Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:24 PM EDT

PDB ID	:	1ING
Title	:	INFLUENZA A SUBTYPE N2 NEURAMINIDASE COMPLEXED WITH AROMATIC BANA109 INHIBITOR
Authors	:	Jedrzejas, M.J.; Luo, M.
Deposited on	:	1995-07-07
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

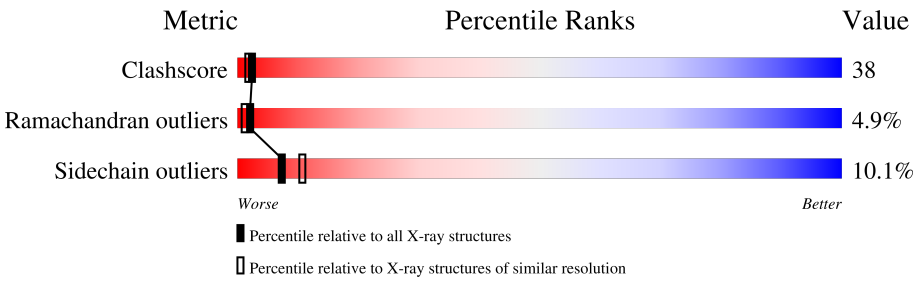
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	388	41% 50% 9% .
1	B	388	40% 51% 9% .
2	C	2	100%
2	F	2	100%
2	G	2	100%
2	J	2	100%
3	D	4	75% 25%
4	E	6	50% 50%

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Mol	Chain	Length	Quality of chain
4	I	6	67% 33%
5	H	4	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
3	FUL	D	4	-	-	X	-
4	NAG	E	1	-	-	X	-
4	MAN	E	4	-	-	X	-
4	MAN	E	6	-	-	X	-
4	NAG	I	1	-	-	X	-
5	FUC	H	4	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8978 atoms, of which 2292 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 INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	388	3745	1866	723	545	588	23	0	0	0
1	B	388	3745	1866	723	545	588	23	0	0	0

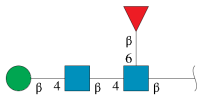
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820
B	339	ASP	ASN	conflict	UNP P06820

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

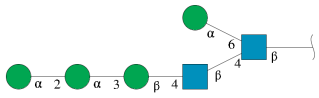
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	55	16	27	2	10	0	0	0
2	F	2	55	16	27	2	10	0	0	0
2	G	2	55	16	27	2	10	0	0	0
2	J	2	55	16	27	2	10	0	0	0

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



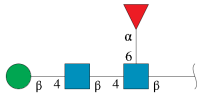
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	D	4	96	28	47	2	19	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	E	6	139	40	67	2	30	0	0	0
			Total	C	H	N	O			
4	I	6	139	40	67	2	30	0	0	0

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



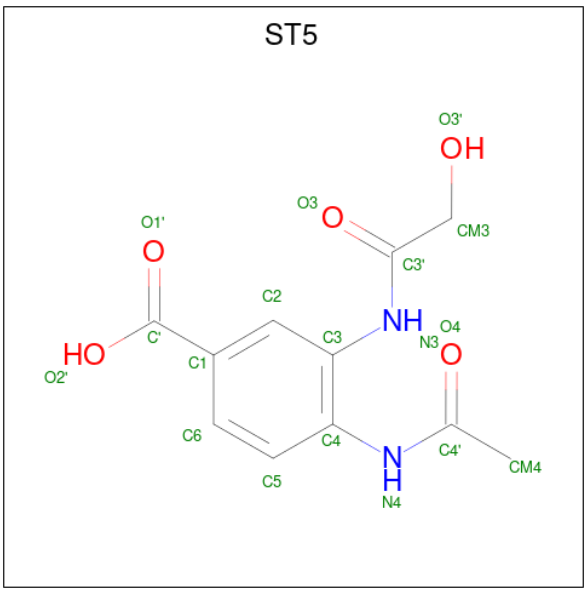
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	H	4	96	28	47	2	19	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is 4-(ACETYLAMINO)-3-[(HYDROXYACETYL)AMINO]BENZOIC ACID

(three-letter code: ST5) (formula: $C_{11}H_{12}N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	A	1	23	11	5	2	5	0	0
			Total	C	H	N	O		
7	B	1	23	11	5	2	5	0	0

- Molecule 8 is water.

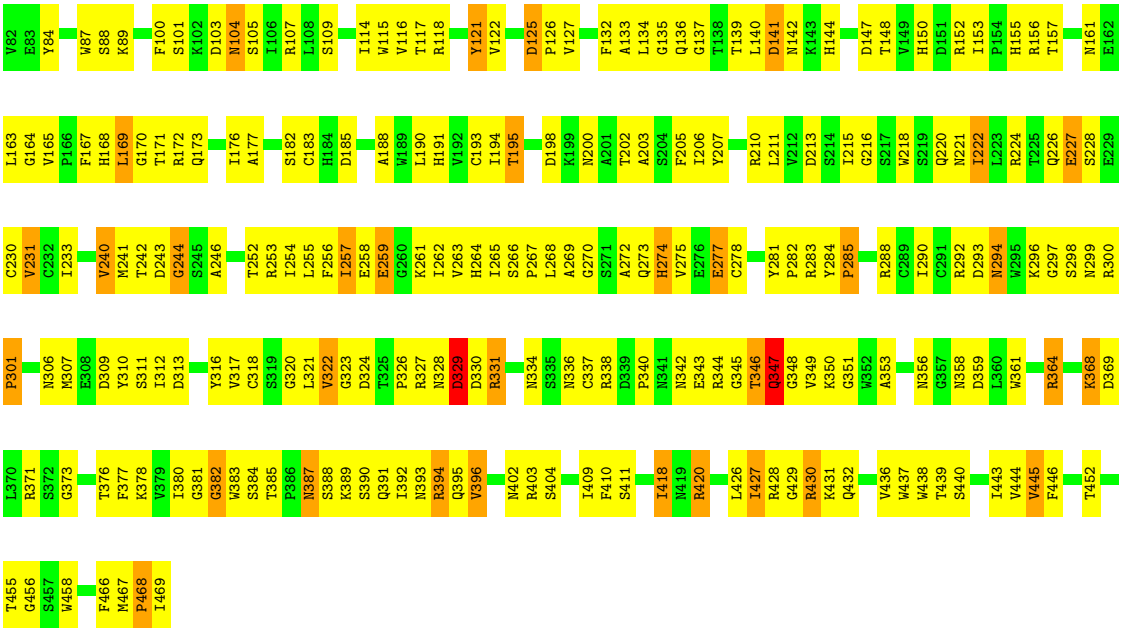
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
8	A	122	366	244	122	0	0
			Total	H	O		
8	B	128	384	256	128	0	0

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.

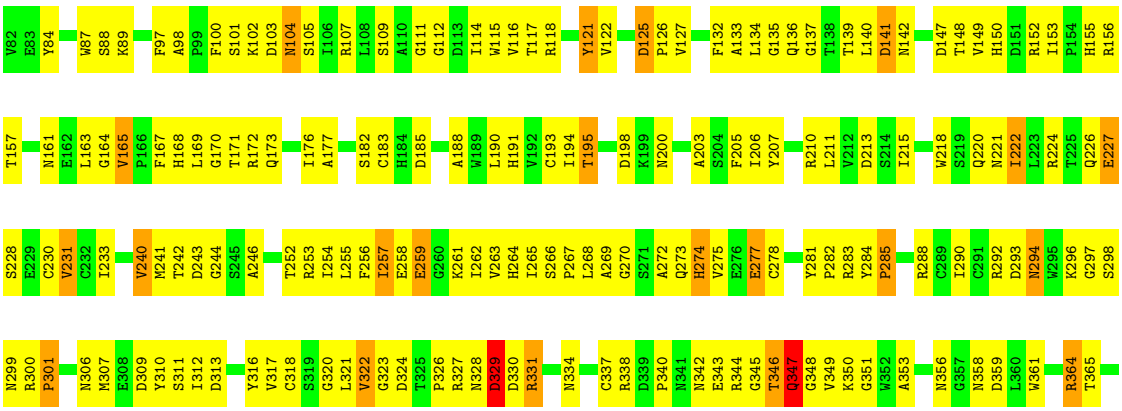
• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

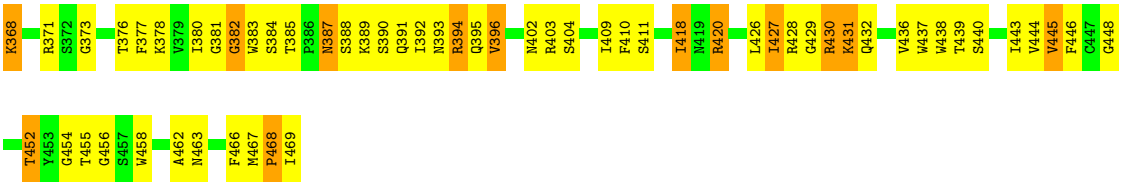
Chain A: 41% 50% 9%



• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain B: 40% 51% 9%





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

Chain C: 100%

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

Chain F: 100%

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

Chain G: 100%

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

Chain J: 100%

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

Chain D: 75% 25%

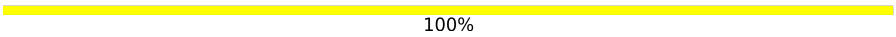
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%

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

Chain I:

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

Chain H: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.42Å 139.06Å 139.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.40 21.23 – 2.34	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.40) 44.6 (21.23-2.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.36Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.163 , (Not available) 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	2.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 122.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUL, MAN, CA, FUC, ST5, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.57	0/3092	0.90	2/4194 (0.0%)
1	B	0.57	0/3092	0.90	2/4194 (0.0%)
All	All	0.57	0/6184	0.90	4/8388 (0.0%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	THR	N-CA-C	-5.15	97.10	111.00
1	B	346	THR	N-CA-C	-5.15	97.10	111.00
1	A	125	ASP	N-CA-C	-5.00	97.49	111.00
1	B	125	ASP	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	TYR	Sidechain
1	B	121	TYR	Sidechain

5.2 Too-close contacts (i)

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	3022	723	2851	229	32
1	B	3022	723	2850	260	12
2	C	28	27	25	0	0
2	F	28	27	25	0	0
2	G	28	27	25	0	0
2	J	28	27	25	0	0
3	D	49	47	43	0	10
4	E	72	67	59	23	10
4	I	72	67	61	1	10
5	H	49	47	43	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	18	5	11	2	0
7	B	18	5	11	2	0
8	A	122	244	0	18	9
8	B	128	256	0	24	21
All	All	6686	2292	6029	470	52

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 38.

