



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:23 PM UTC

PDB ID : 1IVD / pdb_00001ivd
Title : STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS
NEURAMINIDASE
Authors : Jedrzejas, M.J.; Luo, M.
Deposited on : 1994-12-12
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

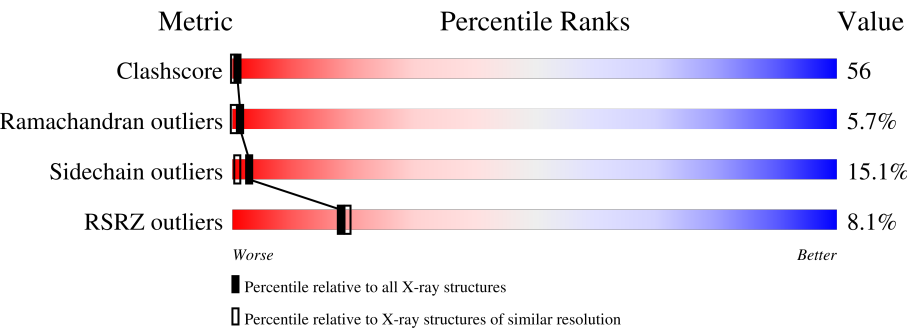
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	8% 27% 53% 17% .
1	B	388	9% 27% 54% 16% .
2	C	2	100%
2	F	2	100%
2	G	2	100%
2	J	2	100%
3	D	4	25% 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	6	 100%
4	I	6	 33% 67%
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
4	NAG	E	1	-	X	X	-
4	MAN	E	6	-	-	X	-
4	NAG	I	1	-	X	-	-
5	FUC	H	4	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8595 atoms, of which 2036 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
1	A	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			
1	B	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			

There are 2 discrepancies between the modelled and reference sequences:

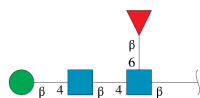
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820
B	339	ASP	ASN	conflict	UNP P06820

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



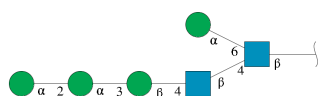
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	F	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	G	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	J	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				

- 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.



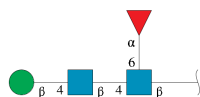
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	0	0	0
			96	28	47	2	19			

- 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
4	E	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			
4	I	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			

- 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.



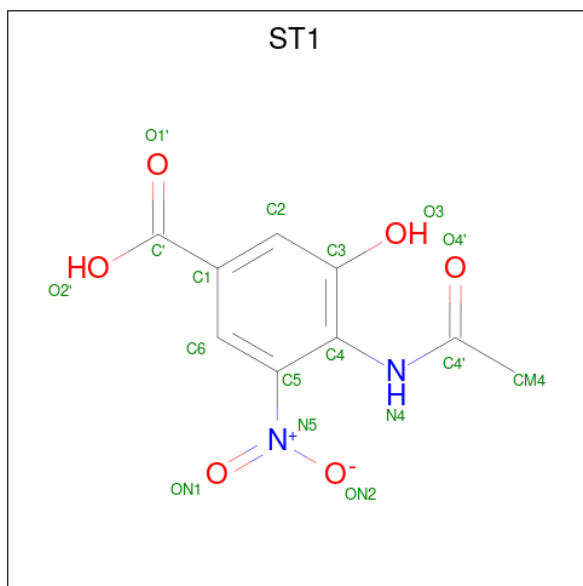
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	4	Total	C	H	N	O	0	0	0
			96	28	47	2	19			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is 4-(ACETYLAMINO)-3-HYDROXY-5-NITROBENZOIC ACID (CCD ID:

ST1) (formula: C₉H₈N₂O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			19	9	2	2	6		
7	B	1	Total	C	H	N	O	0	0
			19	9	2	2	6		

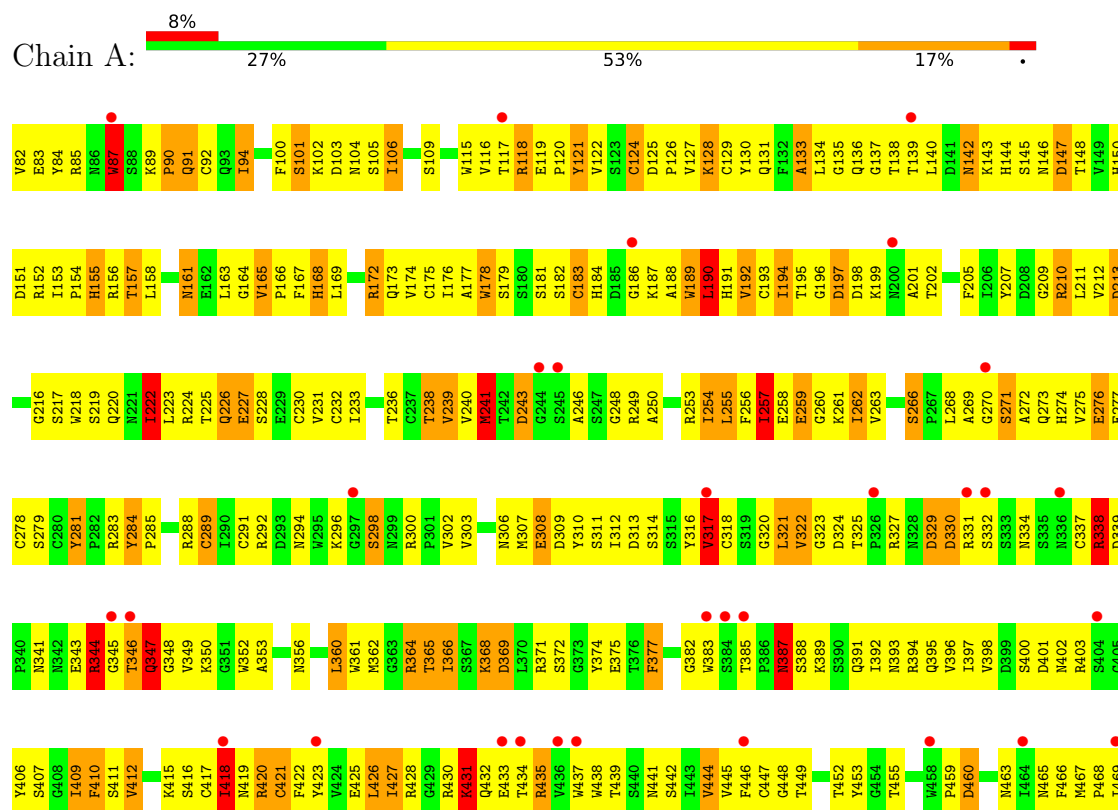
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	121	Total	H	O	1	0
			363	242	121		
8	B	4	Total	H	O	0	0
			12	8	4		

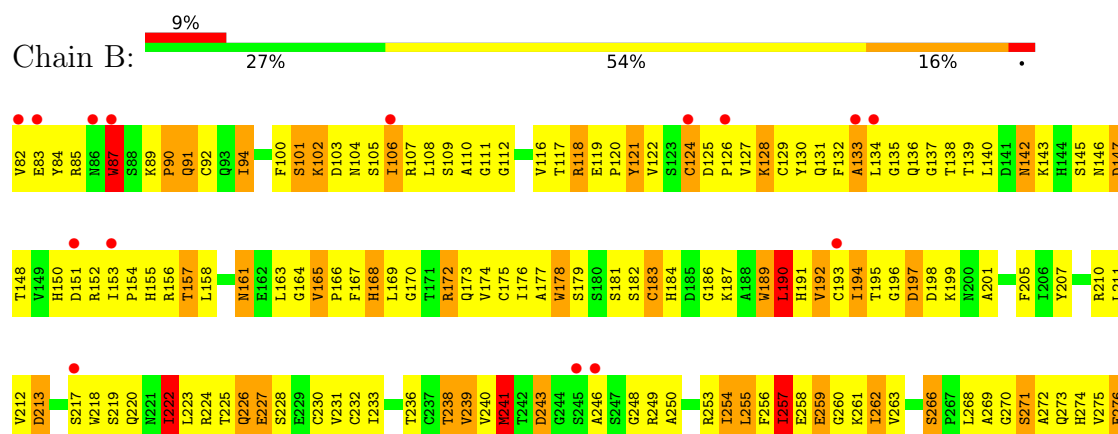
3 Residue-property plots

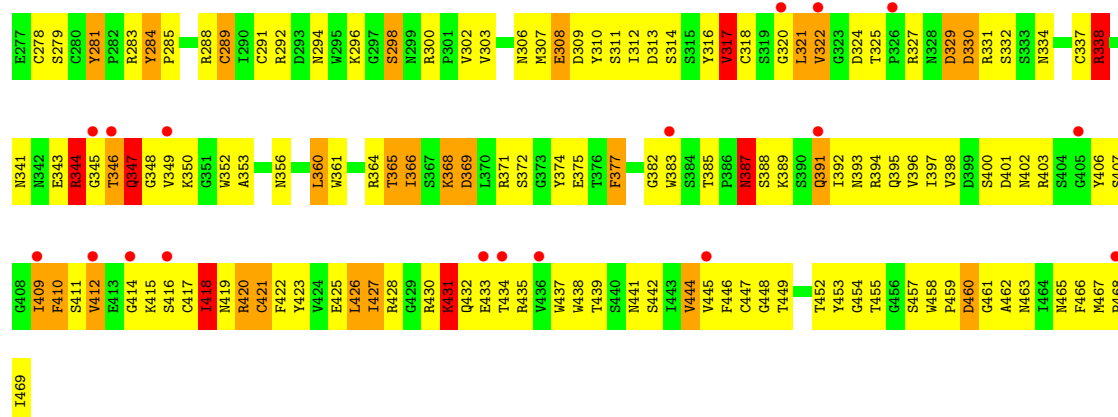
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE



• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE





- 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:  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: 100%



- 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: 33% 67%



- 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: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.42Å 139.83Å 140.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90 5.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-1.90) 28.9 (5.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.76Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.225 , (Not available) 0.287 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	4.1	Xtriage
Anisotropy	3.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 105.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	8595	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, ST1, FUL, MAN, NAG, CA

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	0.81	1/3092 (0.0%)	1.31	38/4194 (0.9%)
1	B	0.81	1/3092 (0.0%)	1.31	38/4194 (0.9%)
All	All	0.81	2/6184 (0.0%)	1.31	76/8388 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	ILE	CA-CB	5.97	1.60	1.53
1	B	418	ILE	CA-CB	5.97	1.60	1.53

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLN	N-CA-C	11.56	123.44	111.07
1	B	226	GLN	N-CA-C	11.56	123.44	111.07
1	A	317	VAL	N-CA-C	7.75	120.00	108.54
1	B	317	VAL	N-CA-C	7.75	120.00	108.54
1	A	266	SER	CA-C-N	7.68	127.44	119.76
1	A	266	SER	C-N-CA	7.68	127.44	119.76
1	B	266	SER	CA-C-N	7.68	127.44	119.76
1	B	266	SER	C-N-CA	7.68	127.44	119.76
1	A	289	CYS	N-CA-C	7.48	121.09	108.90
1	B	289	CYS	N-CA-C	7.48	121.09	108.90
1	A	360	LEU	N-CA-C	7.16	119.19	107.23
1	B	360	LEU	N-CA-C	7.16	119.19	107.23
1	A	243	ASP	N-CA-C	-7.14	95.60	110.80
1	B	243	ASP	N-CA-C	-7.14	95.60	110.80
1	A	344	ARG	N-CA-C	-7.11	102.51	111.90
1	B	344	ARG	N-CA-C	-7.11	102.51	111.90
1	A	194	ILE	N-CA-C	7.08	118.08	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ILE	N-CA-C	7.08	118.08	108.17
1	A	444	VAL	N-CA-C	-7.08	97.35	108.81
1	B	444	VAL	N-CA-C	-7.08	97.35	108.81
1	A	189	TRP	N-CA-C	6.96	121.37	110.17
1	B	189	TRP	N-CA-C	6.96	121.37	110.17
1	A	281	TYR	CA-C-N	6.88	128.44	119.84
1	A	281	TYR	C-N-CA	6.88	128.44	119.84
1	B	281	TYR	CA-C-N	6.88	128.44	119.84
1	B	281	TYR	C-N-CA	6.88	128.44	119.84
1	A	369	ASP	N-CA-C	-6.80	103.00	112.12
1	B	369	ASP	N-CA-C	-6.80	103.00	112.12
1	A	102	LYS	N-CA-C	-6.77	98.74	109.23
1	B	102	LYS	N-CA-C	-6.77	98.74	109.23
1	A	421	CYS	N-CA-C	-6.63	99.51	108.86
1	B	421	CYS	N-CA-C	-6.63	99.51	108.86
1	A	435	ARG	N-CA-C	-6.54	103.99	112.23
1	B	435	ARG	N-CA-C	-6.54	103.99	112.23
1	A	338	ARG	N-CA-C	6.45	124.45	114.64
1	B	338	ARG	N-CA-C	6.45	124.45	114.64
1	A	197	ASP	N-CA-C	-6.34	101.99	110.55
1	B	197	ASP	N-CA-C	-6.34	101.99	110.55
1	A	227	GLU	N-CA-C	-6.26	103.53	111.92
1	B	227	GLU	N-CA-C	-6.26	103.53	111.92
1	A	168	HIS	N-CA-C	6.18	119.61	110.46
1	B	168	HIS	N-CA-C	6.18	119.61	110.46
1	A	460	ASP	N-CA-C	-6.07	104.58	111.07
1	B	460	ASP	N-CA-C	-6.07	104.58	111.07
1	A	257	ILE	N-CA-C	5.99	115.98	106.88
1	B	257	ILE	N-CA-C	5.99	115.98	106.88
1	A	190	LEU	N-CA-C	-5.91	99.27	108.90
1	B	190	LEU	N-CA-C	-5.91	99.27	108.90
1	A	84	TYR	N-CA-C	5.87	119.52	110.42
1	B	84	TYR	N-CA-C	5.87	119.52	110.42
1	A	101	SER	N-CA-C	5.65	118.42	108.75
1	B	101	SER	N-CA-C	5.65	118.42	108.75
1	A	222	ILE	N-CA-C	5.58	120.96	109.34
1	B	222	ILE	N-CA-C	5.58	120.96	109.34
1	A	241	MET	N-CA-C	5.53	118.10	108.76
1	B	241	MET	N-CA-C	5.53	118.10	108.76
1	A	106	ILE	CB-CA-C	-5.52	104.79	112.02
1	B	106	ILE	CB-CA-C	-5.52	104.79	112.02
1	A	151	ASP	N-CA-C	5.46	118.15	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASP	N-CA-C	5.46	118.15	111.82
1	A	298	SER	N-CA-C	-5.45	104.31	112.54
1	B	298	SER	N-CA-C	-5.45	104.31	112.54
1	A	271	SER	N-CA-C	-5.28	106.34	112.89
1	B	271	SER	N-CA-C	-5.28	106.34	112.89
1	A	91	GLN	N-CA-C	-5.22	103.64	110.53
1	B	91	GLN	N-CA-C	-5.22	103.64	110.53
1	A	213	ASP	N-CA-C	5.21	115.41	108.38
1	B	213	ASP	N-CA-C	5.21	115.41	108.38
1	A	366	ILE	N-CA-C	-5.20	105.64	110.53
1	B	366	ILE	N-CA-C	-5.20	105.64	110.53
1	A	90	PRO	N-CA-C	5.15	119.18	111.14
1	B	90	PRO	N-CA-C	5.15	119.18	111.14
1	A	87	TRP	N-CA-C	5.14	121.76	110.80
1	B	87	TRP	N-CA-C	5.14	121.76	110.80
1	A	377	PHE	N-CA-C	5.07	115.23	108.38
1	B	377	PHE	N-CA-C	5.07	115.23	108.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	723	2850	343	5
1	B	3022	723	2850	360	4
2	C	28	27	25	6	0
2	F	28	27	25	6	0
2	G	28	27	25	5	0
2	J	28	27	25	5	0
3	D	49	47	42	2	5
4	E	72	67	60	27	6
4	I	72	67	60	4	4
5	H	49	47	42	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	17	2	7	1	0
7	B	17	2	7	1	0
8	A	121	242	0	27	2
8	B	4	8	0	5	0
All	All	6559	2036	6018	696	13

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 56.

