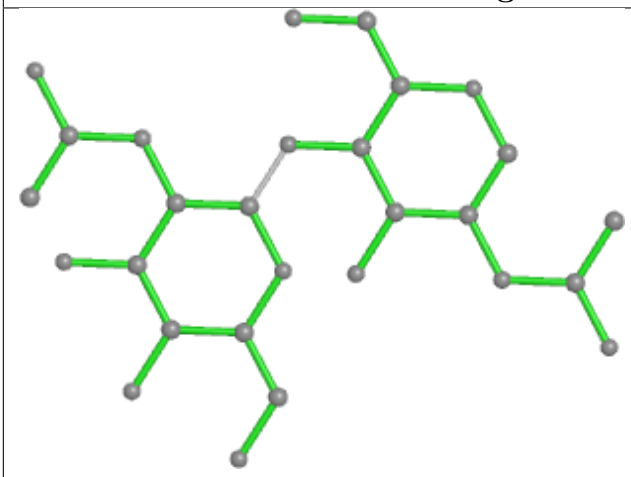


Torsions

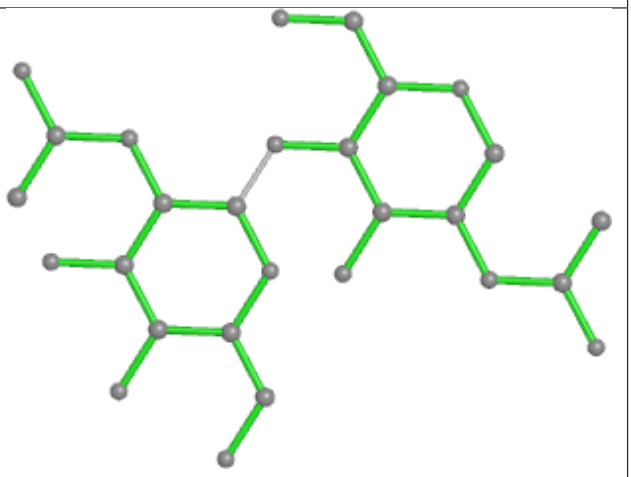


Rings

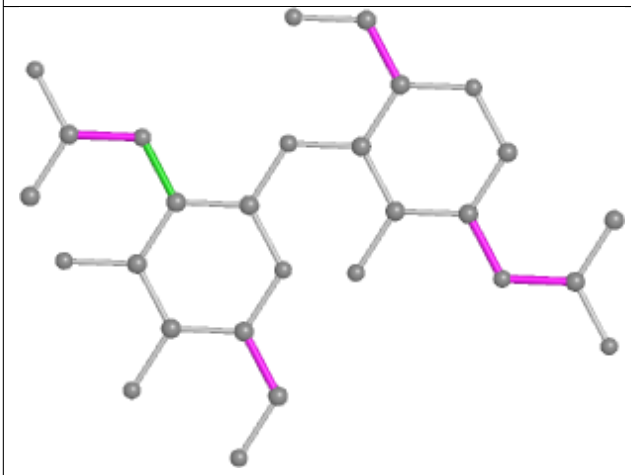
Oligosaccharide Chain L



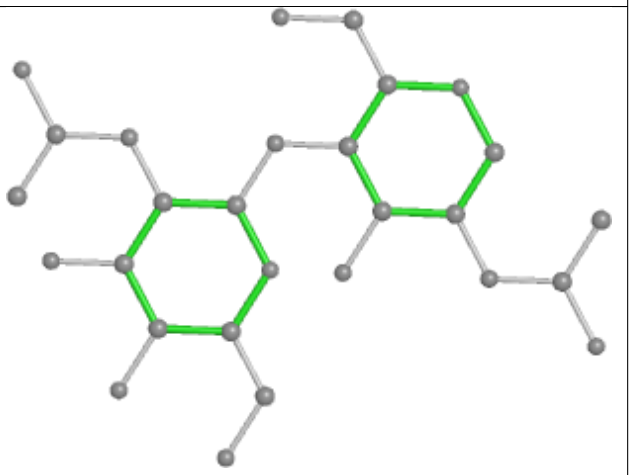
Bond lengths



Bond angles

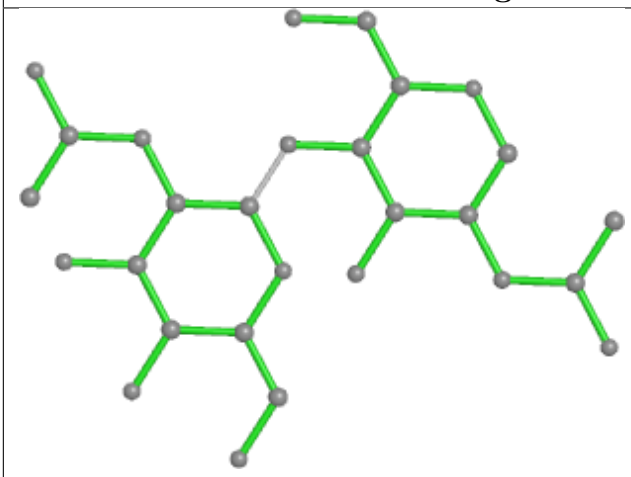


Torsions

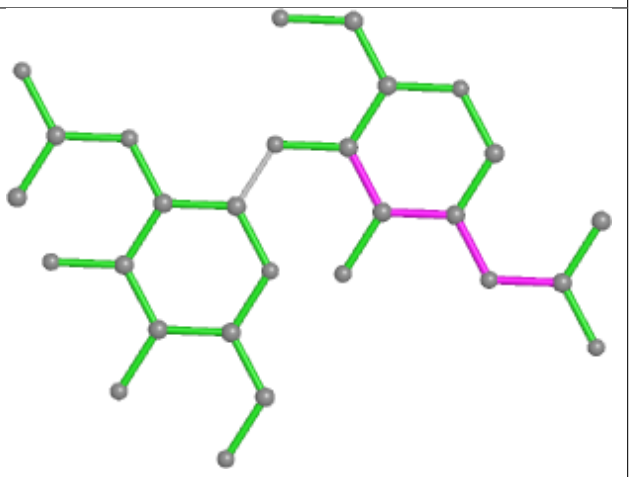


Rings

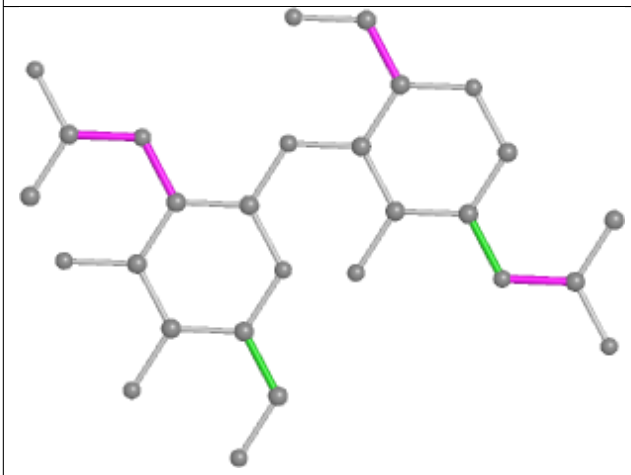
Oligosaccharide Chain O



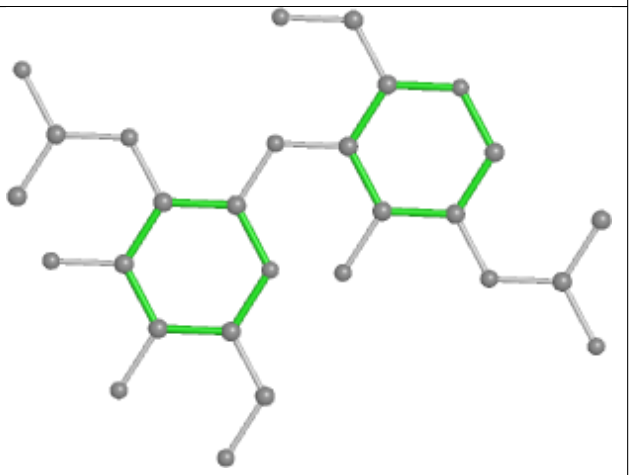
Bond lengths



Bond angles

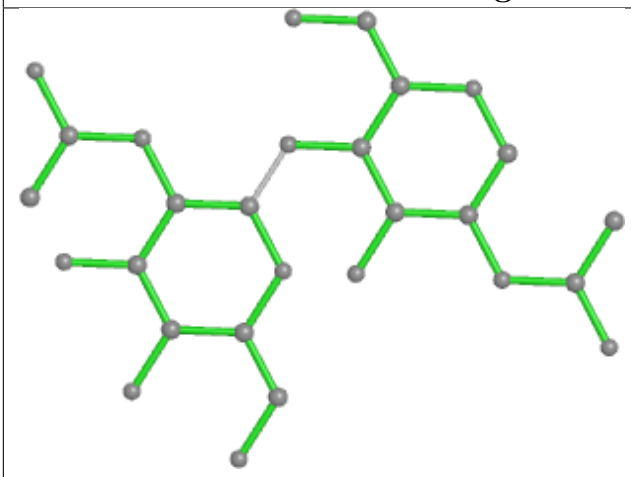


Torsions

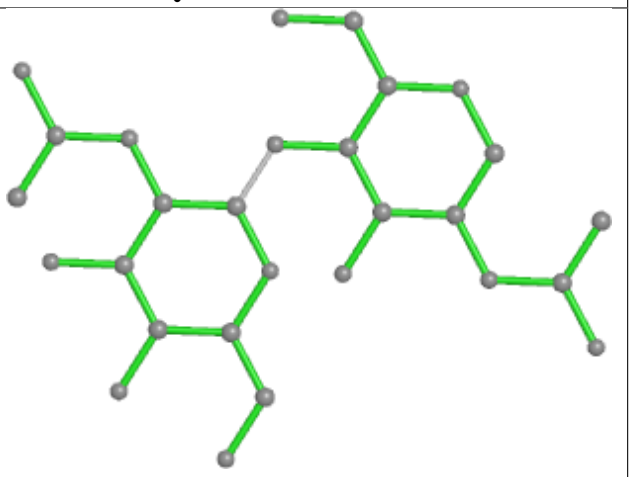


Rings

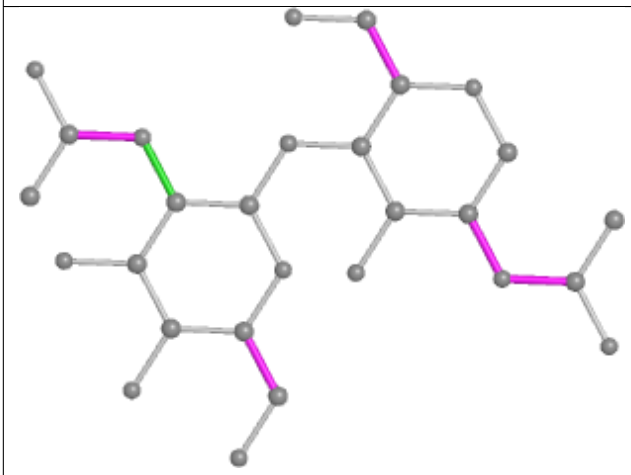
Oligosaccharide Chain Q



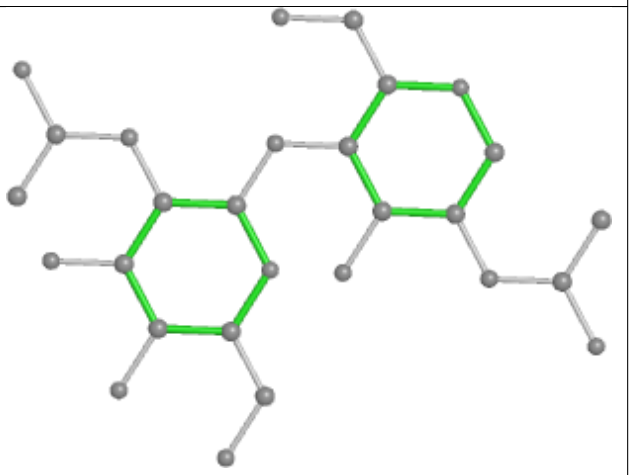
Bond lengths



Bond angles

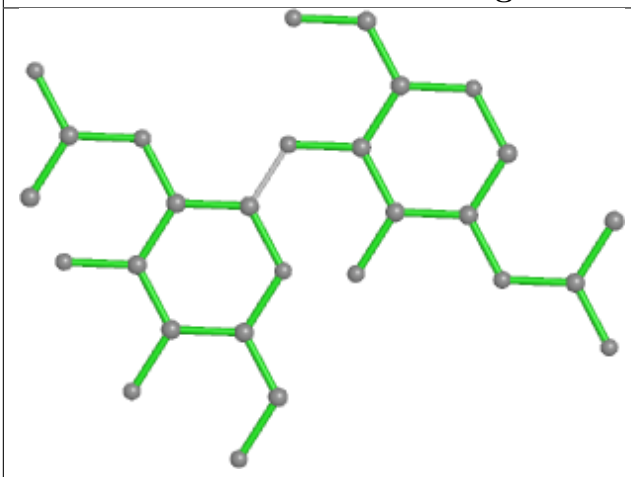


Torsions

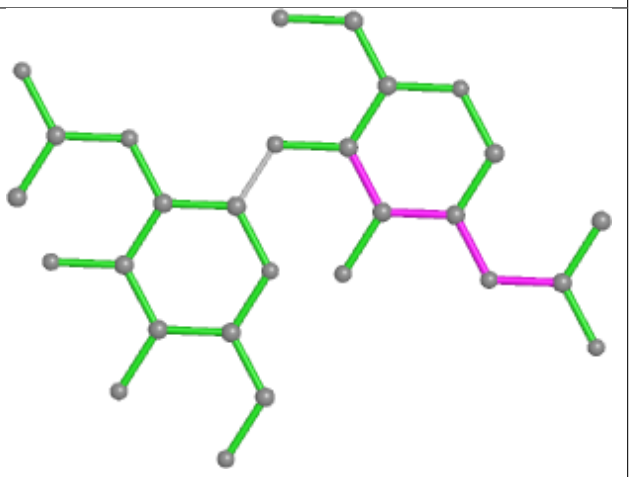


Rings

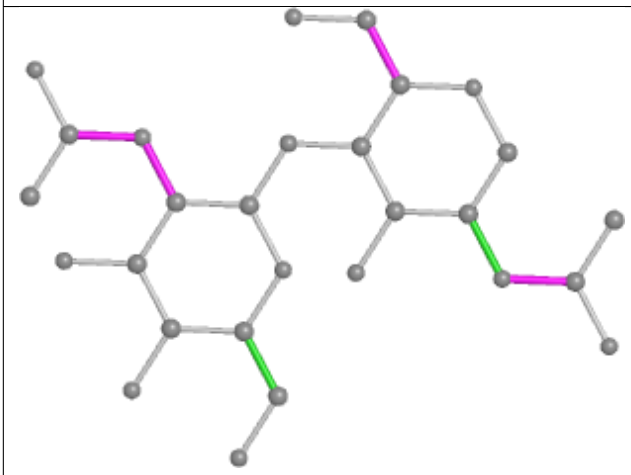
Oligosaccharide Chain T



Bond lengths



Bond angles



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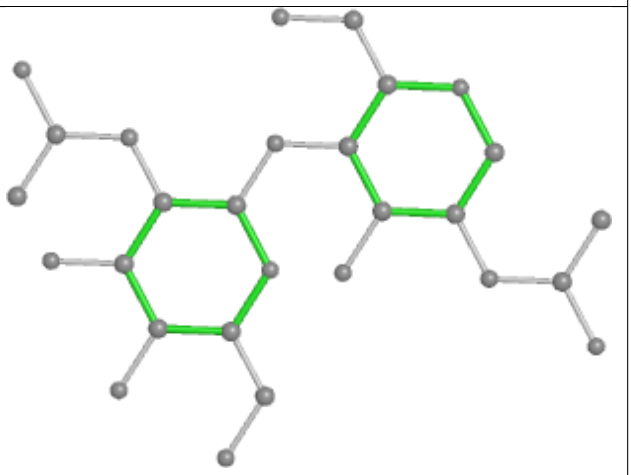
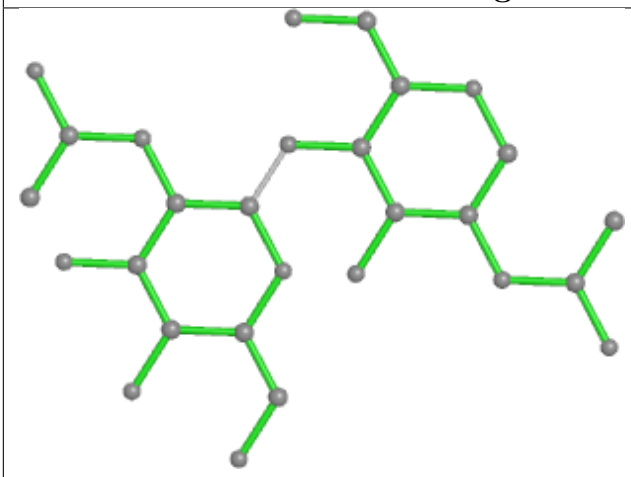
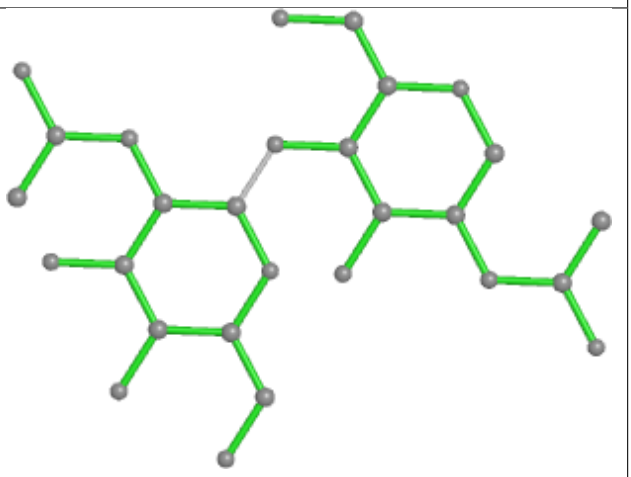