All (470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:THR:OG1	4:E:1:NAG:C6	1.65	1.44
1:B:455:THR:CB	4:E:1:NAG:C6	2.15	1.23
1:B:102:LYS:HE3	8:B:488:HOH:O	1.45	1.14
1:B:455:THR:HG21	4:E:1:NAG:H5	1.32	1.09
1:B:455:THR:HG23	4:E:1:NAG:C1	1.81	1.09
1:A:136:GLN:HG3	1:A:148:THR:HG23	1.44	0.99
1:B:455:THR:HG21	4:E:1:NAG:C5	1.93	0.97
1:B:136:GLN:HG3	1:B:148:THR:HG23	1.44	0.96
1:B:455:THR:OG1	4:E:1:NAG:C5	2.13	0.95
1:B:455:THR:CG2	4:E:1:NAG:C1	2.45	0.94
1:A:173:GLN:HG3	1:B:164:GLY:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:HD2	1:B:466:PHE:HD2	1.20	0.90
1:A:169:LEU:HD11	1:B:112:GLY:HA3	1.52	0.89
1:A:326:PRO:HD2	1:A:347:GLN:HB2	1.55	0.89
1:B:455:THR:HB	4:E:1:NAG:C6	2.00	0.88
1:B:455:THR:OG1	4:E:1:NAG:O5	1.91	0.87
1:B:326:PRO:HD2	1:B:347:GLN:HB2	1.55	0.87
1:B:371:ARG:O	1:B:404:SER:HB3	1.75	0.86
1:A:371:ARG:O	1:A:404:SER:HB3	1.75	0.85
1:B:455:THR:CG2	4:E:1:NAG:C5	2.54	0.85
1:B:222:ILE:HB	8:B:597:HOH:O	1.78	0.82
1:A:222:ILE:HB	8:A:585:HOH:O	1.78	0.81
1:B:176:ILE:HG22	1:B:195:THR:HG21	1.62	0.80
1:B:411:SER:HB3	1:B:418:ILE:CD1	2.12	0.79
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.62	0.79
1:B:102:LYS:CE	8:B:488:HOH:O	2.14	0.79
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.12	0.78
1:A:391:GLN:HG2	1:A:392:ILE:N	1.97	0.78
1:B:391:GLN:HG2	1:B:392:ILE:N	1.97	0.78
1:A:317:VAL:HG23	8:A:534:HOH:O	1.84	0.77
1:B:317:VAL:HG23	8:B:549:HOH:O	1.84	0.77
1:B:254:ILE:HD13	1:B:312:ILE:HD13	1.67	0.76
1:A:254:ILE:HD13	1:A:312:ILE:HD13	1.67	0.75
1:B:455:THR:HB	4:E:1:NAG:O6	1.88	0.74
1:B:233:ILE:HD12	1:B:307:MET:HG3	1.70	0.73
1:B:411:SER:HB3	1:B:418:ILE:HD11	1.71	0.73
1:A:411:SER:HB3	1:A:418:ILE:HD11	1.71	0.72
1:A:202:THR:HB	1:B:454:GLY:H	1.54	0.72
1:A:321:LEU:HD22	1:A:389:LYS:HA	1.72	0.72
1:B:427:ILE:HD11	1:B:439:THR:HG23	1.72	0.71
1:A:427:ILE:HD11	1:A:439:THR:HG23	1.72	0.71
1:A:144:HIS:CD2	1:B:466:PHE:HD2	2.06	0.71
1:A:346:THR:O	1:A:347:GLN:HB3	1.90	0.70
1:B:346:THR:O	1:B:347:GLN:HB3	1.90	0.70
1:A:233:ILE:HD12	1:A:307:MET:HG3	1.70	0.70
1:B:321:LEU:HD22	1:B:389:LYS:HA	1.72	0.70
1:A:104:ASN:HD22	1:A:107:ARG:HD3	1.57	0.70
1:B:218:TRP:NE1	1:B:243:ASP:HB3	2.07	0.69
1:B:327:ARG:NH1	1:B:368:LYS:HA	2.07	0.69
1:A:327:ARG:NH1	1:A:368:LYS:HA	2.07	0.69
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.57	0.69
1:A:105:SER:HB3	8:A:548:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:SER:HB3	8:B:562:HOH:O	1.92	0.69
1:A:218:TRP:NE1	1:A:243:ASP:HB3	2.07	0.68
1:A:338:ARG:HH11	1:A:338:ARG:HG2	1.59	0.68
1:B:134:LEU:HB2	1:B:156:ARG:HH21	1.59	0.68
1:B:334:ASN:HA	1:B:387:ASN:HD21	1.57	0.68
1:A:134:LEU:HB2	1:A:156:ARG:HH21	1.59	0.68
1:B:338:ARG:HG2	1:B:338:ARG:HH11	1.59	0.68
1:B:104:ASN:HD22	1:B:107:ARG:HD3	1.57	0.67
1:A:294:ASN:O	1:A:346:THR:HA	1.95	0.66
1:B:294:ASN:O	1:B:346:THR:HA	1.95	0.66
1:A:328:ASN:O	1:A:329:ASP:HB3	1.95	0.66
1:A:169:LEU:HD11	1:B:112:GLY:CA	2.26	0.65
1:B:359:ASP:OD1	1:B:380:ILE:HA	1.97	0.65
1:B:328:ASN:O	1:B:329:ASP:HB3	1.95	0.65
1:A:183:CYS:HB3	1:A:230:CYS:O	1.97	0.64
1:B:200:ASN:HB3	4:I:1:NAG:O5	1.98	0.64
1:B:455:THR:CB	4:E:1:NAG:C5	2.69	0.64
1:A:327:ARG:HE	1:A:364:ARG:HH21	1.45	0.64
1:B:394:ARG:HG3	1:B:395:GLN:N	2.12	0.64
1:A:228:SER:HB2	1:A:350:LYS:HE2	1.79	0.64
1:B:183:CYS:HB3	1:B:230:CYS:O	1.97	0.64
1:A:328:ASN:OD1	1:A:343:GLU:HB3	1.98	0.64
1:A:205:PHE:HD2	1:A:257:ILE:HD12	1.62	0.64
1:A:359:ASP:OD1	1:A:380:ILE:HA	1.97	0.64
1:B:228:SER:HB2	1:B:350:LYS:HE2	1.79	0.64
1:B:205:PHE:HD2	1:B:257:ILE:HD12	1.62	0.63
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.80	0.63
1:B:267:PRO:O	1:B:312:ILE:HD12	1.98	0.63
1:B:327:ARG:HE	1:B:364:ARG:HH21	1.45	0.63
1:B:328:ASN:OD1	1:B:343:GLU:HB3	1.98	0.63
1:A:394:ARG:HG3	1:A:395:GLN:N	2.12	0.63
1:A:200:ASN:HB3	4:E:1:NAG:O5	1.98	0.63
1:A:144:HIS:HD2	1:B:466:PHE:CD2	2.10	0.63
1:A:267:PRO:O	1:A:312:ILE:HD12	1.98	0.62
1:A:134:LEU:HB2	1:A:156:ARG:NH2	2.14	0.62
1:B:320:GLY:HA2	1:B:387:ASN:HD22	1.64	0.62
1:A:256:PHE:O	1:A:263:VAL:HG22	2.00	0.62
1:B:134:LEU:HB2	1:B:156:ARG:NH2	2.14	0.62
1:B:272:ALA:HA	1:B:316:TYR:CE1	2.35	0.62
1:A:272:ALA:HA	1:A:316:TYR:CE1	2.35	0.61
1:A:320:GLY:HA2	1:A:387:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.80	0.61
7:A:471:ST5:HM31	8:A:571:HOH:O	2.01	0.61
1:A:257:ILE:HA	1:A:262:ILE:HA	1.83	0.60
1:B:139:THR:HB	1:B:142:ASN:OD1	2.01	0.60
1:B:256:PHE:O	1:B:263:VAL:HG22	2.00	0.60
1:A:116:VAL:CG1	1:A:148:THR:HG21	2.31	0.60
1:A:152:ARG:HD3	7:A:471:ST5:HM41	1.83	0.60
1:B:125:ASP:HB2	1:B:126:PRO:HD2	1.83	0.60
1:B:152:ARG:HD3	7:B:471:ST5:HM41	1.83	0.60
1:A:198:ASP:HB3	1:A:222:ILE:HG12	1.83	0.60
1:B:273:GLN:O	1:B:274:HIS:HB2	2.02	0.60
7:B:471:ST5:HM31	8:B:583:HOH:O	2.01	0.60
1:A:144:HIS:CE1	1:B:462:ALA:HA	2.36	0.60
1:A:380:ILE:HD12	1:A:380:ILE:H	1.66	0.60
1:A:430:ARG:HD3	1:A:436:VAL:O	2.02	0.60
1:B:380:ILE:HD12	1:B:380:ILE:H	1.66	0.60
1:B:396:VAL:HG11	4:E:6:MAN:H4	1.84	0.60
1:B:430:ARG:HD3	1:B:436:VAL:O	2.02	0.60
1:B:116:VAL:CG1	1:B:148:THR:HG21	2.31	0.59
1:B:396:VAL:HG12	8:B:560:HOH:O	2.02	0.59
1:B:198:ASP:HB3	1:B:222:ILE:HG12	1.83	0.59
1:A:396:VAL:HG12	8:A:546:HOH:O	2.02	0.59
1:A:125:ASP:HB2	1:A:126:PRO:HD2	1.83	0.59
1:B:121:TYR:HE2	8:B:515:HOH:O	1.85	0.59
1:A:139:THR:HB	1:A:142:ASN:OD1	2.01	0.59
1:B:117:THR:HA	1:B:135:GLY:HA2	1.85	0.59
1:B:257:ILE:HA	1:B:262:ILE:HA	1.83	0.59
1:A:327:ARG:HB3	8:A:583:HOH:O	2.03	0.58
1:B:327:ARG:HB3	8:B:595:HOH:O	2.03	0.58
1:A:272:ALA:HA	1:A:316:TYR:HE1	1.68	0.58
1:B:326:PRO:HB2	1:B:344:ARG:CZ	2.34	0.58
1:A:121:TYR:HE2	8:A:506:HOH:O	1.85	0.58
1:A:283:ARG:NH1	1:A:288:ARG:HE	2.01	0.58
1:A:326:PRO:HB2	1:A:344:ARG:CZ	2.34	0.58
1:A:334:ASN:HA	1:A:387:ASN:ND2	2.19	0.58
1:B:116:VAL:HG11	1:B:148:THR:HG21	1.85	0.58
1:A:116:VAL:HG11	1:A:148:THR:HG21	1.85	0.58
1:A:273:GLN:O	1:A:274:HIS:HB2	2.02	0.58
1:B:150:HIS:HB3	8:B:588:HOH:O	2.03	0.58
1:A:117:THR:HA	1:A:135:GLY:HA2	1.85	0.57
1:A:150:HIS:HB3	8:A:576:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:HA	1:B:316:TYR:HE1	1.68	0.57
1:B:334:ASN:HA	1:B:387:ASN:ND2	2.19	0.57
1:A:326:PRO:HD2	1:A:347:GLN:CB	2.32	0.57
1:A:392:ILE:HG12	1:A:393:ASN:H	1.69	0.57
1:B:326:PRO:HD2	1:B:347:GLN:CB	2.32	0.57
1:B:283:ARG:NH1	1:B:288:ARG:HE	2.01	0.57
1:B:380:ILE:HD11	1:B:392:ILE:HB	1.87	0.57
1:B:396:VAL:HG13	4:E:6:MAN:HO2	1.70	0.57
1:B:392:ILE:HG12	1:B:393:ASN:H	1.69	0.57
1:B:455:THR:HB	4:E:6:MAN:C2	2.35	0.56
1:A:205:PHE:CD2	1:A:257:ILE:HD12	2.40	0.56
1:B:283:ARG:HH11	1:B:288:ARG:HE	1.52	0.56
1:B:436:VAL:HB	1:B:438:TRP:NE1	2.20	0.56
1:B:437:TRP:HB2	1:B:469:ILE:HG21	1.88	0.56
1:B:456:GLY:N	4:E:6:MAN:O2	2.38	0.56
1:A:253:ARG:C	1:A:254:ILE:HD12	2.26	0.56
1:A:283:ARG:HH11	1:A:288:ARG:HE	1.52	0.56
1:A:436:VAL:HB	1:A:438:TRP:NE1	2.20	0.56
1:B:253:ARG:C	1:B:254:ILE:HD12	2.26	0.56
1:B:288:ARG:NH1	1:B:383:TRP:CZ2	2.74	0.56
1:B:263:VAL:O	1:B:264:HIS:HB2	2.06	0.56
1:A:380:ILE:HD11	1:A:392:ILE:HB	1.87	0.56
1:B:205:PHE:CD2	1:B:257:ILE:HD12	2.40	0.56
1:A:437:TRP:H	1:A:469:ILE:HG21	1.71	0.56
1:B:283:ARG:HH12	1:B:288:ARG:HH21	1.54	0.56
1:A:136:GLN:OE1	1:A:156:ARG:HG2	2.06	0.55
1:A:210:ARG:NH2	1:B:126:PRO:O	2.39	0.55
1:A:155:HIS:HB3	1:B:104:ASN:HD21	1.71	0.55
1:B:228:SER:HB2	1:B:350:LYS:CE	2.36	0.55
1:A:283:ARG:HH12	1:A:288:ARG:HH21	1.54	0.55
1:A:282:PRO:O	1:A:420:ARG:NH2	2.38	0.55
1:A:288:ARG:NH1	1:A:383:TRP:CZ2	2.74	0.55
1:A:437:TRP:HB2	1:A:469:ILE:HG21	1.88	0.55
1:A:101:SER:HB2	1:A:445:VAL:HG13	1.89	0.55
1:B:437:TRP:H	1:B:469:ILE:HG21	1.71	0.55
1:B:136:GLN:OE1	1:B:156:ARG:HG2	2.06	0.55
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.72	0.55
1:B:172:ARG:HD2	8:B:524:HOH:O	2.07	0.55
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.72	0.54
1:B:101:SER:HB2	1:B:445:VAL:HG13	1.89	0.54
1:B:282:PRO:O	1:B:420:ARG:NH2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:O	1:A:264:HIS:HB2	2.06	0.54
1:B:455:THR:CG2	4:E:1:NAG:C6	2.80	0.54
1:A:203:ALA:HB3	1:A:215:ILE:HG22	1.90	0.54
1:A:228:SER:HB2	1:A:350:LYS:CE	2.36	0.54
1:B:326:PRO:N	1:B:347:GLN:HG3	2.23	0.54
1:B:321:LEU:O	1:B:322:VAL:HB	2.08	0.54
1:A:306:ASN:HB3	1:A:311:SER:OG	2.08	0.54
1:A:321:LEU:O	1:A:322:VAL:HB	2.08	0.54
1:B:227:GLU:HA	8:B:527:HOH:O	2.08	0.54
1:A:144:HIS:HE1	1:B:462:ALA:HA	1.72	0.53
1:B:306:ASN:HB3	1:B:311:SER:OG	2.08	0.53
1:A:227:GLU:HA	8:A:512:HOH:O	2.08	0.53
1:A:172:ARG:HD2	8:B:494:HOH:O	2.07	0.53
1:A:144:HIS:CD2	1:B:466:PHE:CD2	2.91	0.53
1:B:206:ILE:HD12	1:B:206:ILE:N	2.23	0.53
1:B:455:THR:CG2	4:E:1:NAG:O5	2.56	0.53
1:A:206:ILE:N	1:A:206:ILE:HD12	2.23	0.52
1:B:358:ASN:HB3	1:B:384:SER:OG	2.09	0.52
1:B:391:GLN:CG	1:B:392:ILE:N	2.72	0.52
1:A:326:PRO:N	1:A:347:GLN:HG3	2.23	0.52
1:A:358:ASN:HB3	1:A:384:SER:OG	2.09	0.52
1:A:437:TRP:HD1	1:A:469:ILE:HG23	1.75	0.52
1:A:391:GLN:HG2	1:A:392:ILE:H	1.72	0.52
1:B:203:ALA:HB3	1:B:215:ILE:HG22	1.90	0.52
1:B:377:PHE:HB3	1:B:394:ARG:HB2	1.92	0.52
1:B:391:GLN:HG2	1:B:392:ILE:H	1.72	0.52
1:B:312:ILE:HG22	1:B:313:ASP:N	2.25	0.52
1:A:115:TRP:HZ3	1:A:137:GLY:CA	2.23	0.52
1:B:324:ASP:OD1	1:B:348:GLY:HA2	2.09	0.52
1:B:89:LYS:HB2	1:B:418:ILE:HG22	1.92	0.52
1:A:283:ARG:NH1	1:A:288:ARG:HH21	2.08	0.52
1:A:324:ASP:OD1	1:A:348:GLY:HA2	2.09	0.52
1:B:115:TRP:HZ3	1:B:137:GLY:CA	2.23	0.52
1:B:403:ARG:NH1	1:B:432:GLN:HB3	2.25	0.52
1:A:242:THR:HG22	1:A:243:ASP:N	2.24	0.52
1:B:376:THR:O	1:B:394:ARG:HA	2.10	0.52
1:B:437:TRP:HD1	1:B:469:ILE:HG23	1.75	0.52
1:A:168:HIS:O	1:A:170:GLY:N	2.43	0.51
1:A:211:LEU:HD11	1:B:98:ALA:HB3	1.91	0.51
1:B:242:THR:HG22	1:B:243:ASP:N	2.24	0.51
1:A:312:ILE:HG22	1:A:313:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:TRP:HD1	1:A:469:ILE:CG2	2.23	0.51
1:B:437:TRP:HD1	1:B:469:ILE:CG2	2.23	0.51
1:A:403:ARG:NH1	1:A:432:GLN:HB3	2.25	0.51
1:B:207:TYR:CE2	1:B:259:GLU:HG3	2.46	0.51
1:B:349:VAL:HG23	1:B:371:ARG:HH21	1.76	0.51
1:A:216:GLY:N	1:B:452:THR:HB	2.26	0.51
1:B:298:SER:HB3	8:B:595:HOH:O	2.10	0.51
1:A:298:SER:HB3	8:A:583:HOH:O	2.10	0.51
1:B:168:HIS:O	1:B:170:GLY:N	2.43	0.51
1:A:136:GLN:CD	1:A:156:ARG:HH11	2.14	0.51
1:A:377:PHE:HB3	1:A:394:ARG:HB2	1.92	0.51
1:B:281:TYR:OH	1:B:288:ARG:HD2	2.11	0.51
1:B:283:ARG:NH1	1:B:288:ARG:HH21	2.08	0.51
1:A:292:ARG:HG2	1:A:293:ASP:H	1.76	0.51
1:A:327:ARG:HH12	1:A:368:LYS:HA	1.76	0.51
1:A:429:GLY:HA3	1:A:439:THR:HA	1.92	0.51
1:B:136:GLN:CD	1:B:156:ARG:HH11	2.14	0.51
