Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:48 AM BST

PDB ID	:	1M1X
Title	:	CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN ALPHA VBETA3 BOUND TO MN2+
Authors	:	Xiong, J.-P.; Stehle, T.; Zhang, R.; Joachimiak, A.; Frech, M.; Goodman, S.L.; Arnaout, M.A.
Deposited on	:	2002-06-20
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

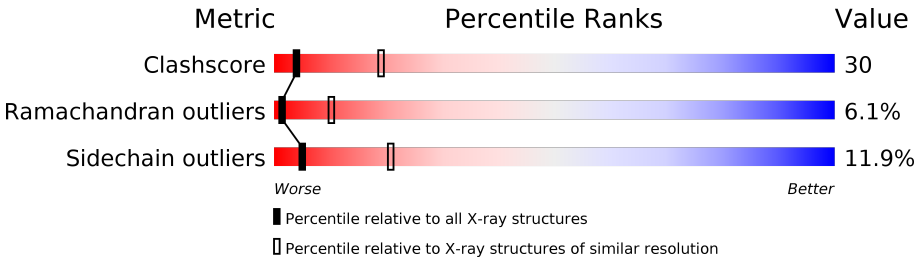
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	49% 40% 7%
2	B	692	35% 33% 9% 22%
3	C	2	50% 50%
3	D	2	100%
3	E	2	50% 50%
3	G	2	100%
4	F	2	50% 50%
4	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	I	2	

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
3	NAG	C	1	-	-	X	-
3	NAG	C	2	-	-	X	-
4	NDG	I	2	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11656 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	927	Total	C	N	O	S	0	0	0
			7216	4568	1224	1389	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	539	Total	C	N	O	S	0	0	0
			4182	2594	700	842	46			

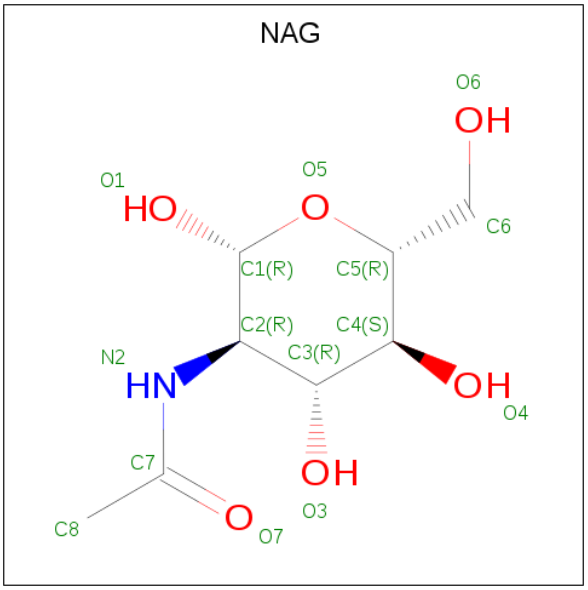
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

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

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



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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mn 1 1	0	0
6	A	5	Total Mn 5 5	0	0

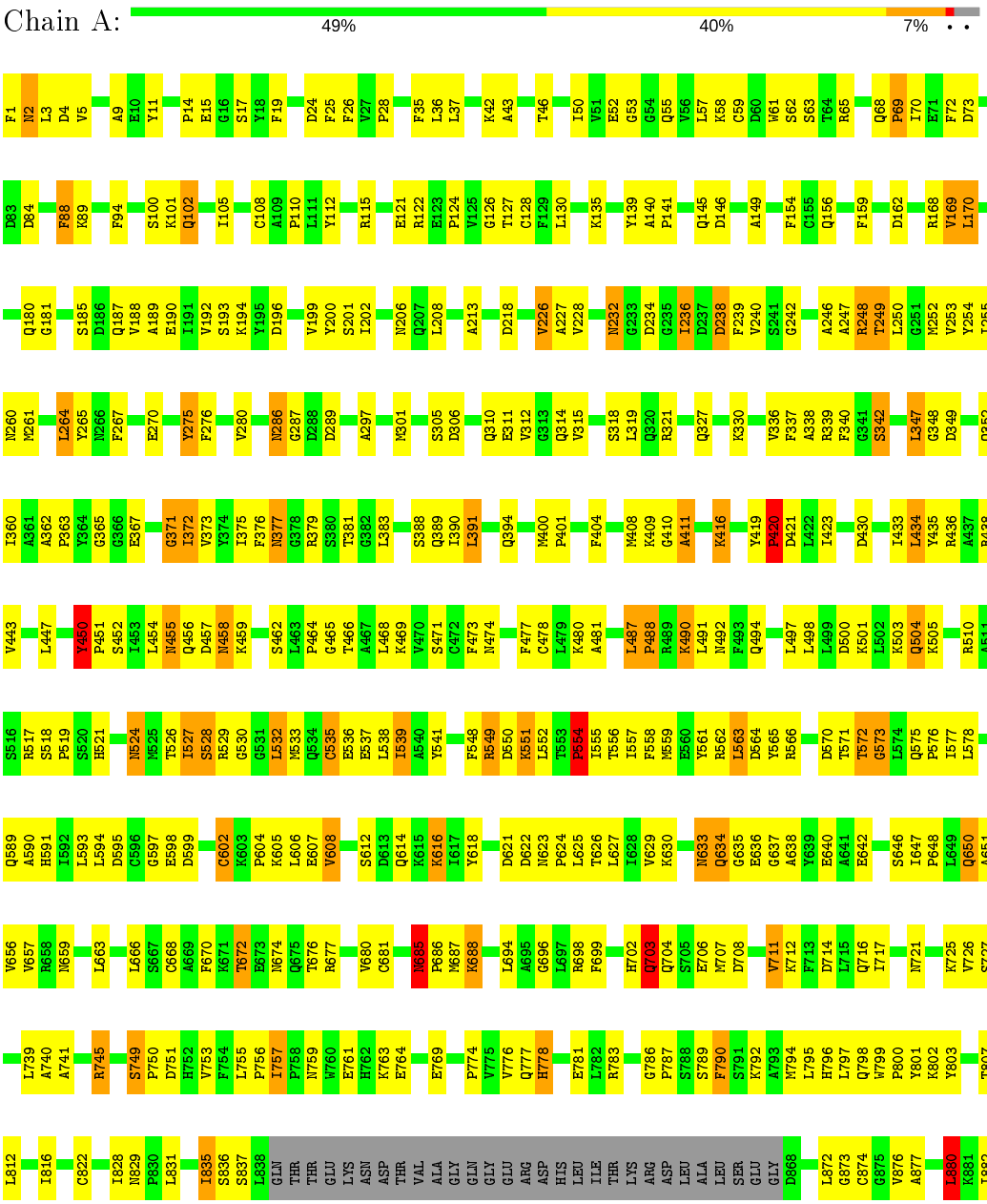
3 Residue-property plots (i)

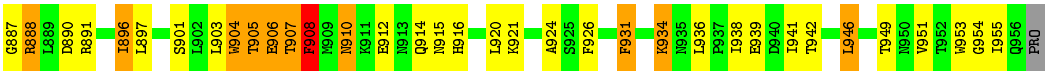
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: Integrin alpha-V

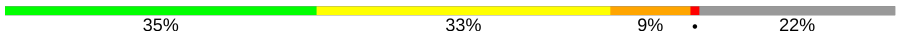
Chain A:

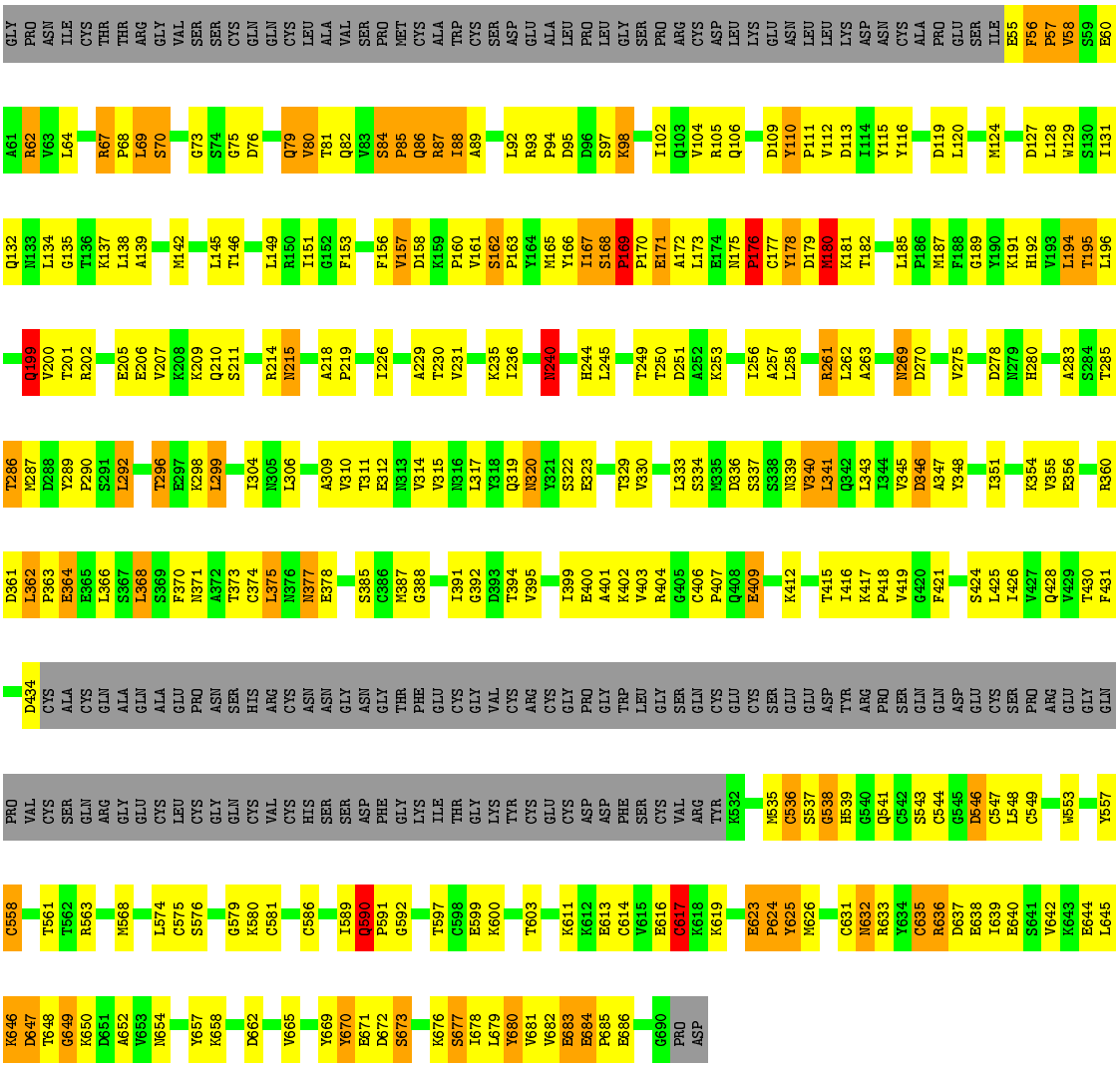




• Molecule 2: Integrin beta-3

Chain B:



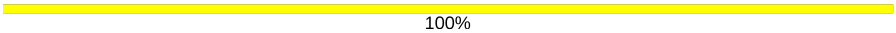


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain D:

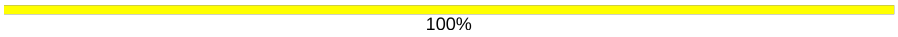


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain G:



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

Chain F:

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

Chain H:

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

Chain I:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.40Å 130.40Å 310.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.244 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11656	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NAG, 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	0.47	0/7372	0.79	7/9994 (0.1%)
2	B	0.46	0/4256	0.80	4/5754 (0.1%)
All	All	0.46	0/11628	0.79	11/15748 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	912	GLU	N-CA-C	8.13	132.95	111.00
1	A	880	LEU	N-CA-C	-6.37	93.81	111.00
1	A	450	TYR	C-N-CD	6.21	141.45	128.40
2	B	590	GLN	N-CA-C	5.73	126.46	111.00
2	B	180	MET	N-CA-C	-5.71	95.60	111.00
1	A	598	GLU	N-CA-C	5.69	126.35	111.00
2	B	378	GLU	N-CA-C	-5.31	96.67	111.00
1	A	338	ALA	N-CA-C	-5.29	96.73	111.00
1	A	672	THR	N-CA-C	-5.28	96.74	111.00
2	B	169	PRO	C-N-CD	5.08	139.07	128.40
1	A	703	GLN	N-CA-C	5.07	124.70	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	625	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7216	0	7036	403	0
2	B	4182	0	4028	279	0
3	C	28	0	25	7	0
3	D	28	0	25	3	0
3	E	28	0	25	2	0
3	G	28	0	25	5	0
4	F	28	0	24	6	0
4	H	28	0	24	1	0
4	I	28	0	24	11	0
5	A	28	0	26	9	0
5	B	28	0	26	10	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
All	All	11656	0	11288	694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (694) 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)
4:F:1:NAG:H2	4:F:1:NAG:H61	1.28	1.14
1:A:753:VAL:HG22	1:A:951:VAL:HG12	1.36	1.07
1:A:800:PRO:HB3	1:A:873:GLY:HA2	1.37	1.04
1:A:685:ASN:HB3	1:A:686:PRO:HD3	1.40	0.98
1:A:585:ASN:ND2	3:E:1:NAG:H61	1.79	0.97
2:B:371:ASN:ND2	5:B:3371:NAG:H62	1.80	0.96
1:A:835:ILE:HG12	1:A:836:SER:H	1.28	0.96
1:A:77:ASN:HD21	1:A:89:LYS:H	1.06	0.95
2:B:366:LEU:HB3	2:B:403:VAL:HG12	1.47	0.95
1:A:438:ARG:HH21	1:A:577:ILE:HB	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.51	0.92
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.51	0.92
1:A:100:SER:HB2	1:A:105:ILE:HG22	1.52	0.91
2:B:388:GLY:HA2	2:B:636:ARG:HH22	1.37	0.90
1:A:556:THR:HG22	1:A:589:GLN:HG2	1.54	0.90
1:A:558:PHE:HD1	1:A:587:SER:HB3	1.38	0.89
1:A:339:ARG:O	1:A:362:ALA:HA	1.74	0.87
2:B:403:VAL:HG11	2:B:431:PHE:HE2	1.40	0.87
1:A:751:ASP:HB2	3:G:1:NAG:H81	1.55	0.87
1:A:781:GLU:HG3	1:A:896:ILE:HD13	1.56	0.87
2:B:88:ILE:HG23	2:B:425:LEU:HD11	1.59	0.85
2:B:194:LEU:HB2	2:B:206:GLU:HG3	1.58	0.84
1:A:745:ARG:HB3	1:A:745:ARG:HH11	1.42	0.84
2:B:613:GLU:HB3	2:B:625:TYR:CE2	2.13	0.84
4:F:1:NAG:H2	4:F:1:NAG:C6	2.06	0.83
1:A:604:PRO:HA	1:A:635:GLY:HA3	1.60	0.83
2:B:625:TYR:HB3	2:B:631:CYS:HB2	1.60	0.82
2:B:68:PRO:HD3	2:B:84:SER:HB2	1.62	0.82
1:A:3:LEU:HD13	1:A:435:TYR:HB3	1.61	0.82
2:B:648:THR:HA	4:I:2:NDG:C1	2.11	0.81
2:B:648:THR:HG22	4:I:2:NDG:H2	1.62	0.80
1:A:498:LEU:HD23	1:A:501:LYS:HD3	1.63	0.80
4:F:1:NAG:H61	4:F:1:NAG:C2	2.04	0.80
2:B:87:ARG:HG3	2:B:87:ARG:HH11	1.45	0.80
1:A:286:ASN:HD22	1:A:286:ASN:H	1.29	0.79
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.17	0.79
2:B:157:VAL:HG12	2:B:189:GLY:H	1.47	0.79
2:B:85:PRO:O	2:B:425:LEU:HD13	1.83	0.79
1:A:260:ASN:HD22	5:A:2260:NAG:H61	1.47	0.78
1:A:286:ASN:N	1:A:286:ASN:HD22	1.81	0.78
2:B:229:ALA:HA	2:B:236:ILE:HD11	1.65	0.78
2:B:391:ILE:HD12	2:B:391:ILE:H	1.47	0.78
2:B:56:PHE:CD2	2:B:56:PHE:N	2.52	0.78
2:B:69:LEU:HD13	2:B:81:THR:H	1.49	0.78
1:A:480:LYS:HB2	1:A:533:MET:HB3	1.66	0.77
1:A:674:ASN:HB3	1:A:676:THR:HG22	1.66	0.77
2:B:88:ILE:HG13	2:B:89:ALA:N	2.00	0.77
2:B:112:VAL:HG23	2:B:146:THR:HG21	1.64	0.77
2:B:341:LEU:C	2:B:343:LEU:H	1.87	0.76
2:B:250:THR:HG22	2:B:310:VAL:HG12	1.68	0.76
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ILE:HD13	2:B:306:LEU:HD21	1.69	0.74
1:A:169:VAL:O	1:A:185:SER:HA	1.88	0.74
1:A:563:LEU:HD12	1:A:564:ASP:H	1.53	0.74
2:B:168:SER:H	2:B:169:PRO:HD3	1.52	0.74
2:B:169:PRO:HB2	2:B:170:PRO:CD	2.18	0.74
1:A:9:ALA:HB3	1:A:434:LEU:HB2	1.68	0.74
1:A:745:ARG:HB2	2:B:603:THR:HG21	1.70	0.74
2:B:230:THR:HG23	2:B:304:ILE:HG13	1.70	0.73
2:B:418:PRO:HB2	2:B:421:PHE:CD2	2.24	0.73
3:C:1:NAG:H4	3:C:2:NAG:H62	1.69	0.73
2:B:56:PHE:HD2	2:B:56:PHE:N	1.87	0.73
2:B:388:GLY:HA2	2:B:636:ARG:NH2	2.03	0.73
2:B:67:ARG:NE	2:B:67:ARG:H	1.86	0.73
2:B:84:SER:HB3	2:B:85:PRO:HD3	1.71	0.73
3:C:1:NAG:C4	3:C:2:NAG:H62	2.19	0.72
2:B:170:PRO:HG3	2:B:178:TYR:CE2	2.24	0.72
1:A:451:PRO:HG3	5:A:2458:NAG:H83	1.71	0.72
2:B:240:ASN:HD22	2:B:240:ASN:H	1.35	0.72
1:A:955:ILE:HG13	2:B:686:GLU:HB3	1.70	0.72
2:B:62:ARG:NH2	2:B:85:PRO:HB3	2.05	0.72
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.18	0.72
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.71	0.72
1:A:816:ILE:HD11	1:A:822:CYS:SG	2.31	0.71
2:B:639:ILE:H	2:B:639:ILE:HD12	1.56	0.71
1:A:774:PRO:HD2	1:A:903:LEU:HB3	1.73	0.71
1:A:626:THR:HG22	1:A:698:ARG:HB3	1.73	0.71
2:B:639:ILE:N	2:B:639:ILE:HD12	2.05	0.71
2:B:170:PRO:HD2	2:B:173:LEU:HD12	1.72	0.71
1:A:127:THR:HG22	1:A:140:ALA:HB2	1.72	0.70
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.73	0.70
2:B:403:VAL:HG11	2:B:431:PHE:CE2	2.24	0.70
1:A:236:ILE:HD12	1:A:236:ILE:H	1.55	0.70
1:A:608:VAL:HG13	1:A:717:ILE:HD11	1.73	0.70
2:B:574:LEU:HD21	2:B:581:CYS:HB2	1.73	0.70
1:A:474:ASN:ND2	1:A:539:ILE:HG23	2.07	0.70
2:B:116:TYR:OH	2:B:340:VAL:HG21	1.90	0.70
2:B:616:GLU:HG2	2:B:657:TYR:OH	1.92	0.69
1:A:835:ILE:HG12	1:A:836:SER:N	2.06	0.69
1:A:349:ASP:H	1:A:420:PRO:HG2	1.58	0.69
1:A:77:ASN:HD21	1:A:89:LYS:N	1.87	0.69
1:A:466:THR:HB	1:A:468:LEU:HG	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:SER:HB3	1:A:890:ASP:HA	1.75	0.68
1:A:914:GLN:HB3	1:A:916:HIS:CE1	2.28	0.68
4:I:1:NAG:H4	4:I:2:NDG:HA	1.58	0.68
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.73	0.68
1:A:112:TYR:HB3	1:A:126:GLY:HA2	1.75	0.68
2:B:683:GLU:O	2:B:684:GLU:HB2	1.92	0.68
1:A:373:VAL:HG23	1:A:404:PHE:HE2	1.57	0.68
1:A:955:ILE:HD11	2:B:686:GLU:O	1.93	0.68
2:B:82:GLN:HG3	2:B:105:ARG:O	1.93	0.68
2:B:105:ARG:HB3	2:B:394:THR:HG23	1.75	0.68
2:B:657:TYR:CE2	2:B:665:VAL:HB	2.29	0.68
2:B:129:TRP:O	2:B:132:GLN:HG2	1.95	0.67
4:F:2:NDG:H6C2	4:F:2:NDG:H2	1.76	0.67
1:A:554:PRO:HG3	1:A:591:HIS:NE2	2.09	0.67
2:B:400:GLU:HG2	2:B:401:ALA:N	2.09	0.67
1:A:122:ARG:HD3	2:B:168:SER:HB3	1.75	0.66
1:A:247:ALA:HB3	1:A:250:LEU:HB2	1.77	0.66
2:B:62:ARG:CZ	2:B:85:PRO:HB3	2.25	0.66
5:B:3320:NAG:N2	5:B:3320:NAG:H5	2.11	0.66
1:A:312:VAL:HG12	1:A:336:VAL:HA	1.78	0.66
1:A:260:ASN:ND2	5:A:2260:NAG:H61	2.11	0.65
1:A:180:GLN:HG2	1:A:218:ASP:HA	1.77	0.65
1:A:72:PHE:HZ	1:A:105:ILE:HG13	1.62	0.65
1:A:751:ASP:HB2	3:G:1:NAG:C8	2.25	0.65
1:A:189:ALA:HA	1:A:192:VAL:HB	1.79	0.65
1:A:9:ALA:HB3	1:A:434:LEU:CB	2.26	0.65
2:B:119:ASP:HB3	2:B:124:MET:SD	2.36	0.65
2:B:361:ASP:O	2:B:362:LEU:HB3	1.95	0.65
1:A:373:VAL:HG23	1:A:404:PHE:CE2	2.32	0.65
1:A:906:GLU:C	1:A:908:PHE:H	2.01	0.65
1:A:377:ASN:HD22	1:A:377:ASN:N	1.95	0.65
1:A:3:LEU:CD1	1:A:435:TYR:HB3	2.26	0.65
2:B:157:VAL:HG13	2:B:158:ASP:H	1.61	0.64
1:A:647:ILE:HD12	1:A:651:ALA:HB3	1.79	0.64
1:A:81:ALA:HB3	1:A:84:ASP:HB3	1.77	0.64
4:F:2:NDG:C6	4:F:2:NDG:H2	2.27	0.64
1:A:808:LEU:O	1:A:809:LEU:HB2	1.97	0.64
2:B:169:PRO:HB2	2:B:170:PRO:HD3	1.78	0.64
1:A:455:ASN:C	1:A:455:ASN:HD22	2.01	0.64
1:A:208:LEU:HD21	1:A:259:LYS:O	1.98	0.63
2:B:162:SER:OG	2:B:163:PRO:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.80	0.63
1:A:551:LYS:HA	1:A:551:LYS:NZ	2.13	0.63
1:A:555:ILE:HB	1:A:590:ALA:HB3	1.80	0.63
2:B:134:LEU:HA	2:B:137:LYS:HE2	1.80	0.62
1:A:904:TRP:CZ3	1:A:906:GLU:HG2	2.34	0.62
1:A:438:ARG:NH2	1:A:577:ILE:HB	2.10	0.62
1:A:188:VAL:C	1:A:190:GLU:H	2.03	0.62
1:A:260:ASN:ND2	5:A:2260:NAG:C6	2.62	0.62
1:A:375:ILE:O	1:A:375:ILE:HG13	1.97	0.62
1:A:416:LYS:H	1:A:416:LYS:HD2	1.65	0.62
1:A:657:VAL:O	1:A:657:VAL:HG13	1.99	0.62
1:A:672:THR:HG22	1:A:677:ARG:HA	1.81	0.62
1:A:798:GLN:HB3	1:A:874:CYS:SG	2.40	0.62
1:A:441:ILE:HD12	1:A:563:LEU:HD21	1.80	0.62
2:B:175:ASN:HB2	2:B:176:PRO:HD3	1.80	0.62