Rings

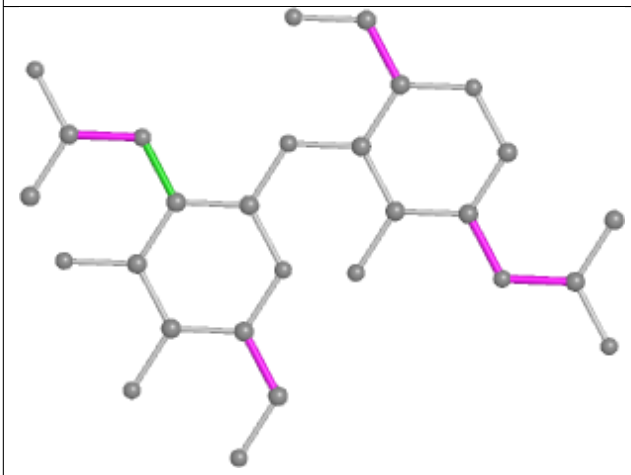
Oligosaccharide Chain V



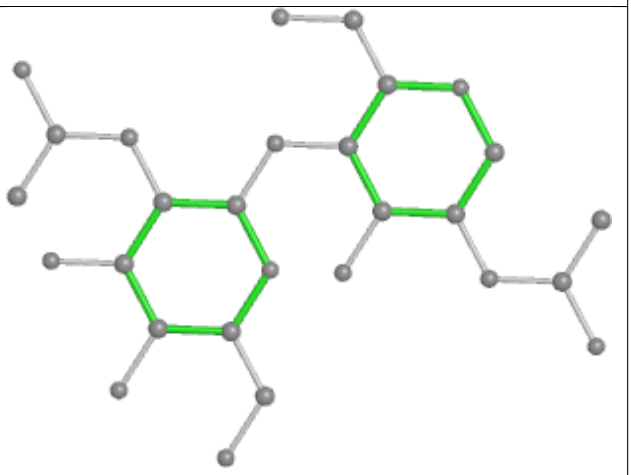
Bond lengths



Bond angles

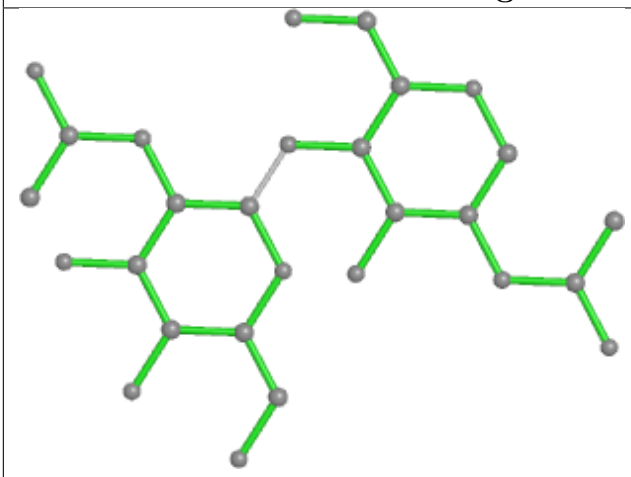


Torsions

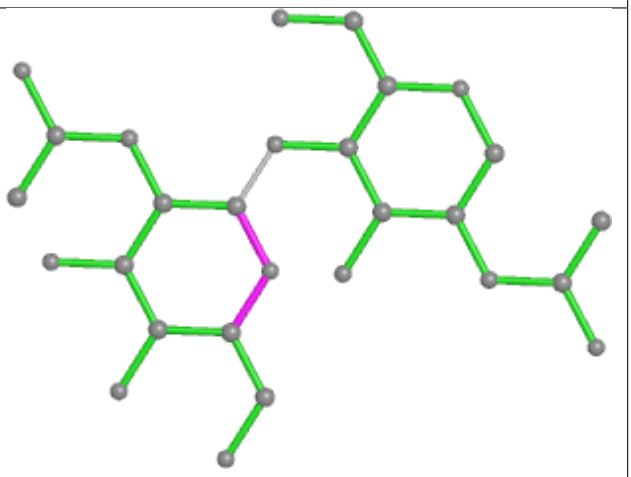


Rings

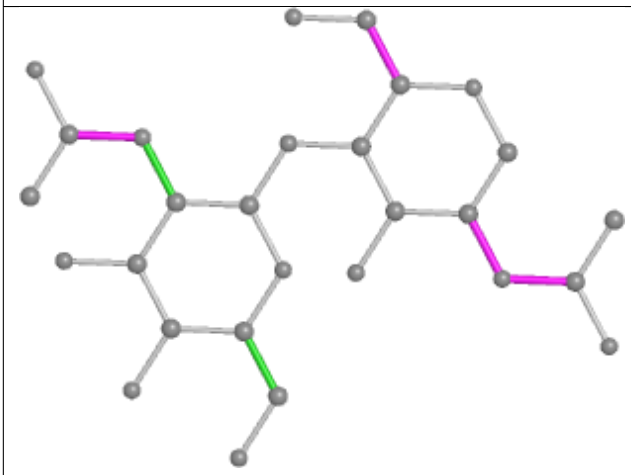
Oligosaccharide Chain F



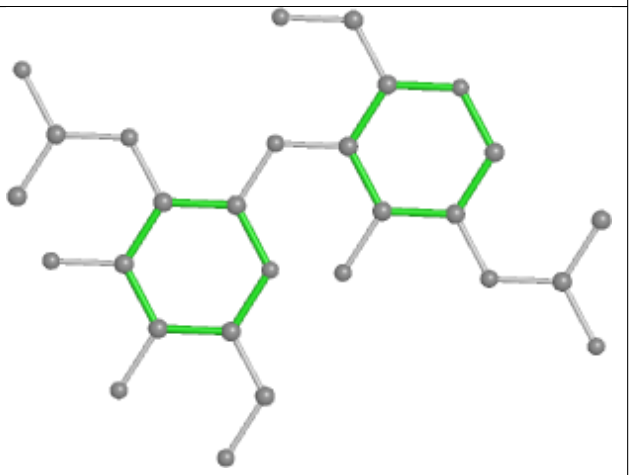
Bond lengths



Bond angles

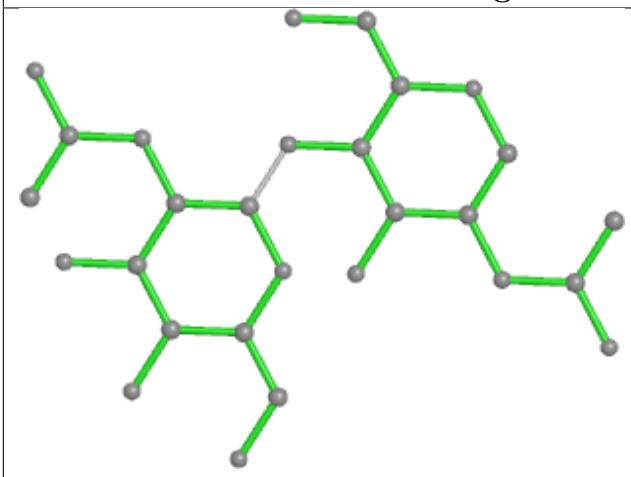


Torsions

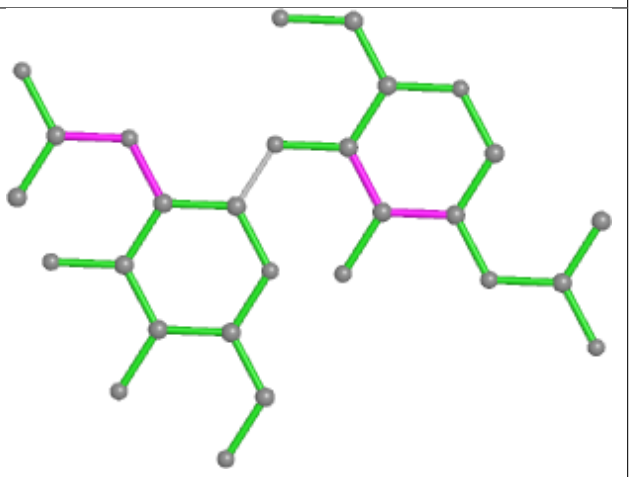


Rings

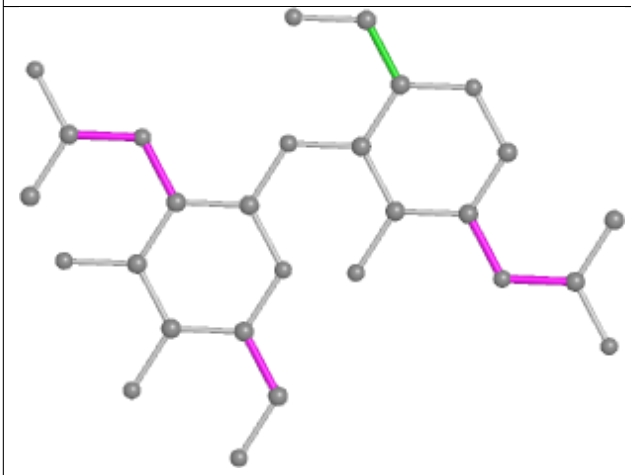
Oligosaccharide Chain H



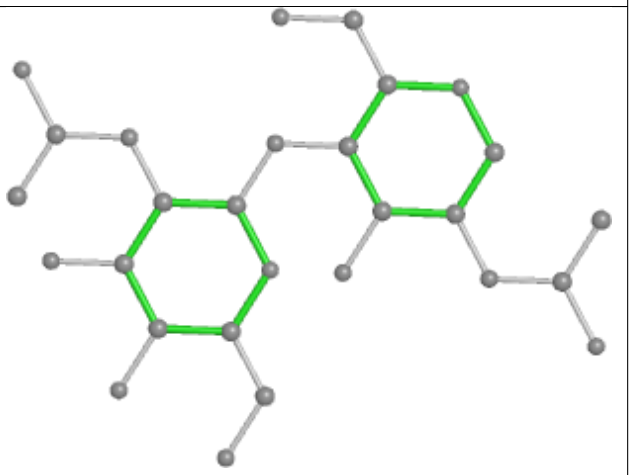
Bond lengths



Bond angles

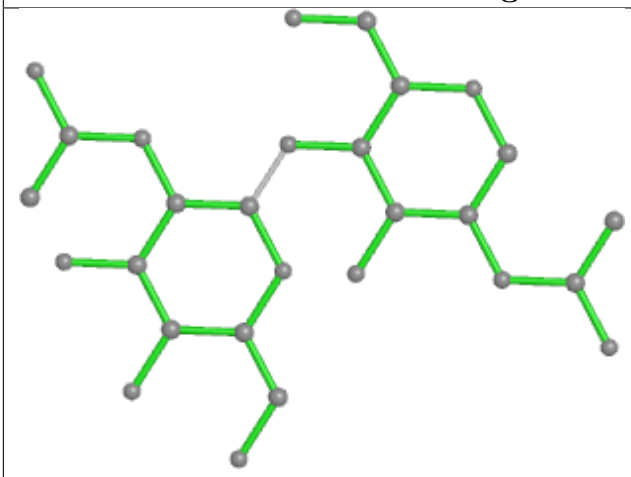


Torsions

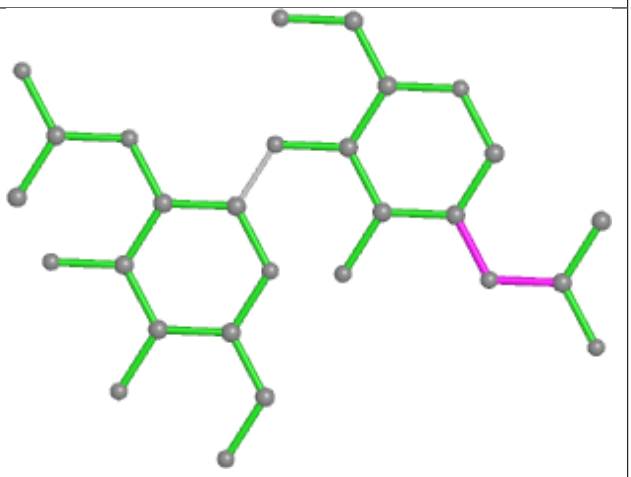


Rings

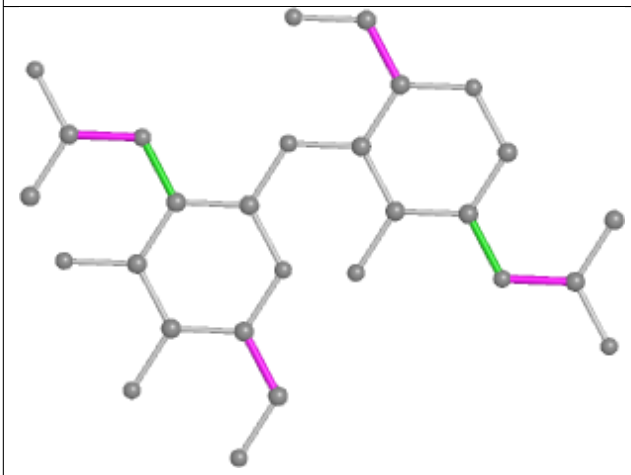
Oligosaccharide Chain I



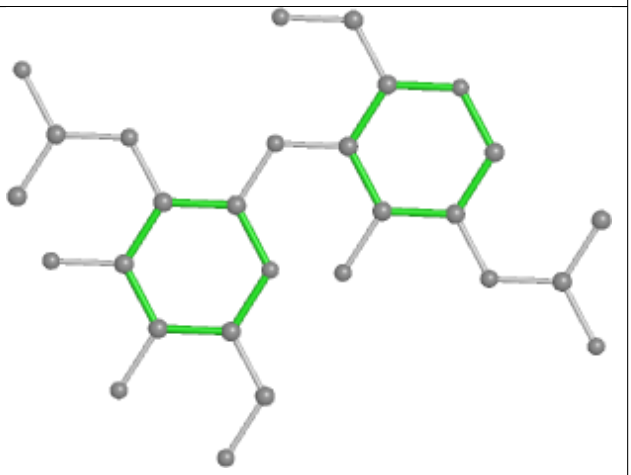
Bond lengths



Bond angles

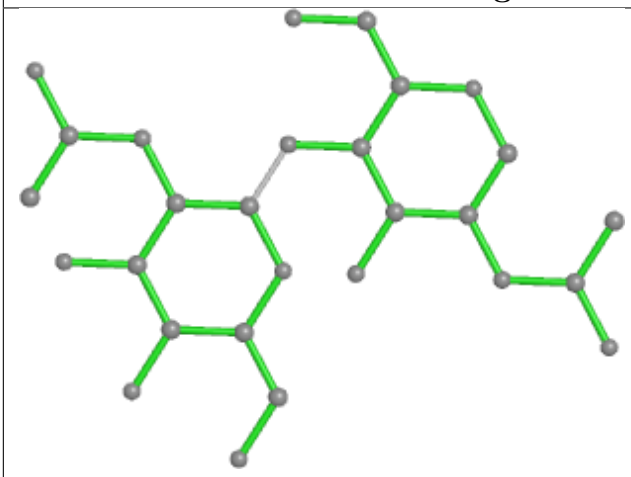


Torsions

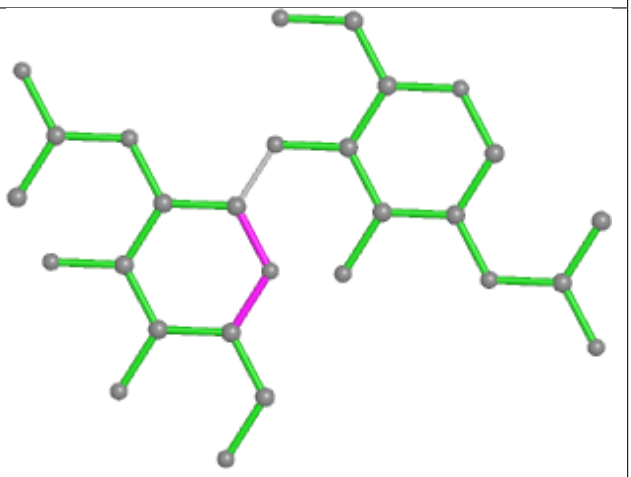


Rings

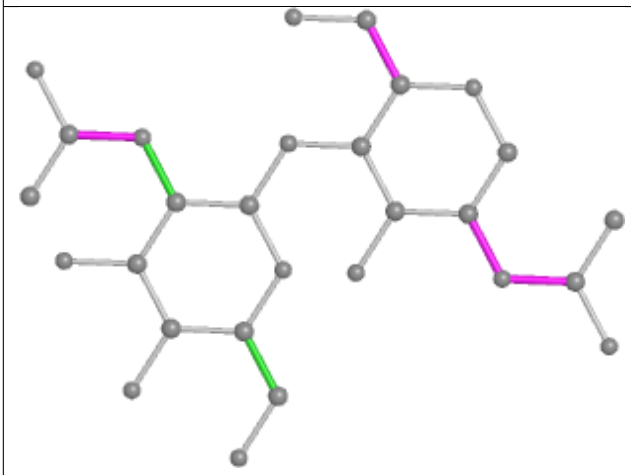
Oligosaccharide Chain K



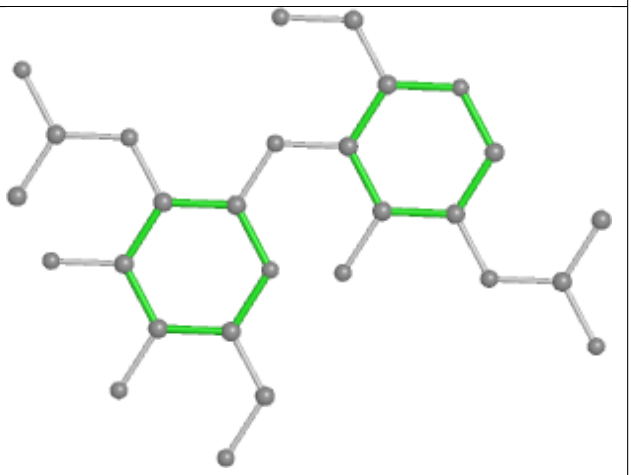
Bond lengths



Bond angles

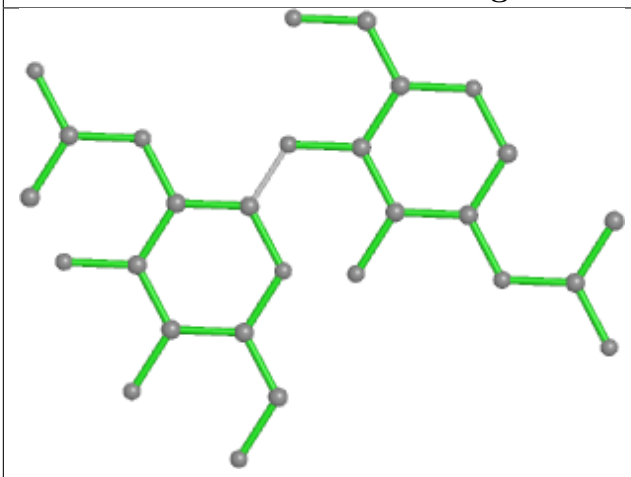


Torsions

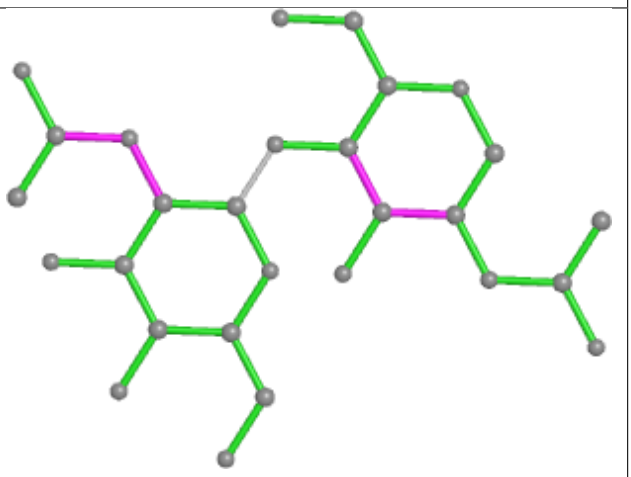


Rings

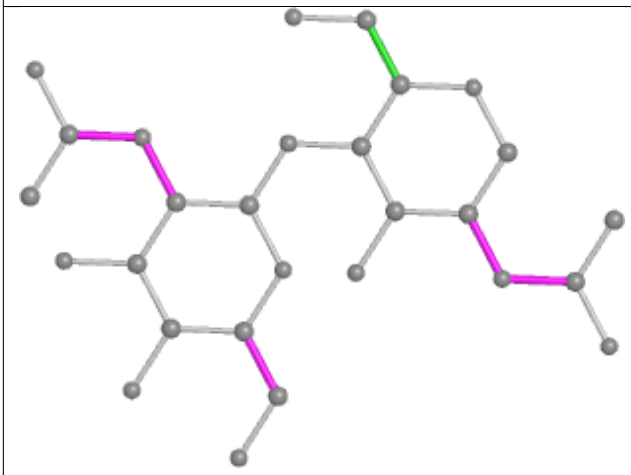
Oligosaccharide Chain M



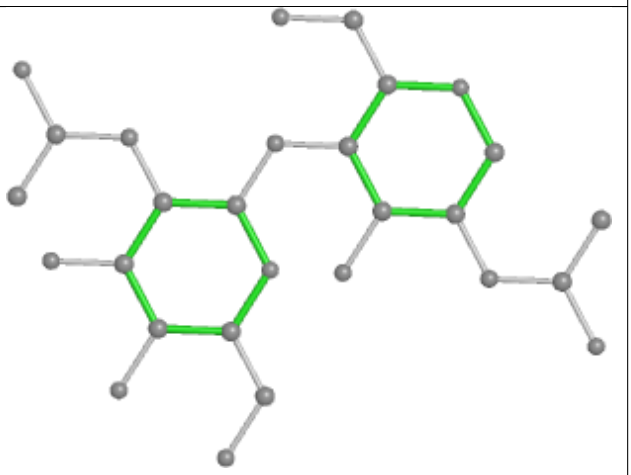
Bond lengths



Bond angles

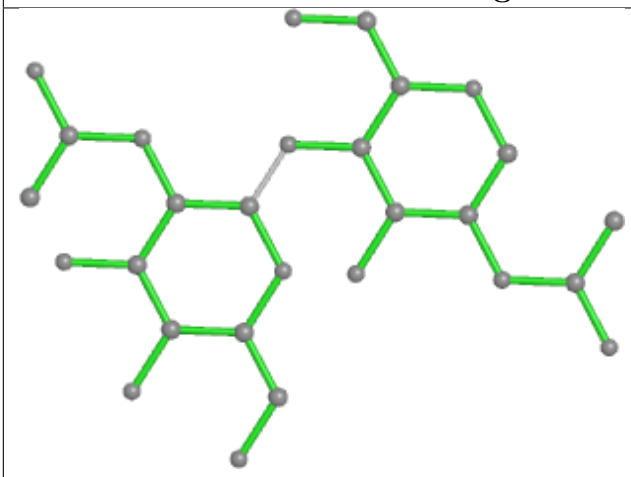


Torsions

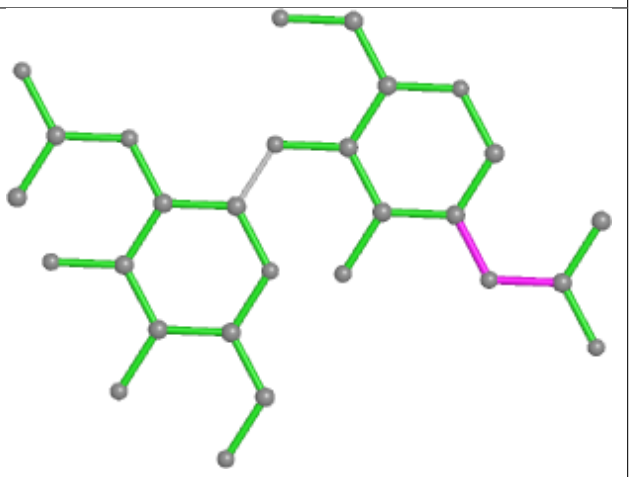


Rings

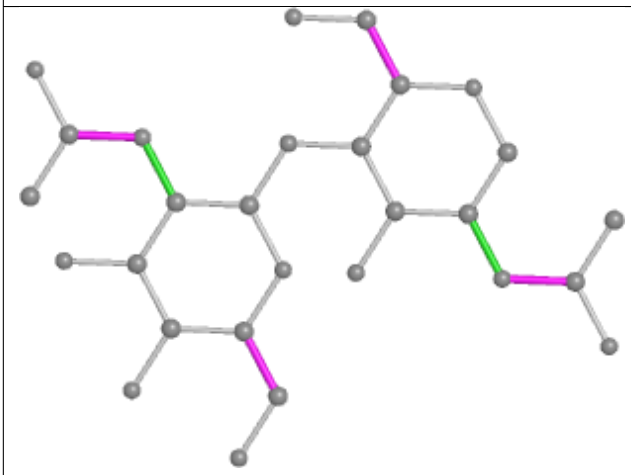
Oligosaccharide Chain N



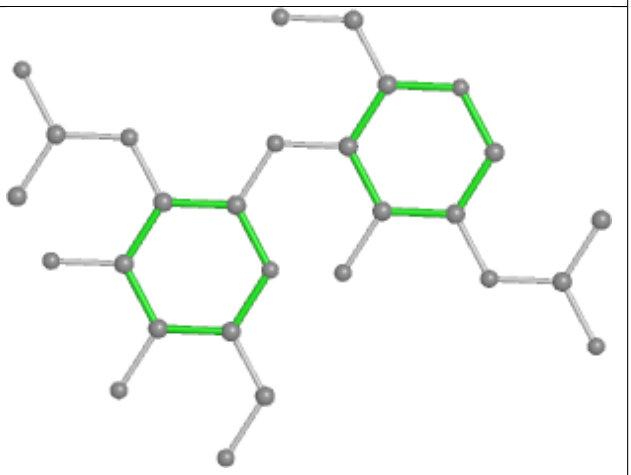
Bond lengths



Bond angles

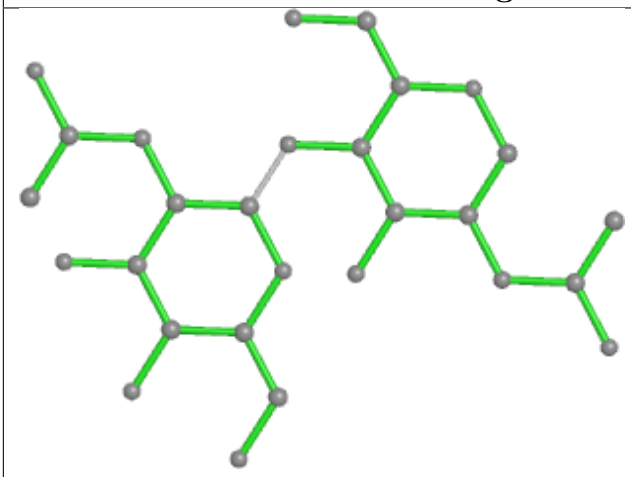


Torsions

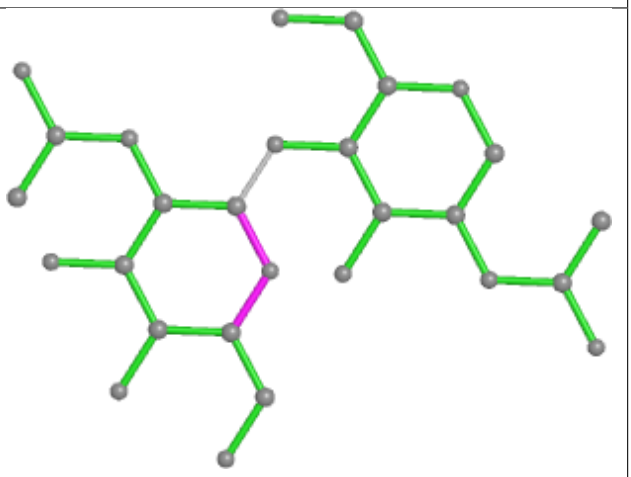


Rings

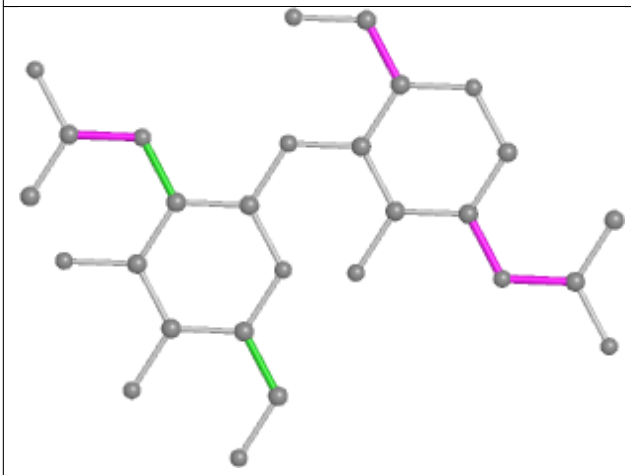
Oligosaccharide Chain P



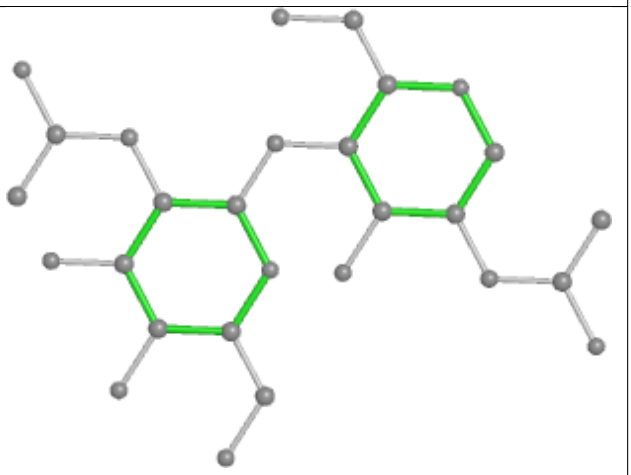
Bond lengths



Bond angles

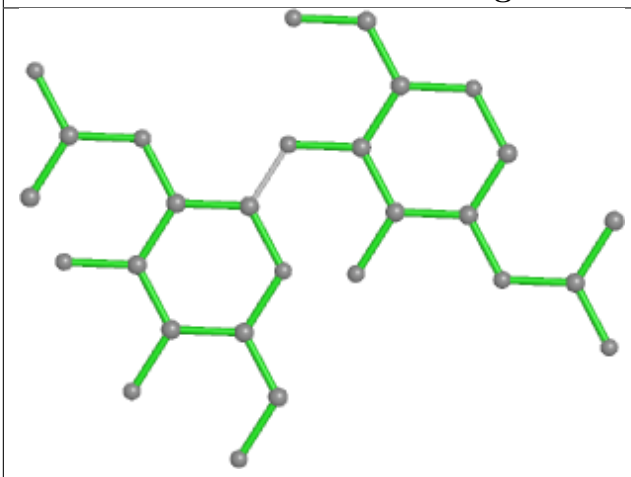


Torsions

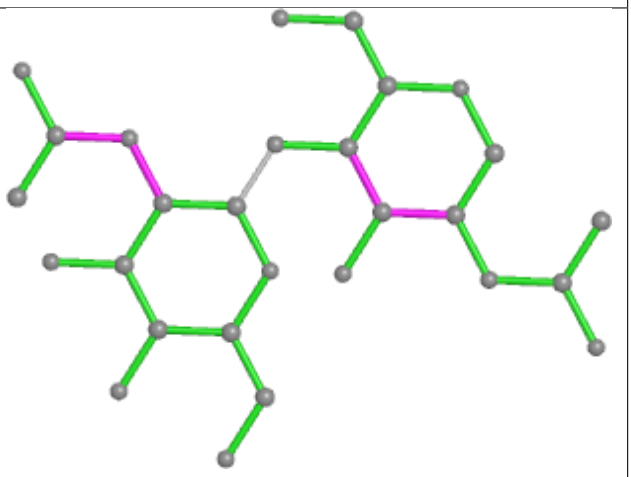