1:B:320:GLY:HA2	1:B:387:ASN:ND2	2.26	0.51
1:A:320:GLY:HA2	1:A:387:ASN:ND2	2.26	0.50
1:A:376:THR:O	1:A:394:ARG:HA	2.10	0.50
1:A:136:GLN:OE1	1:A:136:GLN:HA	2.11	0.50
1:A:182:SER:HB2	8:A:506:HOH:O	2.12	0.50
1:A:207:TYR:CE2	1:A:259:GLU:HG3	2.46	0.50
1:A:349:VAL:HG23	1:A:371:ARG:HH21	1.76	0.50
1:B:136:GLN:OE1	1:B:136:GLN:HA	2.11	0.50
1:B:182:SER:HB2	8:B:515:HOH:O	2.12	0.50
1:B:429:GLY:HA3	1:B:439:THR:HA	1.92	0.50
1:B:455:THR:HG21	4:E:1:NAG:C1	2.37	0.50
1:A:182:SER:OG	1:A:191:HIS:HD2	1.94	0.50
1:A:274:HIS:HD2	1:A:294:ASN:H	1.60	0.50
1:A:321:LEU:CD2	1:A:389:LYS:HA	2.40	0.50
1:A:468:PRO:O	1:A:469:ILE:HB	2.12	0.50
1:B:226:GLN:O	1:B:227:GLU:HB2	2.11	0.50
1:A:281:TYR:OH	1:A:288:ARG:HD2	2.11	0.50
1:B:182:SER:OG	1:B:191:HIS:HD2	1.94	0.50
1:A:117:THR:HB	1:A:133:ALA:HB1	1.94	0.50
1:A:89:LYS:HB2	1:A:418:ILE:HG22	1.92	0.50
1:B:378:LYS:O	1:B:392:ILE:HG22	2.11	0.50
1:A:226:GLN:O	1:A:227:GLU:HB2	2.11	0.49
1:B:292:ARG:HG2	1:B:293:ASP:H	1.76	0.49
1:B:298:SER:O	1:B:324:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:HH12	1:B:368:LYS:HA	1.76	0.49
1:A:298:SER:O	1:A:324:ASP:HB2	2.12	0.49
1:B:117:THR:HB	1:B:133:ALA:HB1	1.94	0.49
1:A:240:VAL:HB	1:A:254:ILE:HG13	1.93	0.49
1:B:240:VAL:HB	1:B:254:ILE:HG13	1.93	0.49
1:A:296:LYS:O	1:A:340:PRO:HB2	2.13	0.49
1:A:446:PHE:HZ	1:A:458:TRP:CE3	2.31	0.49
1:B:446:PHE:HZ	1:B:458:TRP:CE3	2.31	0.49
1:B:103:ASP:OD2	1:B:443:ILE:HG12	2.13	0.49
1:B:321:LEU:CD2	1:B:389:LYS:HA	2.40	0.49
1:A:378:LYS:O	1:A:392:ILE:HG22	2.11	0.49
1:A:283:ARG:O	1:A:284:TYR:C	2.50	0.48
1:A:290:ILE:HG12	1:A:353:ALA:HB3	1.95	0.48
1:B:283:ARG:O	1:B:284:TYR:C	2.50	0.48
1:B:297:GLY:N	1:B:345:GLY:HA3	2.28	0.48
1:B:455:THR:CG2	4:E:1:NAG:H5	2.18	0.48
1:B:468:PRO:O	1:B:469:ILE:HB	2.12	0.48
1:B:290:ILE:HG12	1:B:353:ALA:HB3	1.95	0.48
1:A:391:GLN:CG	1:A:392:ILE:N	2.72	0.48
1:A:103:ASP:OD2	1:A:443:ILE:HG12	2.13	0.48
1:A:153:ILE:HG13	1:A:155:HIS:H	1.78	0.48
1:A:297:GLY:N	1:A:345:GLY:HA3	2.28	0.48
1:B:139:THR:HG22	1:B:141:ASP:H	1.79	0.48
1:A:211:LEU:HD23	1:A:211:LEU:C	2.33	0.48
1:A:318:CYS:HB2	1:A:382:GLY:O	2.14	0.48
1:B:320:GLY:CA	1:B:387:ASN:HD22	2.27	0.48
1:A:427:ILE:HD11	1:A:439:THR:CG2	2.42	0.48
1:B:211:LEU:C	1:B:211:LEU:HD23	2.33	0.48
1:A:258:GLU:O	1:A:259:GLU:HB3	2.14	0.48
1:B:258:GLU:O	1:B:259:GLU:HB3	2.14	0.48
1:A:246:ALA:O	1:A:274:HIS:NE2	2.47	0.47
1:B:100:PHE:HB3	1:B:445:VAL:O	2.14	0.47
1:B:246:ALA:O	1:B:274:HIS:NE2	2.47	0.47
1:B:274:HIS:HD2	1:B:294:ASN:H	1.60	0.47
1:B:318:CYS:HB2	1:B:382:GLY:O	2.14	0.47
1:A:100:PHE:HB3	1:A:445:VAL:O	2.14	0.47
1:B:396:VAL:HG13	4:E:6:MAN:O2	2.13	0.47
1:B:153:ILE:HG13	1:B:155:HIS:H	1.78	0.47
1:A:139:THR:HG22	1:A:141:ASP:H	1.79	0.47
1:A:142:ASN:ND2	1:B:107:ARG:O	2.48	0.47
1:A:283:ARG:HH12	1:A:288:ARG:NH2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TYR:CD1	1:A:285:PRO:HA	2.50	0.47
1:A:411:SER:CB	1:A:418:ILE:HD11	2.43	0.47
1:B:296:LYS:O	1:B:340:PRO:HB2	2.13	0.47
1:B:403:ARG:HB3	8:B:584:HOH:O	2.15	0.47
1:A:188:ALA:HB1	8:A:507:HOH:O	2.15	0.47
1:A:320:GLY:CA	1:A:387:ASN:HD22	2.27	0.47
1:A:378:LYS:HB3	1:A:392:ILE:CG2	2.44	0.47
1:B:284:TYR:CD1	1:B:285:PRO:HA	2.50	0.46
1:B:378:LYS:HB3	1:B:392:ILE:CG2	2.44	0.46
1:B:411:SER:CB	1:B:418:ILE:HD11	2.43	0.46
1:A:343:GLU:O	1:A:344:ARG:HB2	2.15	0.46
1:B:296:LYS:HA	1:B:345:GLY:HA3	1.97	0.46
1:B:309:ASP:O	1:B:310:TYR:HB2	2.15	0.46
1:B:343:GLU:O	1:B:344:ARG:HB2	2.15	0.46
1:B:427:ILE:HD11	1:B:439:THR:CG2	2.42	0.46
1:B:188:ALA:HB1	8:B:516:HOH:O	2.15	0.46
1:A:309:ASP:O	1:A:310:TYR:HB2	2.15	0.46
1:B:381:GLY:O	1:B:383:TRP:N	2.48	0.46
1:A:381:GLY:O	1:A:383:TRP:N	2.48	0.46
1:A:293:ASP:HB2	1:A:301:PRO:HG2	1.98	0.45
1:A:403:ARG:HB3	8:A:572:HOH:O	2.15	0.45
1:B:114:ILE:O	1:B:139:THR:HG23	2.16	0.45
1:B:326:PRO:CD	1:B:347:GLN:HG3	2.46	0.45
1:A:226:GLN:HA	1:A:277:GLU:HA	1.98	0.45
1:A:114:ILE:O	1:A:139:THR:HG23	2.16	0.45
1:A:125:ASP:OD1	1:A:127:VAL:HG22	2.17	0.45
1:A:395:GLN:HB3	8:A:545:HOH:O	2.16	0.45
1:A:446:PHE:HZ	1:A:458:TRP:CZ3	2.34	0.45
1:A:254:ILE:HD12	1:A:254:ILE:N	2.31	0.45
1:A:292:ARG:O	1:A:301:PRO:HG2	2.17	0.45
1:B:125:ASP:OD1	1:B:127:VAL:HG22	2.17	0.45
1:B:283:ARG:HH12	1:B:288:ARG:NH2	2.13	0.45
1:A:426:LEU:HD11	1:A:444:VAL:CG2	2.47	0.45
1:B:254:ILE:HD12	1:B:254:ILE:N	2.31	0.45
1:A:296:LYS:HA	1:A:345:GLY:HA3	1.97	0.45
1:A:326:PRO:CD	1:A:347:GLN:HG3	2.46	0.45
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.85	0.45
1:A:136:GLN:OE1	1:A:156:ARG:NH1	2.49	0.45
1:B:395:GLN:HB3	8:B:559:HOH:O	2.16	0.45
1:B:426:LEU:HD11	1:B:444:VAL:CG2	2.47	0.45
1:B:306:ASN:HB3	1:B:311:SER:HG	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ALA:HB3	1:A:167:PHE:CE2	2.52	0.45
1:B:222:ILE:HG22	1:B:222:ILE:O	2.17	0.45
1:B:266:SER:HB2	1:B:312:ILE:HD11	1.99	0.44
1:A:84:TYR:HE1	1:A:185:ASP:OD2	2.01	0.44
1:B:226:GLN:HA	1:B:277:GLU:HA	1.98	0.44
1:A:132:PHE:CD1	1:A:132:PHE:N	2.86	0.44
1:A:296:LYS:HB2	1:A:342:ASN:OD1	2.18	0.44
1:B:133:ALA:HB3	1:B:167:PHE:CE2	2.52	0.44
1:B:218:TRP:CD1	1:B:243:ASP:HB3	2.52	0.44
1:A:268:LEU:HD12	1:A:269:ALA:N	2.33	0.44
1:B:293:ASP:HB2	1:B:301:PRO:HG2	1.98	0.44
1:B:84:TYR:HE1	1:B:185:ASP:OD2	2.01	0.44
1:A:222:ILE:HG22	1:A:222:ILE:O	2.17	0.44
1:B:446:PHE:HZ	1:B:458:TRP:CZ3	2.34	0.44
1:A:172:ARG:HB2	1:B:165:VAL:HG12	2.00	0.44
1:A:218:TRP:CD1	1:A:243:ASP:HB3	2.52	0.44
1:A:254:ILE:HD13	1:A:312:ILE:CD1	2.44	0.44
1:A:258:GLU:OE1	1:A:263:VAL:HG21	2.17	0.44
1:A:155:HIS:HB3	1:B:104:ASN:ND2	2.32	0.44
1:B:132:PHE:CD1	1:B:132:PHE:N	2.86	0.44
1:B:254:ILE:HD13	1:B:312:ILE:CD1	2.44	0.44
1:B:258:GLU:OE1	1:B:263:VAL:HG21	2.17	0.44
1:A:266:SER:HB2	1:A:312:ILE:HD11	1.99	0.43
1:B:109:SER:HB3	1:B:140:LEU:HD22	2.00	0.43
1:B:292:ARG:O	1:B:301:PRO:HG2	2.17	0.43
1:A:306:ASN:HB3	1:A:311:SER:HG	1.82	0.43
1:A:331:ARG:HA	1:A:331:ARG:NE	2.33	0.43
1:B:255:LEU:HD22	1:B:265:ILE:HG12	2.01	0.43
1:B:268:LEU:HD12	1:B:269:ALA:H	1.84	0.43
1:B:275:VAL:CG1	1:B:278:CYS:SG	3.07	0.43
1:A:161:ASN:ND2	1:A:171:THR:HG23	2.34	0.43
1:A:275:VAL:CG1	1:A:278:CYS:SG	3.07	0.43
1:A:255:LEU:HD22	1:A:265:ILE:HG12	2.01	0.43
1:A:437:TRP:N	1:A:469:ILE:HG21	2.33	0.43
1:B:258:GLU:HB3	1:B:263:VAL:HG13	2.01	0.43
1:A:109:SER:HB3	1:A:140:LEU:HD22	2.00	0.43
1:B:268:LEU:HD12	1:B:269:ALA:N	2.33	0.43
1:B:161:ASN:ND2	1:B:171:THR:HG23	2.34	0.42
1:B:288:ARG:NH1	1:B:383:TRP:HZ2	2.16	0.42
1:B:296:LYS:HB2	1:B:342:ASN:OD1	2.18	0.42
1:B:331:ARG:HA	1:B:331:ARG:NE	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:PHE:CD1	1:B:466:PHE:N	2.86	0.42
1:B:351:GLY:N	8:B:539:HOH:O	2.49	0.42
1:A:144:HIS:CE1	1:B:463:ASN:H	2.37	0.42
1:B:300:ARG:HA	1:B:301:PRO:HD3	1.86	0.42
1:A:194:ILE:HD11	1:A:241:MET:CE	2.50	0.42
1:B:152:ARG:CZ	1:B:222:ILE:HD13	2.50	0.42
1:B:456:GLY:N	4:E:6:MAN:C2	2.82	0.42
1:A:117:THR:HG22	1:A:135:GLY:HA2	2.02	0.42
1:A:258:GLU:HB3	1:A:263:VAL:CG1	2.50	0.42
1:B:116:VAL:HG22	1:B:140:LEU:HD12	2.01	0.42
1:B:299:ASN:HB3	1:B:322:VAL:HG22	2.02	0.42
1:B:117:THR:HG22	1:B:135:GLY:HA2	2.02	0.42
1:B:136:GLN:CD	1:B:156:ARG:NH1	2.73	0.42
1:A:136:GLN:CD	1:A:156:ARG:NH1	2.73	0.42
1:A:268:LEU:HD12	1:A:269:ALA:H	1.84	0.42
1:A:345:GLY:O	1:A:347:GLN:N	2.53	0.42
1:A:467:MET:HA	1:A:468:PRO:HD3	1.79	0.42
1:B:345:GLY:O	1:B:347:GLN:N	2.53	0.42
1:A:242:THR:OG1	1:A:252:THR:HG23	2.20	0.42
1:A:299:ASN:HB3	1:A:322:VAL:HG22	2.02	0.42
1:B:116:VAL:HG13	1:B:440:SER:HB2	2.02	0.42
1:B:136:GLN:OE1	1:B:156:ARG:NH1	2.49	0.42
1:A:84:TYR:CE1	1:A:185:ASP:OD2	2.73	0.41
1:B:338:ARG:HH11	1:B:338:ARG:CG	2.30	0.41
1:B:392:ILE:HG12	1:B:393:ASN:N	2.34	0.41
1:A:231:VAL:HA	8:A:504:HOH:O	2.20	0.41
1:A:466:PHE:N	1:A:466:PHE:CD1	2.86	0.41
1:B:380:ILE:HD12	1:B:390:SER:O	2.20	0.41
1:B:84:TYR:CE1	1:B:185:ASP:OD2	2.73	0.41
1:B:103:ASP:HB3	8:B:509:HOH:O	2.20	0.41
1:A:103:ASP:HB3	8:A:499:HOH:O	2.20	0.41
1:B:149:VAL:HG22	1:B:430:ARG:HB2	2.03	0.41
1:B:231:VAL:HA	8:B:513:HOH:O	2.20	0.41
1:B:242:THR:OG1	1:B:252:THR:HG23	2.20	0.41
1:B:258:GLU:HB3	1:B:263:VAL:CG1	2.50	0.41
1:B:292:ARG:HG2	1:B:293:ASP:N	2.36	0.41
1:B:292:ARG:HE	1:B:348:GLY:HA3	1.86	0.41
1:B:427:ILE:HD12	1:B:428:ARG:H	1.85	0.41
1:B:437:TRP:CD1	1:B:469:ILE:CG2	3.03	0.41
1:B:437:TRP:N	1:B:469:ILE:HG21	2.33	0.41
1:A:155:HIS:ND1	1:B:102:LYS:HE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:HB3	1:A:263:VAL:HG13	2.01	0.41
1:A:292:ARG:HG2	1:A:293:ASP:N	2.36	0.41
1:A:380:ILE:HD12	1:A:390:SER:O	2.20	0.41
1:B:326:PRO:HA	1:B:368:LYS:O	2.21	0.41
1:B:361:TRP:CZ3	1:B:378:LYS:HB2	2.56	0.41
1:A:115:TRP:HZ3	1:A:137:GLY:HA2	1.85	0.41
1:A:221:ASN:HD22	1:A:244:GLY:H	1.69	0.41
1:B:100:PHE:CE2	1:B:163:LEU:CD2	3.04	0.41
1:A:116:VAL:HG22	1:A:140:LEU:HD12	2.01	0.41
1:A:205:PHE:HD2	1:A:257:ILE:CD1	2.32	0.41
1:B:194:ILE:HD11	1:B:241:MET:CE	2.50	0.41
1:B:324:ASP:N	8:B:595:HOH:O	2.51	0.41
1:A:100:PHE:CE2	1:A:163:LEU:CD2	3.04	0.41
1:A:152:ARG:CZ	1:A:222:ILE:HD13	2.50	0.41
1:A:195:THR:HB	1:B:458:TRP:HE1	1.86	0.41
1:A:300:ARG:NE	1:A:323:GLY:O	2.54	0.41
1:A:324:ASP:N	8:A:583:HOH:O	2.51	0.41
1:A:326:PRO:HA	1:A:368:LYS:O	2.21	0.41
1:A:361:TRP:CZ3	1:A:378:LYS:HB2	2.56	0.41
1:B:97:PHE:CD1	1:B:448:GLY:HA2	2.56	0.41
1:B:115:TRP:HZ3	1:B:137:GLY:HA2	1.85	0.41
1:B:300:ARG:NE	1:B:323:GLY:O	2.54	0.41
1:B:361:TRP:CH2	1:B:378:LYS:HB2	2.56	0.41
1:B:365:THR:HG21	1:B:371:ARG:HA	2.03	0.41
1:B:427:ILE:HD12	1:B:428:ARG:N	2.36	0.41
1:A:275:VAL:HG13	1:A:278:CYS:SG	2.61	0.41
1:A:344:ARG:HH22	1:A:369:ASP:CG	2.25	0.41
1:A:427:ILE:HD12	1:A:428:ARG:N	2.36	0.41
1:A:116:VAL:HG13	1:A:440:SER:HB2	2.02	0.40
1:A:213:ASP:HB2	1:A:261:LYS:HD2	2.03	0.40
1:A:361:TRP:CH2	1:A:378:LYS:HB2	2.56	0.40
1:B:221:ASN:ND2	8:B:597:HOH:O	2.54	0.40
1:B:275:VAL:HG13	1:B:278:CYS:SG	2.61	0.40
1:A:148:THR:O	1:A:148:THR:HG22	2.21	0.40
1:A:351:GLY:N	8:A:524:HOH:O	2.49	0.40
1:A:409:ILE:HG12	1:A:410:PHE:N	2.37	0.40
1:B:205:PHE:HD2	1:B:257:ILE:CD1	2.32	0.40
1:A:288:ARG:NH1	1:A:383:TRP:HZ2	2.16	0.40
1:A:338:ARG:HH11	1:A:338:ARG:CG	2.30	0.40
1:B:104:ASN:ND2	8:B:488:HOH:O	2.54	0.40
1:B:213:ASP:HB2	1:B:261:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:O	1:B:431:LYS:HB2	2.22	0.40
1:B:467:MET:HA	1:B:468:PRO:HD3	1.79	0.40
1:A:377:PHE:HB3	1:A:394:ARG:CB	2.52	0.40
1:A:125:ASP:O	1:A:126:PRO:C	2.60	0.40
1:A:142:ASN:OD1	1:B:111:GLY:HA3	2.21	0.40
1:A:320:GLY:CA	1:A:387:ASN:ND2	2.84	0.40
1:B:409:ILE:HG12	1:B:410:PHE:N	2.37	0.40
1:B:437:TRP:HB2	1:B:469:ILE:HD13	2.03	0.40