2:B:191:LYS:HB3	2:B:280:HIS:CE1	2.35	0.62
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.81	0.62
3:C:1:NAG:H61	3:C:2:NAG:O5	2.00	0.62
1:A:375:ILE:HG12	1:A:389:GLN:HB3	1.83	0.61
1:A:625:LEU:HD11	1:A:734:VAL:HG21	1.83	0.61
1:A:629:VAL:O	1:A:694:LEU:HA	1.99	0.61
1:A:740:ALA:HA	1:A:786:GLY:HA3	1.83	0.61
2:B:62:ARG:NE	2:B:85:PRO:HB3	2.16	0.60
1:A:565:TYR:HB3	1:A:575:GLN:NE2	2.16	0.60
2:B:56:PHE:N	2:B:57:PRO:HD3	2.17	0.60
2:B:58:VAL:CG1	2:B:93:ARG:HG2	2.32	0.60
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.83	0.60
2:B:58:VAL:HG13	2:B:93:ARG:HG2	1.82	0.60
1:A:721:ASN:O	1:A:725:LYS:HE2	2.00	0.60
1:A:36:LEU:CB	1:A:59:CYS:HB2	2.32	0.60
1:A:242:GLY:HA2	1:A:253:VAL:HG22	1.84	0.60
1:A:745:ARG:NH1	1:A:745:ARG:HB3	2.13	0.60
2:B:157:VAL:HG13	2:B:158:ASP:N	2.17	0.60
2:B:215:ASN:HD22	2:B:215:ASN:H	1.48	0.59
2:B:88:ILE:CG2	2:B:425:LEU:HD11	2.29	0.59
1:A:721:ASN:O	1:A:725:LYS:HB3	2.02	0.59
1:A:781:GLU:HG3	1:A:896:ILE:CD1	2.29	0.59
2:B:244:HIS:C	2:B:245:LEU:HD12	2.22	0.59
2:B:269:ASN:HD22	2:B:270:ASP:N	1.99	0.59
3:C:1:NAG:O4	3:C:2:NAG:H62	2.02	0.59
5:B:3320:NAG:HN2	5:B:3320:NAG:H5	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:OD2	1:A:436:ARG:HA	2.02	0.59
2:B:112:VAL:HG12	2:B:113:ASP:N	2.17	0.59
2:B:132:GLN:HA	2:B:207:VAL:HG12	1.85	0.59
1:A:110:PRO:O	1:A:156:GLN:HG2	2.03	0.59
2:B:649:GLY:HA3	2:B:670:TYR:OH	2.02	0.58
1:A:180:GLN:HE22	1:A:213:ALA:H	1.49	0.58
1:A:616:LYS:N	1:A:616:LYS:HD3	2.17	0.58
1:A:751:ASP:CB	3:G:1:NAG:H81	2.31	0.58
1:A:246:ALA:HB3	1:A:252:MET:HB2	1.86	0.58
2:B:646:LYS:O	4:I:2:NDG:H8C3	2.02	0.58
2:B:613:GLU:HB3	2:B:625:TYR:HE2	1.66	0.58
2:B:371:ASN:CG	5:B:3371:NAG:H62	2.24	0.58
1:A:276:PHE:HA	1:A:297:ALA:HB2	1.86	0.58
1:A:920:LEU:HD23	1:A:920:LEU:N	2.19	0.58
1:A:602:CYS:O	1:A:604:PRO:HD3	2.03	0.58
1:A:515:TYR:HE1	1:A:539:ILE:HD13	1.68	0.57
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.85	0.57
1:A:605:LYS:HD3	1:A:634:GLN:HB3	1.86	0.57
2:B:632:ASN:HD22	2:B:633:ARG:H	1.52	0.57
1:A:704:GLN:HB3	1:A:707:MET:SD	2.44	0.57
2:B:652:ALA:HB1	2:B:669:TYR:O	2.04	0.57
2:B:356:GLU:HB3	2:B:419:VAL:HG22	1.86	0.57
1:A:792:LYS:HA	1:A:887:GLY:HA2	1.86	0.57
1:A:252:MET:HA	1:A:267:PHE:O	2.05	0.57
1:A:112:TYR:CD2	1:A:127:THR:HG23	2.40	0.57
1:A:377:ASN:O	1:A:383:LEU:HD12	2.04	0.57
2:B:341:LEU:C	2:B:343:LEU:N	2.57	0.57
2:B:124:MET:HA	2:B:127:ASP:OD1	2.05	0.56
2:B:171:GLU:C	2:B:173:LEU:H	2.08	0.56
2:B:67:ARG:H	2:B:67:ARG:HE	1.52	0.56
1:A:375:ILE:CD1	1:A:389:GLN:HB3	2.35	0.56
2:B:320:ASN:OD1	5:B:3320:NAG:H2	2.06	0.56
1:A:562:ARG:HG2	1:A:563:LEU:N	2.21	0.56
1:A:554:PRO:HG3	1:A:591:HIS:CD2	2.41	0.56
2:B:84:SER:CB	2:B:85:PRO:HD3	2.35	0.56
1:A:886:VAL:HG12	1:A:887:GLY:N	2.20	0.56
3:G:1:NAG:C6	3:G:2:NAG:O5	2.54	0.56
1:A:19:PHE:HB3	1:A:430:ASP:HB3	1.87	0.56
1:A:240:VAL:HG22	1:A:255:ILE:HD13	1.88	0.56
1:A:25:PHE:HE1	1:A:410:GLY:HA2	1.71	0.56
1:A:336:VAL:O	1:A:337:PHE:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ASN:HD22	5:B:3371:NAG:H62	1.66	0.56
1:A:704:GLN:OE1	1:A:707:MET:SD	2.64	0.56
3:G:1:NAG:H61	3:G:2:NAG:O5	2.06	0.56
1:A:249:THR:CG2	2:B:256:ILE:HD13	2.36	0.56
1:A:921:LYS:HD2	1:A:946:LEU:HD12	1.88	0.56
1:A:887:GLY:O	1:A:888:ARG:CB	2.53	0.55
2:B:292:LEU:O	2:B:296:THR:HB	2.07	0.55
2:B:173:LEU:HA	2:B:176:PRO:HD2	1.88	0.55
2:B:151:ILE:O	2:B:196:LEU:HA	2.06	0.55
1:A:159:PHE:CZ	2:B:261:ARG:HD2	2.40	0.55
2:B:98:LYS:HA	2:B:98:LYS:HE3	1.87	0.55
3:D:1:NAG:O7	3:D:1:NAG:H3	2.07	0.55
2:B:167:ILE:O	2:B:168:SER:HB2	2.07	0.55
2:B:62:ARG:HH21	2:B:85:PRO:HB3	1.72	0.55
2:B:58:VAL:HG23	2:B:98:LYS:NZ	2.22	0.55
4:I:1:NAG:C4	4:I:2:NDG:HA	2.18	0.55
1:A:286:ASN:N	1:A:286:ASN:ND2	2.53	0.55
2:B:115:TYR:CE1	2:B:236:ILE:HG23	2.42	0.55
2:B:319:GLN:O	2:B:322:SER:HB3	2.06	0.55
1:A:451:PRO:HD2	1:A:473:PHE:HA	1.88	0.55
1:A:640:GLU:H	1:A:685:ASN:ND2	2.05	0.55
1:A:711:VAL:HG23	1:A:734:VAL:HG23	1.89	0.55
1:A:739:LEU:O	1:A:787:PRO:HD2	2.07	0.55
1:A:802:LYS:HB3	1:A:807:THR:HA	1.89	0.55
2:B:157:VAL:CG1	2:B:189:GLY:H	2.17	0.55
1:A:246:ALA:CB	1:A:252:MET:HB2	2.37	0.55
1:A:510:ARG:HD2	1:A:548:PHE:CD1	2.41	0.55
1:A:127:THR:HG22	1:A:140:ALA:CB	2.37	0.54
2:B:185:LEU:HD11	2:B:211:SER:HB3	1.90	0.54
1:A:526:THR:HG22	1:A:527:ILE:N	2.21	0.54
2:B:134:LEU:CA	2:B:137:LYS:HE2	2.37	0.54
2:B:218:ALA:CB	2:B:219:PRO:HD3	2.30	0.54
2:B:426:ILE:HD12	2:B:426:ILE:N	2.23	0.54
1:A:450:TYR:HB2	1:A:451:PRO:HD3	1.89	0.54
2:B:180:MET:HB3	2:B:182:THR:HG22	1.89	0.54
2:B:257:ALA:HA	2:B:289:TYR:HB2	1.88	0.54
2:B:648:THR:HA	4:I:2:NDG:C2	2.37	0.54
1:A:657:VAL:HG11	1:A:663:LEU:HD13	1.88	0.54
1:A:654:ILE:HB	1:A:698:ARG:HG3	1.88	0.54
2:B:340:VAL:HG13	2:B:340:VAL:O	2.08	0.54
1:A:629:VAL:O	1:A:694:LEU:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LEU:HD22	1:A:936:LEU:N	2.22	0.54
1:A:612:SER:HA	1:A:732:HIS:CE1	2.43	0.54
1:A:365:GLY:H	1:A:371:GLY:HA2	1.72	0.54
2:B:157:VAL:CG1	2:B:158:ASP:H	2.20	0.54
2:B:363:PRO:HB2	2:B:366:LEU:CD2	2.38	0.54
2:B:417:LYS:HB3	2:B:424:SER:HB3	1.90	0.54
2:B:654:ASN:ND2	4:I:1:NAG:H61	2.22	0.54
1:A:443:VAL:HG23	1:A:481:ALA:HB2	1.91	0.53
2:B:624:PRO:C	2:B:626:MET:H	2.12	0.53
4:F:2:NDG:C6	4:F:2:NDG:C2	2.86	0.53
1:A:375:ILE:CG1	1:A:389:GLN:HB3	2.38	0.53
1:A:946:LEU:HD23	1:A:946:LEU:H	1.73	0.53
1:A:267:PHE:HE2	1:A:318:SER:HG	1.56	0.53
1:A:725:LYS:HG3	1:A:726:VAL:HG13	1.89	0.53
2:B:134:LEU:HG	2:B:135:GLY:N	2.23	0.53
1:A:375:ILE:HD11	1:A:389:GLN:HB3	1.89	0.53
2:B:366:LEU:HB3	2:B:403:VAL:CG1	2.30	0.53
2:B:58:VAL:HG23	2:B:98:LYS:HZ3	1.74	0.53
1:A:188:VAL:HG12	1:A:189:ALA:H	1.73	0.53
1:A:555:ILE:HD12	1:A:555:ILE:H	1.74	0.53
2:B:632:ASN:ND2	2:B:633:ARG:H	2.06	0.53
1:A:1:PHE:CD2	1:A:2:ASN:HB2	2.44	0.53
1:A:227:ALA:O	1:A:240:VAL:HB	2.09	0.53
1:A:170:LEU:HG	1:A:239:PHE:CD2	2.44	0.53
2:B:590:GLN:C	2:B:592:GLY:H	2.12	0.53
2:B:635:CYS:O	2:B:635:CYS:SG	2.66	0.53
1:A:946:LEU:HD23	1:A:946:LEU:N	2.24	0.53
2:B:283:ALA:HA	2:B:286:THR:HG23	1.89	0.53
1:A:2:ASN:HA	1:A:389:GLN:OE1	2.09	0.53
1:A:340:PHE:C	1:A:342:SER:H	2.12	0.52
1:A:578:LEU:HD22	1:A:578:LEU:N	2.25	0.52
1:A:249:THR:HG21	2:B:256:ILE:HG21	1.90	0.52
3:C:1:NAG:C6	3:C:2:NAG:C1	2.87	0.52
1:A:471:SER:OG	5:A:2458:NAG:H61	2.10	0.52
2:B:192:HIS:CE1	2:B:195:THR:HA	2.44	0.52
1:A:559:MET:HB3	1:A:586:ILE:CG2	2.39	0.52
1:A:627:LEU:O	1:A:696:GLY:HA2	2.09	0.52
1:A:227:ALA:HB2	1:A:280:VAL:HG23	1.92	0.52
1:A:716:GLN:HG3	1:A:727:SER:O	2.09	0.52
1:A:789:SER:CB	1:A:890:ASP:HA	2.39	0.52
1:A:311:GLU:O	1:A:336:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ALA:HB3	1:A:687:MET:HB3	1.92	0.52
1:A:513:PHE:CE1	1:A:521:HIS:HB3	2.44	0.52
2:B:167:ILE:HG13	2:B:169:PRO:HD3	1.91	0.52
2:B:678:ILE:HD12	2:B:680:TYR:OH	2.09	0.52
2:B:192:HIS:HE2	2:B:195:THR:HG22	1.74	0.52
1:A:526:THR:O	1:A:527:ILE:HG23	2.09	0.52
1:A:537:GLU:HG2	1:A:538:LEU:N	2.24	0.52
1:A:608:VAL:HG13	1:A:717:ILE:CD1	2.39	0.52
1:A:257:ASP:HB3	1:A:261:MET:H	1.75	0.51
1:A:487:LEU:H	1:A:488:PRO:CD	2.23	0.51
1:A:556:THR:HG22	1:A:589:GLN:CG	2.35	0.51
1:A:593:LEU:HD23	1:A:594:LEU:N	2.25	0.51
1:A:657:VAL:O	1:A:657:VAL:CG1	2.58	0.51
1:A:666:LEU:O	2:B:535:MET:SD	2.68	0.51
1:A:907:THR:HG21	1:A:951:VAL:HG21	1.92	0.51
2:B:269:ASN:HD22	2:B:270:ASP:H	1.57	0.51
2:B:249:THR:HA	2:B:309:ALA:O	2.09	0.51
2:B:92:LEU:HD12	2:B:403:VAL:HG13	1.91	0.51
1:A:112:TYR:CE2	1:A:127:THR:HG23	2.45	0.51
1:A:802:LYS:O	1:A:877:ALA:HB1	2.10	0.51
1:A:951:VAL:O	1:A:951:VAL:HG23	2.11	0.51
2:B:356:GLU:O	2:B:418:PRO:HA	2.11	0.51
1:A:88:PHE:CD1	1:A:88:PHE:N	2.78	0.51
1:A:275:TYR:CD1	2:B:256:ILE:HD11	2.46	0.51
2:B:269:ASN:OD1	2:B:290:PRO:HB3	2.10	0.51
2:B:406:CYS:HB2	2:B:431:PHE:HB3	1.92	0.51
1:A:552:LEU:O	1:A:554:PRO:HD3	2.10	0.51
1:A:562:ARG:HG2	1:A:563:LEU:H	1.74	0.51
1:A:703:GLN:H	1:A:703:GLN:NE2	2.07	0.51
1:A:799:TRP:HZ2	1:A:901:SER:OG	1.94	0.51
1:A:621:ASP:HB3	1:A:891:ARG:HH21	1.75	0.51
1:A:657:VAL:HG11	1:A:663:LEU:CD1	2.41	0.51
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.92	0.51