Rings

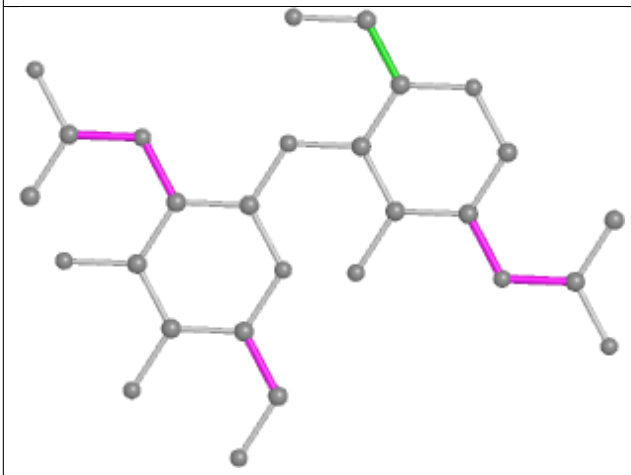
Oligosaccharide Chain R



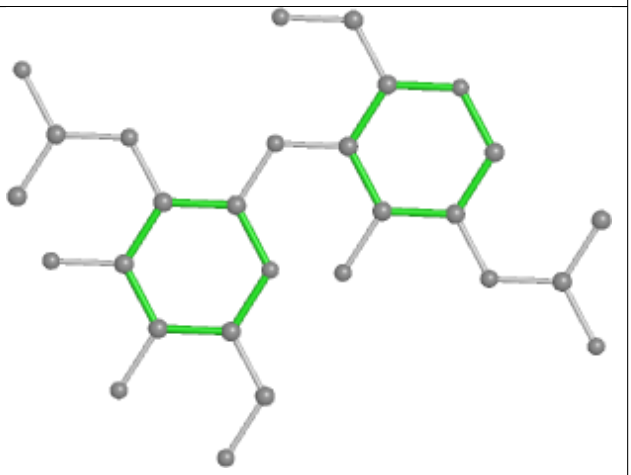
Bond lengths



Bond angles

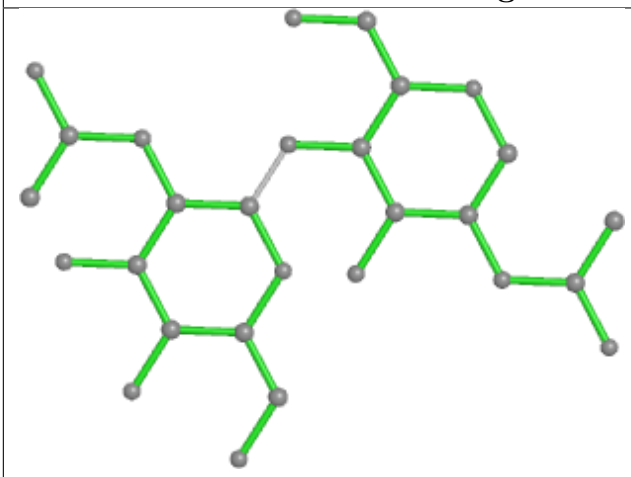


Torsions

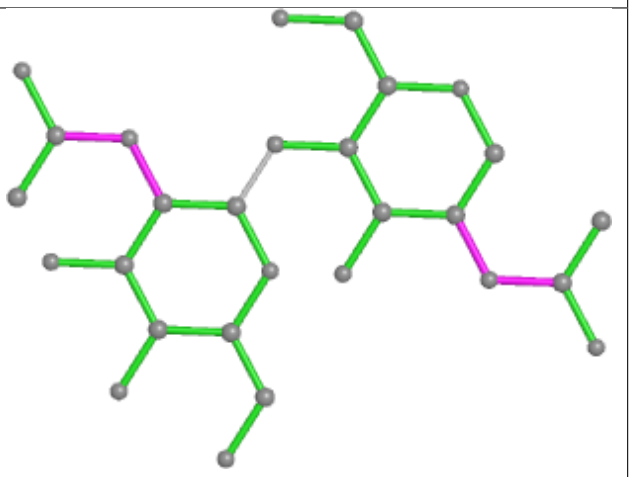


Rings

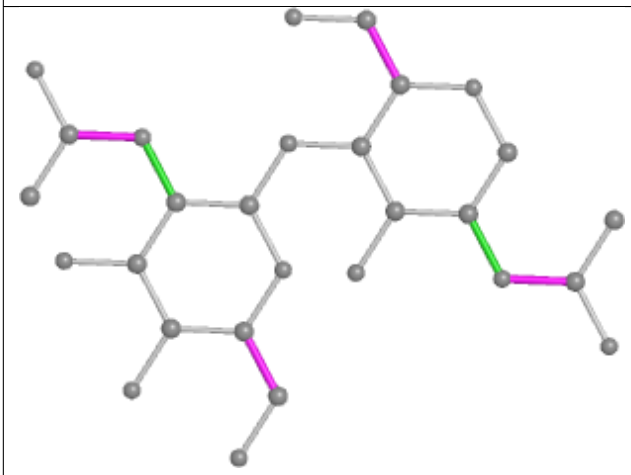
Oligosaccharide Chain S



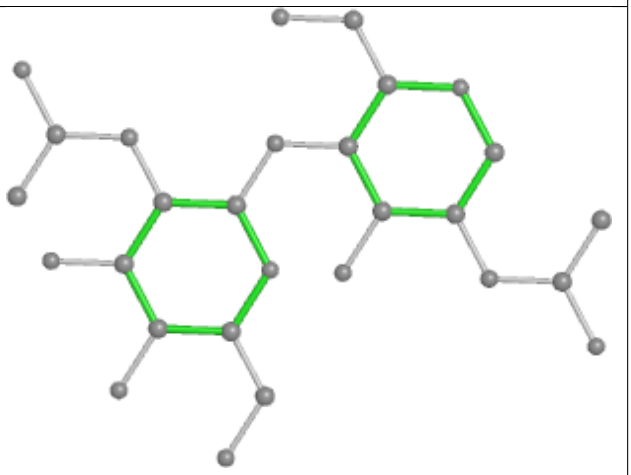
Bond lengths



Bond angles

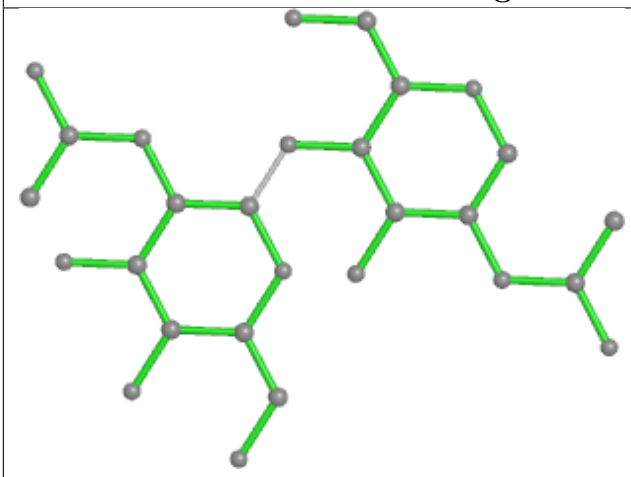


Torsions

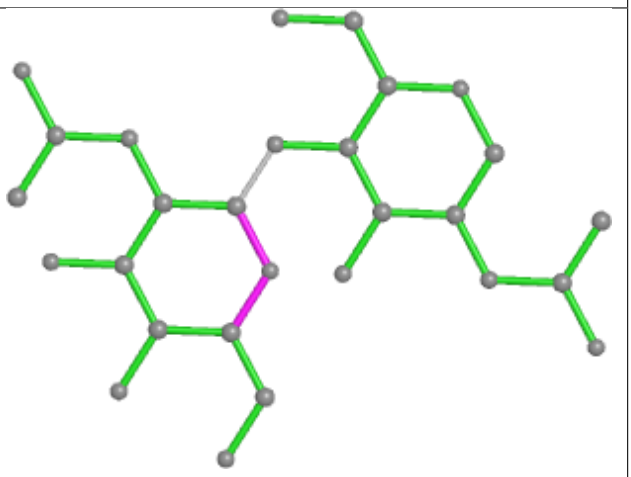


Rings

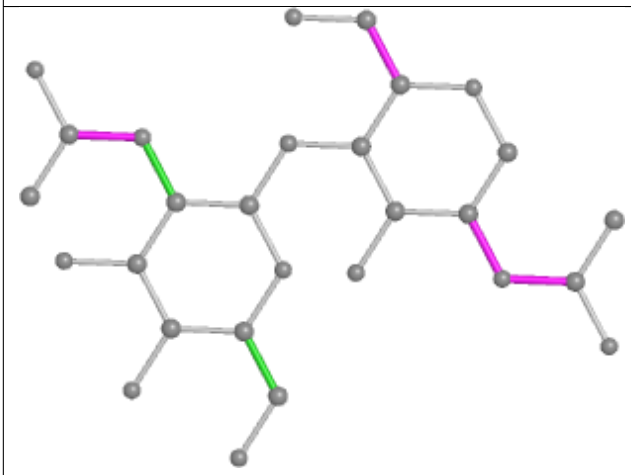
Oligosaccharide Chain U



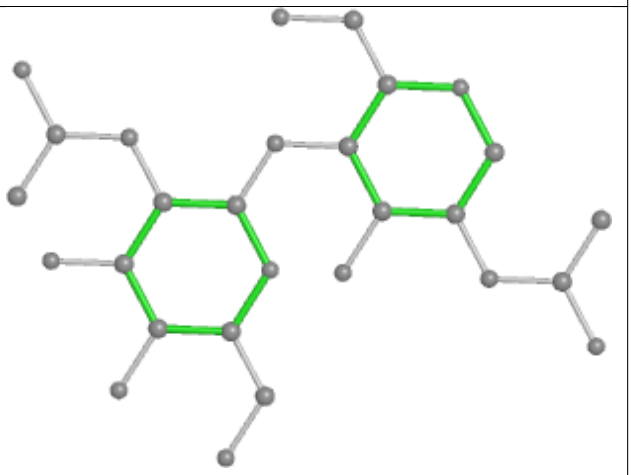
Bond lengths



Bond angles

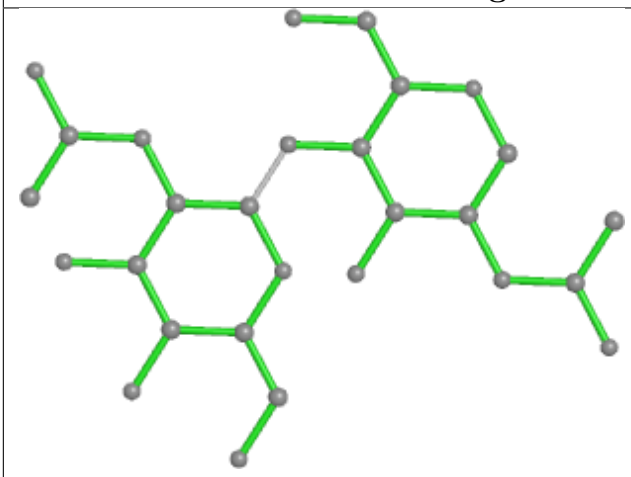


Torsions

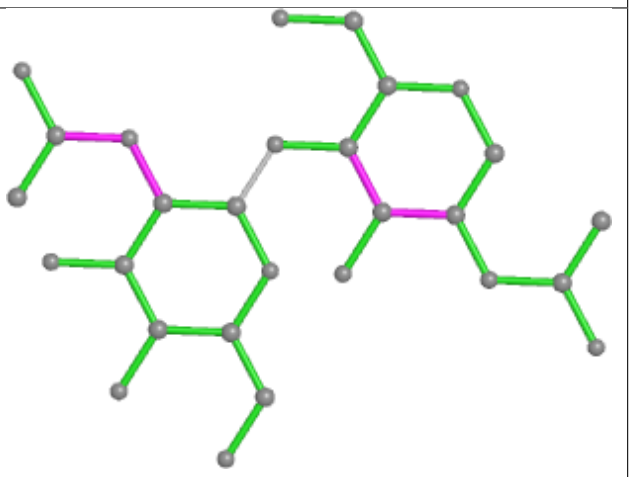


Rings

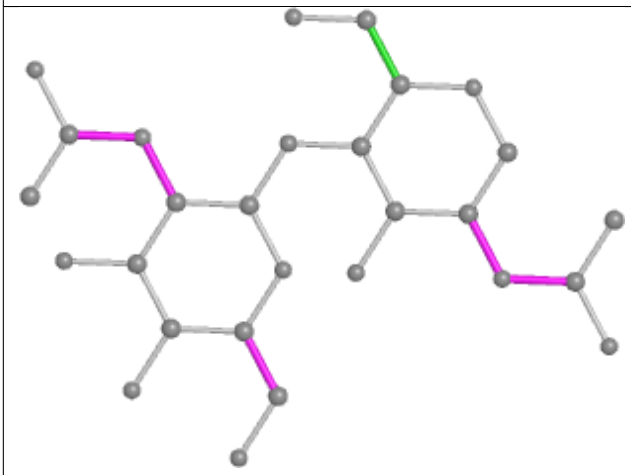
Oligosaccharide Chain W



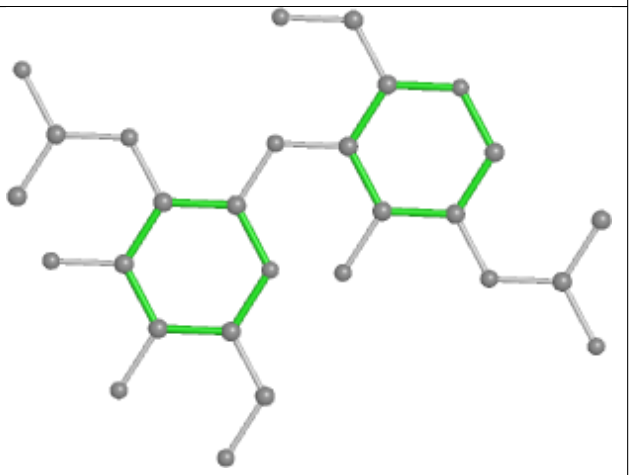
Bond lengths



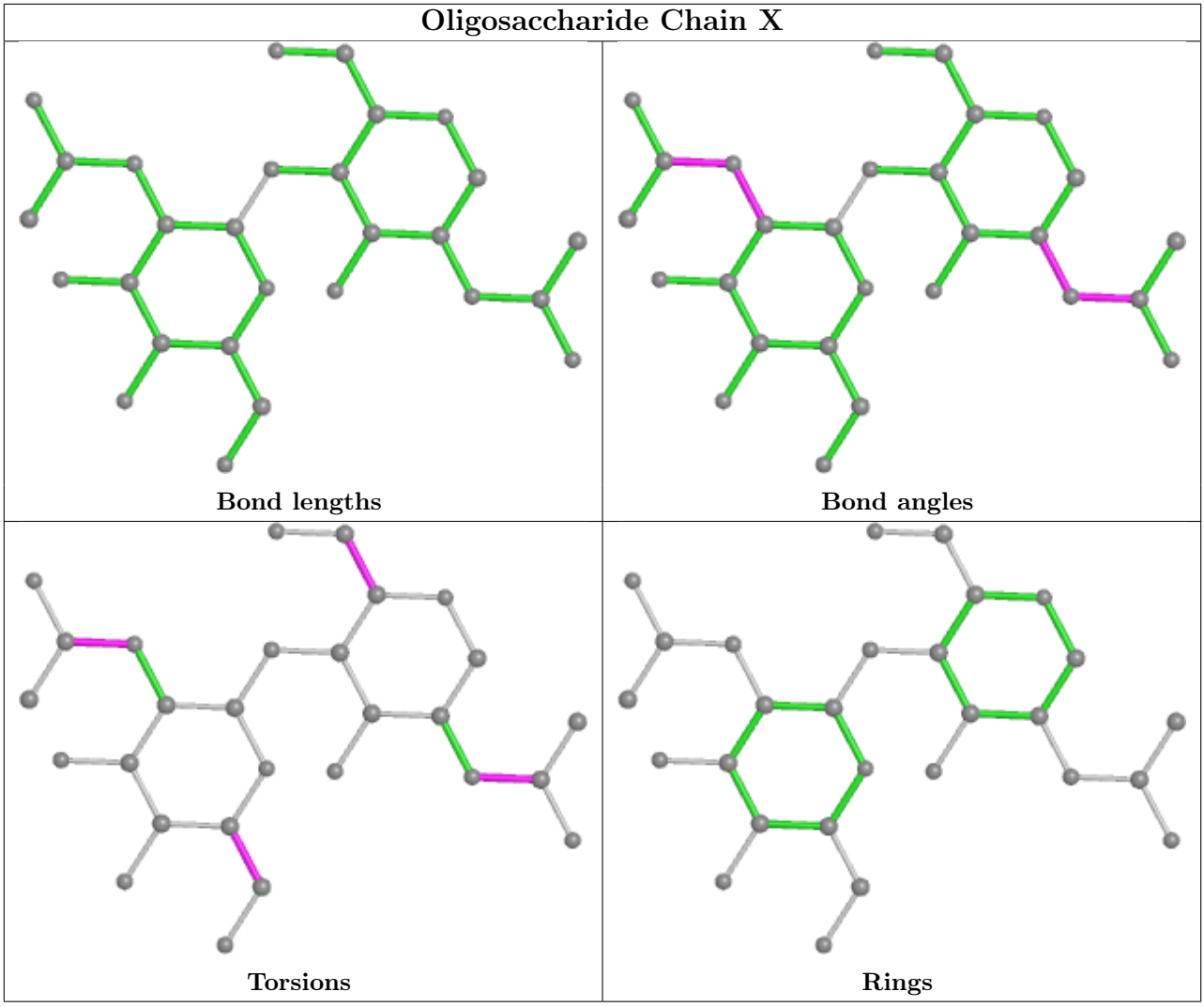
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	2759	1	14,14,15	0.80	0	17,19,21	0.76	0
4	NAG	A	1759	1	14,14,15	0.80	0	17,19,21	0.76	0
4	NAG	D	4760	1	14,14,15	0.91	1 (7%)	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	4759	1	14,14,15	0.80	0	17,19,21	0.76	0
4	NAG	B	2760	1	14,14,15	0.91	1 (7%)	17,19,21	0.71	0
4	NAG	C	3760	1	14,14,15	0.92	1 (7%)	17,19,21	0.71	0
4	NAG	C	3759	1	14,14,15	0.80	0	17,19,21	0.76	0
4	NAG	A	1760	1	14,14,15	0.91	1 (7%)	17,19,21	0.70	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
4	NAG	B	2759	1	-	6/6/23/26	0/1/1/1
4	NAG	A	1759	1	-	6/6/23/26	0/1/1/1
4	NAG	D	4760	1	-	6/6/23/26	0/1/1/1
4	NAG	D	4759	1	-	6/6/23/26	0/1/1/1
4	NAG	B	2760	1	-	6/6/23/26	0/1/1/1
4	NAG	C	3760	1	-	6/6/23/26	0/1/1/1
4	NAG	C	3759	1	-	6/6/23/26	0/1/1/1
4	NAG	A	1760	1	-	6/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4760	NAG	C1-C2	2.70	1.56	1.52
4	C	3760	NAG	C1-C2	2.67	1.56	1.52
4	B	2760	NAG	C1-C2	2.65	1.56	1.52
4	A	1760	NAG	C1-C2	2.65	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1759	NAG	C8-C7-N2-C2