All (52) 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:A:170:GLY:CA	8:A:602:HOH:O[4_555]	0.79	1.41
3:D:4:FUL:H3	4:E:4:MAN:H4[3_654]	0.40	1.20
1:A:394:ARG:CA	8:B:517:HOH:O[4_555]	1.06	1.14
1:B:368:LYS:HZ1	8:B:613:HOH:H1[3_654]	0.46	1.14
3:D:4:FUL:C4	4:E:4:MAN:H61[3_654]	0.59	1.01
1:A:394:ARG:N	8:B:517:HOH:O[4_555]	1.21	0.99
1:A:456:GLY:O	4:I:6:MAN:O3[4_555]	1.34	0.86
1:A:170:GLY:CA	8:A:602:HOH:H2[4_555]	0.76	0.84
1:A:456:GLY:O	4:I:6:MAN:HO3[4_555]	0.80	0.80
1:A:455:THR:OG1	4:I:1:NAG:H61[4_555]	0.81	0.79
1:B:328:ASN:O	8:B:576:HOH:H2[3_654]	0.84	0.76
3:D:4:FUL:H5	4:E:4:MAN:H62[3_654]	0.93	0.67
1:B:329:ASP:N	8:B:576:HOH:H1[3_654]	0.96	0.64
1:A:170:GLY:C	8:A:602:HOH:H2[4_555]	0.97	0.63
1:A:394:ARG:C	8:B:517:HOH:O[4_555]	1.57	0.63
1:A:170:GLY:C	8:A:602:HOH:O[4_555]	1.59	0.61
1:A:394:ARG:N	8:B:517:HOH:H2[4_555]	0.99	0.61
1:B:328:ASN:C	8:B:576:HOH:H1[3_654]	0.99	0.61
1:B:210:ARG:HH21	8:A:553:HOH:H1[4_555]	1.03	0.57
1:A:394:ARG:H	8:B:517:HOH:H2[4_555]	1.05	0.55
1:A:455:THR:OG1	4:I:1:NAG:C6[4_555]	1.65	0.55
3:D:4:FUL:H4	4:E:4:MAN:H61[3_654]	1.06	0.54
1:B:368:LYS:NZ	8:B:613:HOH:H1[3_654]	1.09	0.51
3:D:4:FUL:H3	4:E:4:MAN:C4[3_654]	1.19	0.41
1:A:394:ARG:CA	8:B:517:HOH:H2[4_555]	1.20	0.40
3:D:4:FUL:C5	4:E:4:MAN:H61[3_654]	1.22	0.38
3:D:4:FUL:H4	4:E:4:MAN:C6[3_654]	1.27	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:FUL:C3	4:E:4:MAN:H4[3_654]	1.30	0.30
1:A:455:THR:OG1	4:I:1:NAG:O5[4_555]	1.91	0.29
3:D:4:FUL:H5	4:E:4:MAN:C6[3_654]	1.33	0.27
1:A:170:GLY:CA	8:A:602:HOH:H1[4_555]	1.34	0.26
1:A:394:ARG:O	8:B:517:HOH:O[4_555]	1.94	0.26
1:A:455:THR:CB	4:I:1:NAG:H61[4_555]	1.34	0.26
1:A:394:ARG:CB	8:B:517:HOH:O[4_555]	1.95	0.25
1:A:456:GLY:C	4:I:6:MAN:O3[4_555]	2.02	0.18
1:B:328:ASN:O	8:B:576:HOH:H1[3_654]	1.42	0.18
1:A:394:ARG:CA	8:B:517:HOH:H1[4_555]	1.48	0.12
1:A:170:GLY:N	8:A:602:HOH:O[4_555]	2.09	0.11
3:D:4:FUL:C5	4:E:4:MAN:H62[3_654]	1.49	0.11
1:A:163:LEU:O	8:B:524:HOH:H1[4_555]	1.51	0.09
1:A:394:ARG:C	8:B:517:HOH:H1[4_555]	1.53	0.07
1:A:455:THR:CG2	4:I:1:NAG:H1[4_555]	1.53	0.07
1:A:455:THR:OG1	4:I:1:NAG:C5[4_555]	2.13	0.07
1:A:455:THR:CB	4:I:1:NAG:C6[4_555]	2.15	0.05
1:B:329:ASP:CA	8:B:576:HOH:H1[3_654]	1.56	0.04
1:A:170:GLY:O	8:A:602:HOH:O[4_555]	2.17	0.03
1:A:336:ASN:O	8:B:550:HOH:O[7_554]	2.17	0.03
1:B:368:LYS:CE	8:B:613:HOH:H2[3_654]	1.57	0.03
1:B:368:LYS:NZ	8:B:613:HOH:H2[3_654]	1.58	0.02
1:A:170:GLY:C	8:A:602:HOH:H1[4_555]	1.59	0.01
1:A:313:ASP:OD1	1:B:338:ARG:HH12[7_554]	1.59	0.01
1:A:164:GLY:O	1:B:173:GLN:H[4_555]	1.60	0.00