All (696) 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:CG2	4:E:1:NAG:H61	1.57	1.35
8:A:515:HOH:O	1:B:100:PHE:CZ	1.83	1.31
1:B:107:ARG:CZ	8:B:497:HOH:O	1.78	1.31
1:B:455:THR:CG2	4:E:1:NAG:C6	2.15	1.24
1:B:205:PHE:HD2	1:B:257:ILE:HD12	1.08	1.17
1:B:455:THR:HG21	4:E:1:NAG:C6	1.75	1.15
1:A:205:PHE:HD2	1:A:257:ILE:HD12	1.08	1.12
1:B:455:THR:HG22	4:E:1:NAG:H61	1.26	1.09
1:A:169:LEU:HD11	1:B:112:GLY:HA3	1.31	1.07
1:A:115:TRP:CZ2	1:B:108:LEU:HD11	1.90	1.05
1:A:205:PHE:CD2	1:A:257:ILE:HD12	1.95	1.01
1:A:142:ASN:ND2	1:B:110:ALA:HB3	1.74	1.01
1:B:205:PHE:CD2	1:B:257:ILE:HD12	1.95	1.00
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.42	0.99
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.42	0.99
1:A:136:GLN:HG3	1:A:148:THR:HG23	1.46	0.96
1:A:409:ILE:HD11	1:A:420:ARG:HB3	1.47	0.95
1:B:409:ILE:HD11	1:B:420:ARG:HB3	1.47	0.95
8:A:518:HOH:O	1:B:412:VAL:HG23	1.66	0.94
1:A:142:ASN:HD21	1:B:110:ALA:HB3	1.28	0.94
1:B:136:GLN:HG3	1:B:148:THR:HG23	1.46	0.94
1:A:281:TYR:HB3	8:A:525:HOH:O	1.66	0.93
1:B:455:THR:HB	4:E:1:NAG:O5	1.69	0.92
1:A:106:ILE:HG12	8:A:557:HOH:O	1.69	0.91
1:B:396:VAL:CG1	4:E:6:MAN:O2	2.18	0.90
1:A:202:THR:HB	1:B:454:GLY:H	1.35	0.90
1:A:136:GLN:O	1:A:138:THR:HG22	1.72	0.90
1:B:136:GLN:O	1:B:138:THR:HG22	1.72	0.89
1:B:455:THR:CB	4:E:1:NAG:H61	2.03	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:HD11	1:B:260:GLY:HA2	1.55	0.87
1:A:257:ILE:HD11	1:A:260:GLY:HA2	1.55	0.86
1:B:272:ALA:HA	1:B:316:TYR:CE1	2.11	0.86
1:A:272:ALA:HA	1:A:316:TYR:CE1	2.11	0.86
1:A:195:THR:HG21	1:B:458:TRP:HE1	1.43	0.83
1:A:169:LEU:CD1	1:B:112:GLY:HA3	2.09	0.83
1:B:396:VAL:HG11	4:E:6:MAN:O2	1.79	0.82
1:B:455:THR:HG21	4:E:1:NAG:H5	1.60	0.80
1:B:240:VAL:HG12	1:B:254:ILE:HG23	1.63	0.80
1:A:240:VAL:HG12	1:A:254:ILE:HG23	1.63	0.79
1:B:249:ARG:HG3	1:B:250:ALA:H	1.47	0.79
1:B:331:ARG:NH1	1:B:331:ARG:HA	1.99	0.78
1:A:331:ARG:HA	1:A:331:ARG:HH11	1.48	0.78
1:B:331:ARG:HA	1:B:331:ARG:HH11	1.48	0.77
1:B:455:THR:HG21	4:E:1:NAG:C5	2.13	0.77
1:A:249:ARG:HG3	1:A:250:ALA:H	1.47	0.77
1:A:331:ARG:HA	1:A:331:ARG:NH1	1.99	0.77
1:A:138:THR:HA	1:B:108:LEU:HD23	1.64	0.77
1:A:101:SER:HA	8:A:500:HOH:O	1.84	0.76
1:A:272:ALA:HA	1:A:316:TYR:HE1	1.48	0.76
1:B:452:THR:HG22	1:B:453:TYR:H	1.51	0.76
1:A:318:CYS:HB3	1:A:385:THR:O	1.86	0.76
1:A:452:THR:HG22	1:A:453:TYR:H	1.51	0.76
1:A:296:LYS:O	1:A:345:GLY:HA3	1.86	0.76
1:B:318:CYS:HB3	1:B:385:THR:O	1.86	0.75
1:B:272:ALA:HA	1:B:316:TYR:HE1	1.48	0.74
1:B:455:THR:HG22	4:E:1:NAG:C6	2.00	0.74
1:A:115:TRP:HZ2	1:B:108:LEU:HD11	1.51	0.73
1:B:438:TRP:HD1	1:B:469:ILE:HG13	1.53	0.73
1:A:158:LEU:O	1:A:174:VAL:HG12	1.88	0.73
1:B:296:LYS:O	1:B:345:GLY:HA3	1.86	0.73
1:B:271:SER:HB3	1:B:338:ARG:O	1.89	0.73
1:B:158:LEU:O	1:B:174:VAL:HG12	1.88	0.73
1:A:283:ARG:HE	1:A:288:ARG:HE	1.36	0.72
1:A:438:TRP:HD1	1:A:469:ILE:HG13	1.53	0.72
1:B:283:ARG:HE	1:B:288:ARG:HE	1.36	0.72
1:A:271:SER:HB3	1:A:338:ARG:O	1.89	0.72
1:B:455:THR:CB	4:E:1:NAG:C5	2.68	0.71
1:B:338:ARG:HH11	1:B:338:ARG:HB2	1.55	0.71
1:B:257:ILE:HD11	1:B:260:GLY:CA	2.19	0.71
1:A:257:ILE:HD11	1:A:260:GLY:CA	2.19	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:HD12	1:A:312:ILE:HG21	1.73	0.71
1:A:183:CYS:HB2	1:A:232:CYS:SG	2.31	0.70
1:B:183:CYS:HB2	1:B:232:CYS:SG	2.31	0.70
1:B:438:TRP:CD1	1:B:469:ILE:HG13	2.26	0.70
1:A:338:ARG:HH11	1:A:338:ARG:HB2	1.55	0.70
1:A:438:TRP:CD1	1:A:469:ILE:HG13	2.26	0.70
1:B:157:THR:HG22	1:B:176:ILE:HA	1.73	0.70
1:A:125:ASP:HB3	1:A:184:HIS:ND1	2.06	0.70
1:A:394:ARG:HG3	1:A:395:GLN:N	2.06	0.70
1:B:125:ASP:HB3	1:B:184:HIS:ND1	2.06	0.70
8:A:501:HOH:O	1:B:108:LEU:HD22	1.91	0.70
1:A:430:ARG:HD3	1:A:437:TRP:HA	1.72	0.70
1:B:394:ARG:HG3	1:B:395:GLN:N	2.06	0.70
1:B:268:LEU:HD12	1:B:312:ILE:HG21	1.73	0.70
1:A:289:CYS:HB2	1:A:303:VAL:HB	1.74	0.69
1:A:374:TYR:HB3	1:A:398:VAL:HG23	1.74	0.69
1:B:321:LEU:O	1:B:322:VAL:HB	1.93	0.69
1:B:430:ARG:HG3	1:B:431:LYS:H	1.57	0.69
1:B:430:ARG:HD3	1:B:437:TRP:HA	1.72	0.69
1:A:157:THR:HG22	1:A:176:ILE:HA	1.73	0.69
1:B:87:TRP:HD1	1:B:233:ILE:HG12	1.58	0.69
1:B:217:SER:HA	1:B:223:LEU:HD22	1.75	0.69
1:A:155:HIS:HB3	1:B:104:ASN:ND2	2.06	0.69
1:A:430:ARG:HG3	1:A:431:LYS:H	1.57	0.69
1:A:87:TRP:HD1	1:A:233:ILE:HG12	1.58	0.68
1:B:289:CYS:HB2	1:B:303:VAL:HB	1.74	0.68
1:B:455:THR:HB	4:E:1:NAG:C5	2.22	0.68
1:B:419:ASN:HB3	8:B:517:HOH:O	1.92	0.68
1:B:455:THR:OG1	4:E:1:NAG:C1	2.41	0.68
1:A:134:LEU:HB2	1:A:156:ARG:NH2	2.08	0.68
1:B:134:LEU:HB2	1:B:156:ARG:NH2	2.08	0.68
1:A:321:LEU:O	1:A:322:VAL:HB	1.93	0.68
1:A:216:GLY:H	1:B:452:THR:HB	1.59	0.68
1:A:103:ASP:HB3	8:A:502:HOH:O	1.94	0.68
1:A:116:VAL:HG11	1:A:148:THR:HG21	1.76	0.68
1:B:116:VAL:HG11	1:B:148:THR:HG21	1.76	0.67
1:B:374:TYR:HB3	1:B:398:VAL:HG23	1.74	0.67
1:A:321:LEU:HD13	1:A:377:PHE:CE1	2.30	0.67
1:B:396:VAL:O	1:B:396:VAL:HG13	1.95	0.67
1:A:116:VAL:CG1	1:A:148:THR:HG21	2.24	0.67
1:A:396:VAL:O	1:A:396:VAL:HG13	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:SER:HA	1:A:223:LEU:HD22	1.75	0.67
1:B:238:THR:OG1	1:B:307:MET:SD	2.52	0.67
1:B:455:THR:CB	4:E:1:NAG:O5	2.41	0.67
1:A:238:THR:OG1	1:A:307:MET:SD	2.52	0.67
1:B:116:VAL:CG1	1:B:148:THR:HG21	2.24	0.66
1:A:144:HIS:CD2	1:B:466:PHE:HD2	2.13	0.66
1:A:249:ARG:HG3	1:A:250:ALA:N	2.11	0.66
1:B:300:ARG:O	1:B:317:VAL:HG23	1.95	0.66
1:B:321:LEU:HD13	1:B:377:PHE:CE1	2.30	0.66
1:A:300:ARG:O	1:A:317:VAL:HG23	1.95	0.66
1:B:455:THR:HG21	4:E:1:NAG:O6	1.93	0.66
1:B:226:GLN:HE21	1:B:240:VAL:H	1.44	0.66
1:B:455:THR:HB	4:E:1:NAG:H61	1.77	0.65
1:A:412:VAL:HG11	1:A:421:CYS:SG	2.36	0.65
1:B:412:VAL:HG11	1:B:421:CYS:SG	2.36	0.65
1:B:249:ARG:HG3	1:B:250:ALA:N	2.11	0.65
1:B:312:ILE:HG22	1:B:313:ASP:H	1.62	0.65
1:A:419:ASN:HD21	1:A:448:GLY:HA3	1.61	0.65
1:B:419:ASN:HD21	1:B:448:GLY:HA3	1.61	0.65
1:A:312:ILE:HG22	1:A:313:ASP:H	1.62	0.64
1:A:134:LEU:HD11	8:A:521:HOH:O	1.98	0.64
1:B:228:SER:HB2	1:B:350:LYS:NZ	2.13	0.64
1:A:366:ILE:HG21	1:A:400:SER:HB3	1.80	0.64
1:B:366:ILE:HG21	1:B:400:SER:HB3	1.80	0.64
1:A:228:SER:HB2	1:A:350:LYS:NZ	2.13	0.63
1:A:226:GLN:HE21	1:A:240:VAL:H	1.44	0.63
1:B:219:SER:O	1:B:220:GLN:HB2	1.99	0.63
1:B:334:ASN:HA	1:B:387:ASN:HD21	1.63	0.63
1:A:101:SER:HB2	1:A:445:VAL:HG22	1.80	0.63
1:A:115:TRP:CZ2	1:B:108:LEU:CD1	2.76	0.63
1:A:212:VAL:HB	1:A:260:GLY:O	1.98	0.63
1:B:212:VAL:HB	1:B:260:GLY:O	1.98	0.63
1:A:430:ARG:HD2	1:A:434:THR:HA	1.81	0.63
1:B:101:SER:HB2	1:B:445:VAL:HG22	1.80	0.63
1:B:320:GLY:H	1:B:388:SER:H	1.47	0.63
1:A:146:ASN:OD1	1:A:437:TRP:HB3	1.99	0.63
1:A:177:ALA:CB	1:A:193:CYS:HB3	2.24	0.63
1:B:452:THR:HG22	1:B:453:TYR:N	2.14	0.63
1:B:372:SER:HA	1:B:403:ARG:HA	1.81	0.63
1:B:455:THR:CG2	4:E:1:NAG:C5	2.74	0.63
1:A:372:SER:HA	1:A:403:ARG:HA	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:HD2	1:B:434:THR:HA	1.81	0.63
1:B:146:ASN:OD1	1:B:437:TRP:HB3	1.99	0.62
1:A:320:GLY:N	1:A:388:SER:H	1.97	0.62
1:A:409:ILE:HD12	1:A:421:CYS:O	1.99	0.62
1:A:412:VAL:CG1	1:A:421:CYS:SG	2.87	0.62
1:A:190:LEU:HD11	1:A:257:ILE:HD13	1.82	0.62
1:A:317:VAL:HB	8:A:543:HOH:O	1.98	0.62
1:B:412:VAL:CG1	1:B:421:CYS:SG	2.87	0.62
1:B:320:GLY:N	1:B:388:SER:H	1.97	0.62
1:B:455:THR:CB	4:E:1:NAG:C6	2.71	0.62
1:A:117:THR:HG21	1:A:167:PHE:HD2	1.65	0.62
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.63	0.62
1:B:85:ARG:HH12	1:B:125:ASP:HA	1.65	0.62
1:B:409:ILE:HD12	1:B:421:CYS:O	1.99	0.62
1:A:85:ARG:HH12	1:A:125:ASP:HA	1.65	0.62
1:B:117:THR:HG21	1:B:167:PHE:HD2	1.65	0.62
1:A:118:ARG:HA	1:A:441:ASN:OD1	1.99	0.61
1:B:196:GLY:HA3	1:B:201:ALA:HA	1.82	0.61
1:B:118:ARG:HA	1:B:441:ASN:OD1	1.99	0.61
1:A:320:GLY:H	1:A:388:SER:H	1.47	0.61
1:A:146:ASN:O	1:A:147:ASP:HB2	2.01	0.61
1:A:452:THR:HG22	1:A:453:TYR:N	2.14	0.61
1:B:107:ARG:NH2	8:B:497:HOH:O	2.04	0.61
1:B:275:VAL:HG13	1:B:278:CYS:SG	2.41	0.61
1:A:283:ARG:CZ	1:A:288:ARG:HH21	2.14	0.61
1:A:196:GLY:HA3	1:A:201:ALA:HA	1.82	0.61
1:B:283:ARG:CZ	1:B:288:ARG:HH21	2.14	0.61
1:B:302:VAL:HG21	1:B:383:TRP:CZ3	2.36	0.61
1:A:302:VAL:HG21	1:A:383:TRP:CZ3	2.36	0.60
1:B:146:ASN:O	1:B:147:ASP:HB2	2.01	0.60
1:A:463:ASN:HB3	1:A:466:PHE:CG	2.36	0.60
1:B:190:LEU:HD11	1:B:257:ILE:HD13	1.82	0.60
1:A:219:SER:O	1:A:220:GLN:HB2	1.99	0.60
1:B:246:ALA:O	1:B:274:HIS:NE2	2.34	0.60
1:A:275:VAL:HG13	1:A:278:CYS:SG	2.41	0.60
1:B:329:ASP:HA	1:B:368:LYS:HD3	1.84	0.60
1:A:138:THR:HA	1:B:108:LEU:CD2	2.32	0.60
1:B:410:PHE:CD1	1:B:410:PHE:C	2.80	0.60
1:A:246:ALA:O	1:A:274:HIS:NE2	2.34	0.59
1:B:463:ASN:HB3	1:B:466:PHE:CG	2.36	0.59
1:A:172:ARG:HB3	1:B:165:VAL:HG12	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG22	1:A:313:ASP:N	2.17	0.59
1:B:318:CYS:HB3	1:B:385:THR:C	2.28	0.59
1:A:329:ASP:HA	1:A:368:LYS:HD3	1.84	0.59
1:B:257:ILE:HG12	1:B:257:ILE:O	2.03	0.59
1:B:402:ASN:ND2	1:B:459:PRO:HB3	2.18	0.59
1:A:318:CYS:HB3	1:A:385:THR:C	2.28	0.59
1:A:410:PHE:CD1	1:A:410:PHE:C	2.80	0.59
1:A:402:ASN:ND2	1:A:459:PRO:HB3	2.18	0.58
1:B:312:ILE:HG22	1:B:313:ASP:N	2.17	0.58
1:A:291:CYS:O	1:A:300:ARG:HD3	2.03	0.58
1:B:291:CYS:O	1:B:300:ARG:HD3	2.03	0.58
1:B:116:VAL:O	1:B:135:GLY:HA2	2.02	0.58
1:B:396:VAL:HG12	4:E:6:MAN:O2	2.01	0.58
1:A:116:VAL:O	1:A:135:GLY:HA2	2.02	0.58
1:A:258:GLU:O	1:A:259:GLU:HB2	2.03	0.58
1:A:139:THR:O	1:A:142:ASN:HB2	2.04	0.58
1:B:139:THR:O	1:B:142:ASN:HB2	2.04	0.58
1:B:258:GLU:O	1:B:259:GLU:HB2	2.03	0.58
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.68	0.58
2:C:1:NAG:C3	2:C:2:NAG:O5	2.51	0.58
1:B:177:ALA:CB	1:B:193:CYS:HB3	2.24	0.58
1:A:431:LYS:H	1:A:434:THR:HG22	1.69	0.57
1:B:455:THR:CG2	4:E:1:NAG:O6	2.50	0.57
1:A:218:TRP:HH2	1:A:241:MET:HB2	1.69	0.57
1:B:218:TRP:HH2	1:B:241:MET:HB2	1.69	0.57
1:B:131:GLN:NE2	1:B:164:GLY:H	2.02	0.57
1:B:283:ARG:NE	1:B:288:ARG:HH21	2.03	0.57
1:B:431:LYS:H	1:B:434:THR:HG22	1.69	0.57
1:A:131:GLN:NE2	1:A:164:GLY:H	2.02	0.57
1:B:91:GLN:HG3	1:B:420:ARG:NH1	2.20	0.57
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.68	0.57
1:A:283:ARG:NE	1:A:288:ARG:HH21	2.03	0.57
1:A:257:ILE:HG12	1:A:257:ILE:O	2.03	0.56
1:A:142:ASN:ND2	1:B:110:ALA:CB	2.60	0.56
1:A:341:ASN:OD1	1:A:343:GLU:HG3	2.05	0.56
1:A:91:GLN:HG3	1:A:420:ARG:NH1	2.20	0.56
1:A:155:HIS:HE2	1:B:461:GLY:HA3	1.70	0.56
1:B:324:ASP:O	1:B:327:ARG:HD3	2.05	0.56
1:B:430:ARG:HG3	1:B:431:LYS:N	2.21	0.56
1:A:430:ARG:HG3	1:A:431:LYS:N	2.21	0.56
1:B:341:ASN:OD1	1:B:343:GLU:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:SER:C	1:A:389:LYS:HG2	2.30	0.56
2:G:1:NAG:C3	2:G:2:NAG:O5	2.51	0.56
1:A:279:SER:HB3	1:A:409:ILE:HG22	1.87	0.56
1:B:455:THR:HB	4:E:1:NAG:C6	2.34	0.56
1:B:279:SER:HB3	1:B:409:ILE:HG22	1.87	0.56
1:B:388:SER:C	1:B:389:LYS:HG2	2.30	0.56
1:B:136:GLN:HA	1:B:136:GLN:OE1	2.06	0.55
1:B:147:ASP:O	1:B:150:HIS:HD2	1.90	0.55
1:A:197:ASP:O	1:A:201:ALA:HB2	2.07	0.55
1:A:324:ASP:O	1:A:327:ARG:HD3	2.05	0.55
2:G:1:NAG:N2	2:J:2:NAG:H82	2.22	0.55
1:A:150:HIS:HB3	8:A:585:HOH:O	2.05	0.55
1:B:338:ARG:HH11	1:B:338:ARG:CB	2.20	0.55
1:A:276:GLU:O	1:A:292:ARG:HB3	2.07	0.55
1:B:276:GLU:O	1:B:292:ARG:HB3	2.07	0.55
1:B:106:ILE:HG23	1:B:467:MET:HE2	1.89	0.54
1:B:197:ASP:O	1:B:201:ALA:HB2	2.07	0.54
1:B:288:ARG:NH1	1:B:383:TRP:CZ2	2.75	0.54
1:B:395:GLN:HA	8:B:511:HOH:O	2.06	0.54
1:A:136:GLN:OE1	1:A:136:GLN:HA	2.06	0.54
1:A:155:HIS:HB3	1:B:104:ASN:HD21	1.70	0.54
1:B:352:TRP:CD1	1:B:407:SER:HG	2.25	0.54
1:A:168:HIS:CD2	1:A:168:HIS:H	2.25	0.54
1:A:106:ILE:HG23	1:A:467:MET:HE2	1.89	0.54
1:A:212:VAL:HB	1:A:260:GLY:C	2.33	0.54
1:A:352:TRP:CD1	1:A:407:SER:HG	2.26	0.54
1:B:228:SER:HB2	1:B:350:LYS:CE	2.38	0.54
1:A:228:SER:HB2	1:A:350:LYS:CE	2.38	0.54
1:B:212:VAL:HB	1:B:260:GLY:C	2.33	0.54
1:A:147:ASP:O	1:A:150:HIS:HD2	1.90	0.54
1:A:228:SER:HB2	1:A:350:LYS:HE2	1.90	0.54
1:B:346:THR:O	1:B:347:GLN:O	2.26	0.54
1:A:143:LYS:NZ	1:B:466:PHE:HA	2.23	0.53
1:A:213:ASP:OD2	1:A:262:ILE:HG13	2.08	0.53
1:B:168:HIS:H	1:B:168:HIS:CD2	2.25	0.53
2:C:1:NAG:N2	2:F:2:NAG:H82	2.22	0.53
1:A:288:ARG:NH1	1:A:383:TRP:CZ2	2.75	0.53
1:A:411:SER:HB3	1:A:418:ILE:HD11	1.90	0.53
1:A:199:LYS:HA	1:A:220:GLN:O	2.09	0.53
1:B:199:LYS:HA	1:B:220:GLN:O	2.09	0.53
1:B:213:ASP:OD2	1:B:262:ILE:HG13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:PRO:O	1:B:469:ILE:HB	2.08	0.53
1:A:468:PRO:O	1:A:469:ILE:HB	2.08	0.53
1:A:198:ASP:HB3	1:A:222:ILE:HG12	1.91	0.53
1:B:87:TRP:CD1	1:B:233:ILE:HG12	2.43	0.53
1:A:152:ARG:HD3	8:A:578:HOH:O	2.07	0.53
1:A:177:ALA:HB2	1:A:193:CYS:CB	2.28	0.53
1:A:338:ARG:HH11	1:A:338:ARG:CB	2.20	0.53
1:A:409:ILE:HG13	1:A:410:PHE:N	2.23	0.53
1:B:409:ILE:HG13	1:B:410:PHE:N	2.23	0.53
1:A:463:ASN:OD1	1:A:465:ASN:HB2	2.09	0.53
1:B:411:SER:HB3	1:B:418:ILE:HD11	1.90	0.53
1:B:463:ASN:OD1	1:B:465:ASN:HB2	2.09	0.53
1:A:176:ILE:O	1:A:177:ALA:HB2	2.09	0.52
1:A:346:THR:O	1:A:347:GLN:O	2.26	0.52
1:A:441:ASN:C	8:A:557:HOH:O	2.51	0.52
1:A:212:VAL:HG12	1:A:261:LYS:HE2	1.91	0.52
1:B:106:ILE:O	1:B:109:SER:HB2	2.10	0.52
1:A:82:VAL:O	1:A:187:LYS:HE2	2.10	0.52
1:A:155:HIS:NE2	1:B:461:GLY:HA3	2.24	0.52
1:B:228:SER:HB2	1:B:350:LYS:HE2	1.90	0.52
1:B:107:ARG:NH1	8:B:497:HOH:O	2.15	0.52
1:A:106:ILE:O	1:A:109:SER:HB2	2.10	0.52
1:A:421:CYS:HA	1:A:447:CYS:HA	1.92	0.52
1:A:281:TYR:OH	1:A:288:ARG:HD2	2.10	0.52
1:A:402:ASN:HD22	1:A:459:PRO:HB3	1.75	0.52
1:A:209:GLY:O	1:B:100:PHE:HZ	1.93	0.51
1:A:329:ASP:OD1	1:A:330:ASP:N	2.43	0.51
1:B:177:ALA:HB2	1:B:193:CYS:CB	2.28	0.51
1:B:329:ASP:OD1	1:B:330:ASP:N	2.43	0.51
4:I:2:NAG:H5	4:I:3:BMA:O2	2.10	0.51
1:B:134:LEU:HB2	1:B:156:ARG:HH21	1.75	0.51
1:B:281:TYR:OH	1:B:288:ARG:HD2	2.10	0.51
1:B:82:VAL:O	1:B:187:LYS:HE2	2.10	0.51
1:B:128:LYS:HB3	1:B:130:TYR:CZ	2.45	0.51
1:B:402:ASN:HD22	1:B:459:PRO:HB3	1.75	0.51
1:B:198:ASP:HB3	1:B:222:ILE:HG12	1.91	0.51
4:E:2:NAG:H5	4:E:3:BMA:O2	2.10	0.51
1:B:212:VAL:HG12	1:B:261:LYS:HE2	1.91	0.51
1:A:128:LYS:HB3	1:A:130:TYR:CZ	2.45	0.51
1:A:134:LEU:HB2	1:A:156:ARG:HH21	1.75	0.51
1:B:120:PRO:HG2	1:B:423:TYR:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TRP:CD1	1:A:233:ILE:HG12	2.43	0.51
1:A:129:CYS:O	1:A:163:LEU:N	2.45	0.50
1:A:320:GLY:CA	1:A:387:ASN:HD22	2.24	0.50
8:A:515:HOH:O	1:B:100:PHE:CE2	2.36	0.50
1:B:176:ILE:O	1:B:177:ALA:HB2	2.09	0.50
1:B:421:CYS:HA	1:B:447:CYS:HA	1.92	0.50
1:A:120:PRO:HG2	1:A:423:TYR:CE2	2.46	0.50
1:A:142:ASN:OD1	1:B:111:GLY:HA3	2.12	0.50
1:A:410:PHE:C	1:A:410:PHE:HD1	2.19	0.50
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.77	0.50
1:A:101:SER:HB2	1:A:445:VAL:CG2	2.41	0.50
8:A:515:HOH:O	1:B:100:PHE:HZ	1.50	0.50
1:B:352:TRP:NE1	1:B:374:TYR:OH	2.45	0.50
1:B:101:SER:HB2	1:B:445:VAL:CG2	2.41	0.50
1:A:176:ILE:HD11	1:B:102:LYS:HB2	1.93	0.50
1:B:117:THR:HG21	1:B:167:PHE:CD2	2.46	0.50
1:B:227:GLU:O	1:B:350:LYS:HE2	2.12	0.50
1:B:320:GLY:CA	1:B:387:ASN:HD22	2.24	0.50
1:A:199:LYS:O	1:A:220:GLN:HA	2.12	0.50
2:J:1:NAG:O6	2:J:2:NAG:N2	2.45	0.50
1:A:403:ARG:HG2	8:A:550:HOH:O	2.12	0.50
1:B:199:LYS:O	1:B:220:GLN:HA	2.12	0.50
1:B:270:GLY:HA3	1:B:314:SER:OG	2.12	0.50
1:A:125:ASP:HB2	1:A:126:PRO:CD	2.42	0.49
1:B:348:GLY:O	1:B:371:ARG:NH2	2.44	0.49
1:B:419:ASN:ND2	1:B:448:GLY:HA3	2.26	0.49
1:B:423:TYR:HB2	1:B:445:VAL:HG12	1.94	0.49
1:B:125:ASP:HB2	1:B:126:PRO:CD	2.42	0.49
1:B:302:VAL:HG21	1:B:383:TRP:CH2	2.47	0.49
1:B:410:PHE:C	1:B:410:PHE:HD1	2.19	0.49