2:B:194:LEU:HD23	2:B:202:ARG:NH2	2.26	0.51
1:A:450:TYR:CD1	1:A:474:ASN:HB2	2.45	0.51
1:A:504:GLN:HG2	1:A:505:LYS:H	1.75	0.51
1:A:549:ARG:NE	1:A:549:ARG:HA	2.26	0.51
1:A:755:LEU:C	1:A:757:ILE:N	2.62	0.51
1:A:904:TRP:HZ3	1:A:906:GLU:HG2	1.76	0.51
1:A:170:LEU:HD13	1:A:226:VAL:CG2	2.41	0.51
1:A:227:ALA:CB	1:A:280:VAL:HG23	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ARG:NH1	2:B:87:ARG:HG3	2.16	0.51
1:A:621:ASP:HB3	1:A:891:ARG:NH2	2.26	0.50
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.92	0.50
2:B:575:CYS:HB2	2:B:579:GLY:O	2.11	0.50
2:B:132:GLN:HA	2:B:207:VAL:CG1	2.40	0.50
1:A:108:CYS:HA	1:A:128:CYS:HA	1.94	0.50
1:A:238:ASP:HB3	1:A:256:TYR:O	2.12	0.50
1:A:439:PRO:HB2	1:A:576:PRO:HB3	1.93	0.50
1:A:648:PRO:HD2	1:A:651:ALA:HB2	1.94	0.50
1:A:750:PRO:HD2	1:A:777:GLN:H	1.76	0.50
2:B:262:LEU:HD23	2:B:262:LEU:N	2.27	0.50
1:A:53:GLY:O	1:A:94:PHE:HB3	2.10	0.50
2:B:586:CYS:SG	2:B:597:THR:HA	2.51	0.50
1:A:749:SER:HB3	1:A:750:PRO:CD	2.42	0.50
1:A:799:TRP:CZ2	1:A:901:SER:OG	2.64	0.50
2:B:178:TYR:CD1	2:B:179:ASP:N	2.79	0.50
2:B:115:TYR:OH	2:B:192:HIS:ND1	2.45	0.50
2:B:333:LEU:HD11	2:B:337:SER:OG	2.11	0.50
2:B:95:ASP:HA	2:B:403:VAL:O	2.12	0.50
1:A:390:ILE:HG13	1:A:390:ILE:O	2.11	0.50
1:A:753:VAL:CG2	1:A:951:VAL:HG12	2.24	0.50
2:B:250:THR:CG2	2:B:310:VAL:HG12	2.40	0.50
2:B:625:TYR:HB3	2:B:631:CYS:CB	2.35	0.50
3:D:1:NAG:O7	3:D:1:NAG:C3	2.59	0.50
4:I:1:NAG:H4	4:I:2:NDG:N2	2.25	0.50
1:A:451:PRO:HD2	1:A:473:PHE:HB2	1.93	0.49
1:A:494:GLN:O	1:A:561:TYR:HA	2.11	0.49
1:A:740:ALA:O	1:A:941:ILE:HD13	2.12	0.49
5:B:3371:NAG:H3	5:B:3371:NAG:O7	2.12	0.49
1:A:455:ASN:H	5:A:2458:NAG:H62	1.77	0.49
1:A:36:LEU:HD11	1:A:434:LEU:CD2	2.42	0.49
1:A:626:THR:HA	1:A:698:ARG:HA	1.94	0.49
2:B:240:ASN:N	2:B:240:ASN:HD22	2.05	0.49
1:A:462:SER:HA	1:A:468:LEU:O	2.12	0.49
1:A:647:ILE:HB	1:A:651:ALA:CB	2.42	0.49
1:A:480:LYS:HD2	1:A:530:GLY:O	2.11	0.49
2:B:574:LEU:HD23	2:B:575:CYS:SG	2.52	0.49
2:B:676:LYS:HE3	2:B:678:ILE:HG13	1.93	0.49
1:A:372:ILE:H	1:A:372:ILE:HD13	1.77	0.49
2:B:347:ALA:O	2:B:351:ILE:HG13	2.13	0.49
1:A:254:TYR:OH	3:D:1:NAG:H62	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:HG13	2:B:168:SER:H	1.78	0.49
2:B:368:LEU:HA	2:B:400:GLU:O	2.12	0.49
1:A:674:ASN:C	1:A:676:THR:H	2.15	0.49
2:B:134:LEU:HG	2:B:135:GLY:H	1.76	0.49
1:A:490:LYS:HD2	1:A:566:ARG:O	2.13	0.49
1:A:938:ILE:HD12	1:A:938:ILE:O	2.13	0.49
1:A:524:ASN:HD22	1:A:524:ASN:N	2.09	0.49
1:A:526:THR:HG22	1:A:527:ILE:H	1.77	0.49
1:A:886:VAL:CG1	1:A:887:GLY:N	2.76	0.49
2:B:60:GLU:HB3	2:B:98:LYS:HG2	1.94	0.49
1:A:458:ASN:ND2	5:A:2458:NAG:H4	2.28	0.48
1:A:563:LEU:CD1	1:A:564:ASP:H	2.23	0.48
2:B:334:SER:HB2	2:B:339:ASN:HB2	1.95	0.48
2:B:644:GLU:O	2:B:682:VAL:HG13	2.13	0.48
2:B:58:VAL:HG12	2:B:92:LEU:HA	1.95	0.48
1:A:441:ILE:CD1	1:A:563:LEU:HD21	2.44	0.48
1:A:57:LEU:HD12	1:A:57:LEU:N	2.28	0.48
2:B:399:ILE:HD13	2:B:416:ILE:HD13	1.95	0.48
1:A:828:ILE:HD12	1:A:828:ILE:O	2.13	0.48
2:B:97:SER:HB3	2:B:402:LYS:HB2	1.95	0.48
2:B:257:ALA:O	2:B:258:LEU:HB2	2.13	0.48
2:B:657:TYR:O	2:B:665:VAL:N	2.46	0.48
3:C:1:NAG:O4	3:C:2:NAG:C6	2.61	0.48
3:C:1:NAG:H61	3:C:2:NAG:C1	2.42	0.48
1:A:43:ALA:HB3	1:A:55:GLN:HG2	1.95	0.48
2:B:165:MET:HA	2:B:187:MET:CE	2.43	0.48
1:A:9:ALA:O	1:A:433:ILE:HA	2.13	0.48
1:A:439:PRO:HB3	1:A:487:LEU:HD13	1.95	0.48
1:A:512:LEU:HD12	1:A:541:TYR:OH	2.14	0.48
1:A:703:GLN:O	1:A:704:GLN:HB2	2.12	0.48
1:A:58:LYS:HB2	1:A:70:ILE:HD11	1.96	0.48
2:B:249:THR:HG22	2:B:309:ALA:CB	2.43	0.48
1:A:926:PHE:O	1:A:942:THR:HG23	2.14	0.48
2:B:110:TYR:CD1	2:B:111:PRO:HD2	2.48	0.48
2:B:672:ASP:H	2:B:676:LYS:HB3	1.79	0.48
1:A:168:ARG:NH2	1:A:206:ASN:O	2.47	0.48
2:B:112:VAL:CG1	2:B:113:ASP:N	2.76	0.48
2:B:97:SER:HA	2:B:401:ALA:O	2.14	0.48
2:B:536:CYS:SG	2:B:543:SER:O	2.72	0.48
1:A:42:LYS:O	1:A:52:GLU:HG2	2.13	0.47
1:A:776:VAL:HG11	1:A:949:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:MET:CB	2:B:149:LEU:HD22	2.44	0.47
2:B:67:ARG:O	2:B:67:ARG:CZ	2.62	0.47
1:A:247:ALA:HB1	1:A:250:LEU:HD12	1.96	0.47
1:A:910:ASN:HA	1:A:915:ASN:OD1	2.15	0.47
2:B:642:VAL:HG12	2:B:681:VAL:C	2.35	0.47
2:B:64:LEU:HB3	2:B:87:ARG:HB3	1.95	0.47
1:A:650:GLN:N	1:A:650:GLN:NE2	2.62	0.47
2:B:157:VAL:HG12	2:B:189:GLY:N	2.23	0.47
2:B:231:VAL:HG12	2:B:298:LYS:HD2	1.96	0.47
1:A:555:ILE:N	1:A:555:ILE:HD12	2.30	0.47
2:B:611:LYS:O	2:B:614:CYS:HB2	2.14	0.47
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.97	0.47
1:A:464:PRO:HG2	1:A:465:GLY:H	1.79	0.47
1:A:653:PHE:HB3	1:A:670:PHE:HD2	1.79	0.47
1:A:188:VAL:O	1:A:189:ALA:HB3	2.15	0.47
1:A:558:PHE:CE1	1:A:585:ASN:HB3	2.50	0.47
1:A:558:PHE:CD1	1:A:587:SER:HB3	2.31	0.47
1:A:882:ILE:N	1:A:882:ILE:HD12	2.30	0.47
2:B:173:LEU:HD21	2:B:178:TYR:CD1	2.49	0.47
2:B:400:GLU:HG2	2:B:401:ALA:H	1.79	0.47
2:B:599:GLU:HG2	2:B:600:LYS:HG3	1.96	0.47
1:A:101:LYS:HB3	1:A:102:GLN:H	1.44	0.47
1:A:550:ASP:CG	1:A:551:LYS:H	2.18	0.47
1:A:812:LEU:O	1:A:829:ASN:HB2	2.15	0.47
2:B:417:LYS:HB3	2:B:424:SER:CB	2.45	0.47
1:A:17:SER:HB2	1:A:43:ALA:HB2	1.97	0.47
1:A:187:GLN:O	1:A:190:GLU:HB3	2.15	0.47
1:A:588:ARG:HH11	1:A:588:ARG:HG2	1.80	0.47
2:B:169:PRO:HD2	2:B:173:LEU:HD12	1.97	0.47
2:B:314:VAL:HG22	2:B:317:LEU:HD23	1.97	0.46
2:B:178:TYR:O	2:B:180:MET:O	2.32	0.46
2:B:199:GLN:C	2:B:201:THR:H	2.18	0.46
2:B:391:ILE:CD1	2:B:391:ILE:H	2.23	0.46
1:A:26:PHE:HB2	1:A:37:LEU:HG	1.98	0.46
1:A:797:LEU:HD13	1:A:924:ALA:HB2	1.97	0.46
2:B:557:TYR:O	2:B:558:CYS:HB2	2.16	0.46
2:B:70:SER:HA	2:B:105:ARG:NH1	2.31	0.46
1:A:650:GLN:HB2	1:A:702:HIS:HB2	1.97	0.46
2:B:599:GLU:HG2	2:B:600:LYS:N	2.29	0.46
2:B:684:GLU:N	2:B:685:PRO:HD3	2.29	0.46
1:A:14:PRO:HB2	1:A:17:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HH22	5:B:3320:NAG:H3	1.80	0.46
1:A:232:ASN:HB2	1:A:264:LEU:HG	1.98	0.46
1:A:232:ASN:HB2	1:A:264:LEU:HD11	1.96	0.46
1:A:232:ASN:HD22	1:A:264:LEU:HD11	1.81	0.46
2:B:142:MET:HB3	2:B:149:LEU:HD22	1.97	0.46
2:B:92:LEU:O	2:B:431:PHE:HA	2.16	0.46
2:B:176:PRO:HB2	2:B:177:CYS:H	1.55	0.46
2:B:548:LEU:O	2:B:548:LEU:HD12	2.15	0.46
1:A:139:TYR:CE1	1:A:141:PRO:HD3	2.51	0.46
1:A:521:HIS:CE1	1:A:538:LEU:HD11	2.51	0.46
1:A:551:LYS:HA	1:A:551:LYS:HZ3	1.80	0.46
1:A:668:CYS:HA	1:A:680:VAL:O	2.16	0.46
1:A:188:VAL:HG12	1:A:189:ALA:N	2.31	0.46
2:B:142:MET:SD	2:B:345:VAL:HG22	2.56	0.46
2:B:157:VAL:CG1	2:B:158:ASP:N	2.79	0.46
1:A:455:ASN:HD22	1:A:456:GLN:N	2.14	0.45
1:A:803:TYR:HE2	1:A:876:VAL:HG12	1.81	0.45
2:B:366:LEU:HA	2:B:402:LYS:O	2.16	0.45
2:B:67:ARG:NE	2:B:67:ARG:N	2.61	0.45
1:A:487:LEU:O	1:A:488:PRO:O	2.34	0.45
1:A:630:LYS:HB2	1:A:694:LEU:HD13	1.98	0.45
1:A:906:GLU:C	1:A:908:PHE:N	2.67	0.45
1:A:794:MET:O	1:A:926:PHE:HA	2.15	0.45
2:B:251:ASP:HA	2:B:311:THR:OG1	2.16	0.45
1:A:741:ALA:H	1:A:786:GLY:HA3	1.81	0.45
1:A:790:PHE:C	1:A:790:PHE:CD1	2.90	0.45
2:B:355:VAL:O	2:B:385:SER:HA	2.17	0.45
2:B:391:ILE:HD12	2:B:391:ILE:N	2.23	0.45
1:A:439:PRO:CB	1:A:487:LEU:HD13	2.46	0.45
2:B:168:SER:H	2:B:169:PRO:CD	2.26	0.45
2:B:541:GLN:HG2	2:B:553:TRP:CD1	2.52	0.45
2:B:650:LYS:HG2	4:I:1:NAG:H5	1.98	0.45
1:A:188:VAL:C	1:A:190:GLU:N	2.69	0.45
1:A:193:SER:OG	1:A:193:SER:O	2.35	0.45
1:A:376:PHE:HB3	1:A:383:LEU:HD11	1.97	0.45
1:A:455:ASN:ND2	1:A:455:ASN:C	2.69	0.45
1:A:524:ASN:ND2	1:A:524:ASN:N	2.65	0.45
1:A:149:ALA:HA	1:A:154:PHE:HD1	1.82	0.45
1:A:550:ASP:CG	1:A:551:LYS:N	2.70	0.45
2:B:192:HIS:NE2	2:B:195:THR:HG22	2.32	0.45
2:B:371:ASN:ND2	5:B:3371:NAG:C6	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:HD23	1:A:488:PRO:HD3	1.99	0.45
1:A:68:GLN:O	1:A:69:PRO:O	2.34	0.45
2:B:652:ALA:HB2	2:B:670:TYR:HA	1.97	0.45
1:A:312:VAL:CG1	1:A:336:VAL:HG22	2.47	0.45
1:A:529:ARG:HB2	1:A:532:LEU:HB2	1.99	0.45
2:B:426:ILE:HD12	2:B:426:ILE:H	1.82	0.45
1:A:458:ASN:ND2	5:A:2458:NAG:C4	2.80	0.44
1:A:510:ARG:HH11	1:A:510:ARG:HG3	1.82	0.44
1:A:624:PRO:HG2	4:H:2:NDG:H3	1.99	0.44
2:B:68:PRO:HB2	2:B:105:ARG:NH1	2.31	0.44
1:A:154:PHE:O	1:A:175:GLY:HA3	2.17	0.44
1:A:232:ASN:HB2	1:A:264:LEU:CD1	2.48	0.44