4	A	1759	NAG	O7-C7-N2-C2
4	A	1760	NAG	C8-C7-N2-C2
4	A	1760	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	2759	NAG	C8-C7-N2-C2
4	B	2759	NAG	O7-C7-N2-C2
4	B	2760	NAG	C8-C7-N2-C2
4	B	2760	NAG	O7-C7-N2-C2
4	C	3759	NAG	C8-C7-N2-C2
4	C	3759	NAG	O7-C7-N2-C2
4	C	3760	NAG	C8-C7-N2-C2
4	C	3760	NAG	O7-C7-N2-C2
4	D	4759	NAG	C8-C7-N2-C2
4	D	4759	NAG	O7-C7-N2-C2
4	D	4760	NAG	C8-C7-N2-C2
4	D	4760	NAG	O7-C7-N2-C2
4	A	1759	NAG	O5-C5-C6-O6
4	B	2759	NAG	O5-C5-C6-O6
4	C	3759	NAG	O5-C5-C6-O6
4	D	4759	NAG	O5-C5-C6-O6
4	A	1759	NAG	C1-C2-N2-C7
4	B	2759	NAG	C1-C2-N2-C7
4	B	2760	NAG	C1-C2-N2-C7
4	C	3759	NAG	C1-C2-N2-C7
4	D	4759	NAG	C1-C2-N2-C7
4	A	1759	NAG	C4-C5-C6-O6
4	B	2759	NAG	C4-C5-C6-O6
4	C	3759	NAG	C4-C5-C6-O6
4	D	4759	NAG	C4-C5-C6-O6
4	A	1760	NAG	C1-C2-N2-C7
4	D	4760	NAG	C1-C2-N2-C7
4	A	1760	NAG	O5-C5-C6-O6
4	B	2760	NAG	O5-C5-C6-O6
4	C	3760	NAG	O5-C5-C6-O6
4	D	4760	NAG	O5-C5-C6-O6
4	C	3760	NAG	C1-C2-N2-C7
4	A	1760	NAG	C3-C2-N2-C7
4	B	2760	NAG	C3-C2-N2-C7
4	C	3760	NAG	C3-C2-N2-C7
4	D	4760	NAG	C3-C2-N2-C7
4	D	4760	NAG	C4-C5-C6-O6
4	A	1760	NAG	C4-C5-C6-O6
4	B	2760	NAG	C4-C5-C6-O6
4	C	3760	NAG	C4-C5-C6-O6
4	A	1759	NAG	C3-C2-N2-C7
4	B	2759	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	C	3759	NAG	C3-C2-N2-C7
4	D	4759	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2759	NAG	1	0
4	D	4760	NAG	5	0
4	B	2760	NAG	5	0
4	C	3760	NAG	5	0
4	A	1760	NAG	5	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, 95^{th} 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	695/695 (100%)	-0.38	0 100 100	2, 51, 143, 197	0
1	B	695/695 (100%)	-0.36	3 (0%) 92 90	2, 51, 143, 197	0
1	C	695/695 (100%)	-0.44	1 (0%) 95 95	2, 51, 143, 197	0
1	D	695/695 (100%)	-0.33	8 (1%) 79 73	2, 51, 143, 197	0
All	All	2780/2780 (100%)	-0.38	12 (0%) 92 90	2, 51, 144, 197	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	ASN	4.0
1	D	307	GLU	3.7
1	D	308	LYS	3.3
1	D	319	TRP	3.1