1:A:227:GLU:O	1:A:350:LYS:HE2	2.12	0.49
1:A:344:ARG:NH2	1:A:368:LYS:O	2.46	0.49
1:B:134:LEU:CB	1:B:156:ARG:HH21	2.26	0.49
1:B:419:ASN:ND2	1:B:420:ARG:N	2.61	0.49
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.77	0.49
1:A:419:ASN:ND2	1:A:420:ARG:N	2.61	0.49
1:B:211:LEU:C	1:B:211:LEU:HD23	2.37	0.49
1:B:344:ARG:NH2	1:B:368:LYS:O	2.46	0.49
1:A:202:THR:HB	1:B:454:GLY:N	2.16	0.49
1:A:270:GLY:HA3	1:A:314:SER:OG	2.12	0.49
1:A:302:VAL:HG21	1:A:383:TRP:CH2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:ND2	1:A:448:GLY:HA3	2.26	0.49
1:A:423:TYR:HB2	1:A:445:VAL:HG12	1.94	0.49
1:A:348:GLY:O	1:A:371:ARG:NH2	2.44	0.49
1:A:406:TYR:HD2	8:A:488:HOH:O	1.95	0.49
1:B:320:GLY:HA3	1:B:387:ASN:HD22	1.78	0.49
1:B:425:GLU:HB2	1:B:441:ASN:HD22	1.78	0.49
1:A:211:LEU:HD23	1:A:211:LEU:C	2.37	0.49
1:A:320:GLY:HA3	1:A:387:ASN:HD22	1.78	0.49
2:F:1:NAG:O6	2:F:2:NAG:N2	2.45	0.49
1:A:172:ARG:CB	1:B:165:VAL:HG12	2.42	0.49
1:A:403:ARG:NH1	1:A:433:GLU:HG3	2.28	0.49
1:B:419:ASN:ND2	1:B:420:ARG:O	2.45	0.49
1:A:419:ASN:ND2	1:A:420:ARG:O	2.45	0.49
1:A:425:GLU:HB2	1:A:441:ASN:HD22	1.78	0.48
1:B:327:ARG:HG2	1:B:327:ARG:NH1	2.28	0.48
1:B:422:PHE:CE1	1:B:446:PHE:HB2	2.47	0.48
1:A:140:LEU:HD23	1:A:468:PRO:HG2	1.95	0.48
1:A:327:ARG:HG2	1:A:327:ARG:NH1	2.28	0.48
1:A:124:CYS:HB3	1:A:129:CYS:HA	1.96	0.48
1:A:179:SER:HB3	1:A:194:ILE:HB	1.95	0.48
1:A:422:PHE:CE1	1:A:446:PHE:HB2	2.47	0.48
1:A:426:LEU:HD21	1:A:444:VAL:HG23	1.95	0.48
1:B:85:ARG:NH1	1:B:184:HIS:HB3	2.29	0.48
1:B:281:TYR:CZ	1:B:288:ARG:HD2	2.49	0.48
1:A:228:SER:HB2	1:A:350:LYS:HZ3	1.78	0.48
1:A:430:ARG:O	1:A:431:LYS:HB2	2.14	0.48
8:A:501:HOH:O	1:B:108:LEU:HD13	2.14	0.48
1:B:129:CYS:SG	1:B:410:PHE:HZ	2.37	0.48
1:A:128:LYS:HB3	1:A:130:TYR:CE1	2.49	0.48
1:A:134:LEU:CB	1:A:156:ARG:HH21	2.26	0.48
1:A:124:CYS:CB	1:A:129:CYS:HA	2.43	0.48
1:B:192:VAL:HG11	1:B:239:VAL:HG21	1.96	0.48
1:A:138:THR:OG1	1:A:139:THR:N	2.44	0.48
1:A:144:HIS:HE1	1:B:462:ALA:HB1	1.77	0.48
1:A:352:TRP:NE1	1:A:374:TYR:OH	2.45	0.48
1:B:124:CYS:CB	1:B:129:CYS:HA	2.43	0.48
1:B:139:THR:HG22	1:B:140:LEU:N	2.28	0.48
1:B:128:LYS:HB3	1:B:130:TYR:CE1	2.49	0.47
1:B:165:VAL:HG23	1:B:166:PRO:O	2.14	0.47
1:B:410:PHE:O	1:B:421:CYS:N	2.43	0.47
1:B:430:ARG:O	1:B:431:LYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:NAG:H3	2:G:2:NAG:O5	2.14	0.47
1:A:85:ARG:NH1	1:A:184:HIS:HB3	2.29	0.47
1:A:239:VAL:O	1:A:239:VAL:HG13	2.13	0.47
1:B:140:LEU:HD23	1:B:468:PRO:HG2	1.95	0.47
1:B:239:VAL:O	1:B:239:VAL:HG13	2.13	0.47
1:B:129:CYS:O	1:B:163:LEU:N	2.45	0.47
1:B:407:SER:HB2	1:B:423:TYR:O	2.13	0.47
1:A:100:PHE:HB3	1:A:445:VAL:HG23	1.97	0.47
1:B:179:SER:HB3	1:B:194:ILE:HB	1.95	0.47
1:A:165:VAL:HG23	1:A:166:PRO:O	2.14	0.47
1:A:189:TRP:O	1:A:207:TYR:HA	2.14	0.47
1:A:407:SER:HB2	1:A:423:TYR:O	2.13	0.47
1:A:431:LYS:NZ	1:A:431:LYS:HA	2.29	0.47
1:B:125:ASP:HB3	1:B:184:HIS:CE1	2.49	0.47
1:B:153:ILE:O	1:B:153:ILE:HG13	2.14	0.47
1:B:431:LYS:HA	1:B:431:LYS:NZ	2.29	0.47
2:C:1:NAG:H3	2:C:2:NAG:O5	2.14	0.47
1:A:281:TYR:CZ	1:A:288:ARG:HD2	2.49	0.47
1:B:249:ARG:CG	1:B:250:ALA:N	2.78	0.47
1:B:426:LEU:HD21	1:B:444:VAL:HG23	1.95	0.47
1:A:115:TRP:CH2	1:B:108:LEU:HD11	2.47	0.47
1:A:129:CYS:SG	1:A:410:PHE:HZ	2.37	0.47
1:A:139:THR:HG22	1:A:140:LEU:N	2.28	0.47
1:A:177:ALA:HA	1:A:195:THR:OG1	2.15	0.47
1:A:255:LEU:N	1:A:255:LEU:HD23	2.30	0.47
1:A:320:GLY:H	1:A:388:SER:N	2.11	0.47
1:A:410:PHE:O	1:A:421:CYS:N	2.43	0.47
1:B:268:LEU:HG	1:B:269:ALA:N	2.30	0.47
1:B:403:ARG:NH1	1:B:433:GLU:HG3	2.28	0.47
1:A:120:PRO:HG3	1:A:425:GLU:HB3	1.96	0.47
1:A:188:ALA:HB1	8:A:510:HOH:O	2.14	0.47
1:B:120:PRO:HG3	1:B:425:GLU:HB3	1.96	0.47
1:B:426:LEU:HD11	1:B:444:VAL:CG2	2.45	0.47
1:A:153:ILE:O	1:A:153:ILE:HG13	2.14	0.47
1:A:218:TRP:CG	1:A:253:ARG:NH2	2.83	0.47
1:B:138:THR:OG1	1:B:139:THR:N	2.44	0.47
1:A:117:THR:HG21	1:A:167:PHE:CD2	2.46	0.47
1:A:306:ASN:OD1	1:A:308:GLU:HB2	2.15	0.47
1:B:218:TRP:CG	1:B:253:ARG:NH2	2.83	0.47
1:A:152:ARG:O	1:A:153:ILE:HG23	2.15	0.46
1:A:211:LEU:HD23	1:A:211:LEU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HG23	1:A:258:GLU:HG2	1.98	0.46
1:A:284:TYR:OH	2:F:1:NAG:H3	2.15	0.46
1:B:211:LEU:HD23	1:B:211:LEU:O	2.15	0.46
1:A:179:SER:OG	1:A:225:THR:HG22	2.15	0.46
1:A:283:ARG:NE	1:A:288:ARG:HE	2.11	0.46
1:B:100:PHE:HB3	1:B:445:VAL:HG23	1.97	0.46
1:B:124:CYS:HB3	1:B:129:CYS:HA	1.96	0.46
1:B:152:ARG:O	1:B:153:ILE:HG23	2.15	0.46
1:B:189:TRP:O	1:B:207:TYR:HA	2.14	0.46
1:B:457:SER:HB3	4:E:6:MAN:O3	2.15	0.46
1:B:177:ALA:HA	1:B:195:THR:OG1	2.15	0.46
1:B:283:ARG:NE	1:B:288:ARG:HE	2.11	0.46
1:B:431:LYS:HA	1:B:431:LYS:HZ2	1.81	0.46
1:A:248:GLY:O	1:A:274:HIS:CE1	2.69	0.46
1:A:426:LEU:HD11	1:A:444:VAL:CG2	2.45	0.46
1:B:248:GLY:O	1:B:274:HIS:CE1	2.69	0.46
1:B:306:ASN:OD1	1:B:308:GLU:HB2	2.15	0.46
1:A:91:GLN:HG2	1:A:92:CYS:N	2.31	0.46
1:A:106:ILE:HG13	1:A:428:ARG:HG3	1.98	0.46
1:A:125:ASP:HB3	1:A:184:HIS:CE1	2.49	0.46
1:B:255:LEU:N	1:B:255:LEU:HD23	2.30	0.46
1:A:198:ASP:HB3	1:A:222:ILE:CG1	2.46	0.46
1:B:120:PRO:CG	1:B:425:GLU:HB3	2.46	0.46
1:B:284:TYR:OH	2:J:1:NAG:H3	2.15	0.46
1:B:410:PHE:CD1	1:B:411:SER:O	2.69	0.46
1:B:426:LEU:HD13	1:B:460:ASP:N	2.31	0.46
1:A:120:PRO:CG	1:A:425:GLU:HB3	2.46	0.46
1:A:183:CYS:CB	1:A:232:CYS:SG	3.00	0.46
1:A:249:ARG:HA	8:A:526:HOH:O	2.15	0.46
1:A:327:ARG:C	1:A:344:ARG:HE	2.24	0.46
1:B:133:ALA:HB3	1:B:167:PHE:HE2	1.80	0.46
1:A:284:TYR:CE2	1:A:285:PRO:HG3	2.51	0.46
1:B:91:GLN:HG2	1:B:92:CYS:N	2.31	0.46
1:B:143:LYS:HB2	1:B:143:LYS:HE3	1.79	0.46
1:B:432:GLN:O	1:B:434:THR:HG23	2.16	0.46
1:A:321:LEU:O	1:A:322:VAL:CB	2.64	0.45
1:B:284:TYR:CE2	1:B:285:PRO:HG3	2.51	0.45
1:A:192:VAL:HG11	1:A:239:VAL:HG21	1.96	0.45
1:A:426:LEU:HD13	1:A:460:ASP:N	2.31	0.45
1:A:432:GLN:O	1:A:434:THR:HG23	2.16	0.45
1:B:183:CYS:CB	1:B:232:CYS:SG	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:HG12	1:A:393:ASN:N	2.32	0.45
1:B:327:ARG:C	1:B:344:ARG:HE	2.24	0.45
1:A:115:TRP:CH2	1:B:108:LEU:HD21	2.52	0.45
1:B:179:SER:OG	1:B:225:THR:HG22	2.15	0.45
1:B:392:ILE:HG12	1:B:393:ASN:N	2.32	0.45
1:B:106:ILE:HG13	1:B:428:ARG:HG3	1.98	0.45
1:B:288:ARG:HG3	1:B:288:ARG:HH11	1.82	0.45
1:A:133:ALA:HB3	1:A:167:PHE:HE2	1.80	0.45
1:B:198:ASP:HB3	1:B:222:ILE:CG1	2.46	0.45
2:C:2:NAG:C6	2:C:2:NAG:H2	2.46	0.45
2:G:2:NAG:H2	2:G:2:NAG:C6	2.46	0.45
1:A:87:TRP:CZ3	1:A:418:ILE:HD13	2.52	0.45
1:A:144:HIS:CD2	1:B:466:PHE:CD2	3.00	0.45
1:A:387:ASN:HD22	1:A:387:ASN:HA	1.61	0.45
1:A:410:PHE:CD1	1:A:411:SER:O	2.69	0.45
1:B:87:TRP:CZ3	1:B:418:ILE:HD13	2.52	0.45
1:B:181:SER:HB3	1:B:192:VAL:HG13	1.98	0.45
1:B:236:THR:HG23	1:B:258:GLU:HG2	1.98	0.45
1:A:268:LEU:HG	1:A:269:ALA:N	2.30	0.45
1:B:321:LEU:O	1:B:322:VAL:CB	2.64	0.45
1:A:210:ARG:NH2	8:A:518:HOH:O	2.49	0.45
1:A:298:SER:O	1:A:322:VAL:HG13	2.17	0.45
1:B:120:PRO:O	1:B:121:TYR:HB3	2.17	0.45
1:B:298:SER:O	1:B:322:VAL:HG13	2.17	0.45
1:A:140:LEU:CD2	1:A:468:PRO:HG2	2.47	0.44
1:A:178:TRP:CE2	1:A:195:THR:HA	2.53	0.44
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.99	0.44
1:A:442:SER:HB2	1:A:460:ASP:OD1	2.17	0.44
1:B:306:ASN:OD1	1:B:308:GLU:CB	2.65	0.44
1:B:320:GLY:H	1:B:388:SER:N	2.11	0.44
1:A:190:LEU:CD1	1:A:257:ILE:HD13	2.46	0.44
1:B:139:THR:HB	1:B:142:ASN:OD1	2.17	0.44
1:B:184:HIS:HD2	1:B:186:GLY:H	1.64	0.44
1:B:442:SER:HB2	1:B:460:ASP:OD1	2.17	0.44
2:G:1:NAG:HN2	2:J:2:NAG:H82	1.82	0.44
1:A:139:THR:HB	1:A:142:ASN:OD1	2.17	0.44
1:A:184:HIS:HD2	1:A:186:GLY:H	1.64	0.44
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.57	0.44
4:E:2:NAG:O4	4:E:6:MAN:O6	2.35	0.44
1:A:396:VAL:O	1:A:398:VAL:N	2.51	0.44
1:B:181:SER:HB3	1:B:192:VAL:CG1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:THR:HG22	1:B:196:GLY:N	2.33	0.44
1:A:90:PRO:O	1:A:417:CYS:HA	2.18	0.44
1:A:181:SER:HB3	1:A:192:VAL:HG13	1.98	0.44
1:B:90:PRO:O	1:B:417:CYS:HA	2.18	0.44
1:A:181:SER:HB3	1:A:192:VAL:CG1	2.48	0.44
1:A:288:ARG:HG3	1:A:288:ARG:HH11	1.82	0.44
1:A:415:LYS:O	1:A:415:LYS:HG2	2.18	0.44
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.99	0.44
1:A:195:THR:HG22	1:A:196:GLY:N	2.33	0.44
1:A:306:ASN:OD1	1:A:308:GLU:CB	2.65	0.44
1:B:178:TRP:CE2	1:B:195:THR:HA	2.53	0.44
1:B:240:VAL:HG21	1:B:278:CYS:SG	2.57	0.44
1:B:352:TRP:HD1	1:B:407:SER:HG	1.66	0.44
1:B:415:LYS:O	1:B:415:LYS:HG2	2.18	0.44
1:B:199:LYS:HG2	1:B:220:GLN:O	2.18	0.44
1:A:182:SER:C	1:A:230:CYS:SG	3.01	0.44
1:B:182:SER:C	1:B:230:CYS:SG	3.01	0.44
1:B:218:TRP:NE1	1:B:243:ASP:HB3	2.33	0.44
1:A:143:LYS:HZ1	1:B:466:PHE:HA	1.82	0.43
1:A:249:ARG:CG	1:A:250:ALA:N	2.78	0.43
1:B:131:GLN:HE21	1:B:164:GLY:H	1.66	0.43
1:B:140:LEU:CD2	1:B:468:PRO:HG2	2.47	0.43
1:B:190:LEU:CG	1:B:257:ILE:HD13	2.48	0.43
1:B:406:TYR:H	1:B:425:GLU:HG2	1.83	0.43
1:A:406:TYR:H	1:A:425:GLU:HG2	1.83	0.43
1:B:228:SER:HB2	1:B:350:LYS:HZ3	1.82	0.43
1:A:106:ILE:HG23	1:A:467:MET:CE	2.48	0.43
1:A:120:PRO:O	1:A:121:TYR:HB3	2.17	0.43
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.79	0.43
1:B:311:SER:C	1:B:312:ILE:HD13	2.43	0.43
2:C:1:NAG:HN2	2:F:2:NAG:H82	1.82	0.43
1:A:311:SER:C	1:A:312:ILE:HD13	2.43	0.43
1:B:153:ILE:HG12	1:B:156:ARG:HG3	2.01	0.43
1:B:183:CYS:N	1:B:230:CYS:SG	2.91	0.43
1:A:140:LEU:C	1:A:142:ASN:H	2.27	0.43
1:A:183:CYS:N	1:A:230:CYS:SG	2.91	0.43
1:B:153:ILE:CG1	1:B:156:ARG:HG3	2.49	0.43
1:B:396:VAL:O	1:B:398:VAL:N	2.51	0.43
3:D:2:NAG:O6	3:D:3:BMA:O2	2.33	0.43
1:A:105:SER:HB2	1:A:442:SER:HA	2.00	0.43
1:A:153:ILE:HG12	1:A:156:ARG:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:CG	1:A:257:ILE:HD13	2.48	0.43
1:A:324:ASP:H	1:A:327:ARG:HD3	1.84	0.43
1:A:350:LYS:HG2	1:A:407:SER:O	2.18	0.43
1:A:365:THR:HG21	1:A:371:ARG:HA	2.01	0.43
1:B:127:VAL:HG23	1:B:128:LYS:N	2.34	0.43
1:B:324:ASP:H	1:B:327:ARG:HD3	1.84	0.43
1:B:350:LYS:HG2	1:B:407:SER:O	2.18	0.43
4:I:2:NAG:O4	4:I:6:MAN:O6	2.35	0.43
1:A:131:GLN:HE21	1:A:164:GLY:H	1.66	0.43
1:A:153:ILE:CG1	1:A:156:ARG:HG3	2.49	0.43
1:A:161:ASN:HD22	1:A:161:ASN:HA	1.62	0.43
1:A:218:TRP:NE1	1:A:243:ASP:HB3	2.33	0.43
1:A:366:ILE:HG21	1:A:400:SER:CB	2.49	0.43
1:B:300:ARG:HH22	1:B:349:VAL:HG13	1.84	0.43
1:B:309:ASP:O	1:B:310:TYR:HB2	2.19	0.43
1:B:463:ASN:O	1:B:467:MET:HG2	2.19	0.43
1:B:109:SER:HB3	1:B:140:LEU:HD13	2.00	0.42
1:B:153:ILE:HB	1:B:154:PRO:HD2	2.00	0.42
1:A:161:ASN:HB3	1:A:165:VAL:HG22	2.01	0.42
1:B:327:ARG:NH1	1:B:368:LYS:HA	2.34	0.42
1:A:292:ARG:CZ	1:A:294:ASN:HD21	2.32	0.42
1:A:327:ARG:NH1	1:A:368:LYS:HA	2.34	0.42
1:A:332:SER:O	1:A:334:ASN:OD1	2.37	0.42
1:A:442:SER:N	8:A:557:HOH:O	2.53	0.42
1:B:292:ARG:CZ	1:B:294:ASN:HD21	2.32	0.42
1:B:365:THR:HG21	1:B:371:ARG:HA	2.01	0.42
1:A:144:HIS:CE1	1:B:463:ASN:H	2.37	0.42
1:A:153:ILE:HB	1:A:154:PRO:HD2	2.00	0.42
1:A:199:LYS:HG2	1:A:220:GLN:O	2.18	0.42
1:A:463:ASN:O	1:A:467:MET:HG2	2.19	0.42
1:A:325:THR:HG23	1:A:368:LYS:C	2.44	0.42
1:A:409:ILE:HG12	8:A:525:HOH:O	2.19	0.42
1:B:128:LYS:HE2	1:B:128:LYS:HB2	1.82	0.42
1:B:140:LEU:C	1:B:142:ASN:H	2.27	0.42
1:B:184:HIS:C	1:B:186:GLY:H	2.26	0.42
1:B:427:ILE:HD11	1:B:439:THR:HG23	2.02	0.42
1:A:109:SER:HB3	1:A:140:LEU:HD13	2.00	0.42
1:A:302:VAL:HG21	1:A:383:TRP:HZ3	1.84	0.42
1:B:103:ASP:O	1:B:104:ASN:HB2	2.20	0.42
1:B:161:ASN:HB3	1:B:165:VAL:HG22	2.01	0.42
1:B:325:THR:HG23	1:B:368:LYS:C	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:SER:O	1:B:334:ASN:OD1	2.37	0.42
1:A:103:ASP:O	1:A:104:ASN:HB2	2.20	0.42
1:B:105:SER:HB2	1:B:442:SER:HA	2.00	0.42
1:B:106:ILE:HG23	1:B:467:MET:CE	2.48	0.42
4:I:1:NAG:O4	4:I:2:NAG:O6	2.33	0.42
1:A:309:ASP:O	1:A:310:TYR:HB2	2.19	0.42
2:F:1:NAG:H5	2:F:2:NAG:HN2	1.85	0.42
1:A:127:VAL:HG23	1:A:128:LYS:N	2.34	0.42
1:A:323:GLY:HA3	8:A:534:HOH:O	2.19	0.42
1:A:402:ASN:ND2	1:A:459:PRO:CB	2.83	0.42
1:B:157:THR:OG1	1:B:173:GLN:HG2	2.20	0.42
1:A:427:ILE:HD11	1:A:439:THR:HG23	2.02	0.42
1:A:431:LYS:HA	1:A:431:LYS:HZ2	1.85	0.42
1:A:455:THR:HG23	8:A:555:HOH:O	2.20	0.42
1:B:419:ASN:HD21	1:B:448:GLY:CA	2.32	0.42
4:E:2:NAG:O4	4:E:6:MAN:C6	2.68	0.42
1:A:352:TRP:HD1	1:A:407:SER:HG	1.67	0.41
1:A:375:GLU:HA	1:A:395:GLN:O	2.20	0.41
1:B:257:ILE:HG13	1:B:261:LYS:C	2.45	0.41
1:B:402:ASN:ND2	1:B:459:PRO:CB	2.83	0.41
1:A:157:THR:OG1	1:A:173:GLN:HG2	2.20	0.41
1:B:161:ASN:HD22	1:B:161:ASN:HA	1.62	0.41
1:B:302:VAL:HG21	1:B:383:TRP:HZ3	1.84	0.41
1:B:353:ALA:HB1	1:B:360:LEU:HD11	2.02	0.41
4:I:2:NAG:O4	4:I:6:MAN:C6	2.68	0.41
2:J:1:NAG:H5	2:J:2:NAG:HN2	1.85	0.41
1:A:94:ILE:HD11	1:A:361:TRP:CD2	2.55	0.41
1:A:118:ARG:CA	1:A:441:ASN:OD1	2.67	0.41
1:A:158:LEU:HB3	1:A:175:CYS:SG	2.60	0.41
1:A:184:HIS:C	1:A:186:GLY:H	2.26	0.41
1:A:256:PHE:CD2	1:A:310:TYR:CD1	3.08	0.41
1:B:134:LEU:CB	1:B:156:ARG:NH2	2.80	0.41
1:B:190:LEU:CD1	1:B:257:ILE:HD13	2.46	0.41
1:A:136:GLN:O	1:A:138:THR:N	2.54	0.41
1:A:266:SER:OG	1:A:310:TYR:HB3	2.21	0.41
1:A:425:GLU:HB2	1:A:441:ASN:ND2	2.35	0.41
1:A:300:ARG:HH22	1:A:349:VAL:HG13	1.84	0.41
1:A:409:ILE:CG1	8:A:525:HOH:O	2.68	0.41
1:A:435:ARG:HH21	1:A:465:ASN:HA	1.86	0.41
1:A:463:ASN:HB3	1:A:466:PHE:CD2	2.56	0.41
1:B:94:ILE:HD11	1:B:361:TRP:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASP:O	1:B:127:VAL:N	2.54	0.41
1:B:136:GLN:O	1:B:138:THR:N	2.54	0.41
1:B:158:LEU:HB3	1:B:175:CYS:SG	2.60	0.41
1:B:266:SER:OG	1:B:310:TYR:HB3	2.21	0.41
1:B:366:ILE:HG21	1:B:400:SER:CB	2.49	0.41
1:B:375:GLU:HA	1:B:395:GLN:O	2.20	0.41
1:A:257:ILE:HG13	1:A:261:LYS:C	2.45	0.41
1:A:432:GLN:O	1:A:434:THR:N	2.54	0.41
1:A:125:ASP:O	1:A:127:VAL:N	2.54	0.41
1:A:147:ASP:O	1:A:150:HIS:CD2	2.73	0.41
1:A:181:SER:OG	1:A:230:CYS:HB3	2.21	0.41
1:A:191:HIS:O	1:A:193:CYS:SG	2.79	0.41
1:A:218:TRP:CH2	1:A:241:MET:HB2	2.51	0.41
1:A:283:ARG:HD3	1:A:283:ARG:O	2.20	0.41
7:A:471:ST1:HM43	7:A:471:ST1:O3	2.21	0.41
1:B:168:HIS:C	1:B:170:GLY:N	2.79	0.41
1:B:256:PHE:CD2	1:B:310:TYR:CD1	3.08	0.41
1:B:387:ASN:HD22	1:B:387:ASN:HA	1.61	0.41
1:B:391:GLN:HE22	1:B:394:ARG:HB2	1.86	0.41
1:B:425:GLU:HB2	1:B:441:ASN:ND2	2.35	0.41
1:B:463:ASN:HB3	1:B:466:PHE:CD2	2.56	0.41
1:A:216:GLY:N	1:B:452:THR:HB	2.31	0.41
1:B:132:PHE:CD1	1:B:132:PHE:N	2.89	0.41
1:B:191:HIS:O	1:B:193:CYS:SG	2.79	0.41
1:B:283:ARG:O	1:B:283:ARG:HD3	2.20	0.41
1:B:414:GLY:N	1:B:417:CYS:O	2.54	0.41
7:B:471:ST1:HM43	7:B:471:ST1:O3	2.21	0.41
1:A:127:VAL:HG23	1:A:128:LYS:H	1.86	0.40
1:A:296:LYS:C	1:A:345:GLY:HA3	2.45	0.40
1:A:338:ARG:NH1	1:A:339:ASP:OD1	2.55	0.40
1:A:362:MET:CE	1:A:364:ARG:HG2	2.51	0.40
1:B:120:PRO:HG2	1:B:423:TYR:HE2	1.86	0.40
2:C:1:NAG:O3	2:F:2:NAG:C8	2.69	0.40
1:A:277:GLU:N	8:A:522:HOH:O	2.53	0.40
1:A:353:ALA:HB1	1:A:360:LEU:HD11	2.02	0.40
1:B:320:GLY:N	1:B:388:SER:N	2.68	0.40
1:B:432:GLN:O	1:B:434:THR:N	2.54	0.40
4:E:2:NAG:O4	4:E:6:MAN:H61	2.22	0.40
1:A:128:LYS:HE2	1:A:128:LYS:HB2	1.82	0.40
1:A:136:GLN:OE1	1:A:156:ARG:CG	2.69	0.40
1:A:144:HIS:HE1	1:B:462:ALA:CB	2.34	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG21	8:A:535:HOH:O	2.21	0.40
1:A:142:ASN:HD21	1:B:110:ALA:CB	2.14	0.40
1:A:284:TYR:CG	1:A:285:PRO:HA	2.57	0.40
1:B:91:GLN:OE1	1:B:420:ARG:NH1	2.51	0.40
1:B:256:PHE:CD1	1:B:256:PHE:N	2.90	0.40
1:B:368:LYS:NZ	1:B:369:ASP:OD2	2.54	0.40
1:A:368:LYS:NZ	1:A:369:ASP:OD2	2.54	0.40
1:B:136:GLN:OE1	1:B:156:ARG:CG	2.69	0.40
1:B:256:PHE:CD2	1:B:310:TYR:CE1	3.10	0.40
1:B:349:VAL:HG22	1:B:350:LYS:N	2.37	0.40
3:D:2:NAG:H3	3:D:3:BMA:O5	2.22	0.40