1:A:477:PHE:CZ	1:A:536:GLU:HB3	2.52	0.44
1:A:498:LEU:O	1:A:557:ILE:HA	2.17	0.44
1:A:739:LEU:HD12	1:A:739:LEU:HA	1.82	0.44
1:A:836:SER:O	1:A:837:SER:HB3	2.17	0.44
2:B:163:PRO:HG2	2:B:263:ALA:HA	1.98	0.44
2:B:87:ARG:NH1	2:B:428:GLN:OE1	2.50	0.44
1:A:745:ARG:CB	2:B:603:THR:HG21	2.43	0.44
1:A:549:ARG:HA	1:A:549:ARG:HE	1.81	0.44
1:A:931:PHE:CD2	1:A:931:PHE:N	2.85	0.44
2:B:366:LEU:H	2:B:366:LEU:HD23	1.83	0.44
2:B:568:MET:O	2:B:597:THR:HG21	2.18	0.44
2:B:638:GLU:HG3	2:B:638:GLU:O	2.17	0.44
2:B:639:ILE:HG22	2:B:640:GLU:N	2.32	0.44
1:A:11:TYR:HE2	1:A:65:ARG:HA	1.81	0.44
1:A:170:LEU:HD13	1:A:226:VAL:HG22	1.99	0.44
1:A:192:VAL:HG12	1:A:193:SER:N	2.33	0.44
1:A:267:PHE:HE2	1:A:318:SER:OG	2.00	0.44
1:A:319:LEU:HD12	1:A:327:GLN:OE1	2.18	0.44
1:A:755:LEU:HD23	1:A:953:TRP:NE1	2.33	0.44
2:B:104:VAL:HG21	2:B:418:PRO:HG2	1.99	0.44
1:A:451:PRO:CD	1:A:473:PHE:HA	2.48	0.44
1:A:755:LEU:C	1:A:757:ILE:H	2.21	0.44
1:A:872:LEU:HA	1:A:872:LEU:HD23	1.64	0.44
1:A:934:LYS:HE3	1:A:934:LYS:HB3	1.70	0.44
2:B:589:ILE:O	2:B:591:PRO:HD3	2.18	0.44
2:B:683:GLU:O	2:B:684:GLU:CB	2.65	0.44
1:A:36:LEU:HD11	1:A:434:LEU:HD21	1.99	0.44
2:B:639:ILE:CD1	2:B:639:ILE:H	2.26	0.44
1:A:614:GLN:HE22	1:A:616:LYS:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:LYS:HB3	1:A:725:LYS:HE2	1.86	0.44
2:B:120:LEU:HA	2:B:120:LEU:HD12	1.83	0.44
2:B:374:CYS:SG	2:B:395:VAL:CG1	3.06	0.44
1:A:248:ARG:HH12	5:B:3320:NAG:H3	1.83	0.43
2:B:537:SER:HB3	2:B:538:GLY:H	1.67	0.43
2:B:574:LEU:HD21	2:B:581:CYS:CB	2.47	0.43
1:A:314:GLN:NE2	1:A:330:LYS:HG2	2.33	0.43
1:A:423:ILE:HG12	1:A:434:LEU:HD22	2.00	0.43
1:A:524:ASN:H	1:A:524:ASN:HD22	1.67	0.43
1:A:801:TYR:CD2	1:A:802:LYS:HG2	2.53	0.43
2:B:116:TYR:HB3	2:B:153:PHE:CD1	2.53	0.43
1:A:102:GLN:HE21	1:A:102:GLN:HB3	1.59	0.43
1:A:100:SER:CB	1:A:105:ILE:HG22	2.38	0.43
1:A:559:MET:HB3	1:A:586:ILE:HG23	1.99	0.43
1:A:887:GLY:O	1:A:888:ARG:HB3	2.18	0.43
2:B:388:GLY:O	2:B:633:ARG:HG3	2.18	0.43
1:A:255:ILE:HG13	1:A:265:TYR:HB2	2.01	0.43
1:A:61:TRP:O	1:A:63:SER:N	2.42	0.43
2:B:283:ALA:HB1	2:B:287:MET:HB3	2.01	0.43
1:A:642:GLU:HA	1:A:681:CYS:O	2.17	0.43
1:A:711:VAL:O	1:A:733:LYS:HA	2.18	0.43
2:B:356:GLU:HB3	2:B:419:VAL:CG2	2.49	0.43
2:B:636:ARG:CG	2:B:637:ASP:H	2.31	0.43
1:A:622:ASP:O	1:A:624:PRO:HD3	2.18	0.43
2:B:364:GLU:H	2:B:364:GLU:CD	2.21	0.43
1:A:503:LYS:HE3	1:A:510:ARG:NH1	2.33	0.43
1:A:625:LEU:O	1:A:699:PHE:N	2.46	0.43
1:A:750:PRO:CG	1:A:776:VAL:HA	2.49	0.43
1:A:196:ASP:HB3	1:A:199:VAL:HG12	2.01	0.43
1:A:363:PRO:HA	1:A:404:PHE:O	2.19	0.43
2:B:156:PHE:HA	2:B:189:GLY:O	2.19	0.43
2:B:240:ASN:ND2	2:B:240:ASN:H	2.11	0.43
2:B:374:CYS:SG	2:B:395:VAL:HG13	2.59	0.43
1:A:761:GLU:HB2	1:A:763:LYS:NZ	2.34	0.42
1:A:796:HIS:CE1	1:A:883:VAL:HG23	2.54	0.42
1:A:359:ALA:O	1:A:408:MET:HE2	2.20	0.42
1:A:377:ASN:ND2	1:A:377:ASN:N	2.66	0.42
1:A:514:LEU:HB3	1:A:515:TYR:CD1	2.54	0.42
1:A:799:TRP:HZ2	1:A:901:SER:HG	1.64	0.42
2:B:579:GLY:HA2	2:B:589:ILE:HG13	2.01	0.42
2:B:646:LYS:HB2	2:B:647:ASP:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:676:LYS:HG2	2:B:677:SER:N	2.33	0.42
1:A:454:LEU:O	1:A:593:LEU:N	2.44	0.42
1:A:490:LYS:O	1:A:492:ASN:N	2.52	0.42
1:A:559:MET:HB3	1:A:586:ILE:HG22	2.01	0.42
2:B:106:GLN:O	2:B:392:GLY:N	2.51	0.42
2:B:415:THR:HG22	2:B:416:ILE:N	2.35	0.42
2:B:68:PRO:CD	2:B:84:SER:HB2	2.42	0.42
2:B:93:ARG:HB2	2:B:94:PRO:CD	2.35	0.42
1:A:336:VAL:HG12	1:A:337:PHE:CD1	2.54	0.42
1:A:500:ASP:OD1	1:A:510:ARG:HG3	2.19	0.42
1:A:551:LYS:HA	1:A:551:LYS:CE	2.48	0.42
1:A:712:LYS:HE2	1:A:714:ASP:OD1	2.19	0.42
2:B:375:LEU:HG	2:B:633:ARG:HD2	2.00	0.42
2:B:684:GLU:H	2:B:685:PRO:HD3	1.85	0.42
1:A:469:LYS:HD3	1:A:469:LYS:N	2.34	0.42
1:A:703:GLN:H	1:A:703:GLN:CD	2.22	0.42
2:B:145:LEU:HD23	2:B:348:TYR:CD2	2.55	0.42
2:B:128:LEU:HD21	2:B:210:GLN:O	2.19	0.42
1:A:539:ILE:N	1:A:539:ILE:HD12	2.34	0.42
2:B:229:ALA:HA	2:B:236:ILE:CD1	2.42	0.42
2:B:658:LYS:HZ3	2:B:662:ASP:HA	1.82	0.42
2:B:67:ARG:HH11	2:B:67:ARG:HG2	1.84	0.42
1:A:130:LEU:HD21	1:A:188:VAL:HG13	2.01	0.42
2:B:162:SER:CB	2:B:163:PRO:HD3	2.49	0.42
2:B:165:MET:HA	2:B:187:MET:HE1	2.00	0.42
2:B:134:LEU:N	2:B:137:LYS:HE2	2.33	0.42
1:A:379:ARG:HG3	1:A:381:THR:OG1	2.20	0.42
1:A:514:LEU:HB3	1:A:515:TYR:H	1.61	0.42
1:A:594:LEU:O	1:A:595:ASP:HB2	2.19	0.42
1:A:795:LEU:HB3	1:A:884:CYS:HB2	2.01	0.42
1:A:174:PRO:O	1:A:181:GLY:HA2	2.19	0.42
1:A:477:PHE:N	1:A:477:PHE:CD2	2.87	0.42
1:A:447:LEU:HD13	1:A:559:MET:HB2	2.01	0.42
1:A:585:ASN:ND2	3:E:1:NAG:C6	2.63	0.42
1:A:602:CYS:HA	1:A:636:GLU:HG3	2.02	0.42
2:B:127:ASP:O	2:B:131:ILE:HD12	2.20	0.42
1:A:955:ILE:HD13	1:A:955:ILE:HA	1.86	0.41
2:B:205:GLU:O	2:B:209:LYS:HG3	2.20	0.41
2:B:235:LYS:HE3	2:B:275:VAL:HG23	2.01	0.41
1:A:749:SER:CB	1:A:750:PRO:CD	2.98	0.41
2:B:56:PHE:N	2:B:57:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:GLY:HA3	2:B:109:ASP:O	2.21	0.41
1:A:232:ASN:HB2	1:A:264:LEU:CG	2.51	0.41
1:A:633:ASN:ND2	1:A:635:GLY:H	2.18	0.41
1:A:646:SER:HB2	1:A:714:ASP:HB2	2.01	0.41
2:B:646:LYS:C	4:I:2:NDG:H8C3	2.40	0.41
1:A:642:GLU:O	1:A:717:ILE:HA	2.21	0.41
1:A:810:TYR:HE1	1:A:831:LEU:HG	1.86	0.41
1:A:946:LEU:N	1:A:946:LEU:CD2	2.84	0.41
2:B:678:ILE:HG22	2:B:679:LEU:N	2.35	0.41
1:A:61:TRP:C	1:A:63:SER:H	2.21	0.41
2:B:85:PRO:HG2	2:B:102:ILE:HA	2.03	0.41
2:B:340:VAL:O	2:B:341:LEU:HB2	2.20	0.41
2:B:648:THR:HA	4:I:2:NDG:H2	2.01	0.41
2:B:84:SER:O	2:B:86:GLN:N	2.53	0.41
1:A:139:TYR:CD1	1:A:141:PRO:HD3	2.55	0.41
1:A:305:SER:O	2:B:563:ARG:HD2	2.21	0.41
1:A:527:ILE:HB	1:A:528:SER:H	1.71	0.41
1:A:778:HIS:HE1	1:A:949:THR:OG1	2.03	0.41
1:A:914:GLN:HB3	1:A:916:HIS:ND1	2.36	0.41
2:B:314:VAL:CG2	2:B:317:LEU:HD23	2.51	0.41
2:B:617:CYS:C	2:B:619:LYS:H	2.24	0.41
1:A:149:ALA:O	1:A:177:PHE:O	2.39	0.41
1:A:799:TRP:CD2	1:A:800:PRO:HD2	2.55	0.41
2:B:110:TYR:HD1	2:B:111:PRO:HD2	1.85	0.41
2:B:299:LEU:HA	2:B:299:LEU:HD12	1.88	0.41
2:B:580:LYS:HB2	2:B:580:LYS:HE2	1.93	0.41
1:A:618:TYR:O	1:A:623:ASN:ND2	2.54	0.41
1:A:769:GLU:OE1	1:A:835:ILE:HA	2.20	0.41
2:B:160:PRO:HG2	2:B:285:THR:CG2	2.51	0.41
2:B:173:LEU:HD11	2:B:178:TYR:CE1	2.56	0.41
2:B:323:GLU:O	2:B:323:GLU:HG2	2.19	0.41
1:A:518:SER:OG	1:A:519:PRO:HD2	2.21	0.41
1:A:577:ILE:HG13	1:A:578:LEU:O	2.19	0.41
1:A:556:THR:CG2	1:A:589:GLN:HE21	2.34	0.41
1:A:5:VAL:O	1:A:5:VAL:HG12	2.21	0.41
1:A:349:ASP:HA	1:A:357:ASP:OD1	2.21	0.41
1:A:480:LYS:HE2	1:A:480:LYS:HB3	1.87	0.41
1:A:572:THR:O	1:A:573:GLY:C	2.58	0.41
1:A:672:THR:HA	1:A:676:THR:O	2.21	0.41
1:A:755:LEU:HD23	1:A:953:TRP:CE2	2.55	0.41
2:B:370:PHE:CD1	2:B:370:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:SER:HB3	2:B:402:LYS:HE2	2.03	0.41
1:A:388:SER:O	1:A:389:GLN:HB2	2.21	0.41
1:A:410:GLY:O	1:A:411:ALA:HB2	2.21	0.41
1:A:529:ARG:HD2	1:A:532:LEU:HG	2.02	0.41
1:A:880:LEU:C	1:A:880:LEU:HD12	2.41	0.41
2:B:683:GLU:HG2	2:B:684:GLU:HG2	2.03	0.41
1:A:26:PHE:CE1	1:A:28:PRO:HG3	2.55	0.40
1:A:301:MET:HA	1:A:310:GLN:O	2.21	0.40
1:A:606:LEU:CB	1:A:727:SER:HB3	2.51	0.40
2:B:404:ARG:NH1	2:B:548:LEU:O	2.54	0.40
2:B:623:GLU:CB	2:B:624:PRO:CD	2.99	0.40
1:A:458:ASN:HD22	5:A:2458:NAG:H4	1.85	0.40
1:A:636:GLU:HB2	1:A:637:GLY:H	1.73	0.40
1:A:936:LEU:H	1:A:936:LEU:HD22	1.86	0.40
2:B:134:LEU:CG	2:B:135:GLY:N	2.84	0.40
1:A:478:CYS:N	1:A:535:CYS:SG	2.95	0.40
1:A:910:ASN:HA	1:A:915:ASN:CG	2.42	0.40
2:B:134:LEU:CG	2:B:135:GLY:H	2.34	0.40
2:B:180:MET:O	2:B:181:LYS:HD2	2.21	0.40
1:A:124:PRO:O	1:A:124:PRO:HG2	2.21	0.40
1:A:776:VAL:O	1:A:901:SER:HB2	2.20	0.40
1:A:347:LEU:HA	1:A:410:GLY:O	2.21	0.40
1:A:423:ILE:HG12	1:A:434:LEU:CD2	2.51	0.40
1:A:477:PHE:CE2	1:A:497:LEU:HD11	2.56	0.40
1:A:562:ARG:HB3	1:A:562:ARG:NH1	2.36	0.40
1:A:588:ARG:NH1	1:A:588:ARG:HG2	2.36	0.40
2:B:312:GLU:O	2:B:315:VAL:HG12	2.21	0.40
2:B:617:CYS:C	2:B:619:LYS:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	923/957 (96%)	728 (79%)	152 (16%)	43 (5%)	2 14
2	B	535/692 (77%)	407 (76%)	82 (15%)	46 (9%)	1 5
All	All	1458/1649 (88%)	1135 (78%)	234 (16%)	89 (6%)	1 10