1	D	336	ASN	3.1
1	D	309	MET	2.6
1	D	328	ASN	2.6
1	D	505	GLU	2.6
1	D	198	GLY	2.3
1	C	541	TRP	2.3
1	B	546	PHE	2.3
1	B	340	GLN	2.0

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 (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, 95^{th} 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
2	NAG	V	1	14/15	0.23	0.57	197,197,197,197	0
2	NAG	L	1	14/15	0.25	0.67	197,197,197,197	0
2	NDG	V	2	14/15	0.32	0.38	189,189,189,189	0
3	NAG	M	2	14/15	0.44	0.35	197,197,197,197	0
3	NAG	U	2	14/15	0.51	0.34	196,196,196,196	0
3	NAG	P	2	14/15	0.58	0.37	196,196,196,196	0
3	NAG	K	2	14/15	0.61	0.36	196,196,196,196	0
3	NAG	W	2	14/15	0.66	0.34	197,197,197,197	0
2	NAG	G	1	14/15	0.68	0.31	197,197,197,197	0
2	NDG	Q	2	14/15	0.69	0.33	189,189,189,189	0
2	NAG	Q	1	14/15	0.69	0.50	197,197,197,197	0
3	NAG	U	1	14/15	0.70	0.23	173,173,173,173	0
3	NAG	H	2	14/15	0.71	0.53	197,197,197,197	0
3	NAG	F	2	14/15	0.74	0.28	196,196,196,196	0
2	NDG	G	2	14/15	0.74	0.37	189,189,189,189	0
3	NAG	F	1	14/15	0.76	0.26	173,173,173,173	0
3	NAG	P	1	14/15	0.76	0.24	173,173,173,173	0
2	NDG	L	2	14/15	0.77	0.35	189,189,189,189	0
2	NDG	T	2	14/15	0.77	0.28	142,142,142,142	0
3	NAG	K	1	14/15	0.78	0.18	173,173,173,173	0
3	NAG	R	2	14/15	0.79	0.24	197,197,197,197	0
2	NDG	J	2	14/15	0.80	0.30	142,142,142,142	0
3	NAG	S	2	14/15	0.81	0.27	111,111,111,111	0
2	NDG	O	2	14/15	0.82	0.25	142,142,142,142	0
2	NDG	E	2	14/15	0.83	0.21	142,142,142,142	0
3	NAG	N	2	14/15	0.83	0.27	111,111,111,111	0
3	NAG	M	1	14/15	0.83	0.23	117,117,117,117	0
3	NAG	R	1	14/15	0.84	0.19	117,117,117,117	0
3	NAG	H	1	14/15	0.84	0.22	117,117,117,117	0
2	NAG	J	1	14/15	0.85	0.17	77,77,77,77	0
2	NAG	E	1	14/15	0.86	0.17	77,77,77,77	0
3	NAG	X	2	14/15	0.86	0.23	111,111,111,111	0
2	NAG	T	1	14/15	0.88	0.18	77,77,77,77	0
3	NAG	W	1	14/15	0.89	0.19	117,117,117,117	0
3	NAG	I	2	14/15	0.89	0.26	111,111,111,111	0
3	NAG	N	1	14/15	0.89	0.18	88,88,88,88	0
3	NAG	I	1	14/15	0.91	0.19	88,88,88,88	0