All (13) 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:B:463:ASN:HD22	4:E:5:MAN:H62[3_654]	1.02	0.58
3:D:4:FUL:H1	4:E:4:MAN:O3[3_654]	1.02	0.58
3:D:4:FUL:H3	4:E:4:MAN:HO3[3_654]	1.04	0.56
3:D:4:FUL:C1	4:E:4:MAN:O3[3_654]	1.85	0.35
1:A:455:THR:OG1	4:I:1:NAG:H1[4_555]	1.42	0.18
1:A:455:THR:CG2	4:I:1:NAG:H61[4_555]	1.43	0.17
1:B:270:GLY:CA	8:A:489:HOH:O[7_544]	2.10	0.10
1:A:164:GLY:O	1:B:173:GLN:H[4_555]	1.54	0.06
1:A:455:THR:CG2	4:I:1:NAG:C6[4_555]	2.15	0.05
3:D:4:FUL:H3	4:E:4:MAN:O2[3_654]	1.56	0.04
1:A:396:VAL:CG1	4:I:6:MAN:O2[4_555]	2.18	0.02
1:B:270:GLY:C	8:A:489:HOH:O[7_544]	2.18	0.02
3:D:4:FUL:H5	4:E:4:MAN:O5[3_654]	1.58	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	294 (76%)	70 (18%)	22 (6%)	1	0
1	B	386/388 (100%)	294 (76%)	70 (18%)	22 (6%)	1	0
All	All	772/776 (100%)	588 (76%)	140 (18%)	44 (6%)	1	0