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	PRO
1	A	82	LYS
1	A	411	ALA
1	A	420	PRO
1	A	450	TYR
1	A	487	LEU
1	A	488	PRO
1	A	504	GLN
1	A	514	LEU
1	A	527	ILE
1	A	554	PRO
1	A	656	VAL
1	A	835	ILE
1	A	888	ARG
1	A	908	PHE
2	B	80	VAL
2	B	84	SER
2	B	162	SER
2	B	167	ILE
2	B	168	SER
2	B	176	PRO
2	B	240	ASN
2	B	341	LEU
2	B	671	GLU
2	B	673	SER
1	A	62	SER
1	A	194	LYS
1	A	371	GLY
1	A	528	SER
1	A	572	THR
1	A	573	GLY
1	A	688	LYS
1	A	759	ASN
1	A	954	GLY
2	B	70	SER

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Mol	Chain	Res	Type
2	B	75	GLY
2	B	79	GLN
2	B	169	PRO
2	B	195	THR
2	B	346	ASP
2	B	377	ASN
2	B	546	ASP
2	B	547	CYS
2	B	617	CYS
2	B	636	ARG
1	A	202	ILE
1	A	491	LEU
1	A	517	ARG
1	A	570	ASP
1	A	571	THR
1	A	659	ASN
1	A	685	ASN
1	A	749	SER
1	A	809	LEU
1	A	910	ASN
2	B	57	PRO
2	B	172	ALA
2	B	194	LEU
2	B	199	GLN
2	B	340	VAL
2	B	362	LEU
2	B	409	GLU
2	B	558	CYS
1	A	201	SER
1	A	708	ASP
1	A	905	THR
2	B	407	PRO
2	B	412	LYS
2	B	549	CYS
2	B	576	SER
2	B	623	GLU
1	A	287	GLY
1	A	348	GLY
2	B	76	ASP
2	B	157	VAL
2	B	180	MET
2	B	253	LYS

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Mol	Chain	Res	Type
2	B	590	GLN
2	B	677	SER
2	B	680	TYR
2	B	684	GLU
1	A	515	TYR
1	A	652	ASP
1	A	757	ILE
1	A	597	GLY
2	B	85	PRO
2	B	538	GLY
2	B	624	PRO
2	B	649	GLY

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	787/812 (97%)	696 (88%)	91 (12%)	5	22
2	B	484/616 (79%)	424 (88%)	60 (12%)	4	19
All	All	1271/1428 (89%)	1120 (88%)	151 (12%)	5	21

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	ASP
1	A	15	GLU
1	A	46	THR
1	A	73	ASP
1	A	88	PHE
1	A	102	GLN
1	A	115	ARG
1	A	121	GLU
1	A	135	LYS
1	A	145	GLN

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Mol	Chain	Res	Type
1	A	146	ASP
1	A	162	ASP
1	A	169	VAL
1	A	170	LEU
1	A	200	TYR
1	A	226	VAL
1	A	228	VAL
1	A	232	ASN
1	A	234	ASP
1	A	236	ILE
1	A	238	ASP
1	A	248	ARG
1	A	249	THR
1	A	264	LEU
1	A	270	GLU
1	A	275	TYR
1	A	286	ASN
1	A	289	ASP
1	A	306	ASP
1	A	321	ARG
1	A	342	SER
1	A	347	LEU
1	A	352	GLN
1	A	357	ASP
1	A	367	GLU
1	A	372	ILE
1	A	377	ASN
1	A	391	LEU
1	A	394	GLN
1	A	416	LYS
1	A	420	PRO
1	A	434	LEU
1	A	452	SER
1	A	455	ASN
1	A	457	ASP
1	A	458	ASN
1	A	459	LYS
1	A	490	LYS
1	A	514	LEU
1	A	524	ASN
1	A	532	LEU
1	A	535	CYS

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Mol	Chain	Res	Type
1	A	539	ILE
1	A	549	ARG
1	A	551	LYS
1	A	554	PRO
1	A	563	LEU
1	A	599	ASP
1	A	602	CYS
1	A	607	GLU
1	A	608	VAL
1	A	616	LYS
1	A	633	ASN
1	A	634	GLN
1	A	650	GLN
1	A	685	ASN
1	A	688	LYS
1	A	703	GLN
1	A	706	GLU
1	A	711	VAL
1	A	734	VAL
1	A	745	ARG
1	A	756	PRO
1	A	764	GLU
1	A	778	HIS
1	A	783	ARG
1	A	790	PHE
1	A	808	LEU
1	A	880	LEU
1	A	896	ILE
1	A	897	LEU
1	A	904	TRP
1	A	905	THR
1	A	906	GLU
1	A	907	THR
1	A	908	PHE
1	A	931	PHE
1	A	934	LYS
1	A	939	GLU
1	A	946	LEU
2	B	55	GLU
2	B	56	PHE
2	B	58	VAL
2	B	62	ARG

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Mol	Chain	Res	Type
2	B	67	ARG
2	B	69	LEU
2	B	79	GLN
2	B	86	GLN
2	B	87	ARG
2	B	88	ILE
2	B	98	LYS
2	B	110	TYR
2	B	138	LEU
2	B	161	VAL
2	B	166	TYR
2	B	171	GLU
2	B	176	PRO
2	B	178	TYR
2	B	180	MET
2	B	199	GLN
2	B	214	ARG
2	B	215	ASN
2	B	240	ASN
2	B	261	ARG
2	B	269	ASN
2	B	278	ASP
2	B	286	THR
2	B	292	LEU
2	B	296	THR
2	B	299	LEU
2	B	320	ASN
2	B	329	THR
2	B	330	VAL
2	B	336	ASP
2	B	346	ASP
2	B	354	LYS
2	B	360	ARG
2	B	364	GLU
2	B	368	LEU
2	B	373	THR
2	B	375	LEU
2	B	377	ASN
2	B	387	MET
2	B	409	GLU
2	B	430	THR
2	B	434	ASP

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Mol	Chain	Res	Type
2	B	536	CYS
2	B	539	HIS
2	B	544	CYS
2	B	546	ASP
2	B	561	THR
2	B	617	CYS
2	B	632	ASN
2	B	635	CYS
2	B	645	LEU
2	B	646	LYS
2	B	647	ASP
2	B	670	TYR
2	B	673	SER
2	B	683	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	68	GLN
1	A	77	ASN
1	A	92	GLN
1	A	102	GLN
1	A	113	HIS
1	A	152	GLN
1	A	180	GLN
1	A	182	GLN
1	A	187	GLN
1	A	205	ASN
1	A	206	ASN
1	A	232	ASN
1	A	286	ASN
1	A	314	GLN
1	A	320	GLN
1	A	332	ASN
1	A	352	GLN
1	A	384	ASN
1	A	394	GLN
1	A	444	ASN
1	A	455	ASN
1	A	474	ASN
1	A	524	ASN

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Mol	Chain	Res	Type
1	A	575	GLN
1	A	580	GLN
1	A	614	GLN
1	A	633	ASN
1	A	650	GLN
1	A	685	ASN
1	A	716	GLN
1	A	721	ASN
1	A	732	HIS
1	A	759	ASN
1	A	778	HIS
1	A	806	ASN
1	A	821	ASN
1	A	870	HIS
1	A	935	ASN
2	B	79	GLN
2	B	86	GLN
2	B	132	GLN
2	B	175	ASN
2	B	210	GLN
2	B	215	ASN
2	B	269	ASN
2	B	342	GLN
2	B	376	ASN
2	B	408	GLN
2	B	629	ASN
2	B	632	ASN

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

14 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.61	0	17,19,21	0.77	1 (5%)
3	NAG	C	2	3	14,14,15	0.70	0	17,19,21	0.67	0
3	NAG	D	1	1,3	14,14,15	0.62	0	17,19,21	0.69	0
3	NAG	D	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.75	0
3	NAG	E	1	1,3	14,14,15	0.57	0	17,19,21	0.65	0
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.54	0
4	NAG	F	1	1,4	14,14,15	0.54	0	17,19,21	0.66	1 (5%)
4	NDG	F	2	4	14,14,15	0.60	0	17,19,21	0.74	0
3	NAG	G	1	1,3	14,14,15	0.60	0	17,19,21	0.69	0
3	NAG	G	2	3	14,14,15	0.55	0	17,19,21	0.59	0
4	NAG	H	1	2,4	14,14,15	0.63	0	17,19,21	0.62	0
4	NDG	H	2	4	14,14,15	0.60	0	17,19,21	0.84	0
4	NAG	I	1	2,4	14,14,15	0.71	0	17,19,21	1.12	3 (17%)
4	NDG	I	2	4	14,14,15	0.60	0	17,19,21	0.75	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NDG	F	2	4	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NDG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	2,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	I	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	2.17	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	NAG	C4-C3-C2	-2.47	107.39	111.02
4	I	1	NAG	C1-O5-C5	2.45	115.51	112.19
4	I	1	NAG	C2-N2-C7	-2.07	119.96	122.90
3	C	1	NAG	C4-C3-C2	2.00	113.95	111.02
4	F	1	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	F	2	NDG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6

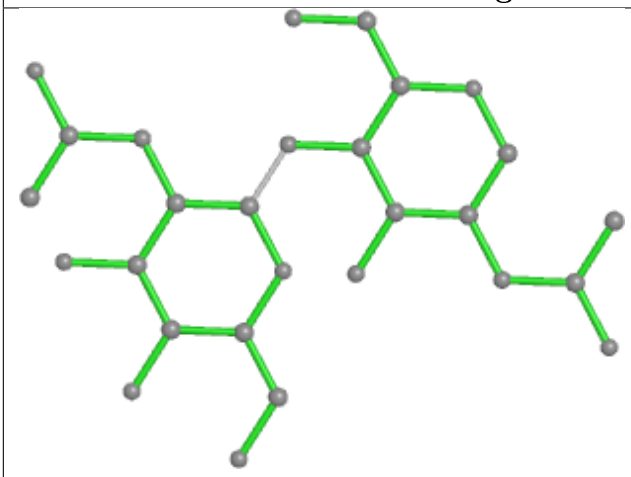
There are no ring outliers.