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	386/388 (100%)	302 (78%)	65 (17%)	19 (5%)	2 1
1	B	386/388 (100%)	302 (78%)	65 (17%)	19 (5%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	772/776 (100%)	604 (78%)	130 (17%)	38 (5%)	2 1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	TRP
1	A	274	HIS
1	A	329	ASP
1	A	356	ASN
1	A	430	ARG
1	B	87	TRP
1	B	274	HIS
1	B	329	ASP
1	B	356	ASN
1	B	430	ARG
1	A	169	LEU
1	A	322	VAL
1	A	330	ASP
1	A	347	GLN
1	A	382	GLY
1	B	169	LEU
1	B	322	VAL
1	B	330	ASP
1	B	347	GLN
1	B	382	GLY
1	A	259	GLU
1	B	259	GLU
1	A	88	SER
1	A	277	GLU
1	A	431	LYS
1	B	88	SER
1	B	277	GLU
1	B	431	LYS
1	A	104	ASN
1	B	104	ASN
1	A	244	GLY
1	A	270	GLY
1	A	373	GLY
1	B	244	GLY
1	B	270	GLY
1	B	373	GLY
1	A	222	ILE

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Mol	Chain	Res	Type
1	B	222	ILE

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	338/338 (100%)	304 (90%)	34 (10%)	7 11
1	B	338/338 (100%)	304 (90%)	34 (10%)	7 11
All	All	676/676 (100%)	608 (90%)	68 (10%)	7 11

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	122	VAL
1	A	141	ASP
1	A	147	ASP
1	A	157	THR
1	A	165	VAL
1	A	190	LEU
1	A	195	THR
1	A	220	GLN
1	A	227	GLU
1	A	231	VAL
1	A	240	VAL
1	A	257	ILE
1	A	285	PRO
1	A	294	ASN
1	A	301	PRO
1	A	329	ASP
1	A	331	ARG
1	A	337	CYS
1	A	347	GLN
1	A	364	ARG
1	A	368	LYS

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Mol	Chain	Res	Type
1	A	385	THR
1	A	387	ASN
1	A	388	SER
1	A	394	ARG
1	A	396	VAL
1	A	402	ASN
1	A	418	ILE
1	A	420	ARG
1	A	427	ILE
1	A	445	VAL
1	A	452	THR
1	A	468	PRO
1	B	118	ARG
1	B	122	VAL
1	B	141	ASP
1	B	147	ASP
1	B	157	THR
1	B	165	VAL
1	B	190	LEU
1	B	195	THR
1	B	220	GLN
1	B	227	GLU
1	B	231	VAL
1	B	240	VAL
1	B	257	ILE
1	B	285	PRO
1	B	294	ASN
1	B	301	PRO
1	B	329	ASP
1	B	331	ARG
1	B	337	CYS
1	B	347	GLN
1	B	364	ARG
1	B	368	LYS
1	B	385	THR
1	B	387	ASN
1	B	388	SER
1	B	394	ARG
1	B	396	VAL
1	B	402	ASN
1	B	418	ILE
1	B	420	ARG

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Mol	Chain	Res	Type
1	B	427	ILE
1	B	445	VAL
1	B	452	THR
1	B	468	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	144	HIS
1	A	161	ASN
1	A	173	GLN
1	A	191	HIS
1	A	220	GLN
1	A	221	ASN
1	A	334	ASN
1	A	347	GLN
1	A	387	ASN
1	A	402	ASN
1	A	465	ASN
1	B	104	ASN
1	B	161	ASN
1	B	173	GLN
1	B	191	HIS
1	B	220	GLN
1	B	221	ASN
1	B	334	ASN
1	B	347	GLN
1	B	387	ASN
1	B	402	ASN
1	B	465	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	1.38	2 (14%)	17,19,21	1.99	3 (17%)
2	NAG	C	2	2	14,14,15	1.48	3 (21%)	17,19,21	2.22	2 (11%)
3	NAG	D	1	3,1	14,14,15	1.96	3 (21%)	17,19,21	2.90	4 (23%)
3	NAG	D	2	3	14,14,15	1.84	2 (14%)	17,19,21	2.20	5 (29%)
3	BMA	D	3	3	11,11,12	1.27	1 (9%)	15,15,17	2.22	4 (26%)
3	FUL	D	4	3	10,10,11	2.05	4 (40%)	14,14,16	1.97	5 (35%)
4	NAG	E	1	4,1	14,14,15	2.00	4 (28%)	17,19,21	2.99	6 (35%)
4	NAG	E	2	4	14,14,15	1.79	3 (21%)	17,19,21	2.60	4 (23%)
4	BMA	E	3	4	11,11,12	1.99	5 (45%)	15,15,17	2.63	4 (26%)
4	MAN	E	4	4	11,11,12	3.06	3 (27%)	15,15,17	2.63	4 (26%)
4	MAN	E	5	4	11,11,12	1.87	4 (36%)	15,15,17	2.49	5 (33%)
4	MAN	E	6	4	11,11,12	1.75	4 (36%)	15,15,17	1.65	3 (20%)
2	NAG	F	1	2,1	14,14,15	0.94	0	17,19,21	2.32	4 (23%)
2	NAG	F	2	2	14,14,15	1.35	2 (14%)	17,19,21	3.57	12 (70%)
2	NAG	G	1	2,1	14,14,15	1.38	2 (14%)	17,19,21	1.99	3 (17%)
2	NAG	G	2	2	14,14,15	1.48	3 (21%)	17,19,21	2.22	2 (11%)
5	NAG	H	1	5,1	14,14,15	1.96	3 (21%)	17,19,21	2.90	4 (23%)
5	NAG	H	2	5	14,14,15	1.84	2 (14%)	17,19,21	2.20	5 (29%)
5	BMA	H	3	5	11,11,12	1.27	1 (9%)	15,15,17	2.22	4 (26%)
5	FUC	H	4	5	10,10,11	2.05	4 (40%)	14,14,16	1.97	5 (35%)
4	NAG	I	1	4,1	14,14,15	2.00	4 (28%)	17,19,21	2.99	6 (35%)
4	NAG	I	2	4	14,14,15	1.79	3 (21%)	17,19,21	2.60	4 (23%)
4	BMA	I	3	4	11,11,12	1.99	5 (45%)	15,15,17	2.63	4 (26%)
4	MAN	I	4	4	11,11,12	3.06	3 (27%)	15,15,17	2.63	4 (26%)
4	MAN	I	5	4	11,11,12	1.87	4 (36%)	15,15,17	2.49	5 (33%)
4	MAN	I	6	4	11,11,12	1.75	4 (36%)	15,15,17	1.65	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	J	1	2,1	14,14,15	0.94	0	17,19,21	2.32	4 (23%)
2	NAG	J	2	2	14,14,15	1.35	2 (14%)	17,19,21	3.57	12 (70%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	FUL	D	4	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	1/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	1/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	FUC	H	4	5	1/1/5/5	-	0/1/1/1
4	NAG	I	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	1/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	1/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	MAN	C2-C3	6.72	1.62	1.52
4	I	4	MAN	C2-C3	6.72	1.62	1.52
4	E	4	MAN	C1-C2	5.63	1.65	1.52
4	I	4	MAN	C1-C2	5.63	1.65	1.52
3	D	1	NAG	C1-C2	-5.50	1.44	1.52
5	H	1	NAG	C1-C2	-5.50	1.44	1.52
3	D	2	NAG	C1-C2	5.30	1.60	1.52
5	H	2	NAG	C1-C2	5.30	1.60	1.52
4	E	1	NAG	C3-C2	4.58	1.62	1.52
4	I	1	NAG	C3-C2	4.58	1.62	1.52
3	D	4	FUL	C4-C5	3.92	1.61	1.52
5	H	4	FUC	C4-C5	3.92	1.61	1.52
4	E	2	NAG	O5-C5	3.85	1.51	1.43
4	I	2	NAG	O5-C5	3.85	1.51	1.43
4	E	4	MAN	C4-C3	3.77	1.61	1.52
4	I	4	MAN	C4-C3	3.77	1.61	1.52
4	E	2	NAG	C3-C2	3.76	1.60	1.52
4	I	2	NAG	C3-C2	3.76	1.60	1.52
4	E	5	MAN	C2-C3	3.65	1.57	1.52
4	I	5	MAN	C2-C3	3.65	1.57	1.52
2	F	2	NAG	C4-C5	3.60	1.60	1.53
2	J	2	NAG	C4-C5	3.60	1.60	1.53
2	C	2	NAG	C4-C5	3.48	1.60	1.53
2	G	2	NAG	C4-C5	3.48	1.60	1.53
4	E	3	BMA	O5-C5	3.22	1.50	1.43
4	I	3	BMA	O5-C5	3.22	1.50	1.43
4	E	1	NAG	C4-C3	3.15	1.60	1.52
4	I	1	NAG	C4-C3	3.15	1.60	1.52
4	E	6	MAN	C4-C5	3.05	1.59	1.53
4	I	6	MAN	C4-C5	3.05	1.59	1.53
4	E	3	BMA	C4-C5	3.04	1.59	1.53
4	I	3	BMA	C4-C5	3.04	1.59	1.53
2	C	1	NAG	C1-C2	-3.03	1.47	1.52
2	G	1	NAG	C1-C2	-3.03	1.47	1.52
4	E	5	MAN	O5-C5	2.97	1.49	1.43
4	I	5	MAN	O5-C5	2.97	1.49	1.43
2	C	1	NAG	O5-C1	-2.97	1.39	1.43
2	G	1	NAG	O5-C1	-2.97	1.39	1.43
2	C	2	NAG	O5-C5	2.89	1.49	1.43
2	G	2	NAG	O5-C5	2.89	1.49	1.43
3	D	1	NAG	C4-C3	2.89	1.59	1.52
5	H	1	NAG	C4-C3	2.89	1.59	1.52
4	E	3	BMA	C1-C2	2.84	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	BMA	C1-C2	2.84	1.58	1.52
4	E	3	BMA	C6-C5	2.83	1.61	1.51
4	I	3	BMA	C6-C5	2.83	1.61	1.51
3	D	2	NAG	C4-C5	2.78	1.58	1.53
5	H	2	NAG	C4-C5	2.78	1.58	1.53
4	E	6	MAN	O5-C5	2.64	1.48	1.43
4	I	6	MAN	O5-C5	2.64	1.48	1.43
3	D	4	FUL	C2-C3	2.61	1.56	1.52
5	H	4	FUC	C2-C3	2.61	1.56	1.52
3	D	1	NAG	O5-C5	2.58	1.48	1.43
5	H	1	NAG	O5-C5	2.58	1.48	1.43
3	D	3	BMA	C4-C3	2.56	1.58	1.52
5	H	3	BMA	C4-C3	2.56	1.58	1.52
3	D	4	FUL	O5-C5	2.56	1.49	1.43
5	H	4	FUC	O5-C5	2.56	1.49	1.43
4	E	2	NAG	C4-C5	2.54	1.58	1.53
4	I	2	NAG	C4-C5	2.54	1.58	1.53
3	D	4	FUL	C4-C3	2.52	1.58	1.52
5	H	4	FUC	C4-C3	2.52	1.58	1.52
4	E	1	NAG	O4-C4	2.48	1.48	1.43
4	I	1	NAG	O4-C4	2.48	1.48	1.43
2	F	2	NAG	C3-C2	2.42	1.57	1.52
2	J	2	NAG	C3-C2	2.42	1.57	1.52
4	E	6	MAN	C1-C2	2.42	1.57	1.52
4	I	6	MAN	C1-C2	2.42	1.57	1.52
4	E	5	MAN	C1-C2	2.32	1.57	1.52
4	I	5	MAN	C1-C2	2.32	1.57	1.52
2	C	2	NAG	O5-C1	2.24	1.47	1.43
2	G	2	NAG	O5-C1	2.24	1.47	1.43
4	E	6	MAN	C6-C5	2.13	1.59	1.51
4	I	6	MAN	C6-C5	2.13	1.59	1.51
4	E	1	NAG	C1-C2	2.12	1.55	1.52
4	I	1	NAG	C1-C2	2.12	1.55	1.52
4	E	3	BMA	O5-C1	2.11	1.47	1.43
4	I	3	BMA	O5-C1	2.11	1.47	1.43
4	E	5	MAN	O5-C1	2.07	1.47	1.43
4	I	5	MAN	O5-C1	2.07	1.47	1.43