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	A	284	TYR
1	A	329	ASP
1	A	346	THR
1	A	347	GLN
1	A	397	ILE
1	A	412	VAL
1	B	145	SER
1	B	284	TYR
1	B	329	ASP
1	B	346	THR
1	B	347	GLN
1	B	397	ILE
1	B	412	VAL
1	A	87	TRP
1	A	118	ARG
1	A	259	GLU
1	A	322	VAL
1	A	416	SER
1	B	87	TRP
1	B	118	ARG
1	B	259	GLU
1	B	322	VAL
1	B	416	SER
1	A	133	ALA
1	A	137	GLY
1	A	147	ASP
1	A	431	LYS
1	B	133	ALA
1	B	137	GLY
1	B	147	ASP
1	B	431	LYS
1	A	356	ASN
1	B	356	ASN
1	A	121	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	222	ILE
1	B	121	TYR
1	B	222	ILE
1	A	239	VAL
1	A	387	ASN
1	B	239	VAL
1	B	387	ASN
1	A	382	GLY
1	B	382	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/338 (100%)	287 (85%)	51 (15%)	3	1
1	B	338/338 (100%)	287 (85%)	51 (15%)	3	1
All	All	676/676 (100%)	574 (85%)	102 (15%)	3	1

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	89	LYS
1	A	94	ILE
1	A	119	GLU
1	A	122	VAL
1	A	124	CYS
1	A	128	LYS
1	A	142	ASN
1	A	155	HIS
1	A	157	THR
1	A	161	ASN
1	A	165	VAL
1	A	172	ARG
1	A	178	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	CYS
1	A	190	LEU
1	A	192	VAL
1	A	210	ARG
1	A	224	ARG
1	A	231	VAL
1	A	238	THR
1	A	241	MET
1	A	254	ILE
1	A	255	LEU
1	A	257	ILE
1	A	262	ILE
1	A	263	VAL
1	A	273	GLN
1	A	276	GLU
1	A	308	GLU
1	A	317	VAL
1	A	321	LEU
1	A	330	ASP
1	A	337	CYS
1	A	338	ARG
1	A	344	ARG
1	A	347	GLN
1	A	364	ARG
1	A	365	THR
1	A	368	LYS
1	A	387	ASN
1	A	391	GLN
1	A	401	ASP
1	A	409	ILE
1	A	410	PHE
1	A	418	ILE
1	A	420	ARG
1	A	426	LEU
1	A	427	ILE
1	A	431	LYS
1	A	449	THR
1	B	83	GLU
1	B	89	LYS
1	B	94	ILE
1	B	119	GLU
1	B	122	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	124	CYS
1	B	128	LYS
1	B	142	ASN
1	B	155	HIS
1	B	157	THR
1	B	161	ASN
1	B	165	VAL
1	B	172	ARG
1	B	178	TRP
1	B	183	CYS
1	B	190	LEU
1	B	192	VAL
1	B	210	ARG
1	B	224	ARG
1	B	231	VAL
1	B	238	THR
1	B	241	MET
1	B	254	ILE
1	B	255	LEU
1	B	257	ILE
1	B	262	ILE
1	B	263	VAL
1	B	273	GLN
1	B	276	GLU
1	B	308	GLU
1	B	317	VAL
1	B	321	LEU
1	B	330	ASP
1	B	337	CYS
1	B	338	ARG
1	B	344	ARG
1	B	347	GLN
1	B	364	ARG
1	B	365	THR
1	B	368	LYS
1	B	387	ASN
1	B	391	GLN
1	B	401	ASP
1	B	409	ILE
1	B	410	PHE
1	B	418	ILE
1	B	420	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	426	LEU
1	B	427	ILE
1	B	431	LYS
1	B	449	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	131	GLN
1	A	144	HIS
1	A	150	HIS
1	A	161	ASN
1	A	173	GLN
1	A	191	HIS
1	A	226	GLN
1	A	334	ASN
1	A	387	ASN
1	A	393	ASN
1	A	402	ASN
1	A	419	ASN
1	B	104	ASN
1	B	131	GLN
1	B	150	HIS
1	B	161	ASN
1	B	168	HIS
1	B	173	GLN
1	B	191	HIS
1	B	226	GLN
1	B	334	ASN
1	B	387	ASN
1	B	393	ASN
1	B	402	ASN
1	B	419	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 ⓘ