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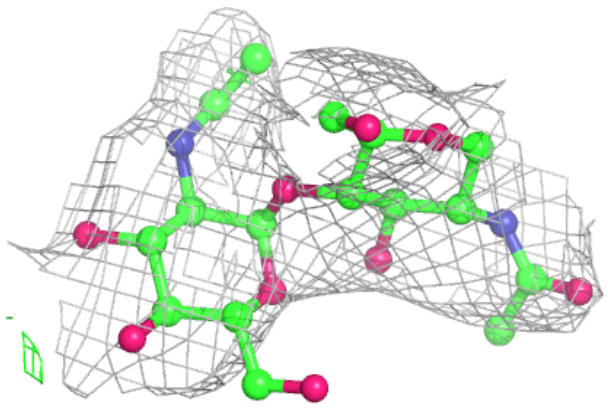
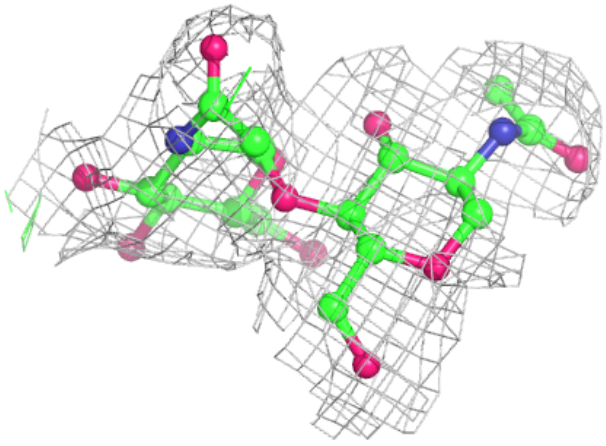
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	O	1	14/15	0.93	0.14	77,77,77,77	0
3	NAG	X	1	14/15	0.93	0.17	88,88,88,88	0
3	NAG	S	1	14/15	0.93	0.17	88,88,88,88	0

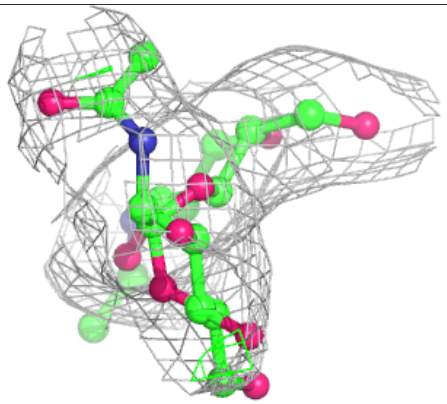
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

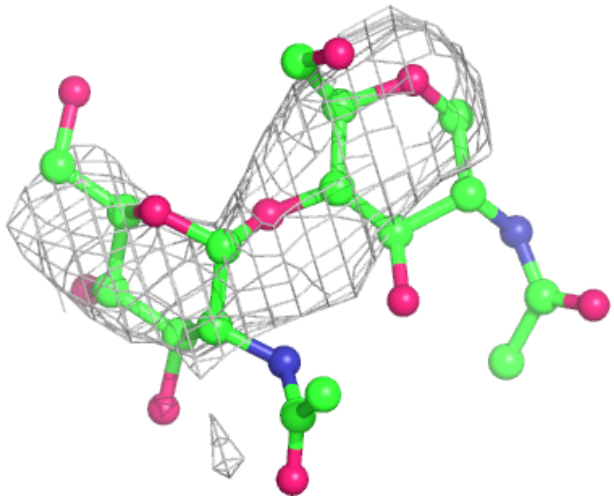


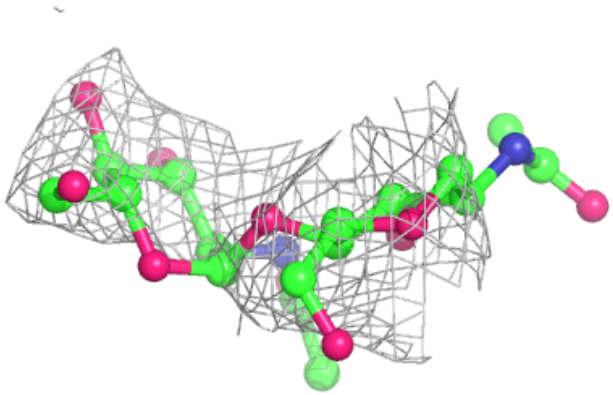


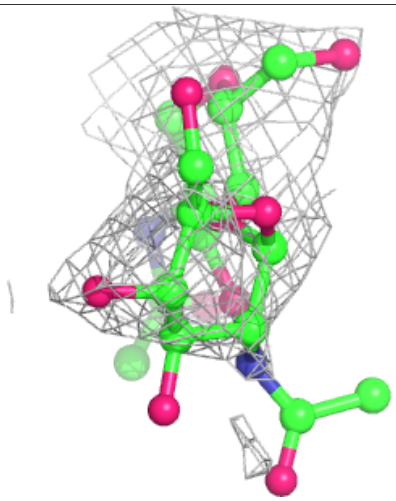


Electron density around Chain G:

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

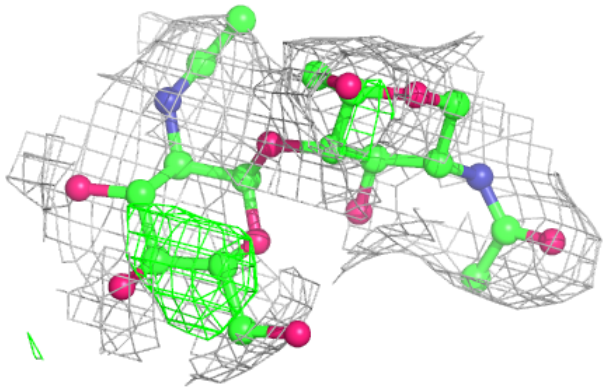


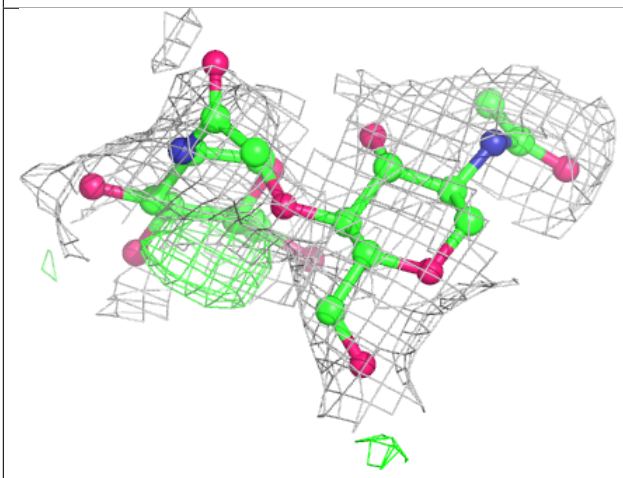


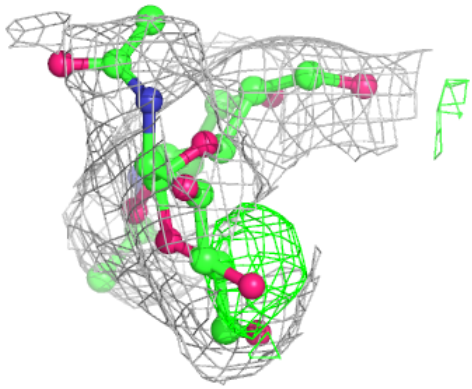


Electron density around Chain J:

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

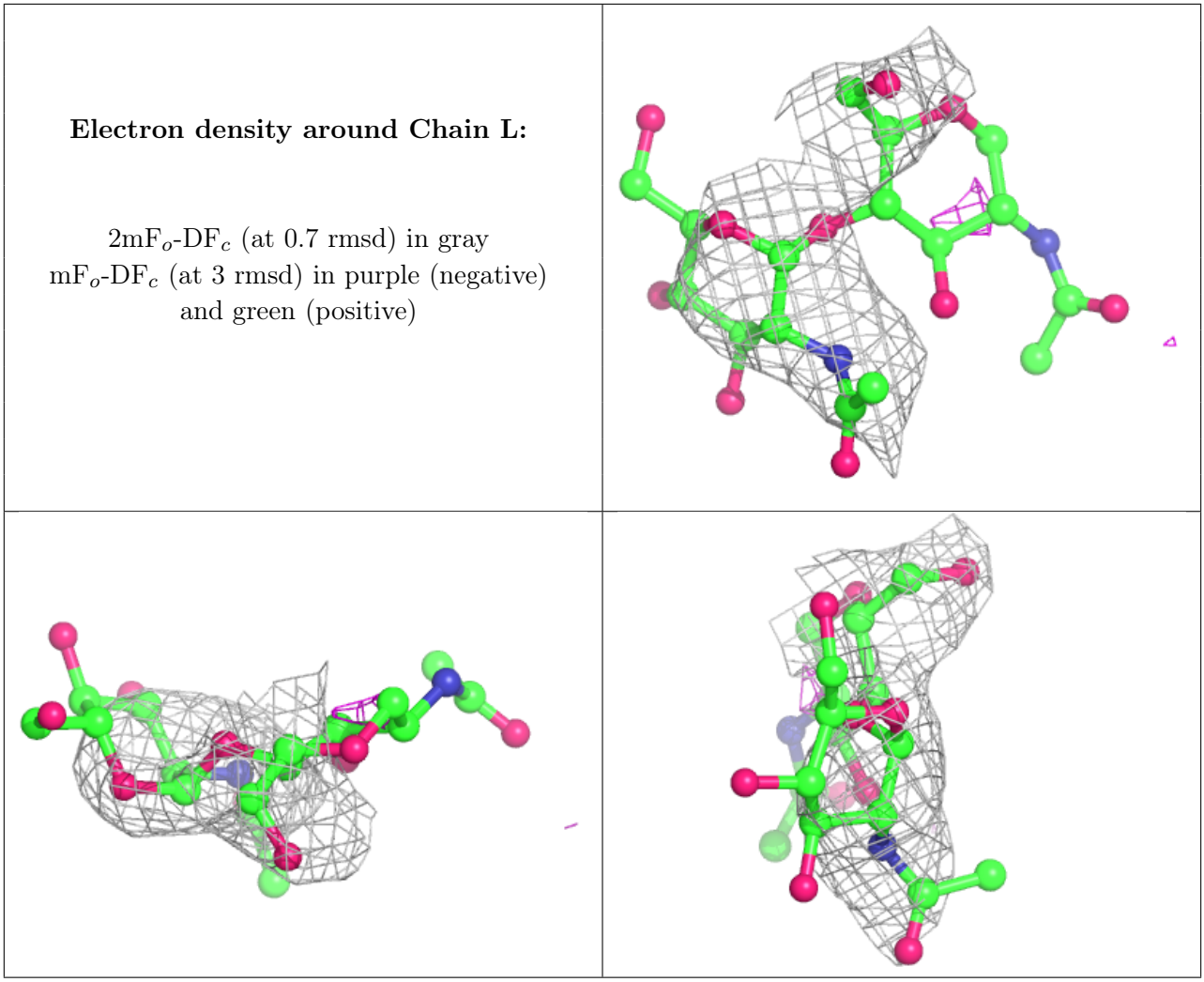






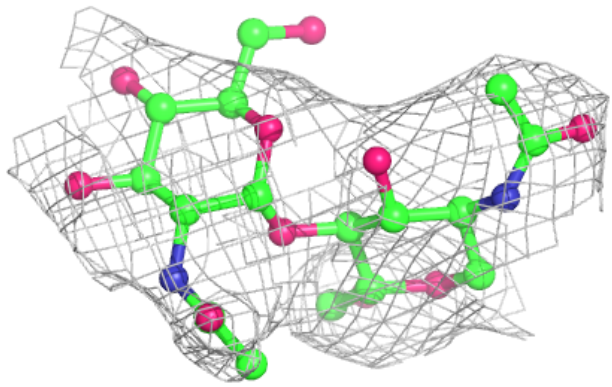
Electron density around Chain L:

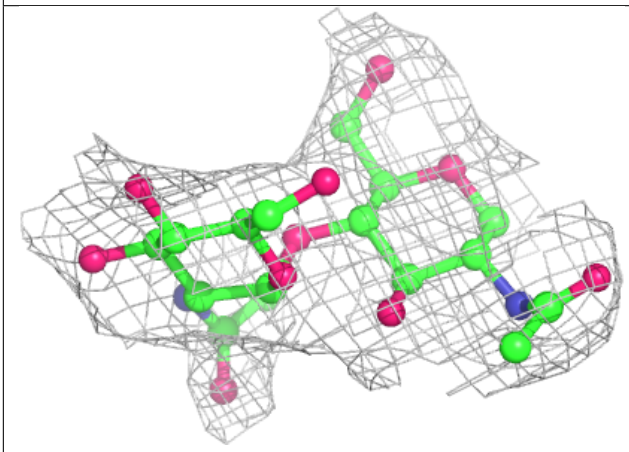
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

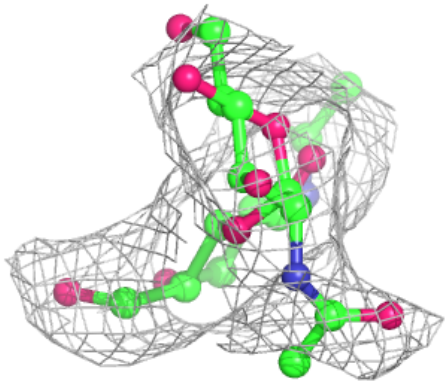


Electron density around Chain O:

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

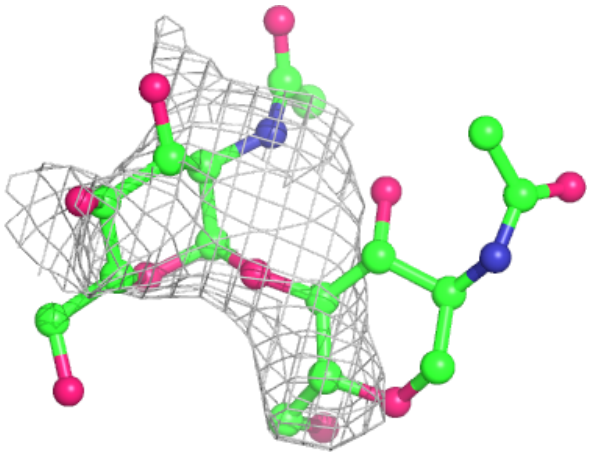


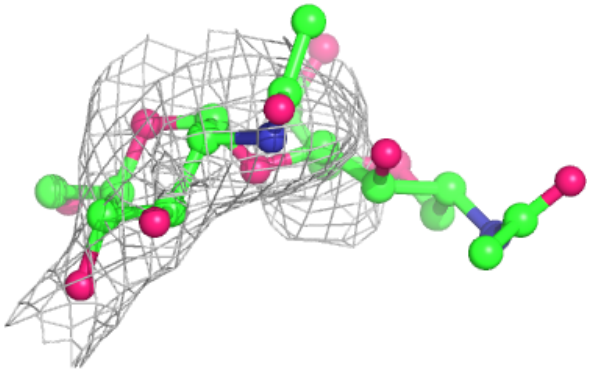


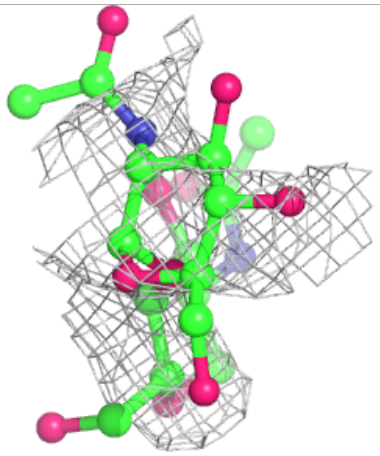


Electron density around Chain Q:

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

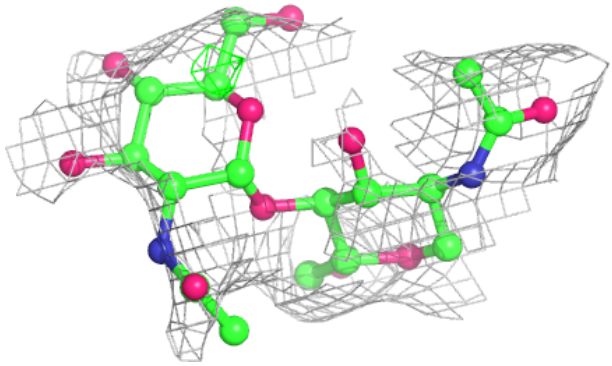


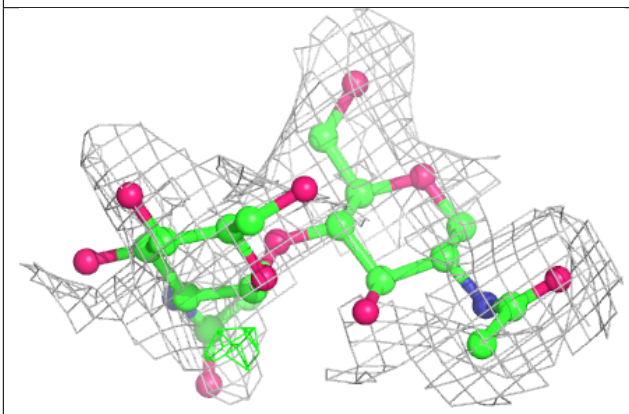


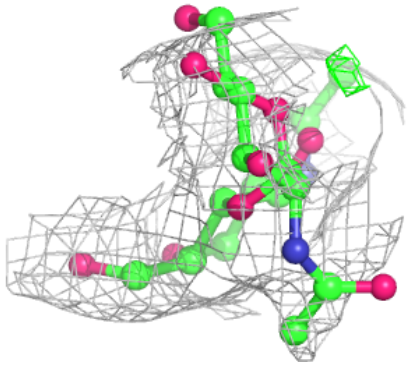


Electron density around Chain T:

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

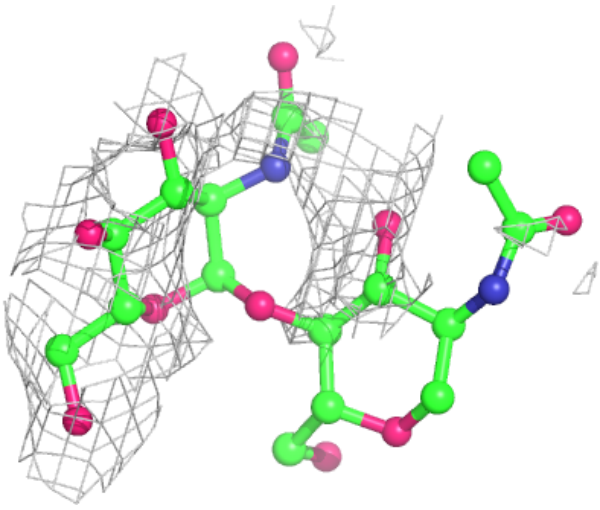


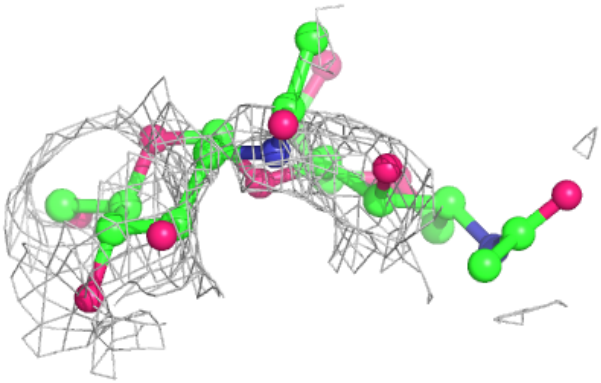


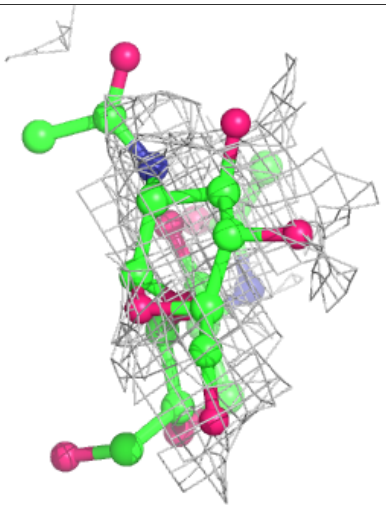


Electron density around Chain V:

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

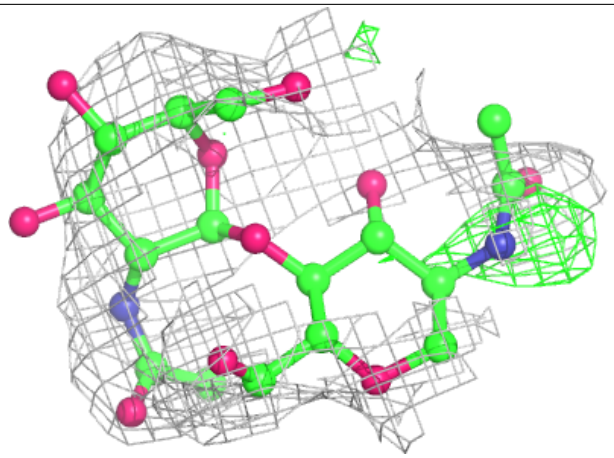


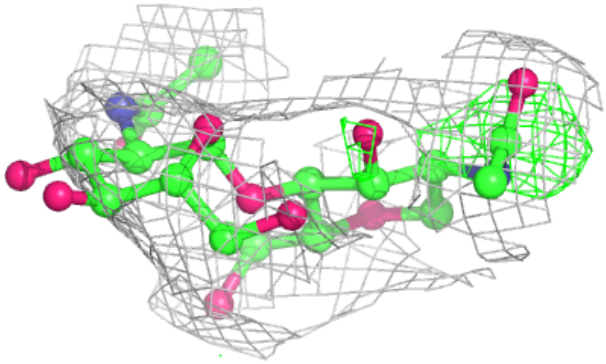


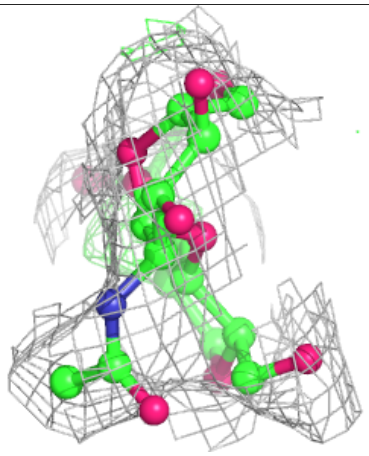


Electron density around Chain F:

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

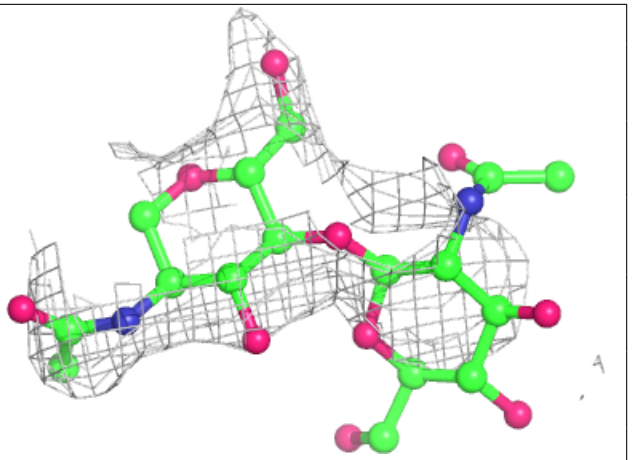


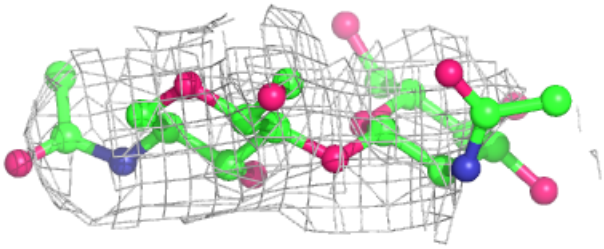


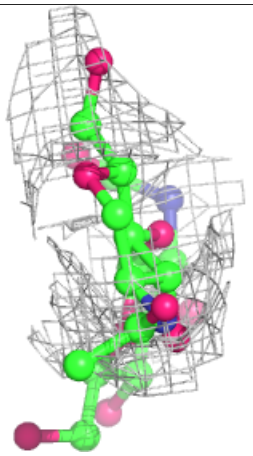


Electron density around Chain H:

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

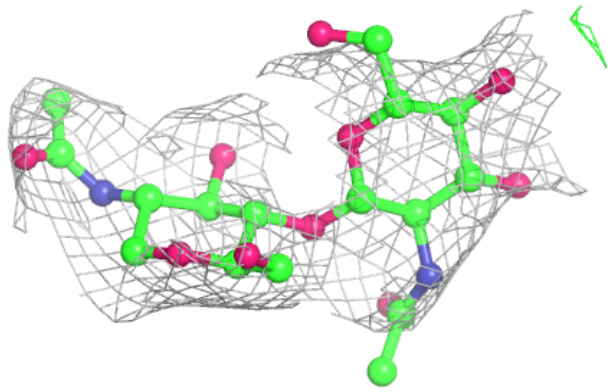


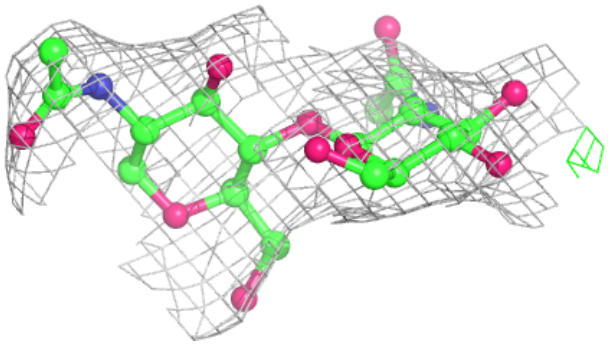


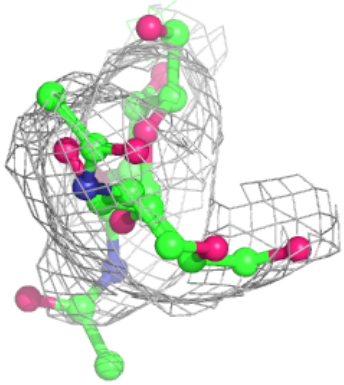


Electron density around Chain I:

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

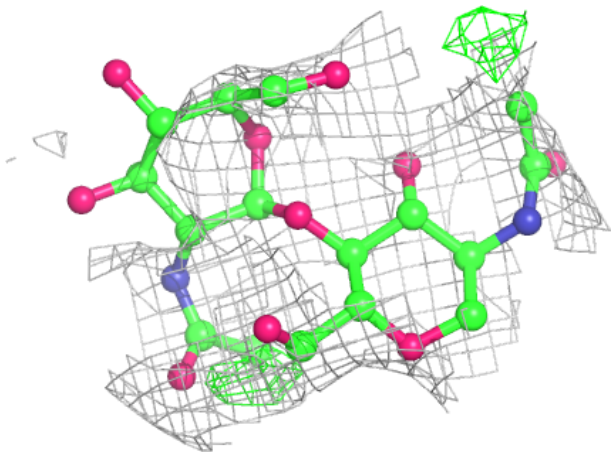


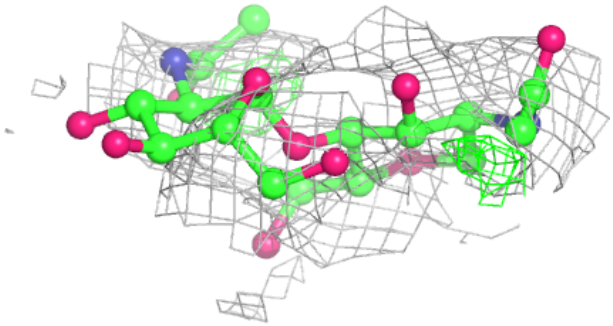


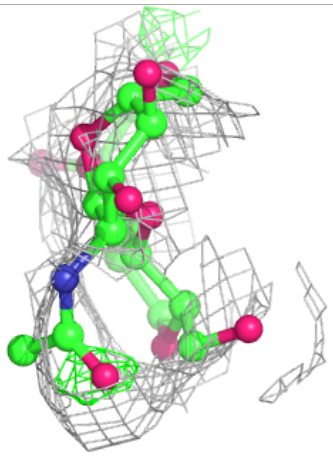


Electron density around Chain K:

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

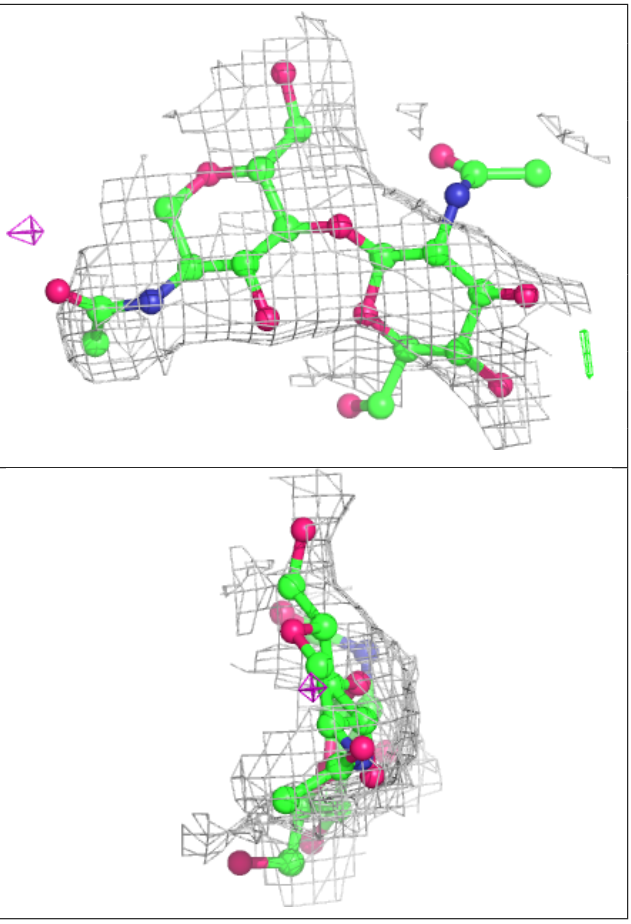






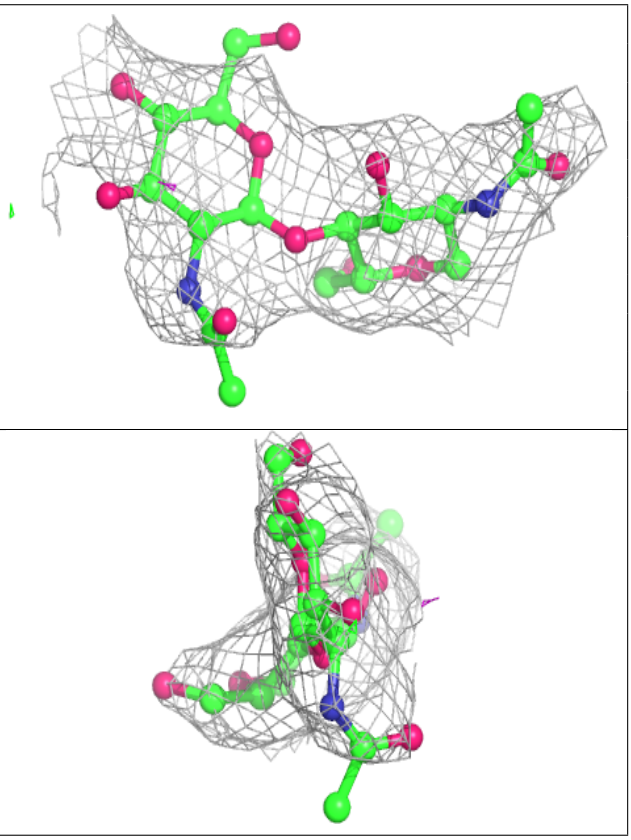
Electron density around Chain M:

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



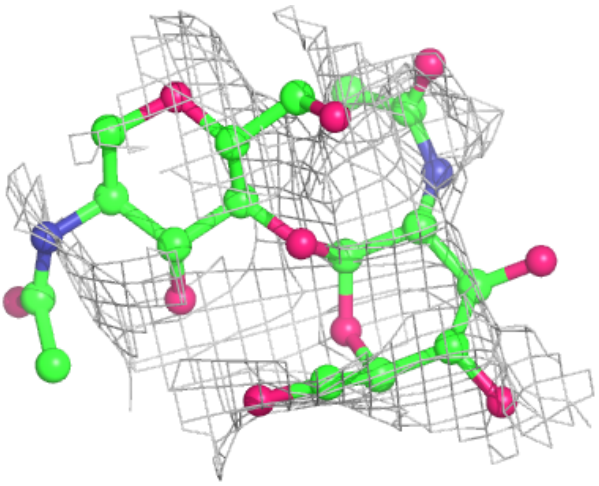
Electron density around Chain N:

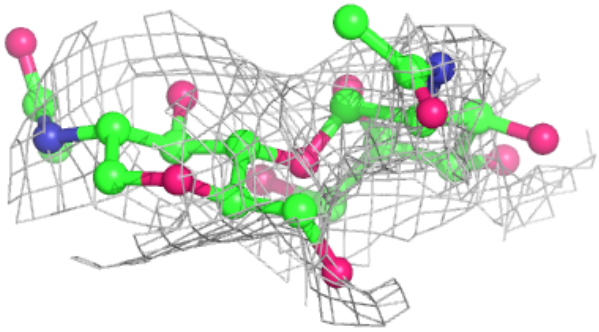
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

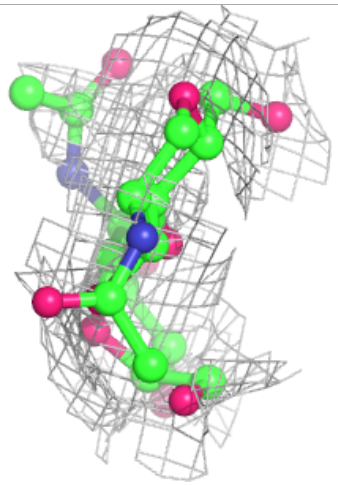


Electron density around Chain P:

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

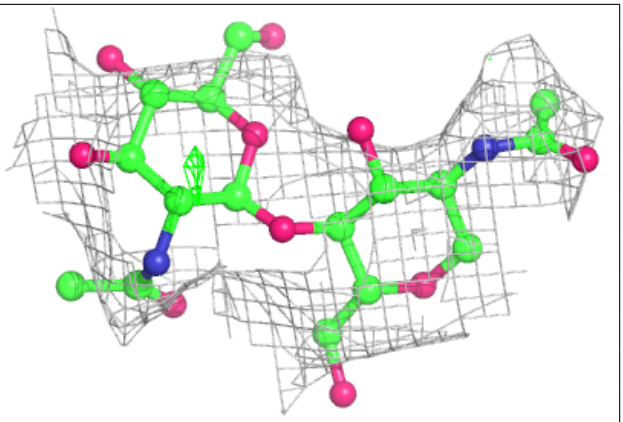


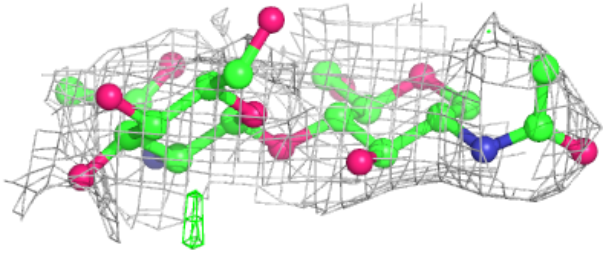


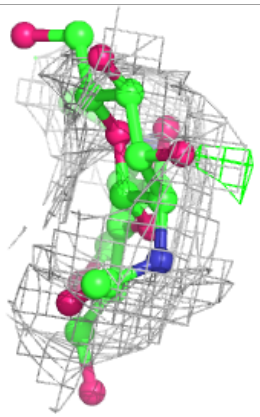


Electron density around Chain R:

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

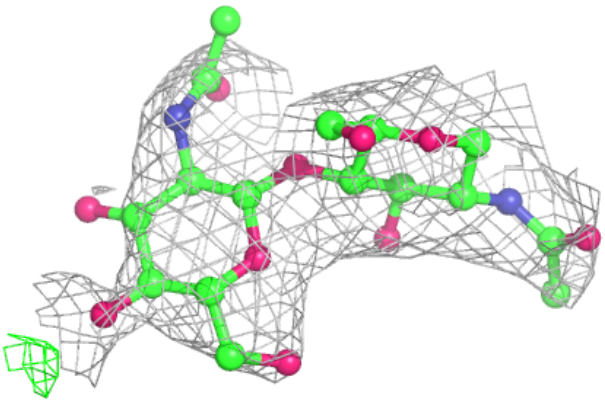


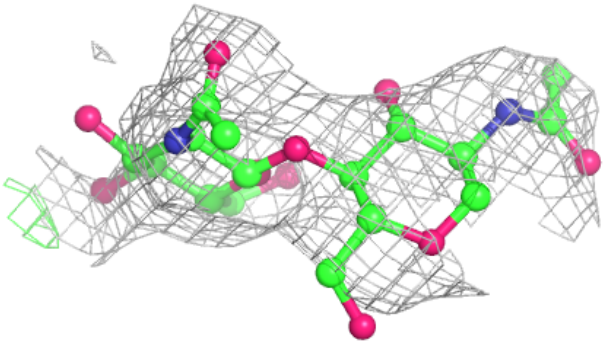


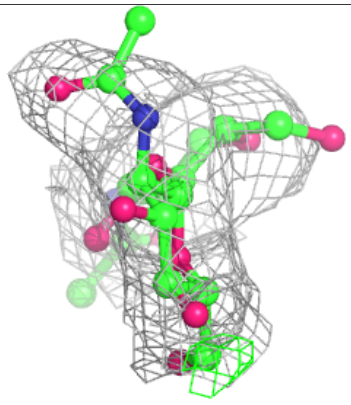


Electron density around Chain S:

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

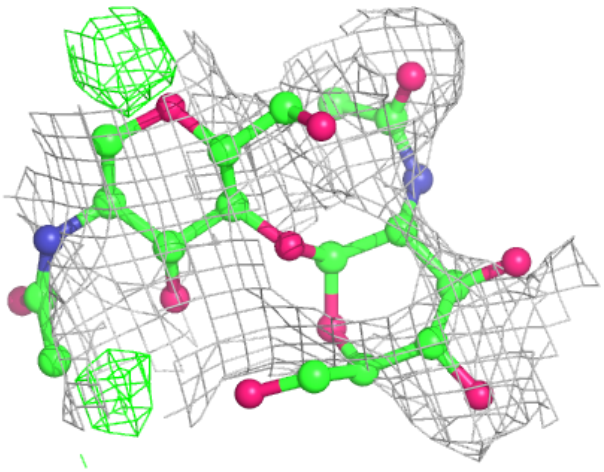


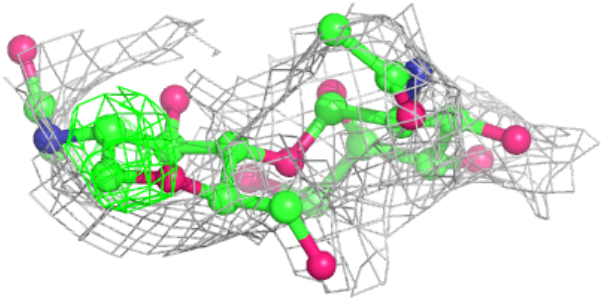


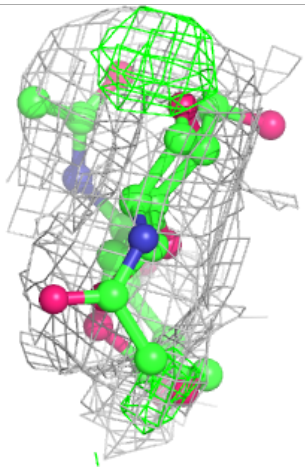


Electron density around Chain U:

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

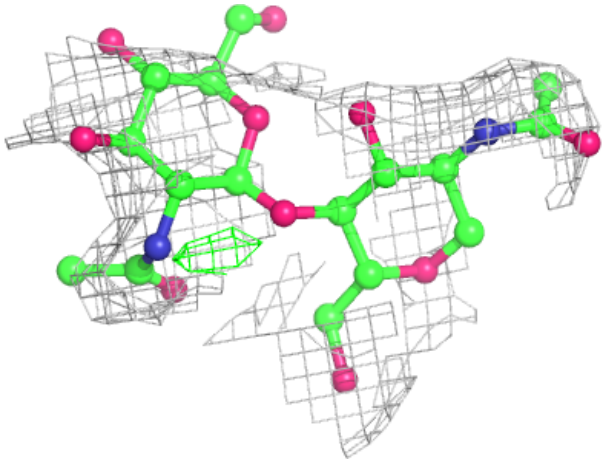


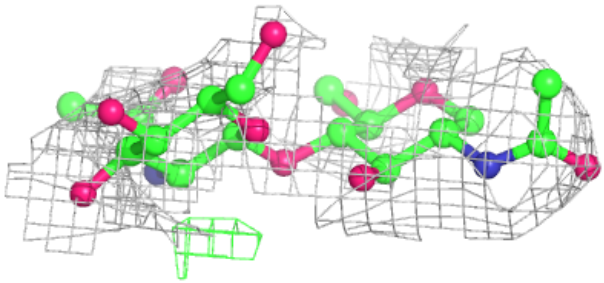


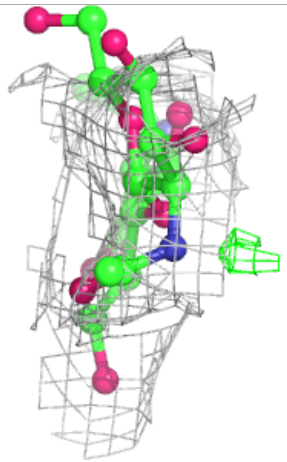


Electron density around Chain W:

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

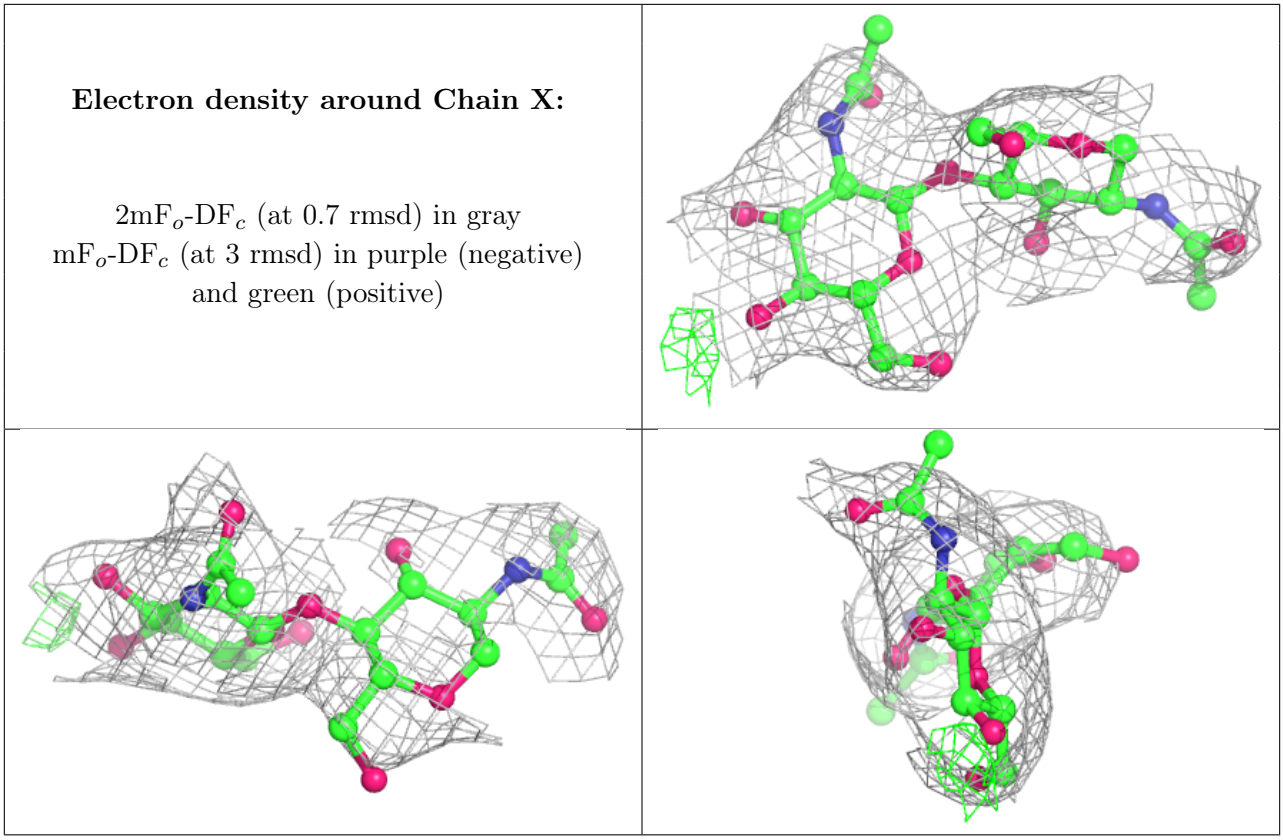






Electron density around Chain X:

$2mF_o$-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, 95^{th} 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	4760	14/15	0.50	0.40	155,155,155,155	0
4	NAG	B	2760	14/15	0.54	0.32	155,155,155,155	0
4	NAG	C	3760	14/15	0.60	0.35	155,155,155,155	0
4	NAG	A	1760	14/15	0.62	0.35	155,155,155,155	0
4	NAG	D	4759	14/15	0.84	0.22	57,57,57,57	0
4	NAG	C	3759	14/15	0.84	0.26	57,57,57,57	0
4	NAG	B	2759	14/15	0.89	0.19	57,57,57,57	0
4	NAG	A	1759	14/15	0.89	0.20	57,57,57,57	0
5	ZN	C	3751	1/1	0.89	0.07	52,52,52,52	0
5	ZN	C	3752	1/1	0.89	0.15	52,52,52,52	0
5	ZN	D	4751	1/1	0.90	0.06	52,52,52,52	0
5	ZN	D	4752	1/1	0.93	0.07	52,52,52,52	0
5	ZN	B	2751	1/1	0.95	0.13	52,52,52,52	0
5	ZN	B	2752	1/1	0.95	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	A	1752	1/1	0.96	0.08	52,52,52,52	0
5	ZN	A	1751	1/1	0.97	0.06	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.