11 monomers are involved in 35 short contacts:

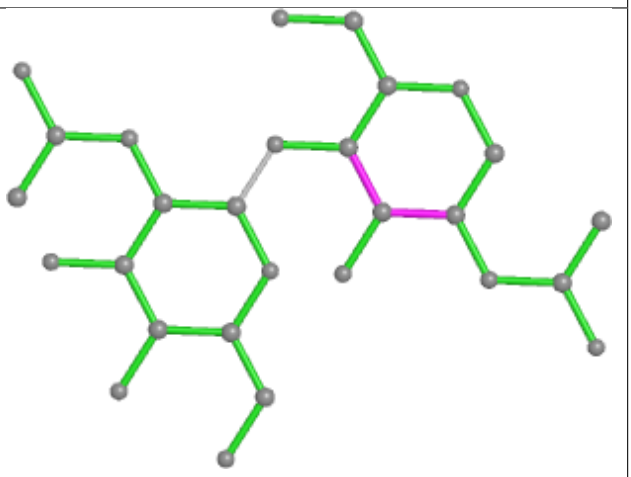
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	5	0
3	D	1	NAG	3	0
3	C	1	NAG	7	0
4	F	1	NAG	3	0
4	I	2	NDG	9	0
4	H	2	NDG	1	0
4	F	2	NDG	3	0
3	G	2	NAG	2	0
4	I	1	NAG	5	0
3	C	2	NAG	7	0
3	E	1	NAG	2	0

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

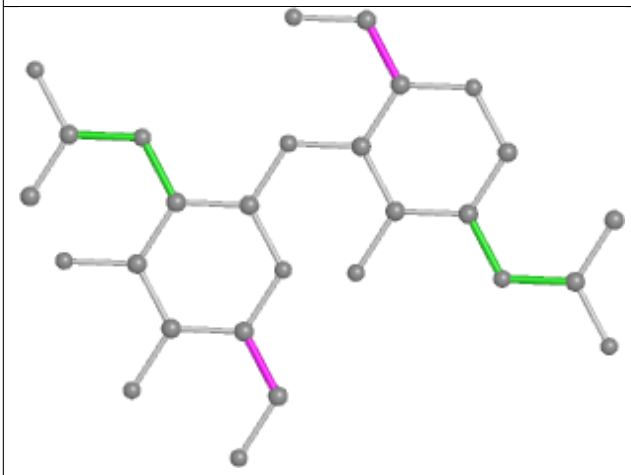
Oligosaccharide Chain C



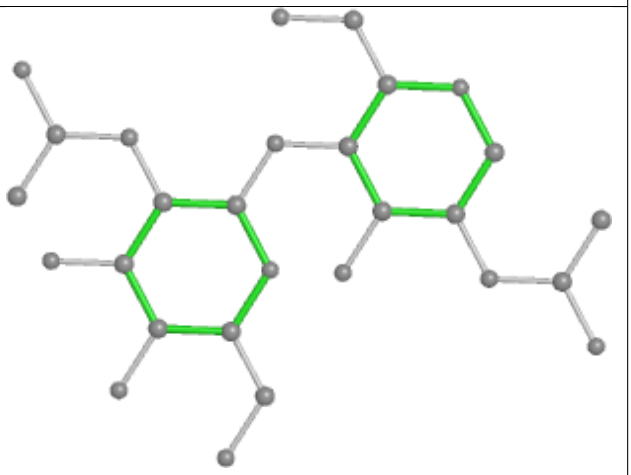
Bond lengths



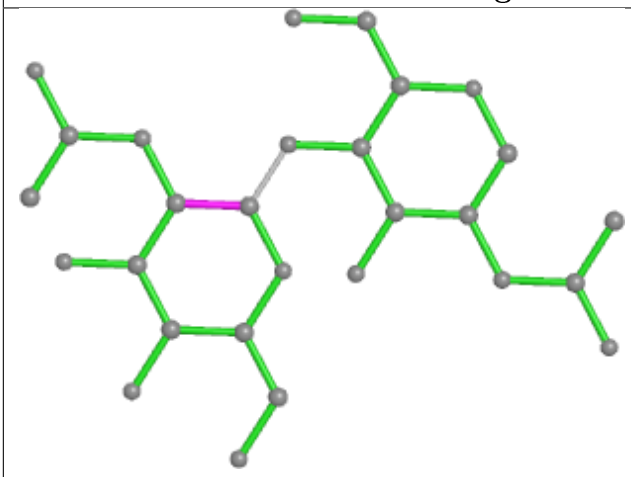
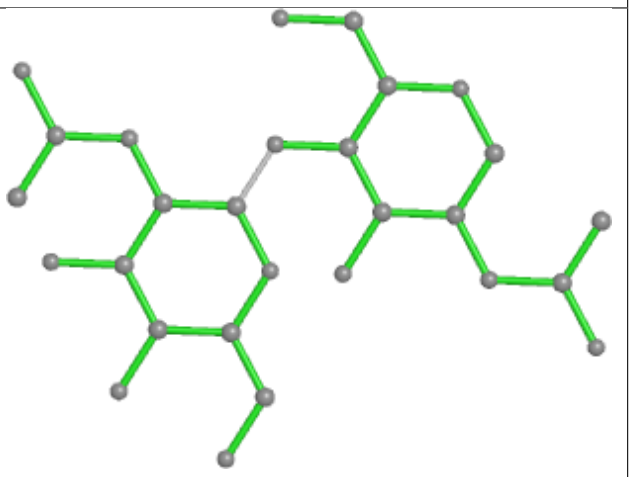
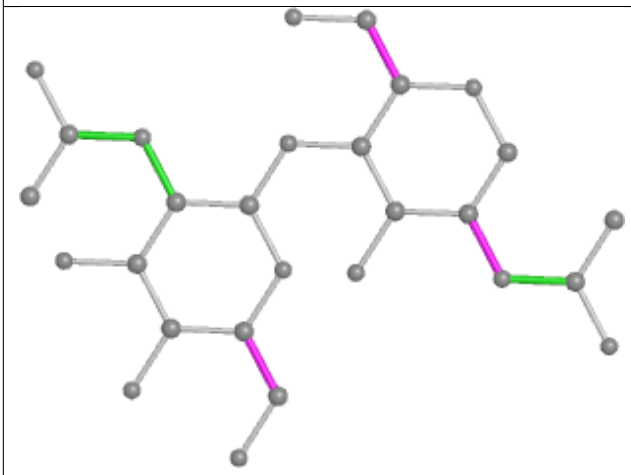
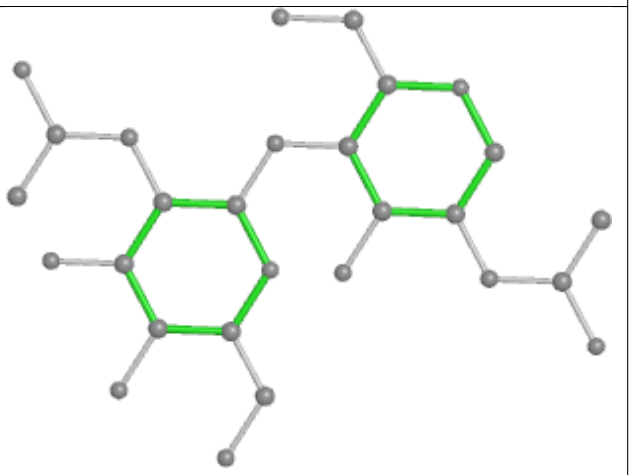
Bond angles



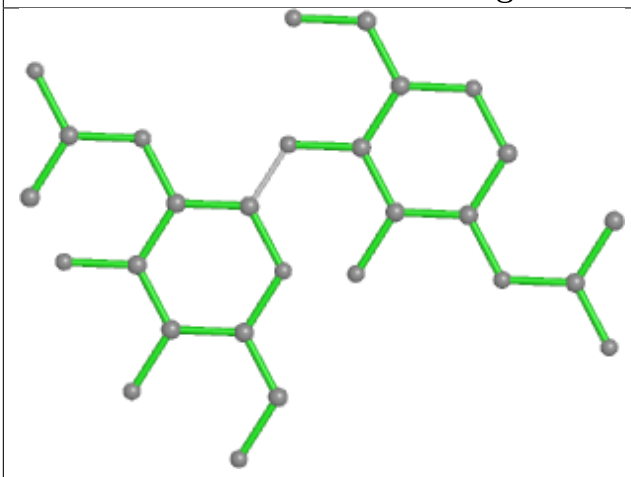
Torsions



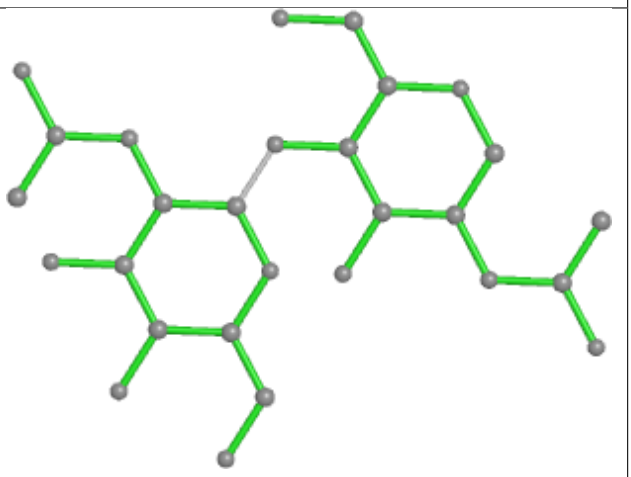
Rings

Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

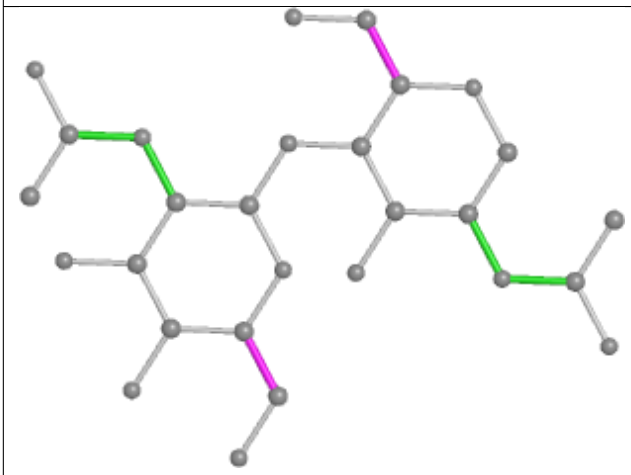
Oligosaccharide Chain E



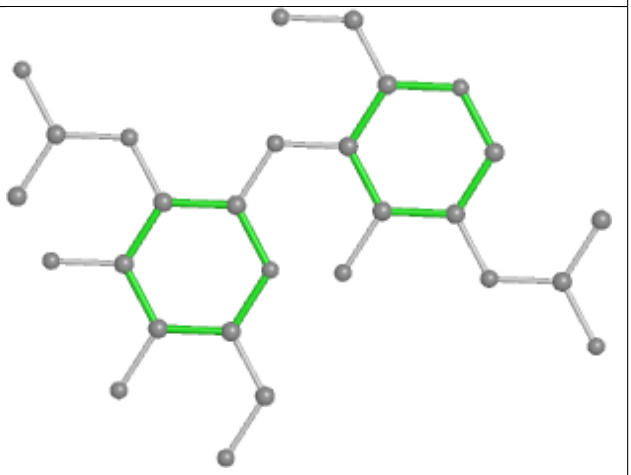
Bond lengths



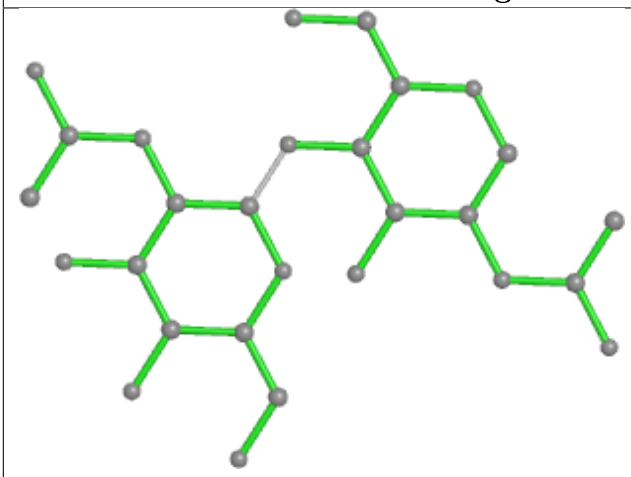
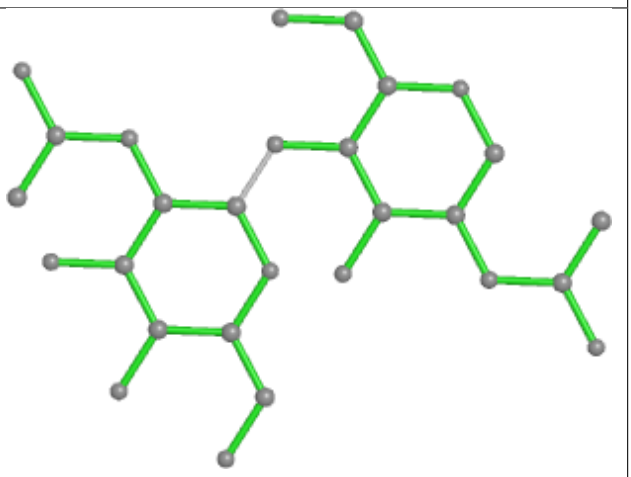
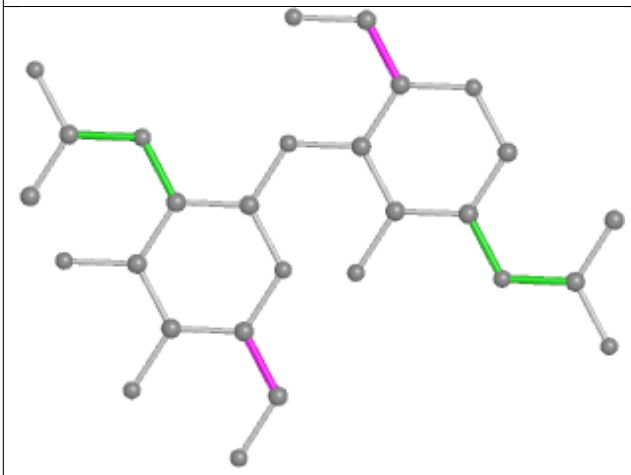
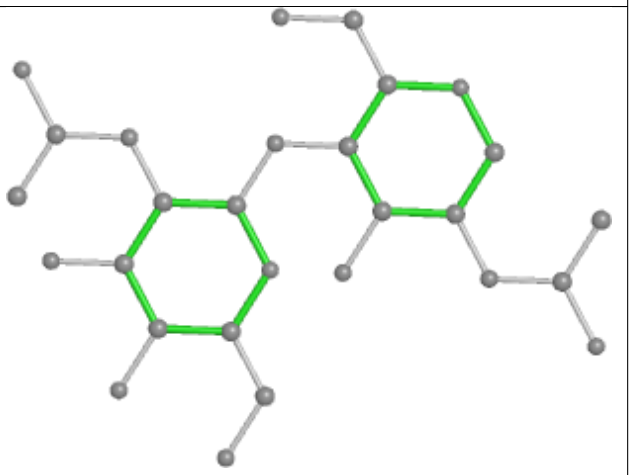
Bond angles