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	1,2	14,14,15	1.78	3 (21%)	17,19,21	2.40	8 (47%)
2	NAG	C	2	2	14,14,15	2.00	4 (28%)	17,19,21	2.76	5 (29%)
3	NAG	D	1	3,1	14,14,15	2.04	3 (21%)	17,19,21	2.66	6 (35%)
3	NAG	D	2	3	14,14,15	1.81	1 (7%)	17,19,21	3.10	7 (41%)
3	BMA	D	3	3	11,11,12	2.16	5 (45%)	15,15,17	2.15	3 (20%)
3	FUL	D	4	3	10,10,11	2.58	4 (40%)	14,14,16	2.53	7 (50%)
4	NAG	E	1	1,4	14,14,15	4.80	9 (64%)	17,19,21	4.10	11 (64%)
4	NAG	E	2	4	14,14,15	1.93	6 (42%)	17,19,21	2.16	8 (47%)
4	BMA	E	3	4	11,11,12	2.42	2 (18%)	15,15,17	2.60	5 (33%)
4	MAN	E	4	4	11,11,12	2.82	5 (45%)	15,15,17	1.90	3 (20%)
4	MAN	E	5	4	11,11,12	2.46	4 (36%)	15,15,17	2.72	4 (26%)
4	MAN	E	6	4	11,11,12	3.27	5 (45%)	15,15,17	2.62	8 (53%)
2	NAG	F	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	2.85	8 (47%)
2	NAG	F	2	2	14,14,15	1.52	4 (28%)	17,19,21	3.62	11 (64%)
2	NAG	G	1	1,2	14,14,15	1.78	3 (21%)	17,19,21	2.40	8 (47%)
2	NAG	G	2	2	14,14,15	2.00	4 (28%)	17,19,21	2.76	5 (29%)
5	NAG	H	1	1,5	14,14,15	2.04	3 (21%)	17,19,21	2.66	6 (35%)
5	NAG	H	2	5	14,14,15	1.81	1 (7%)	17,19,21	3.10	7 (41%)
5	BMA	H	3	5	11,11,12	2.16	5 (45%)	15,15,17	2.15	3 (20%)
5	FUC	H	4	5	10,10,11	2.58	4 (40%)	14,14,16	2.53	7 (50%)
4	NAG	I	1	1,4	14,14,15	4.80	9 (64%)	17,19,21	4.10	11 (64%)
4	NAG	I	2	4	14,14,15	1.93	6 (42%)	17,19,21	2.16	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	I	3	4	11,11,12	2.42	2 (18%)	15,15,17	2.60	5 (33%)
4	MAN	I	4	4	11,11,12	2.82	5 (45%)	15,15,17	1.90	3 (20%)
4	MAN	I	5	4	11,11,12	2.46	4 (36%)	15,15,17	2.72	4 (26%)
4	MAN	I	6	4	11,11,12	3.27	5 (45%)	15,15,17	2.62	8 (53%)
2	NAG	J	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	2.85	8 (47%)
2	NAG	J	2	2	14,14,15	1.52	4 (28%)	17,19,21	3.62	11 (64%)

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	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	1/1/1/1
3	FUL	D	4	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	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	-	1/2/19/22	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	1,2	-	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	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	1/1/1/1
5	FUC	H	4	5	1/1/5/5	-	0/1/1/1
4	NAG	I	1	1,4	-	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	-	1/2/19/22	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	9.55	1.65	1.52
4	I	1	NAG	C1-C2	9.55	1.65	1.52
4	E	6	MAN	C4-C5	7.67	1.69	1.53
4	I	6	MAN	C4-C5	7.67	1.69	1.53
4	E	1	NAG	O5-C1	7.27	1.55	1.43
4	I	1	NAG	O5-C1	7.27	1.55	1.43
4	E	3	BMA	C1-C2	6.46	1.67	1.52
4	I	3	BMA	C1-C2	6.46	1.67	1.52
4	E	1	NAG	C4-C5	6.39	1.66	1.53
4	I	1	NAG	C4-C5	6.39	1.66	1.53
4	E	4	MAN	C2-C3	6.10	1.61	1.52
4	I	4	MAN	C2-C3	6.10	1.61	1.52
4	E	1	NAG	C3-C2	6.03	1.65	1.52
4	I	1	NAG	C3-C2	6.03	1.65	1.52
4	E	6	MAN	O5-C5	5.84	1.54	1.43
4	I	6	MAN	O5-C5	5.84	1.54	1.43
3	D	1	NAG	C1-C2	5.83	1.60	1.52
5	H	1	NAG	C1-C2	5.83	1.60	1.52
3	D	2	NAG	C4-C3	5.55	1.66	1.52
5	H	2	NAG	C4-C3	5.55	1.66	1.52
4	E	1	NAG	O5-C5	5.18	1.53	1.43
4	I	1	NAG	O5-C5	5.18	1.53	1.43
2	C	2	NAG	C4-C3	4.84	1.64	1.52
2	G	2	NAG	C4-C3	4.84	1.64	1.52
4	E	1	NAG	C4-C3	4.83	1.64	1.52
4	I	1	NAG	C4-C3	4.83	1.64	1.52
3	D	4	FUL	C4-C5	4.76	1.63	1.52
5	H	4	FUC	C4-C5	4.76	1.63	1.52
2	F	1	NAG	O5-C1	4.70	1.51	1.43
2	J	1	NAG	O5-C1	4.70	1.51	1.43
2	C	1	NAG	O5-C5	4.54	1.52	1.43
2	G	1	NAG	O5-C5	4.54	1.52	1.43
4	E	4	MAN	O5-C5	4.50	1.52	1.43
4	I	4	MAN	O5-C5	4.50	1.52	1.43
4	E	5	MAN	C4-C5	4.48	1.62	1.53
4	I	5	MAN	C4-C5	4.48	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C6-C5	4.48	1.66	1.51
4	I	1	NAG	C6-C5	4.48	1.66	1.51
4	E	1	NAG	C2-N2	4.32	1.53	1.46
4	I	1	NAG	C2-N2	4.32	1.53	1.46
4	E	5	MAN	O5-C5	4.22	1.51	1.43
4	I	5	MAN	O5-C5	4.22	1.51	1.43
3	D	4	FUL	C4-C3	4.17	1.63	1.52
5	H	4	FUC	C4-C3	4.17	1.63	1.52
4	E	3	BMA	C4-C5	4.16	1.61	1.53
4	I	3	BMA	C4-C5	4.16	1.61	1.53
4	E	2	NAG	C6-C5	4.02	1.65	1.51
4	I	2	NAG	C6-C5	4.02	1.65	1.51
4	E	5	MAN	O5-C1	3.73	1.50	1.43
4	I	5	MAN	O5-C1	3.73	1.50	1.43
3	D	4	FUL	O2-C2	-3.62	1.35	1.43
5	H	4	FUC	O2-C2	-3.62	1.35	1.43
2	F	2	NAG	C3-C2	3.58	1.60	1.52
2	J	2	NAG	C3-C2	3.58	1.60	1.52
3	D	3	BMA	C1-C2	3.34	1.60	1.52
5	H	3	BMA	C1-C2	3.34	1.60	1.52
3	D	3	BMA	C4-C3	3.32	1.61	1.52
5	H	3	BMA	C4-C3	3.32	1.61	1.52
2	C	1	NAG	C4-C3	3.30	1.60	1.52
2	G	1	NAG	C4-C3	3.30	1.60	1.52
4	E	4	MAN	C1-C2	3.20	1.59	1.52
4	I	4	MAN	C1-C2	3.20	1.59	1.52
2	C	2	NAG	C4-C5	3.16	1.59	1.53
2	G	2	NAG	C4-C5	3.16	1.59	1.53
4	E	4	MAN	O4-C4	-3.13	1.35	1.43
4	I	4	MAN	O4-C4	-3.13	1.35	1.43
2	F	1	NAG	O4-C4	3.02	1.50	1.43
2	J	1	NAG	O4-C4	3.02	1.50	1.43
3	D	3	BMA	C2-C3	2.99	1.57	1.52
5	H	3	BMA	C2-C3	2.99	1.57	1.52
2	F	1	NAG	C1-C2	2.95	1.56	1.52
2	J	1	NAG	C1-C2	2.95	1.56	1.52
2	F	1	NAG	C2-N2	2.95	1.51	1.46
2	J	1	NAG	C2-N2	2.95	1.51	1.46
2	F	1	NAG	O5-C5	2.84	1.49	1.43
2	J	1	NAG	O5-C5	2.84	1.49	1.43
4	E	2	NAG	C4-C5	2.83	1.59	1.53
4	I	2	NAG	C4-C5	2.83	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	FUL	C6-C5	2.78	1.58	1.51
5	H	4	FUC	C6-C5	2.78	1.58	1.51
3	D	3	BMA	C4-C5	2.70	1.58	1.53
5	H	3	BMA	C4-C5	2.70	1.58	1.53
4	E	6	MAN	O4-C4	2.70	1.49	1.43
4	I	6	MAN	O4-C4	2.70	1.49	1.43
4	E	6	MAN	C1-C2	2.67	1.58	1.52
4	I	6	MAN	C1-C2	2.67	1.58	1.52
3	D	1	NAG	O5-C5	2.55	1.48	1.43
5	H	1	NAG	O5-C5	2.55	1.48	1.43
4	E	1	NAG	O6-C6	2.54	1.53	1.42
4	I	1	NAG	O6-C6	2.54	1.53	1.42
2	F	2	NAG	C4-C5	2.53	1.58	1.53
2	J	2	NAG	C4-C5	2.53	1.58	1.53
3	D	3	BMA	O5-C1	2.52	1.47	1.43
5	H	3	BMA	O5-C1	2.52	1.47	1.43
2	C	2	NAG	C8-C7	2.45	1.55	1.50
2	G	2	NAG	C8-C7	2.45	1.55	1.50
4	E	2	NAG	O5-C1	-2.42	1.39	1.43
4	I	2	NAG	O5-C1	-2.42	1.39	1.43
2	C	2	NAG	O4-C4	2.41	1.48	1.43
2	G	2	NAG	O4-C4	2.41	1.48	1.43
2	C	1	NAG	C1-C2	2.26	1.55	1.52
2	G	1	NAG	C1-C2	2.26	1.55	1.52
4	E	6	MAN	O2-C2	-2.25	1.38	1.43
4	I	6	MAN	O2-C2	-2.25	1.38	1.43
2	F	2	NAG	C4-C3	2.23	1.58	1.52
2	J	2	NAG	C4-C3	2.23	1.58	1.52
3	D	1	NAG	C4-C5	2.18	1.57	1.53
5	H	1	NAG	C4-C5	2.18	1.57	1.53
2	F	2	NAG	O5-C5	2.15	1.47	1.43
2	J	2	NAG	O5-C5	2.15	1.47	1.43
4	E	2	NAG	C3-C2	2.12	1.57	1.52
4	I	2	NAG	C3-C2	2.12	1.57	1.52
4	E	2	NAG	C4-C3	2.09	1.57	1.52
4	I	2	NAG	C4-C3	2.09	1.57	1.52
4	E	5	MAN	C6-C5	2.09	1.58	1.51
4	I	5	MAN	C6-C5	2.09	1.58	1.51
4	E	4	MAN	O5-C1	2.06	1.47	1.43
4	I	4	MAN	O5-C1	2.06	1.47	1.43
4	E	2	NAG	O5-C5	2.01	1.47	1.43
4	I	2	NAG	O5-C5	2.01	1.47	1.43