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	C1-O5-C5	8.93	124.30	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1	NAG	C1-O5-C5	8.93	124.30	112.19
4	E	3	BMA	C1-O5-C5	8.09	123.15	112.19
4	I	3	BMA	C1-O5-C5	8.09	123.15	112.19
2	C	2	NAG	C1-O5-C5	7.98	123.01	112.19
2	G	2	NAG	C1-O5-C5	7.98	123.01	112.19
2	F	2	NAG	C1-C2-N2	7.08	122.58	110.49
2	J	2	NAG	C1-C2-N2	7.08	122.58	110.49
2	F	1	NAG	C1-O5-C5	6.61	121.14	112.19
2	J	1	NAG	C1-O5-C5	6.61	121.14	112.19
4	E	2	NAG	C1-O5-C5	6.52	121.02	112.19
4	I	2	NAG	C1-O5-C5	6.52	121.02	112.19
4	E	5	MAN	C1-O5-C5	6.42	120.89	112.19
4	I	5	MAN	C1-O5-C5	6.42	120.89	112.19
4	E	1	NAG	C4-C3-C2	6.29	120.23	111.02
4	I	1	NAG	C4-C3-C2	6.29	120.23	111.02
4	E	1	NAG	C6-C5-C4	6.10	127.30	113.00
4	I	1	NAG	C6-C5-C4	6.10	127.30	113.00
4	E	2	NAG	C4-C3-C2	-6.07	102.12	111.02
4	I	2	NAG	C4-C3-C2	-6.07	102.12	111.02
3	D	2	NAG	C1-O5-C5	5.90	120.19	112.19
5	H	2	NAG	C1-O5-C5	5.90	120.19	112.19
4	E	4	MAN	O2-C2-C1	5.58	120.57	109.15
4	I	4	MAN	O2-C2-C1	5.58	120.57	109.15
3	D	3	BMA	C1-C2-C3	5.51	116.43	109.67
5	H	3	BMA	C1-C2-C3	5.51	116.43	109.67
2	F	2	NAG	C4-C3-C2	-5.15	103.47	111.02
2	J	2	NAG	C4-C3-C2	-5.15	103.47	111.02
4	E	4	MAN	C1-C2-C3	5.14	115.99	109.67
4	I	4	MAN	C1-C2-C3	5.14	115.99	109.67
2	C	1	NAG	O5-C1-C2	-5.08	103.27	111.29
2	G	1	NAG	O5-C1-C2	-5.08	103.27	111.29
4	E	1	NAG	C3-C4-C5	-4.92	101.46	110.24
4	I	1	NAG	C3-C4-C5	-4.92	101.46	110.24
3	D	2	NAG	C1-C2-N2	4.83	118.74	110.49
5	H	2	NAG	C1-C2-N2	4.83	118.74	110.49
2	F	2	NAG	C1-O5-C5	4.79	118.68	112.19
2	J	2	NAG	C1-O5-C5	4.79	118.68	112.19
2	F	2	NAG	C3-C4-C5	-4.75	101.77	110.24
2	J	2	NAG	C3-C4-C5	-4.75	101.77	110.24
3	D	1	NAG	C2-N2-C7	4.70	129.60	122.90
5	H	1	NAG	C2-N2-C7	4.70	129.60	122.90
3	D	1	NAG	C4-C3-C2	-4.48	104.45	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1	NAG	C4-C3-C2	-4.48	104.45	111.02
3	D	3	BMA	C1-O5-C5	4.44	118.20	112.19
5	H	3	BMA	C1-O5-C5	4.44	118.20	112.19
4	E	5	MAN	C1-C2-C3	4.41	115.08	109.67
4	I	5	MAN	C1-C2-C3	4.41	115.08	109.67
2	F	2	NAG	O3-C3-C2	4.32	118.39	109.47
2	J	2	NAG	O3-C3-C2	4.32	118.39	109.47
2	C	1	NAG	C1-O5-C5	4.09	117.74	112.19
2	G	1	NAG	C1-O5-C5	4.09	117.74	112.19
2	F	2	NAG	O4-C4-C5	4.05	119.36	109.30
2	J	2	NAG	O4-C4-C5	4.05	119.36	109.30
4	E	4	MAN	O2-C2-C3	-4.00	102.13	110.14
4	I	4	MAN	O2-C2-C3	-4.00	102.13	110.14
2	F	1	NAG	C3-C4-C5	3.98	117.34	110.24
2	J	1	NAG	C3-C4-C5	3.98	117.34	110.24
2	F	2	NAG	O5-C5-C6	-3.83	101.20	107.20
2	J	2	NAG	O5-C5-C6	-3.83	101.20	107.20
2	F	1	NAG	O5-C1-C2	3.77	117.24	111.29
2	J	1	NAG	O5-C1-C2	3.77	117.24	111.29
4	E	5	MAN	O5-C1-C2	3.75	116.56	110.77
4	I	5	MAN	O5-C1-C2	3.75	116.56	110.77
4	E	1	NAG	O3-C3-C4	-3.75	101.69	110.35
4	I	1	NAG	O3-C3-C4	-3.75	101.69	110.35
3	D	4	FUL	C6-C5-C4	3.61	119.75	113.07
5	H	4	FUC	C6-C5-C4	3.61	119.75	113.07
4	E	1	NAG	O5-C5-C4	-3.61	102.05	110.83
4	I	1	NAG	O5-C5-C4	-3.61	102.05	110.83
4	E	1	NAG	O4-C4-C5	3.61	118.25	109.30
4	I	1	NAG	O4-C4-C5	3.61	118.25	109.30
3	D	3	BMA	O2-C2-C3	-3.56	103.00	110.14
5	H	3	BMA	O2-C2-C3	-3.56	103.00	110.14
4	E	4	MAN	C1-O5-C5	3.55	117.00	112.19
4	I	4	MAN	C1-O5-C5	3.55	117.00	112.19
4	E	6	MAN	C1-O5-C5	3.44	116.86	112.19
4	I	6	MAN	C1-O5-C5	3.44	116.86	112.19
4	E	3	BMA	O3-C3-C2	-3.42	103.44	109.99
4	I	3	BMA	O3-C3-C2	-3.42	103.44	109.99
3	D	4	FUL	C1-C2-C3	3.34	113.77	109.67
5	H	4	FUC	C1-C2-C3	3.34	113.77	109.67
3	D	4	FUL	C1-O5-C5	3.25	120.14	112.78
5	H	4	FUC	C1-O5-C5	3.25	120.14	112.78
2	F	2	NAG	C6-C5-C4	3.22	120.54	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	C6-C5-C4	3.22	120.54	113.00
4	E	6	MAN	C3-C4-C5	-3.19	104.56	110.24
4	I	6	MAN	C3-C4-C5	-3.19	104.56	110.24
4	E	2	NAG	C2-N2-C7	3.04	127.23	122.90
4	I	2	NAG	C2-N2-C7	3.04	127.23	122.90
2	F	2	NAG	O7-C7-C8	-2.92	116.64	122.06
2	J	2	NAG	O7-C7-C8	-2.92	116.64	122.06
2	F	2	NAG	C8-C7-N2	2.91	121.03	116.10
2	J	2	NAG	C8-C7-N2	2.91	121.03	116.10
2	C	1	NAG	C1-C2-N2	2.90	115.45	110.49
2	G	1	NAG	C1-C2-N2	2.90	115.45	110.49
4	E	2	NAG	O4-C4-C3	2.86	116.97	110.35
4	I	2	NAG	O4-C4-C3	2.86	116.97	110.35
2	F	2	NAG	O5-C1-C2	-2.77	106.92	111.29
2	J	2	NAG	O5-C1-C2	-2.77	106.92	111.29
3	D	4	FUL	C3-C4-C5	2.59	113.81	109.77
5	H	4	FUC	C3-C4-C5	2.59	113.81	109.77
4	E	3	BMA	C1-C2-C3	2.52	112.77	109.67
4	I	3	BMA	C1-C2-C3	2.52	112.77	109.67
3	D	1	NAG	O3-C3-C4	2.48	116.08	110.35
5	H	1	NAG	O3-C3-C4	2.48	116.08	110.35
2	C	2	NAG	O4-C4-C3	-2.39	104.83	110.35
2	G	2	NAG	O4-C4-C3	-2.39	104.83	110.35
3	D	2	NAG	O5-C1-C2	-2.34	107.60	111.29
5	H	2	NAG	O5-C1-C2	-2.34	107.60	111.29
4	E	5	MAN	C3-C4-C5	2.33	114.40	110.24
4	I	5	MAN	C3-C4-C5	2.33	114.40	110.24
4	E	6	MAN	O4-C4-C5	2.33	115.08	109.30
4	I	6	MAN	O4-C4-C5	2.33	115.08	109.30
2	F	1	NAG	C4-C3-C2	-2.31	107.64	111.02
2	J	1	NAG	C4-C3-C2	-2.31	107.64	111.02
3	D	2	NAG	O4-C4-C3	2.26	115.56	110.35
5	H	2	NAG	O4-C4-C3	2.26	115.56	110.35
4	E	3	BMA	O2-C2-C3	-2.18	105.78	110.14
4	I	3	BMA	O2-C2-C3	-2.18	105.78	110.14
3	D	4	FUL	O3-C3-C2	-2.13	105.91	109.99
5	H	4	FUC	O3-C3-C2	-2.13	105.91	109.99
4	E	5	MAN	O2-C2-C3	-2.08	105.97	110.14
4	I	5	MAN	O2-C2-C3	-2.08	105.97	110.14
2	F	2	NAG	C2-N2-C7	-2.08	119.95	122.90
2	J	2	NAG	C2-N2-C7	-2.08	119.95	122.90
3	D	3	BMA	C6-C5-C4	2.05	117.81	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3	BMA	C6-C5-C4	2.05	117.81	113.00
3	D	2	NAG	C4-C3-C2	-2.03	108.04	111.02
5	H	2	NAG	C4-C3-C2	-2.03	108.04	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	4	FUC	C1

All (24) torsion outliers are listed below:

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

All (2) ring outliers are listed below:

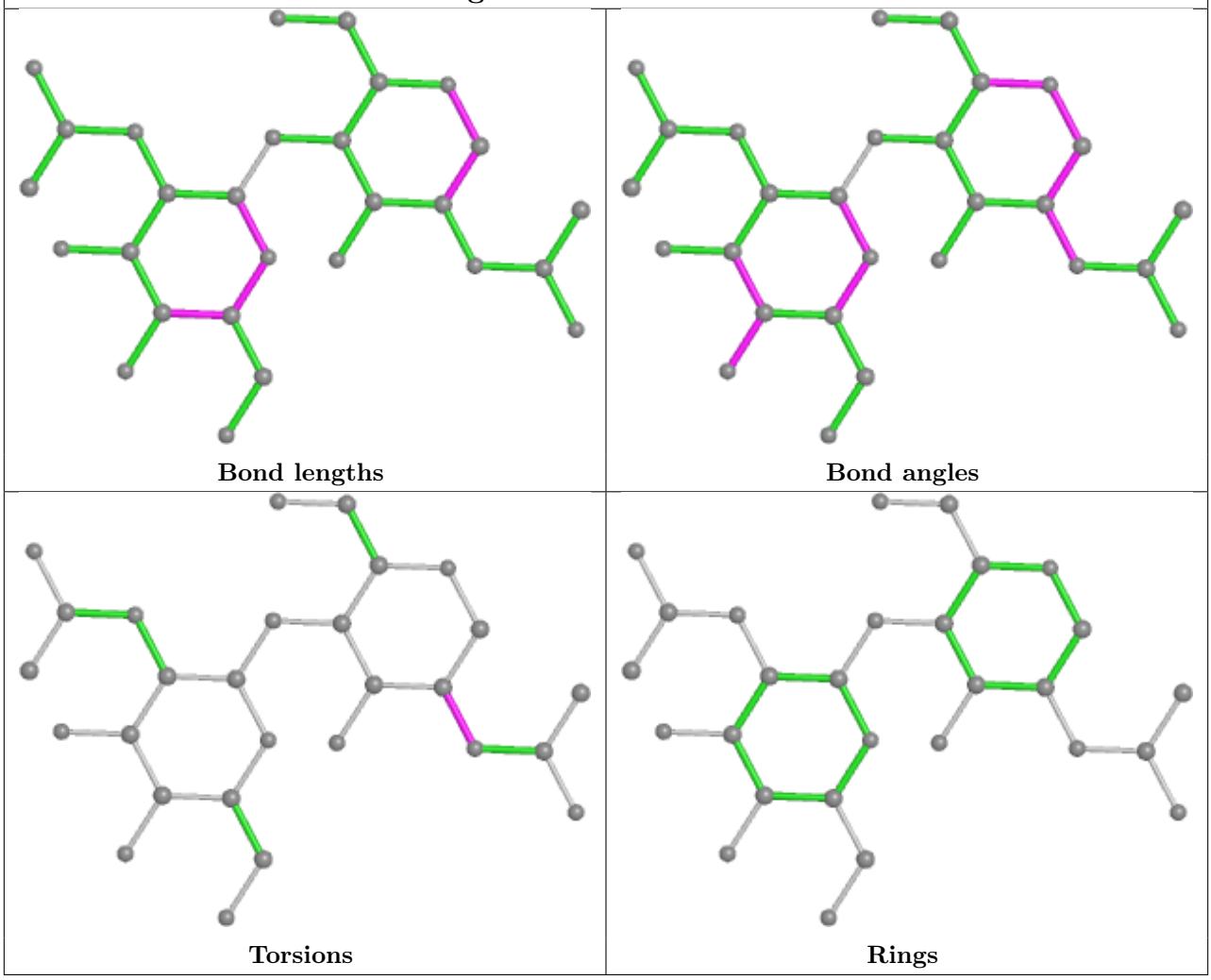
Mol	Chain	Res	Type	Atoms
4	E	6	MAN	C1-C2-C3-C4-C5-O5
4	I	6	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 44 short contacts:

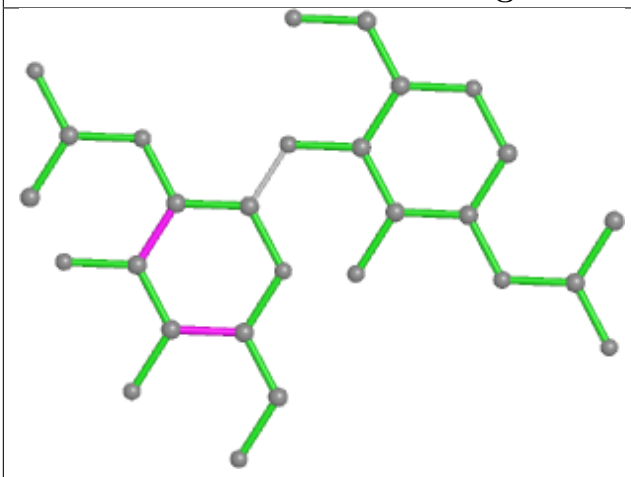
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	MAN	0	10
3	D	4	FUL	0	10
4	E	1	NAG	17	0
4	E	6	MAN	6	0
4	I	1	NAG	1	7
4	I	6	MAN	0	3