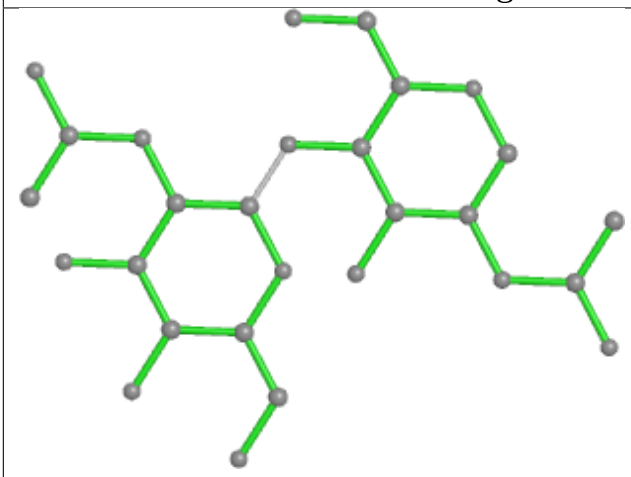
Torsions



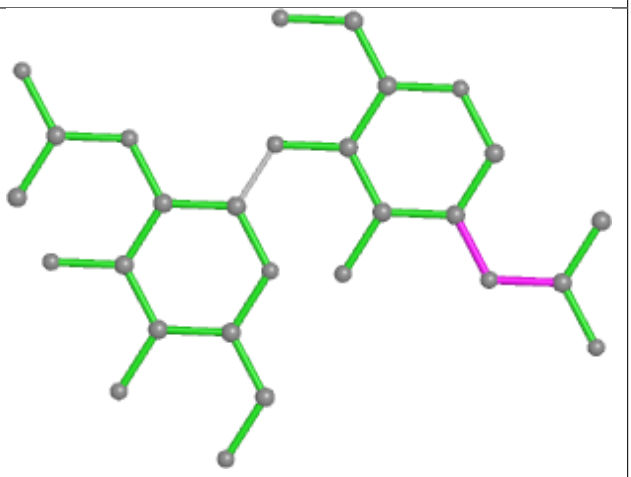
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

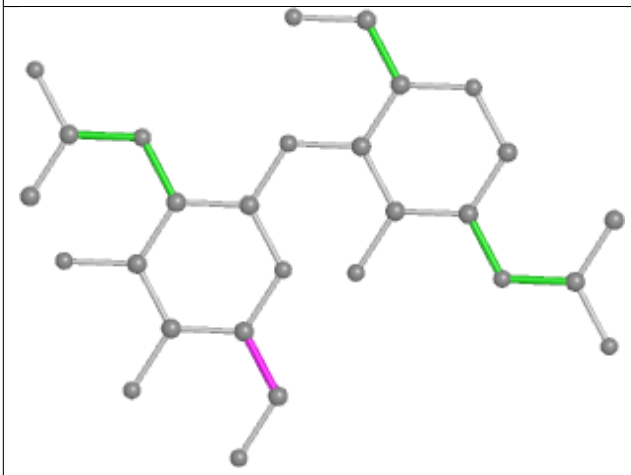
Oligosaccharide Chain F



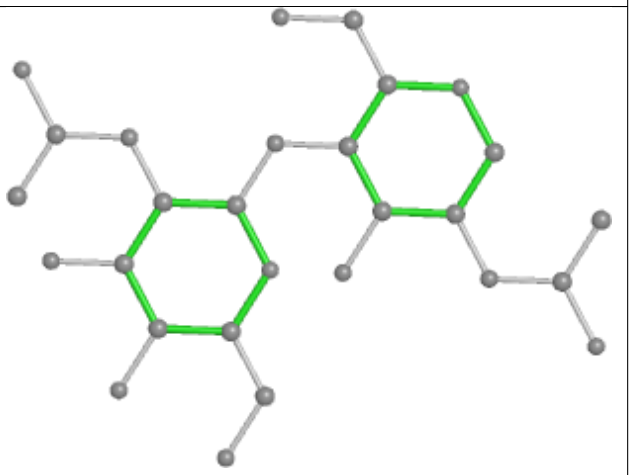
Bond lengths



Bond angles

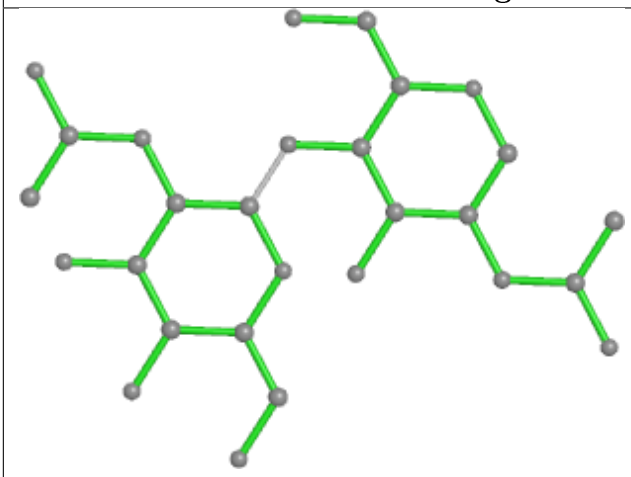


Torsions

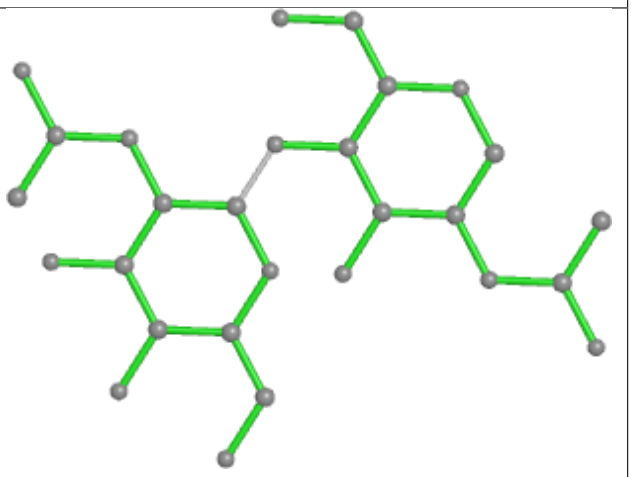


Rings

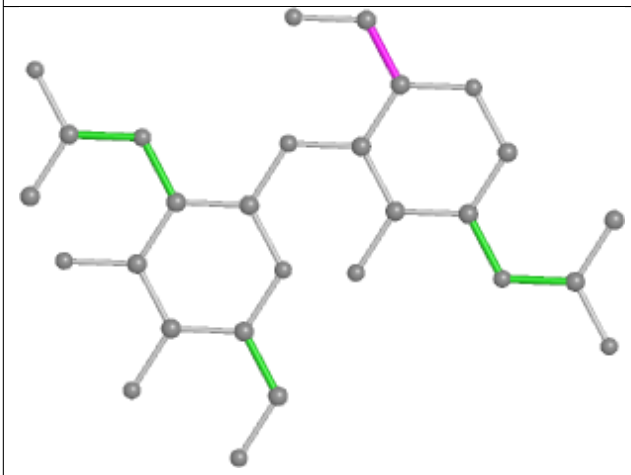
Oligosaccharide Chain H



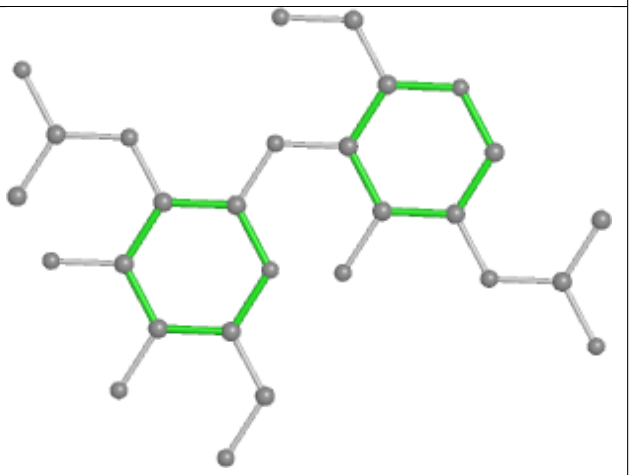
Bond lengths



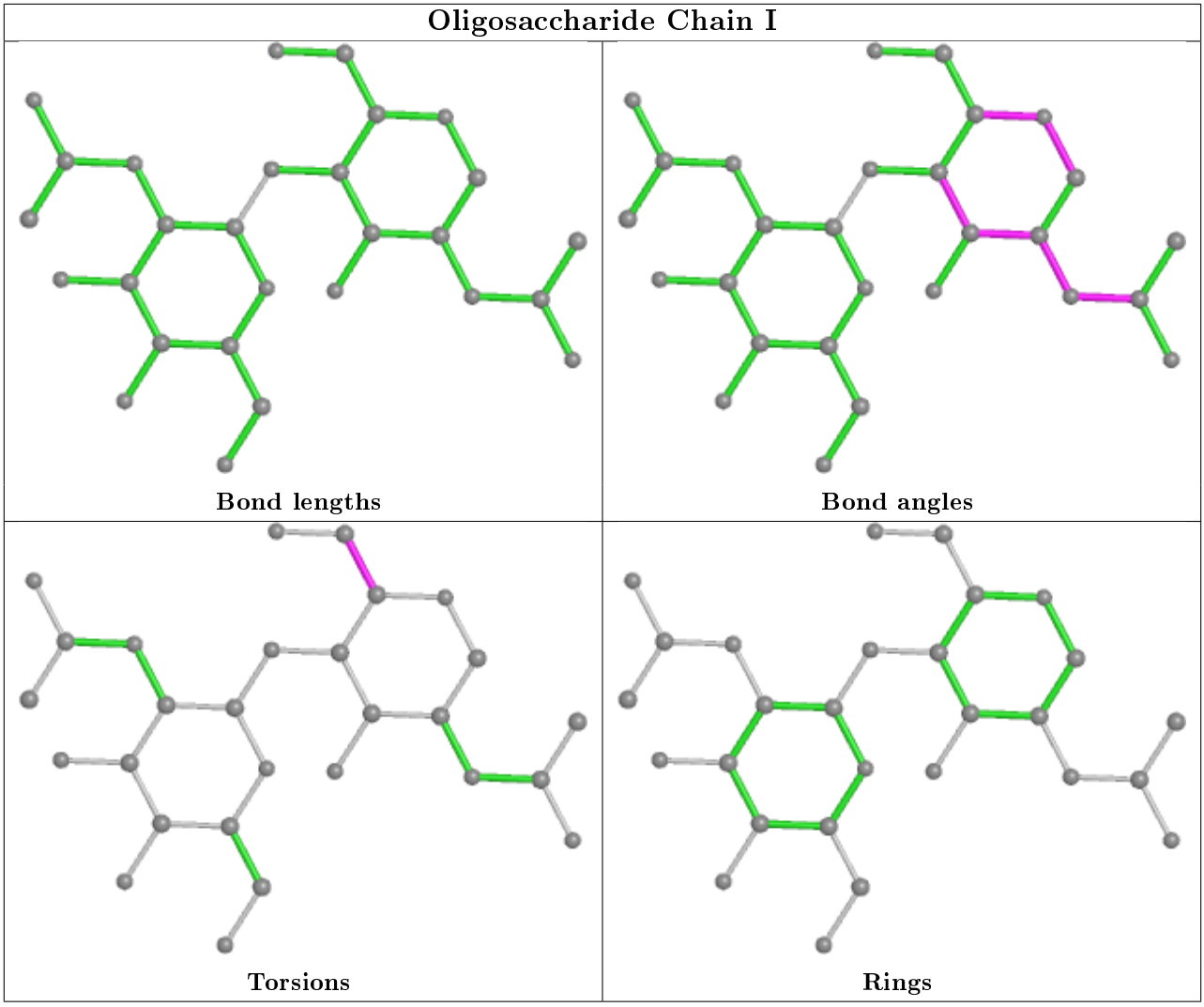
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	NAG	B	3371	2	14,14,15	0.56	0	17,19,21	0.64	0
5	NAG	A	2458	1	14,14,15	0.54	0	17,19,21	0.65	0
5	NAG	A	2260	1	14,14,15	0.53	0	17,19,21	0.64	0
5	NAG	B	3320	2	14,14,15	0.45	0	17,19,21	0.64	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
5	NAG	B	3371	2	-	4/6/23/26	0/1/1/1
5	NAG	A	2458	1	-	3/6/23/26	0/1/1/1
5	NAG	A	2260	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3320	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2458	NAG	O5-C5-C6-O6
5	B	3371	NAG	C4-C5-C6-O6
5	B	3371	NAG	O5-C5-C6-O6
5	B	3371	NAG	C1-C2-N2-C7
5	A	2458	NAG	C4-C5-C6-O6
5	B	3371	NAG	C3-C2-N2-C7
5	A	2458	NAG	C1-C2-N2-C7
5	A	2260	NAG	C1-C2-N2-C7
5	A	2260	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3371	NAG	5	0
5	A	2458	NAG	6	0
5	A	2260	NAG	3	0
5	B	3320	NAG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.