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

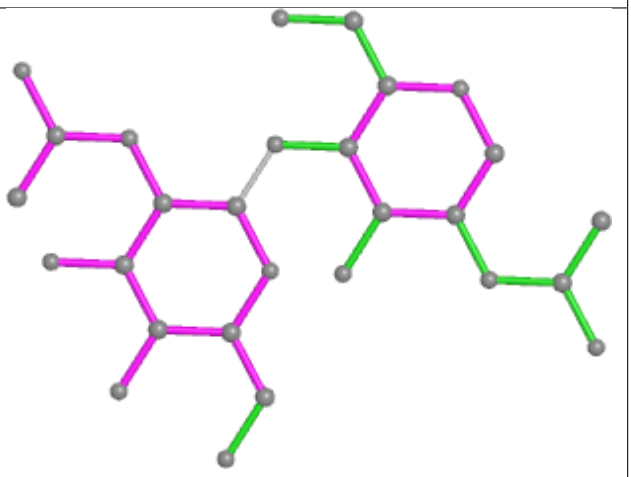
Oligosaccharide Chain C



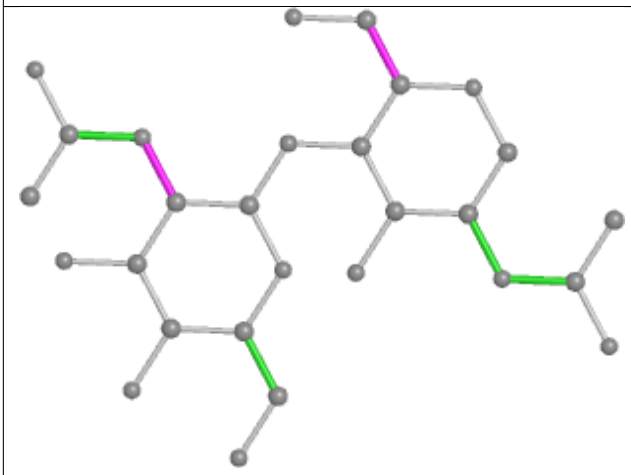
Oligosaccharide Chain F



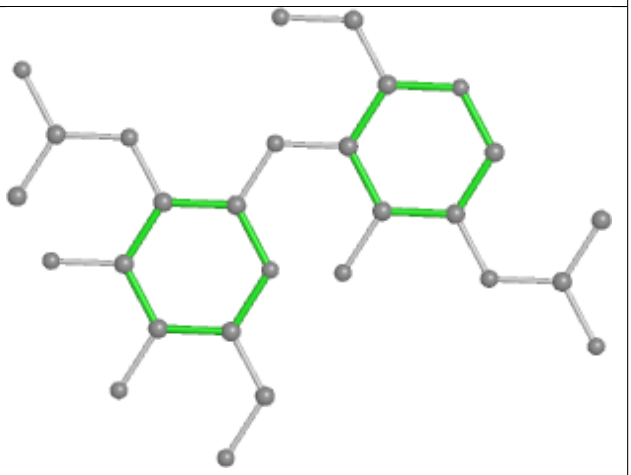
Bond lengths



Bond angles

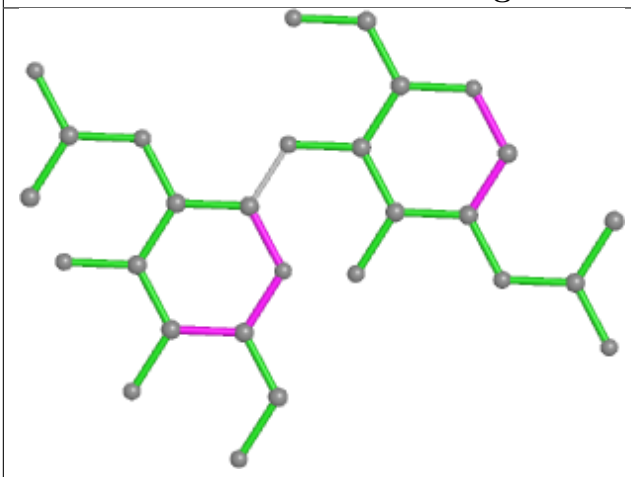


Torsions

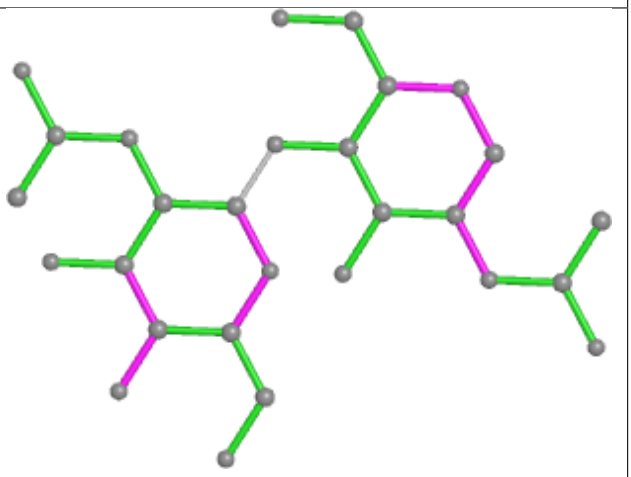


Rings

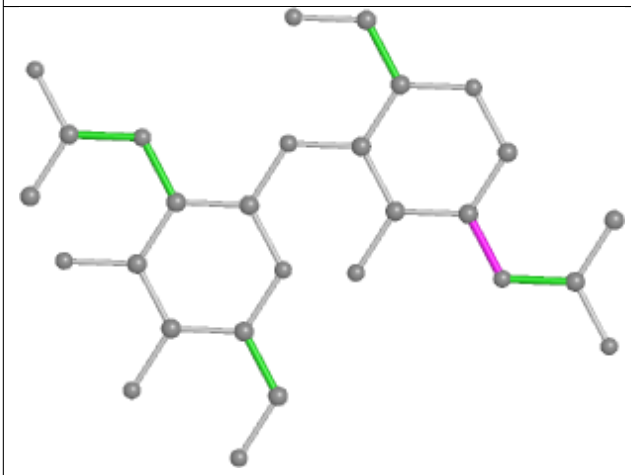
Oligosaccharide Chain G



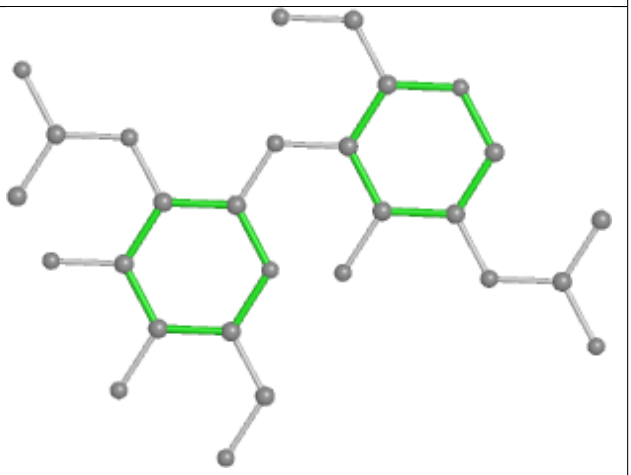
Bond lengths



Bond angles

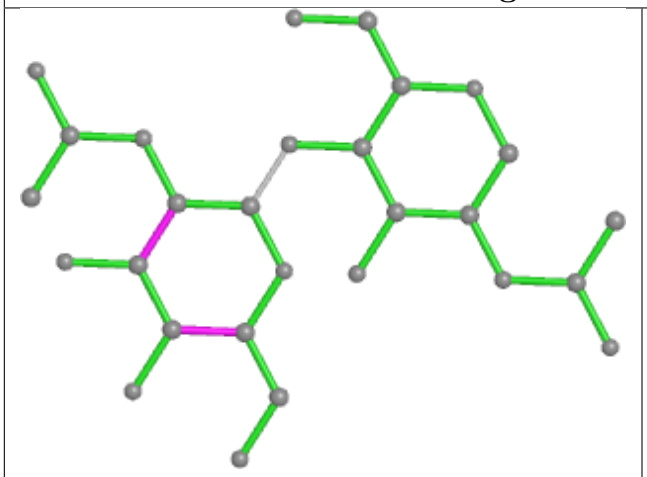


Torsions

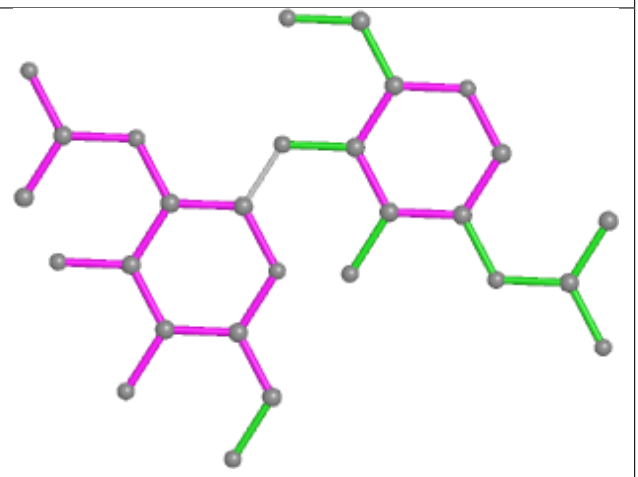


Rings

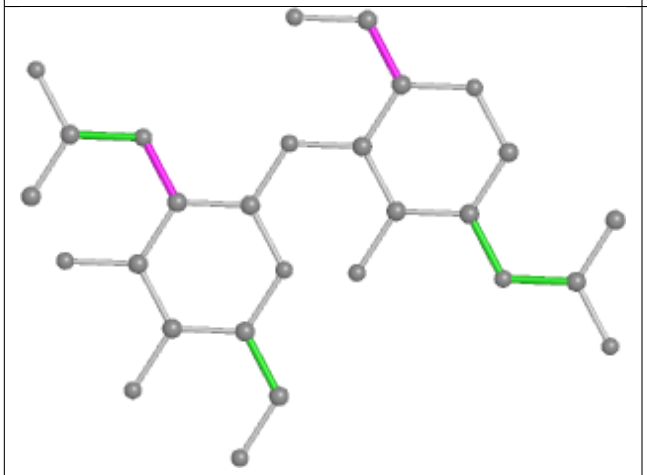
Oligosaccharide Chain J



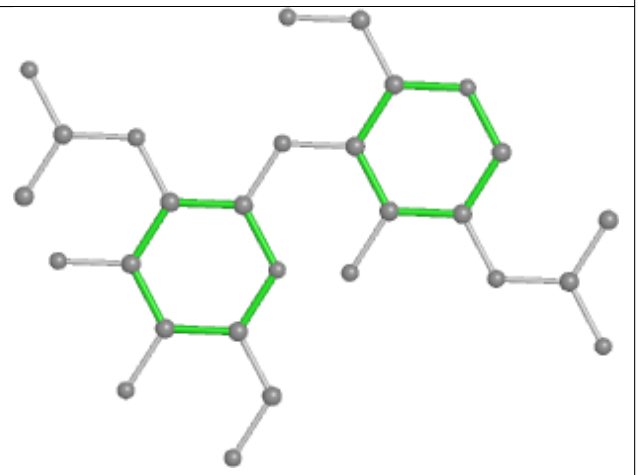
Bond lengths



Bond angles

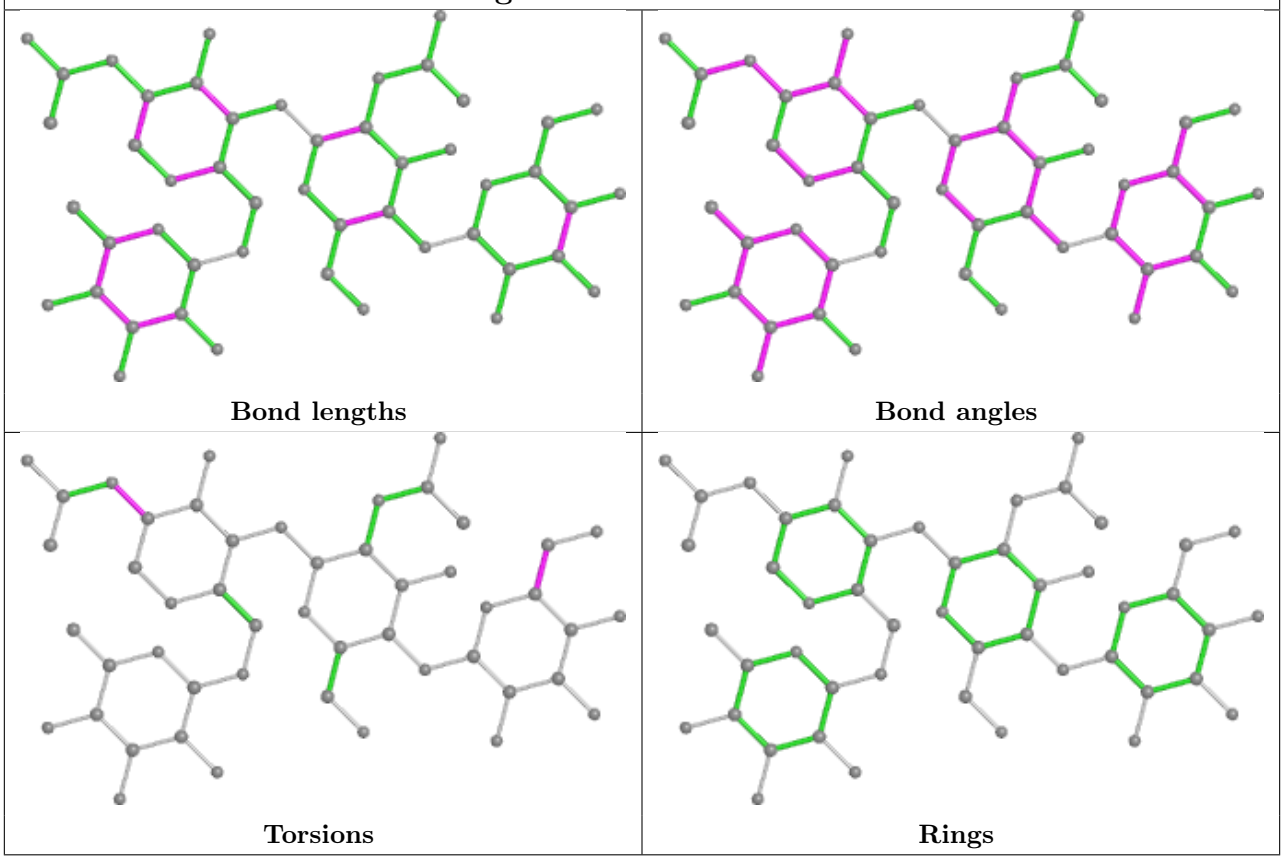


Torsions

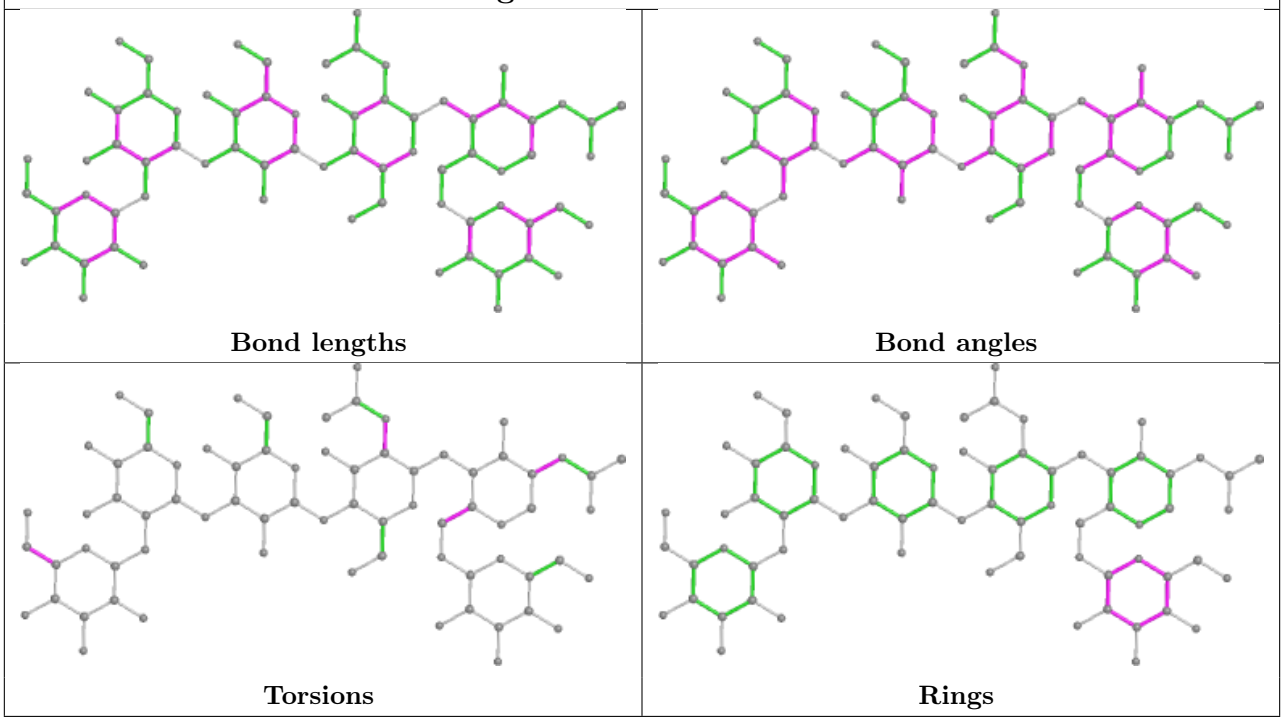


Rings

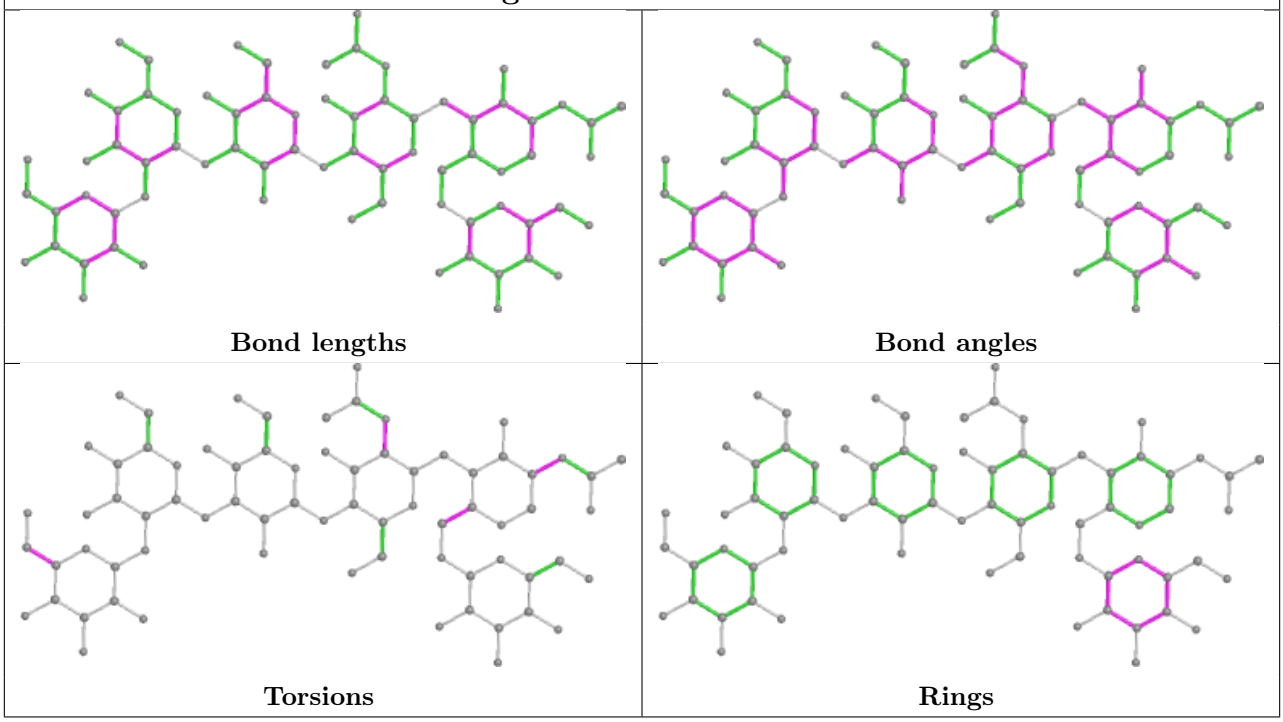
Oligosaccharide Chain D



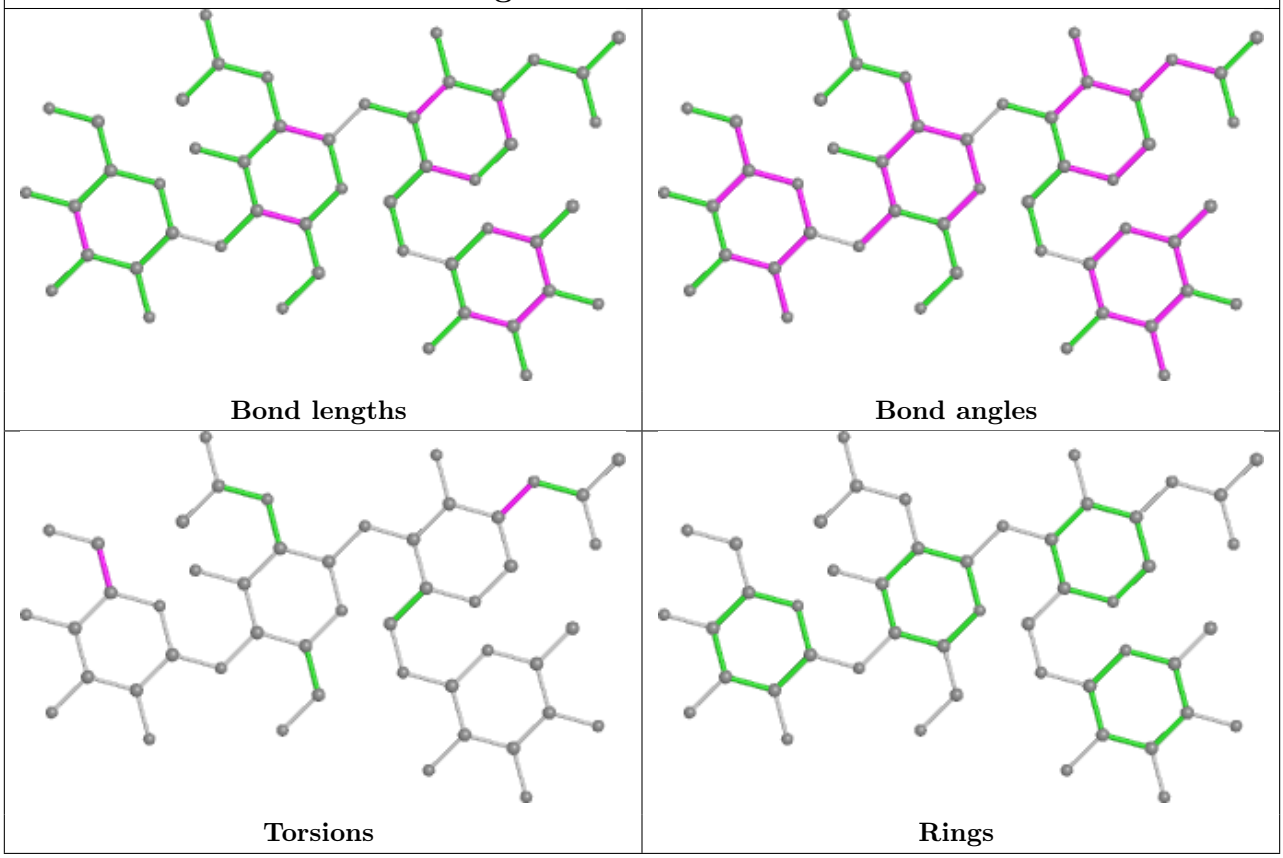
Oligosaccharide Chain E



Oligosaccharide Chain I



Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ST5	A	471	-	18,18,18	1.28	1 (5%)	24,24,24	1.19	2 (8%)
7	ST5	B	471	-	18,18,18	1.28	1 (5%)	24,24,24	1.19	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ST5	A	471	-	-	2/13/14/14	0/1/1/1
7	ST5	B	471	-	-	2/13/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	471	ST5	C1-C'	-4.32	1.40	1.49
7	B	471	ST5	C1-C'	-4.32	1.40	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	471	ST5	CM4-C4'-N4	3.00	119.38	114.98
7	B	471	ST5	CM4-C4'-N4	3.00	119.38	114.98
7	A	471	ST5	C4-N4-C4'	-2.45	121.50	127.49
7	B	471	ST5	C4-N4-C4'	-2.45	121.50	127.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	471	ST5	CM3-C3'-N3-C3
7	B	471	ST5	CM3-C3'-N3-C3
7	A	471	ST5	O3-C3'-N3-C3
7	B	471	ST5	O3-C3'-N3-C3

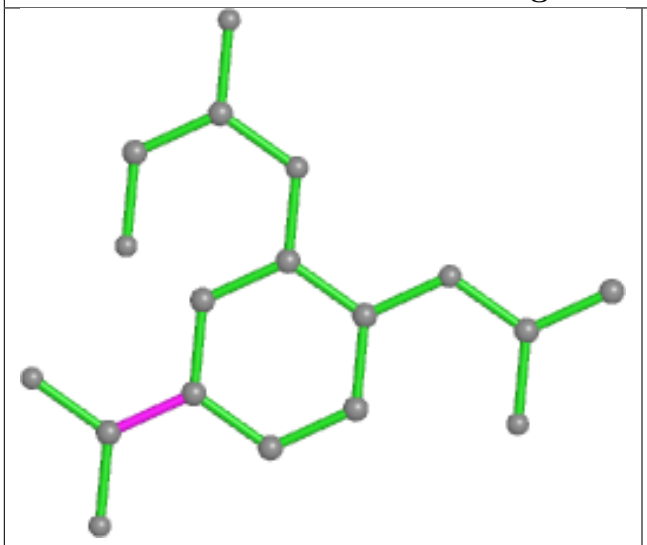
There are no ring outliers.

2 monomers are involved in 4 short contacts:

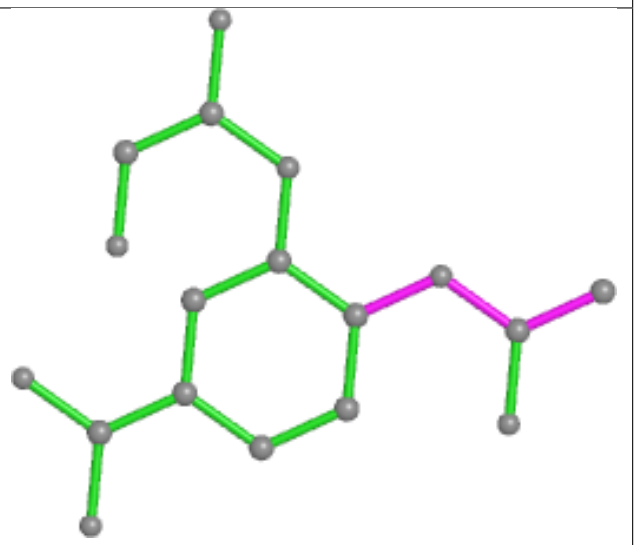
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	471	ST5	2	0
7	B	471	ST5	2	0

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

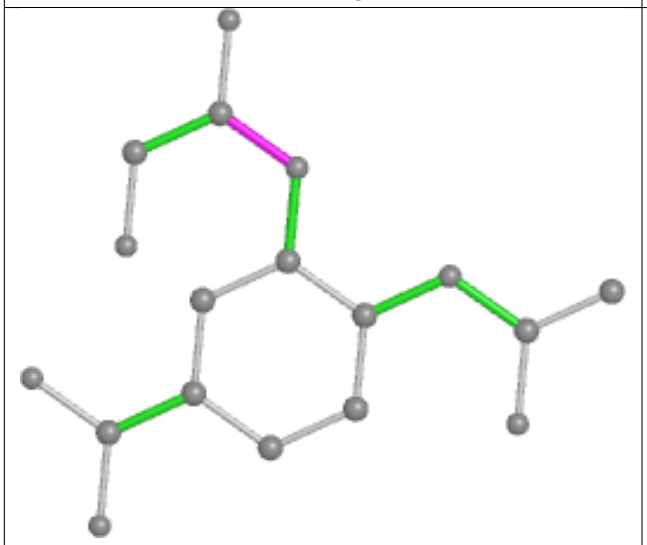
Ligand ST5 A 471



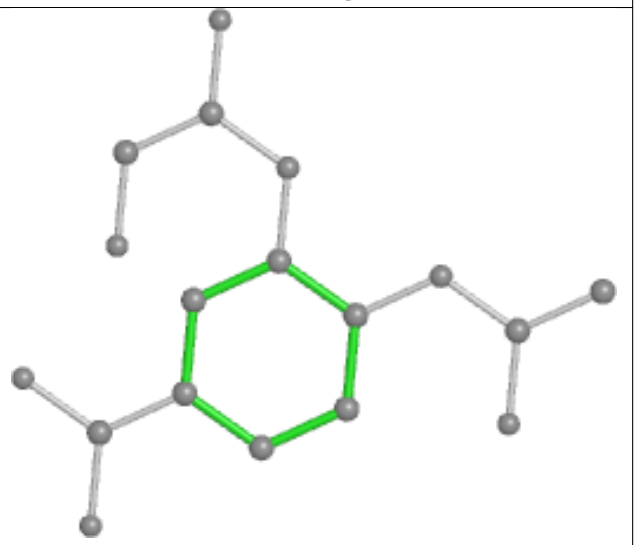
Bond lengths



Bond angles

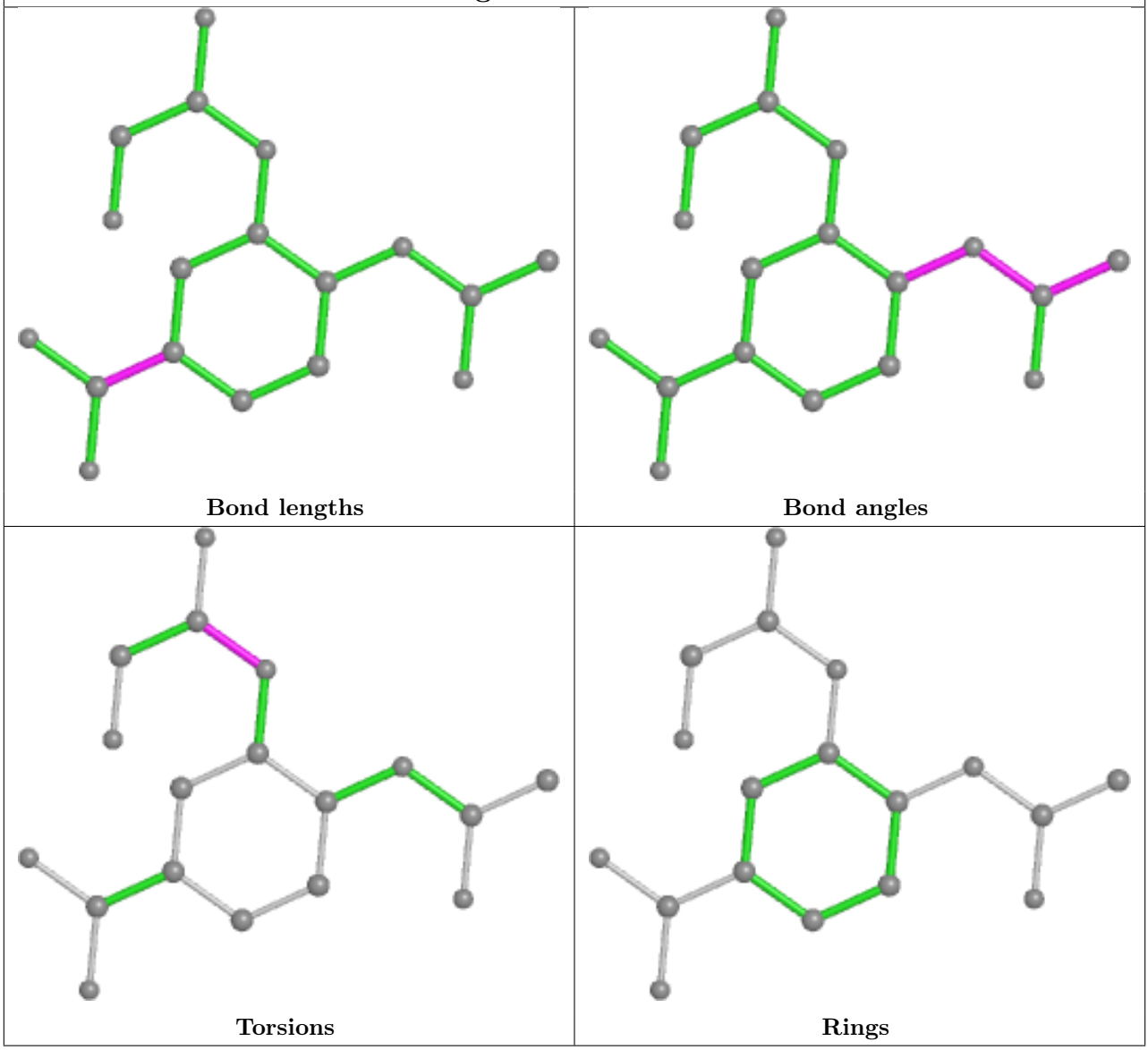


Torsions



Rings

Ligand ST5 B 471



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

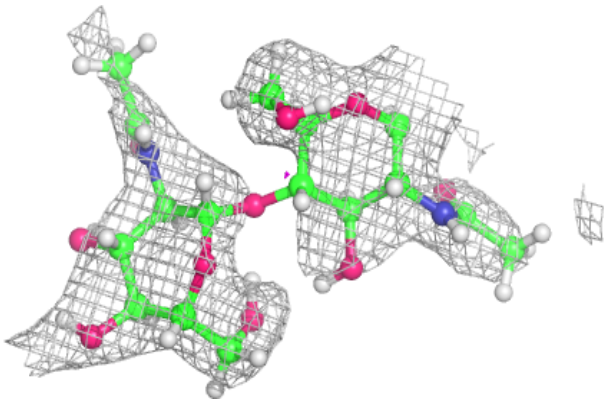
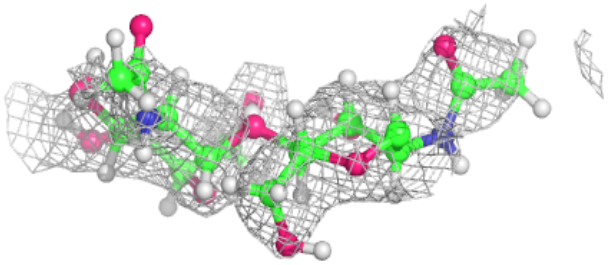
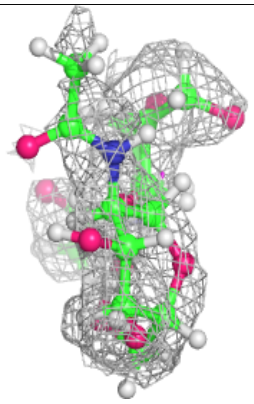
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

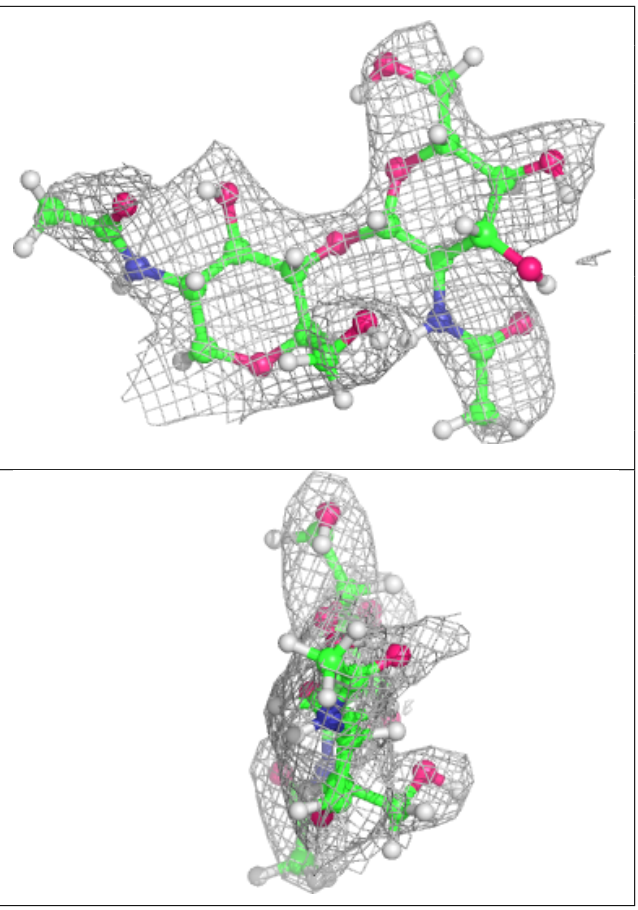
Unable to reproduce the depositors R factor - this section is therefore empty.

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

Electron density around Chain C: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

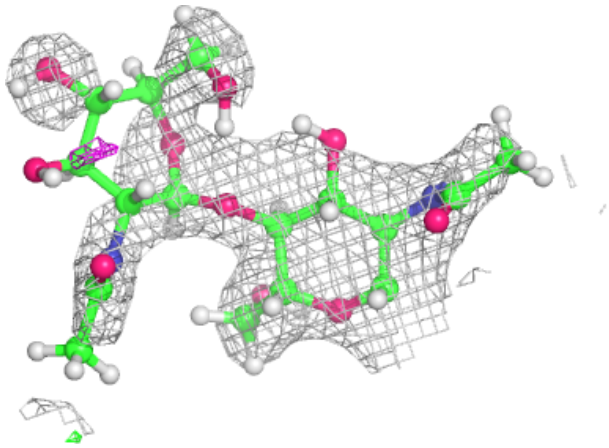
Electron density around Chain F:

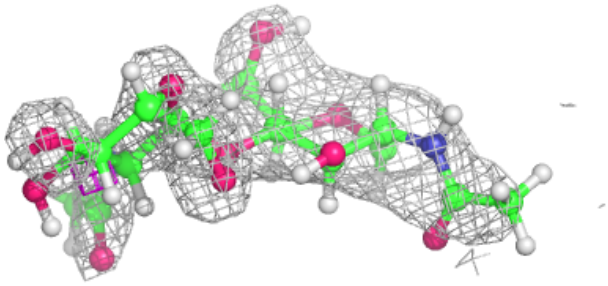
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

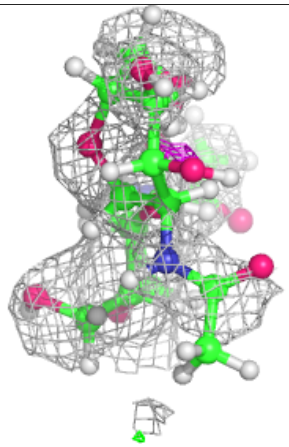


Electron density around Chain G:

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

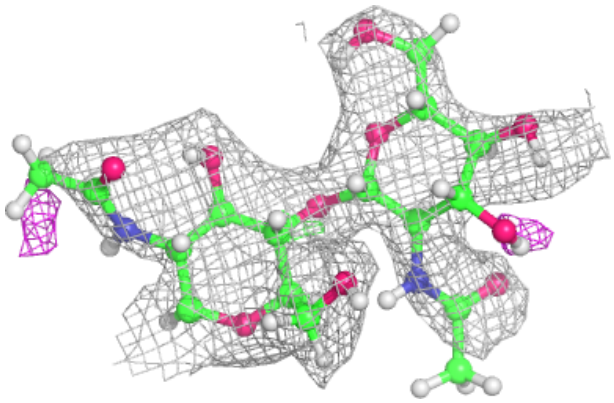


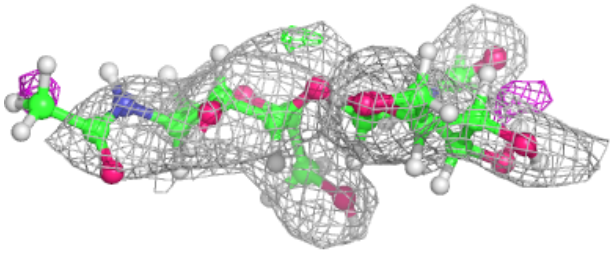


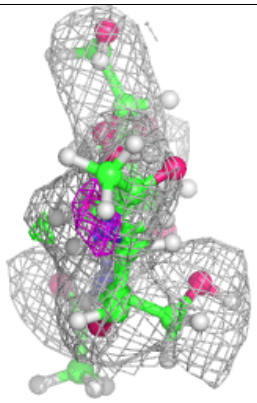


Electron density around Chain J:

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

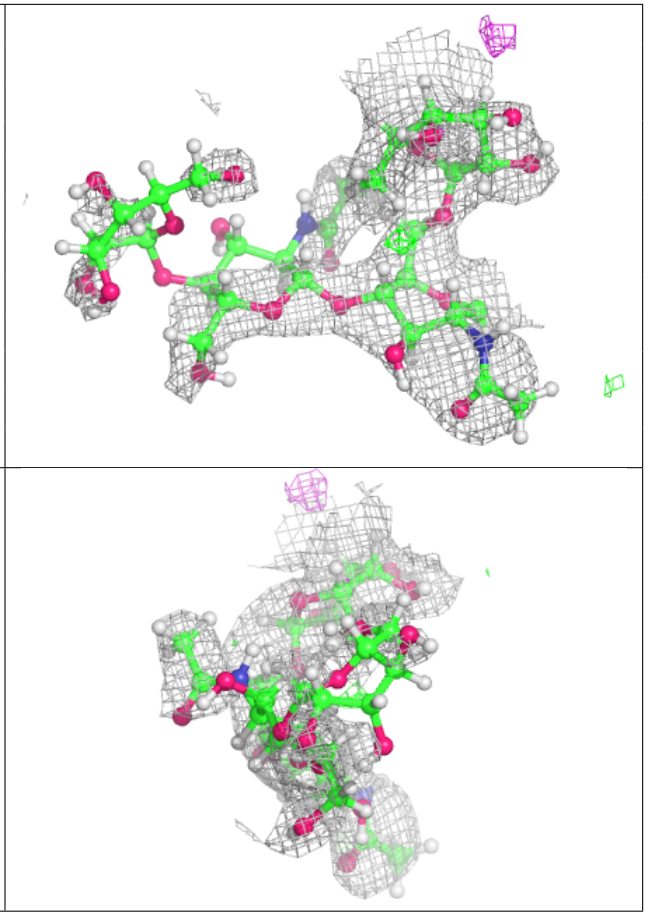






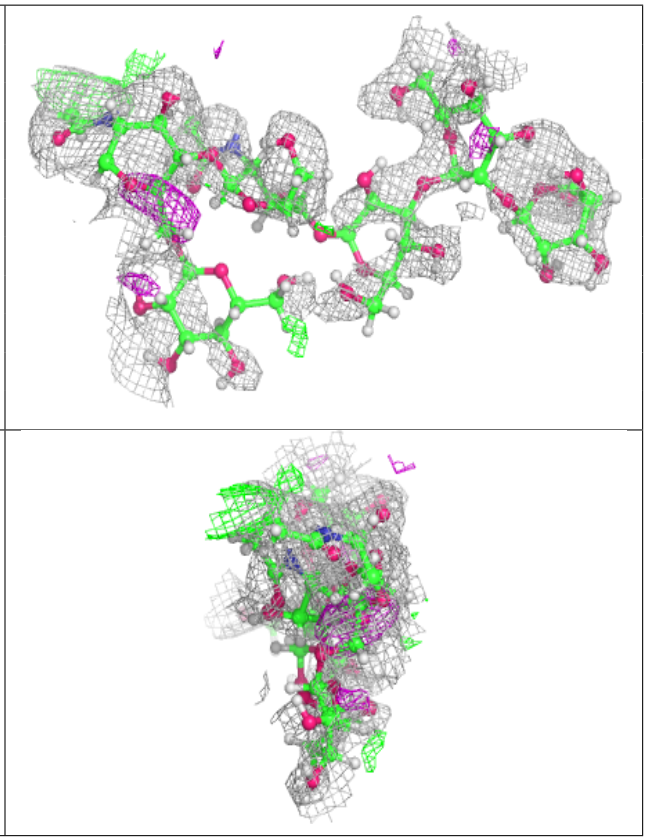
Electron density around Chain D:

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



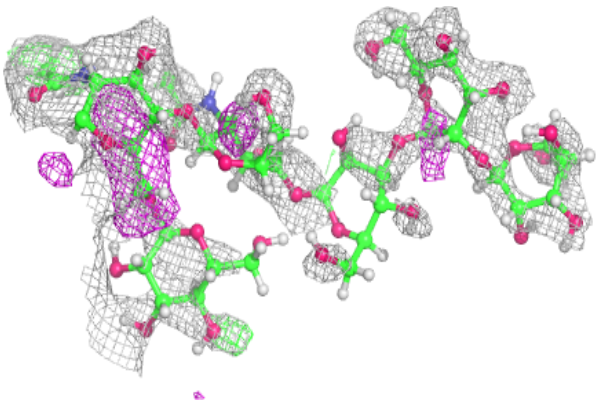
Electron density around Chain E:

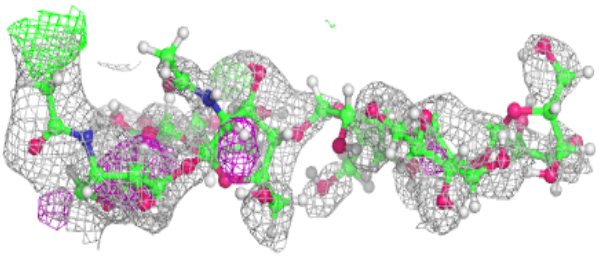
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

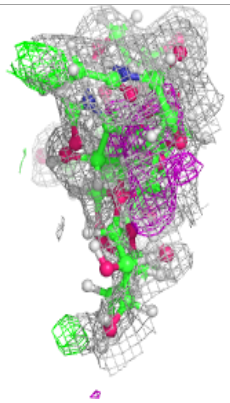


Electron density around Chain I:

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

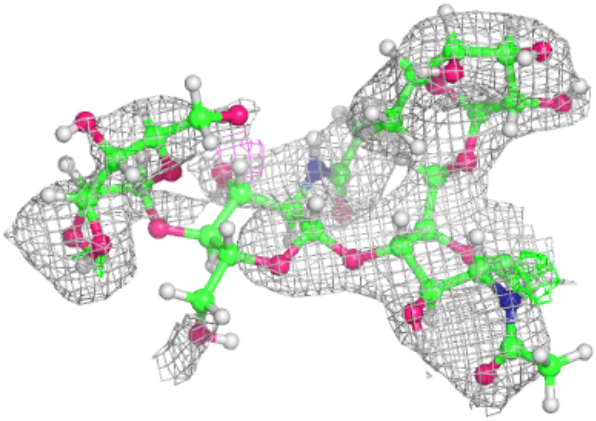


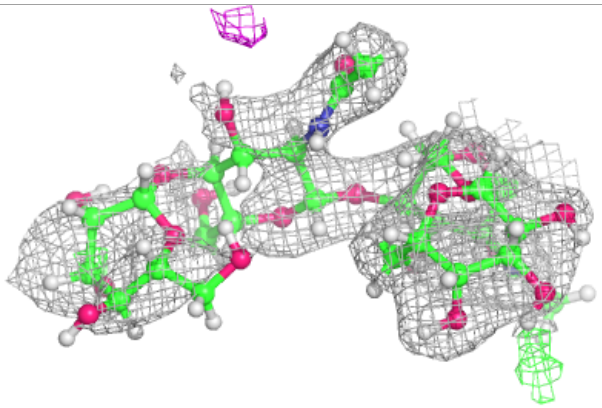


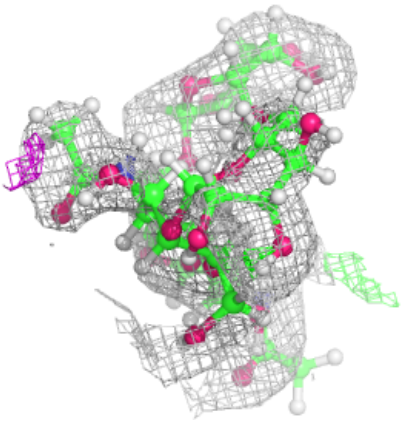


Electron density around Chain H:

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







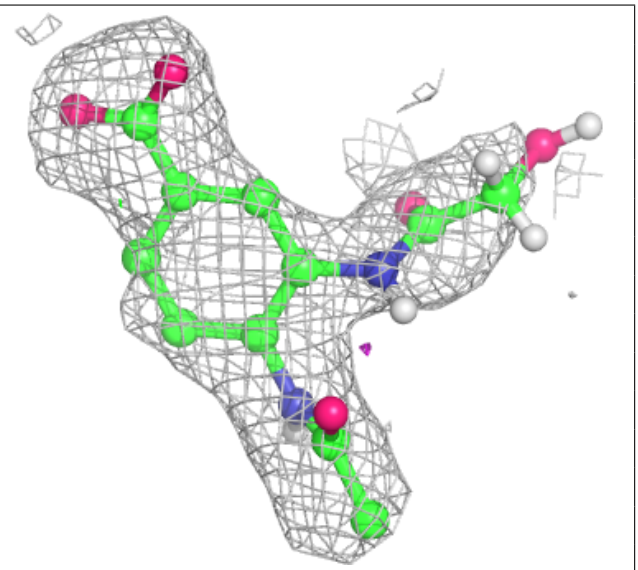
6.4 Ligands (i)

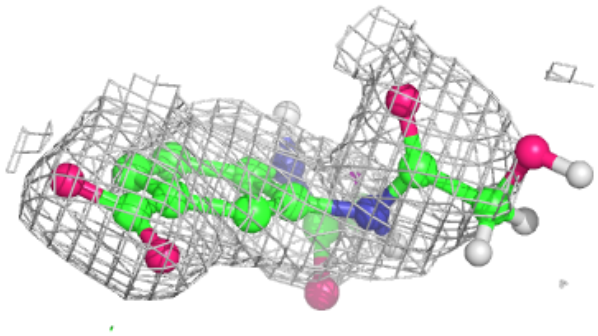
Unable to reproduce the depositors R factor - this section is therefore empty.

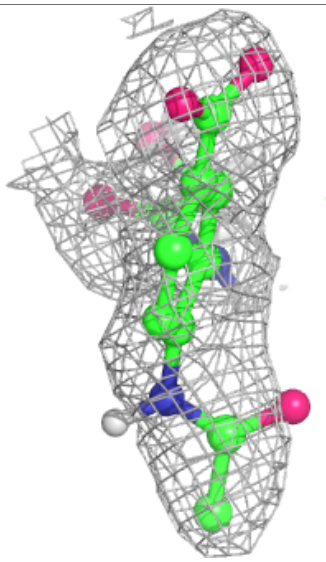
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ST5 A 471:

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

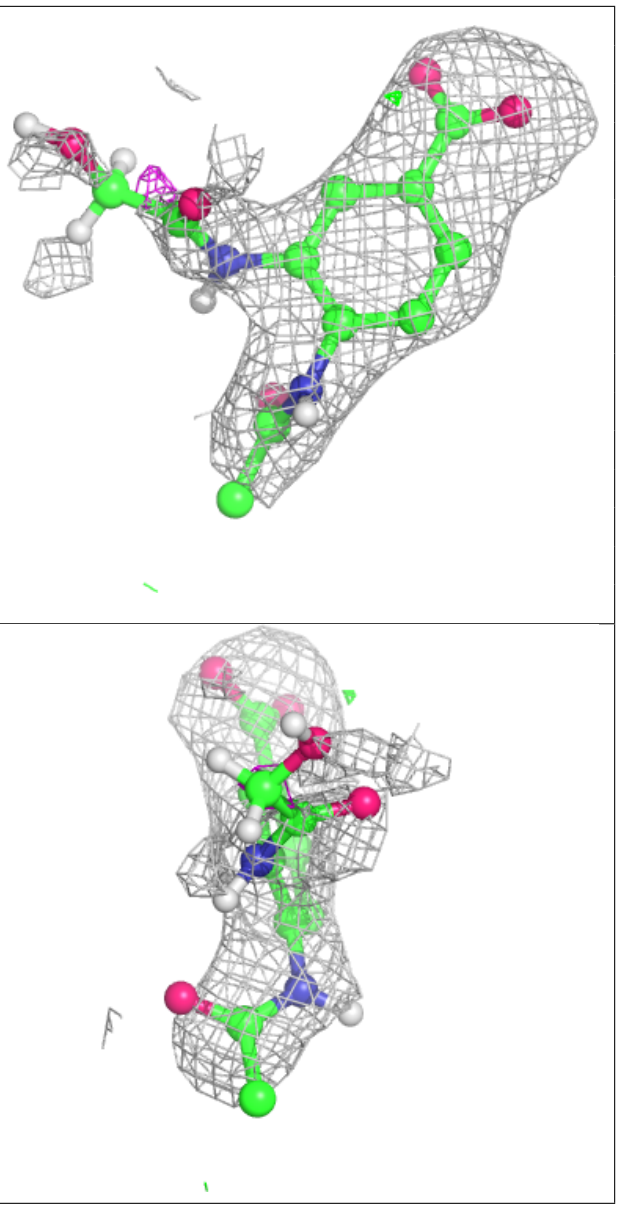






Electron density around ST5 B 471:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.