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	MAN	C1-O5-C5	8.56	123.66	112.19
4	I	5	MAN	C1-O5-C5	8.56	123.66	112.19
3	D	1	NAG	C1-C2-N2	8.47	123.78	110.43
5	H	1	NAG	C1-C2-N2	8.47	123.78	110.43
4	E	1	NAG	O7-C7-C8	-8.14	107.56	122.05
4	I	1	NAG	O7-C7-C8	-8.14	107.56	122.05
2	C	2	NAG	C1-O5-C5	7.89	122.77	112.19
2	G	2	NAG	C1-O5-C5	7.89	122.77	112.19
4	E	1	NAG	C8-C7-N2	7.76	128.98	116.12
4	I	1	NAG	C8-C7-N2	7.76	128.98	116.12
4	E	1	NAG	O5-C1-C2	7.09	122.26	111.29
4	I	1	NAG	O5-C1-C2	7.09	122.26	111.29
2	F	1	NAG	C1-O5-C5	6.87	121.40	112.19
2	J	1	NAG	C1-O5-C5	6.87	121.40	112.19
2	F	2	NAG	C2-N2-C7	-6.87	113.70	122.90
2	J	2	NAG	C2-N2-C7	-6.87	113.70	122.90
3	D	2	NAG	C4-C3-C2	-5.88	102.41	111.02
5	H	2	NAG	C4-C3-C2	-5.88	102.41	111.02
2	F	2	NAG	C4-C3-C2	-5.87	102.41	111.02
2	J	2	NAG	C4-C3-C2	-5.87	102.41	111.02
4	E	6	MAN	C3-C4-C5	-5.80	99.72	110.23
4	I	6	MAN	C3-C4-C5	-5.80	99.72	110.23
4	E	3	BMA	O2-C2-C1	5.58	121.99	109.22
4	I	3	BMA	O2-C2-C1	5.58	121.99	109.22
3	D	2	NAG	O4-C4-C3	5.57	123.52	110.38
5	H	2	NAG	O4-C4-C3	5.57	123.52	110.38
2	F	2	NAG	O3-C3-C2	5.57	120.97	109.40
2	J	2	NAG	O3-C3-C2	5.57	120.97	109.40
2	F	1	NAG	O5-C1-C2	5.55	119.88	111.29
2	J	1	NAG	O5-C1-C2	5.55	119.88	111.29
4	E	1	NAG	C6-C5-C4	5.43	126.35	113.02
4	I	1	NAG	C6-C5-C4	5.43	126.35	113.02
4	E	3	BMA	C1-O5-C5	5.29	119.28	112.19
4	I	3	BMA	C1-O5-C5	5.29	119.28	112.19
3	D	3	BMA	C1-O5-C5	5.22	119.19	112.19
5	H	3	BMA	C1-O5-C5	5.22	119.19	112.19
3	D	2	NAG	O3-C3-C2	-5.14	98.73	109.40
5	H	2	NAG	O3-C3-C2	-5.14	98.73	109.40
2	F	2	NAG	C3-C4-C5	-5.01	101.15	110.23
2	J	2	NAG	C3-C4-C5	-5.01	101.15	110.23
4	E	1	NAG	O5-C5-C4	-4.93	98.83	110.83
4	I	1	NAG	O5-C5-C4	-4.93	98.83	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	6	MAN	O4-C4-C5	4.90	121.39	109.32
4	I	6	MAN	O4-C4-C5	4.90	121.39	109.32
2	C	1	NAG	C4-C3-C2	-4.84	103.92	111.02
2	G	1	NAG	C4-C3-C2	-4.84	103.92	111.02
3	D	3	BMA	O2-C2-C1	4.63	119.82	109.22
5	H	3	BMA	O2-C2-C1	4.63	119.82	109.22
2	F	2	NAG	C6-C5-C4	4.59	124.28	113.02
2	J	2	NAG	C6-C5-C4	4.59	124.28	113.02
3	D	2	NAG	C2-N2-C7	-4.48	116.90	122.90
5	H	2	NAG	C2-N2-C7	-4.48	116.90	122.90
2	F	2	NAG	C1-C2-N2	4.37	117.33	110.43
2	J	2	NAG	C1-C2-N2	4.37	117.33	110.43
4	E	4	MAN	O4-C4-C3	-4.31	100.22	110.38
4	I	4	MAN	O4-C4-C3	-4.31	100.22	110.38
2	C	2	NAG	C6-C5-C4	4.26	123.49	113.02
2	G	2	NAG	C6-C5-C4	4.26	123.49	113.02
3	D	2	NAG	O3-C3-C4	4.17	120.22	110.38
5	H	2	NAG	O3-C3-C4	4.17	120.22	110.38
3	D	4	FUL	C2-C3-C4	-4.13	103.60	110.86
5	H	4	FUC	C2-C3-C4	-4.13	103.60	110.86
2	C	2	NAG	C1-C2-N2	4.09	116.87	110.43
2	G	2	NAG	C1-C2-N2	4.09	116.87	110.43
4	E	2	NAG	O5-C5-C6	4.06	115.56	107.66
4	I	2	NAG	O5-C5-C6	4.06	115.56	107.66
4	E	5	MAN	C1-C2-C3	4.03	115.51	109.64
4	I	5	MAN	C1-C2-C3	4.03	115.51	109.64
3	D	2	NAG	C3-C4-C5	-3.95	103.07	110.23
5	H	2	NAG	C3-C4-C5	-3.95	103.07	110.23
4	E	3	BMA	O5-C1-C2	3.90	120.08	110.79
4	I	3	BMA	O5-C1-C2	3.90	120.08	110.79
4	E	1	NAG	C4-C3-C2	3.87	116.69	111.02
4	I	1	NAG	C4-C3-C2	3.87	116.69	111.02
2	C	2	NAG	O5-C1-C2	-3.84	105.35	111.29
2	G	2	NAG	O5-C1-C2	-3.84	105.35	111.29
3	D	4	FUL	O3-C3-C4	3.75	119.22	110.38
5	H	4	FUC	O3-C3-C4	3.75	119.22	110.38
2	C	1	NAG	O4-C4-C3	3.70	119.11	110.38
2	G	1	NAG	O4-C4-C3	3.70	119.11	110.38
3	D	4	FUL	C3-C4-C5	3.65	115.36	109.81
5	H	4	FUC	C3-C4-C5	3.65	115.36	109.81
2	C	1	NAG	C1-O5-C5	3.63	117.06	112.19
2	G	1	NAG	C1-O5-C5	3.63	117.06	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C3-C4-C5	3.53	116.62	110.23
4	I	4	MAN	C3-C4-C5	3.53	116.62	110.23
4	E	2	NAG	C4-C3-C2	-3.51	105.88	111.02
4	I	2	NAG	C4-C3-C2	-3.51	105.88	111.02
2	F	2	NAG	O4-C4-C5	3.42	117.73	109.32
2	J	2	NAG	O4-C4-C5	3.42	117.73	109.32
2	F	1	NAG	O3-C3-C2	3.40	116.46	109.40
2	J	1	NAG	O3-C3-C2	3.40	116.46	109.40
4	E	6	MAN	O2-C2-C3	-3.34	103.24	110.15
4	I	6	MAN	O2-C2-C3	-3.34	103.24	110.15
2	F	1	NAG	C8-C7-N2	3.34	121.65	116.12
2	J	1	NAG	C8-C7-N2	3.34	121.65	116.12
4	E	6	MAN	C1-C2-C3	3.33	114.49	109.64
4	I	6	MAN	C1-C2-C3	3.33	114.49	109.64
2	C	1	NAG	C2-N2-C7	3.31	127.34	122.90
2	G	1	NAG	C2-N2-C7	3.31	127.34	122.90
3	D	1	NAG	C2-N2-C7	3.29	127.31	122.90
5	H	1	NAG	C2-N2-C7	3.29	127.31	122.90
4	E	1	NAG	O3-C3-C4	-3.28	102.65	110.38
4	I	1	NAG	O3-C3-C4	-3.28	102.65	110.38
2	F	1	NAG	O7-C7-C8	-3.20	116.35	122.05
2	J	1	NAG	O7-C7-C8	-3.20	116.35	122.05
3	D	4	FUL	O5-C1-C2	-3.12	103.34	110.79
5	H	4	FUC	O5-C1-C2	-3.12	103.34	110.79
2	C	1	NAG	C8-C7-N2	-3.12	110.94	116.12
2	G	1	NAG	C8-C7-N2	-3.12	110.94	116.12
4	E	2	NAG	C2-N2-C7	-3.11	118.73	122.90
4	I	2	NAG	C2-N2-C7	-3.11	118.73	122.90
4	E	2	NAG	C1-O5-C5	3.09	116.33	112.19
4	I	2	NAG	C1-O5-C5	3.09	116.33	112.19
2	F	1	NAG	C1-C2-N2	-3.08	105.58	110.43
2	J	1	NAG	C1-C2-N2	-3.08	105.58	110.43
3	D	4	FUL	C1-C2-C3	-3.05	105.20	109.64
5	H	4	FUC	C1-C2-C3	-3.05	105.20	109.64
3	D	1	NAG	C3-C4-C5	3.01	115.69	110.23
5	H	1	NAG	C3-C4-C5	3.01	115.69	110.23
2	F	2	NAG	O5-C1-C2	-3.00	106.64	111.29
2	J	2	NAG	O5-C1-C2	-3.00	106.64	111.29
3	D	4	FUL	O3-C3-C2	-2.96	104.02	110.05
5	H	4	FUC	O3-C3-C2	-2.96	104.02	110.05
4	E	2	NAG	O5-C5-C4	-2.92	103.73	110.83
4	I	2	NAG	O5-C5-C4	-2.92	103.73	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	O3-C3-C2	2.91	115.45	109.40
5	H	1	NAG	O3-C3-C2	2.91	115.45	109.40
2	F	1	NAG	O4-C4-C3	-2.86	103.64	110.38
2	J	1	NAG	O4-C4-C3	-2.86	103.64	110.38
4	E	1	NAG	O4-C4-C5	2.81	116.25	109.32
4	I	1	NAG	O4-C4-C5	2.81	116.25	109.32
4	E	2	NAG	C1-C2-N2	2.80	114.84	110.43
4	I	2	NAG	C1-C2-N2	2.80	114.84	110.43
4	E	1	NAG	O5-C5-C6	2.72	112.95	107.66
4	I	1	NAG	O5-C5-C6	2.72	112.95	107.66
4	E	5	MAN	O2-C2-C3	-2.65	104.66	110.15
4	I	5	MAN	O2-C2-C3	-2.65	104.66	110.15
3	D	1	NAG	O5-C1-C2	-2.55	107.34	111.29
5	H	1	NAG	O5-C1-C2	-2.55	107.34	111.29
3	D	3	BMA	C1-C2-C3	-2.52	105.97	109.64
5	H	3	BMA	C1-C2-C3	-2.52	105.97	109.64
2	C	1	NAG	C3-C4-C5	-2.51	105.69	110.23
2	G	1	NAG	C3-C4-C5	-2.51	105.69	110.23
2	C	1	NAG	O3-C3-C4	2.50	116.28	110.38
2	G	1	NAG	O3-C3-C4	2.50	116.28	110.38
4	E	5	MAN	O2-C2-C1	-2.43	103.65	109.22
4	I	5	MAN	O2-C2-C1	-2.43	103.65	109.22
3	D	4	FUL	C6-C5-C4	2.42	117.50	113.08
5	H	4	FUC	C6-C5-C4	2.42	117.50	113.08
4	E	1	NAG	O6-C6-C5	2.41	119.53	111.33
4	I	1	NAG	O6-C6-C5	2.41	119.53	111.33
2	C	1	NAG	O3-C3-C2	2.38	114.34	109.40
2	G	1	NAG	O3-C3-C2	2.38	114.34	109.40
2	F	2	NAG	O7-C7-C8	-2.37	117.84	122.05
2	J	2	NAG	O7-C7-C8	-2.37	117.84	122.05
2	F	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	J	2	NAG	C8-C7-N2	2.36	120.03	116.12
4	E	4	MAN	O3-C3-C2	2.33	114.81	110.05
4	I	4	MAN	O3-C3-C2	2.33	114.81	110.05
4	E	3	BMA	O2-C2-C3	-2.32	105.34	110.15
4	I	3	BMA	O2-C2-C3	-2.32	105.34	110.15
4	E	6	MAN	C6-C5-C4	2.32	118.72	113.02
4	I	6	MAN	C6-C5-C4	2.32	118.72	113.02
4	E	6	MAN	O3-C3-C2	2.31	114.76	110.05
4	I	6	MAN	O3-C3-C2	2.31	114.76	110.05
4	E	2	NAG	O3-C3-C2	2.20	113.98	109.40
4	I	2	NAG	O3-C3-C2	2.20	113.98	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C3-C4-C5	-2.16	106.32	110.23
4	I	3	BMA	C3-C4-C5	-2.16	106.32	110.23
4	E	2	NAG	O6-C6-C5	2.14	118.63	111.33
4	I	2	NAG	O6-C6-C5	2.14	118.63	111.33
4	E	6	MAN	O6-C6-C5	-2.06	104.31	111.33
4	I	6	MAN	O6-C6-C5	-2.06	104.31	111.33
3	D	2	NAG	O5-C1-C2	-2.05	108.12	111.29
5	H	2	NAG	O5-C1-C2	-2.05	108.12	111.29
3	D	1	NAG	O4-C4-C3	-2.04	105.56	110.38
5	H	1	NAG	O4-C4-C3	-2.04	105.56	110.38
2	C	2	NAG	O5-C5-C4	-2.03	105.88	110.83
2	G	2	NAG	O5-C5-C4	-2.03	105.88	110.83
4	E	1	NAG	C1-C2-N2	2.03	113.63	110.43
4	I	1	NAG	C1-C2-N2	2.03	113.63	110.43
2	F	1	NAG	C2-N2-C7	2.00	125.59	122.90
2	J	1	NAG	C2-N2-C7	2.00	125.59	122.90
4	E	6	MAN	O2-C2-C1	2.00	113.81	109.22
4	I	6	MAN	O2-C2-C1	2.00	113.81	109.22
2	F	2	NAG	O6-C6-C5	-2.00	104.52	111.33
2	J	2	NAG	O6-C6-C5	-2.00	104.52	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	4	FUC	C1

All (34) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

All (4) 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
3	D	3	BMA	C1-C2-C3-C4-C5-O5
5	H	3	BMA	C1-C2-C3-C4-C5-O5

21 monomers are involved in 60 short contacts:

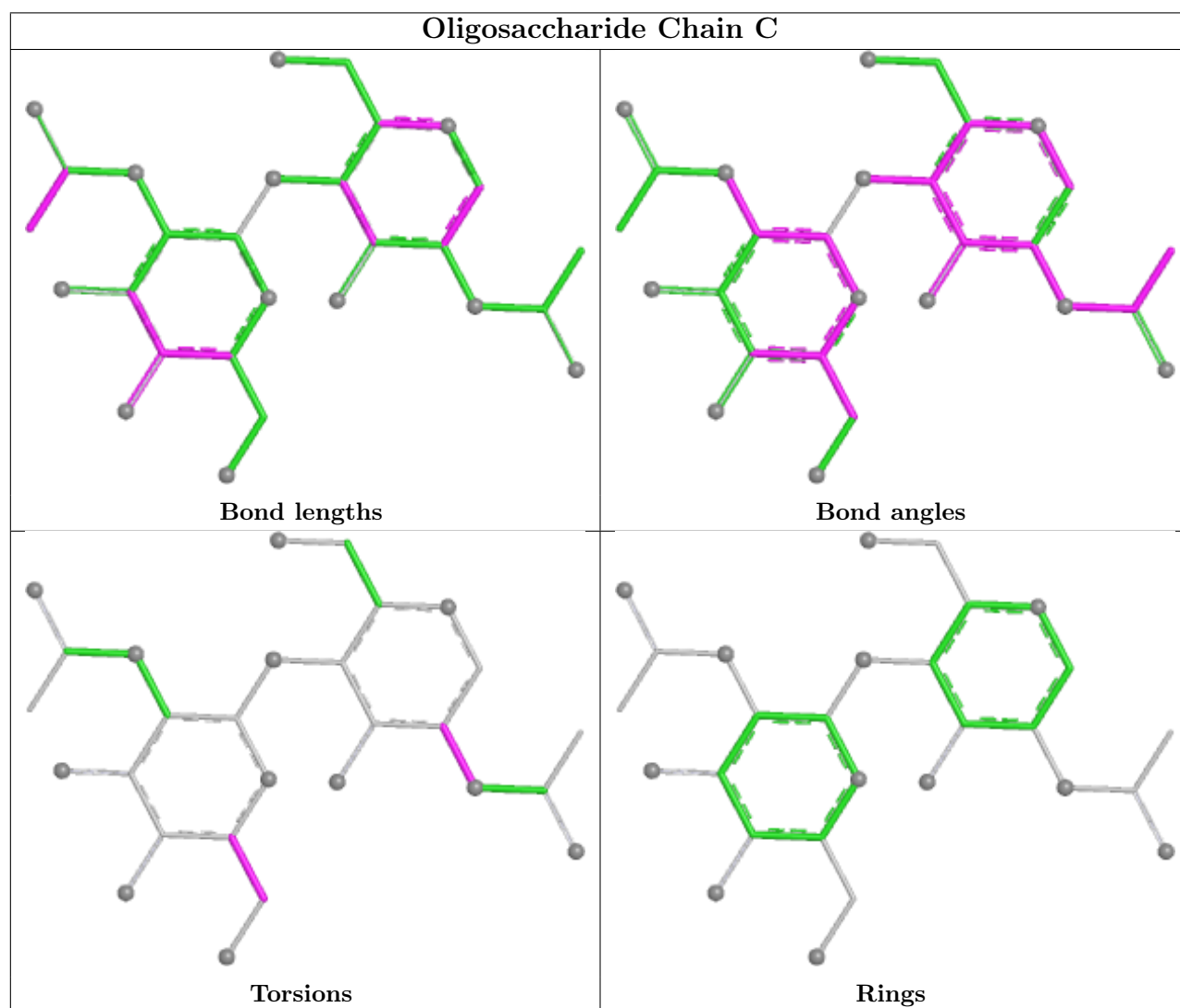
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	5	0
4	I	1	NAG	1	3
2	G	1	NAG	4	0
3	D	4	FUL	0	5
4	E	6	MAN	7	0
4	E	3	BMA	1	0
4	I	2	NAG	4	0
4	I	6	MAN	2	1
3	D	3	BMA	2	0

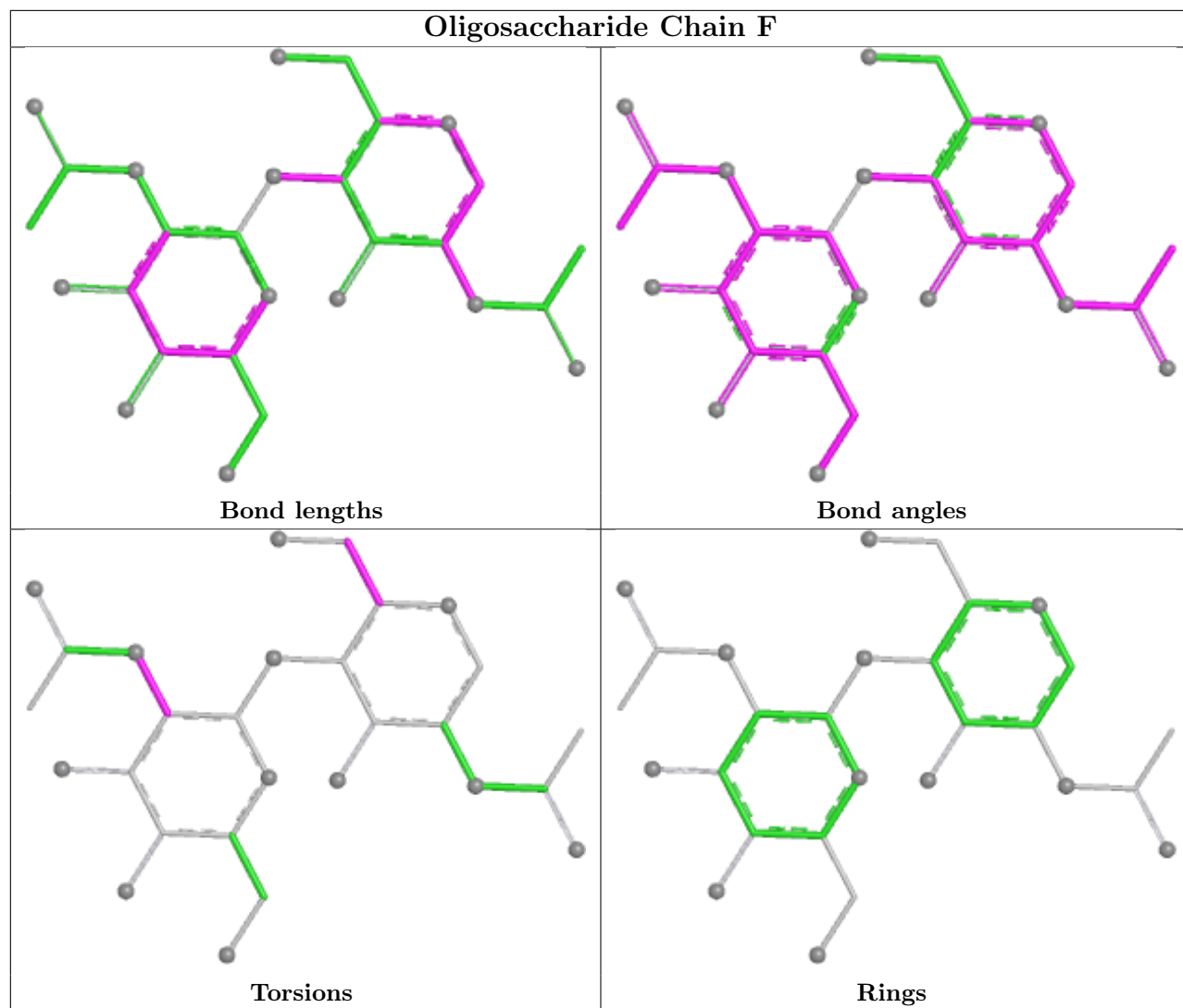
Continued on next page...

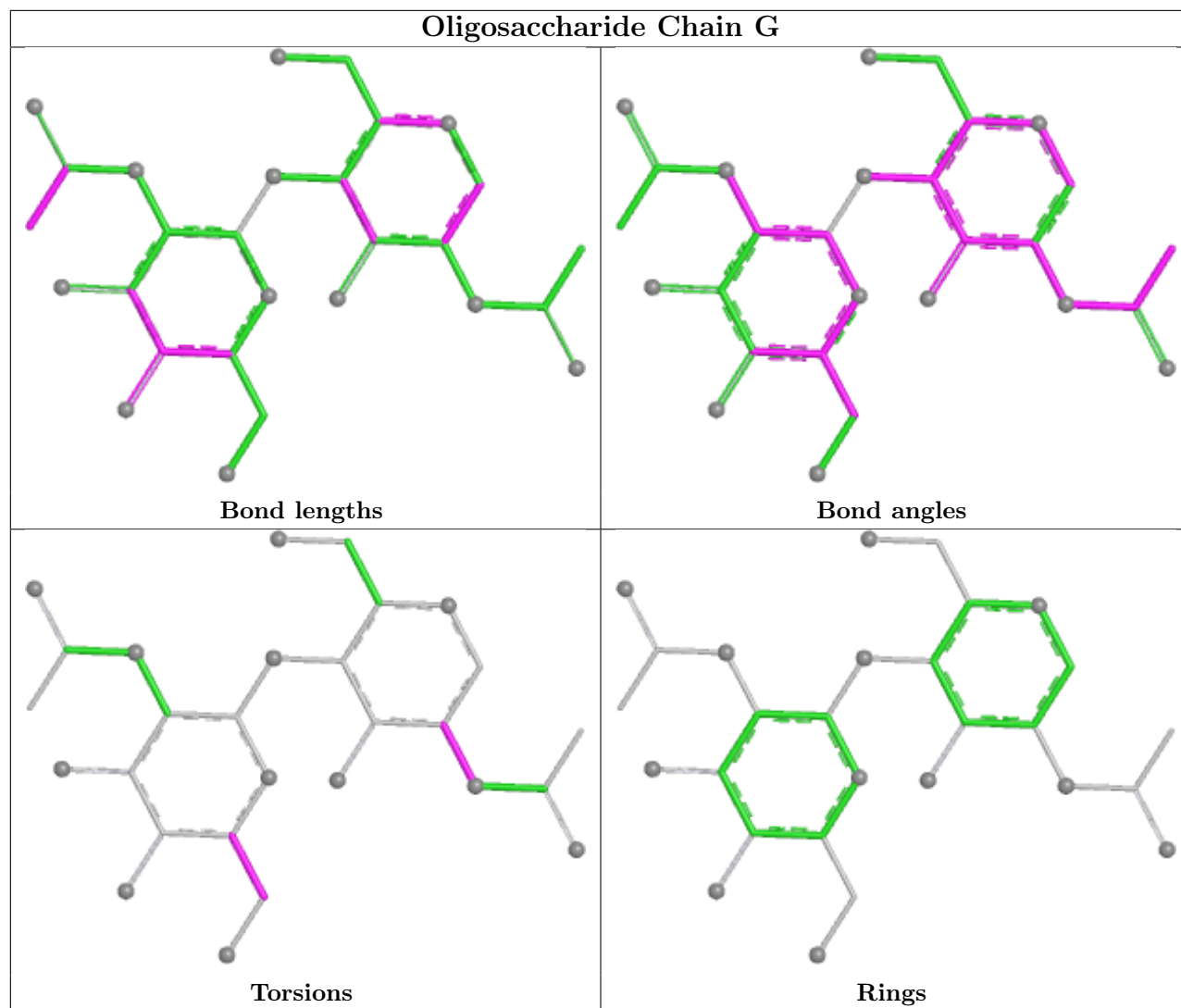
Continued from previous page...

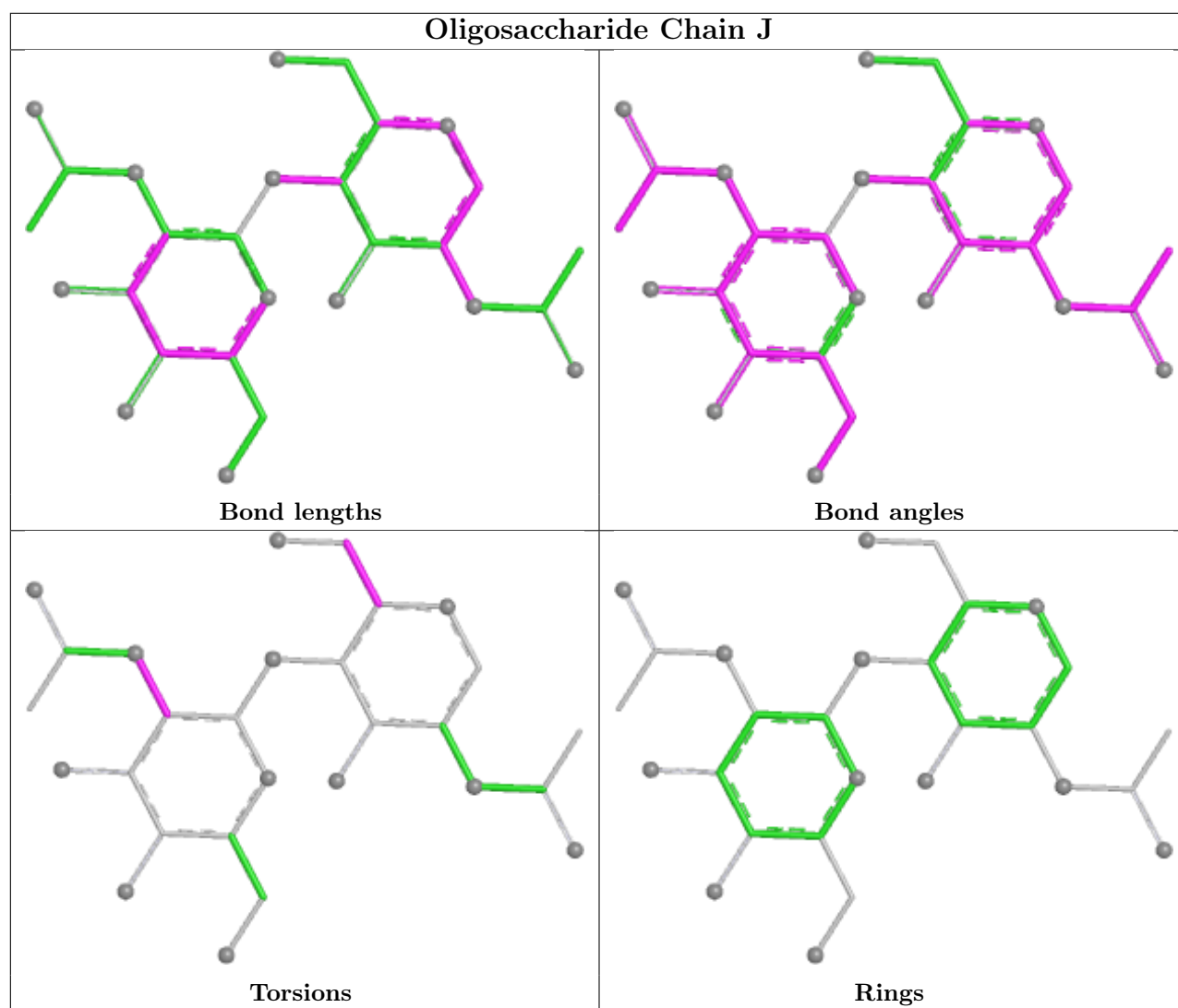
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	3	0
4	E	1	NAG	19	0
2	G	2	NAG	3	0
4	E	2	NAG	4	0
2	F	2	NAG	5	0
4	E	5	MAN	0	1
4	I	3	BMA	1	0
3	D	2	NAG	2	0
2	J	2	NAG	4	0
2	F	1	NAG	3	0
2	C	2	NAG	3	0
4	E	4	MAN	0	5

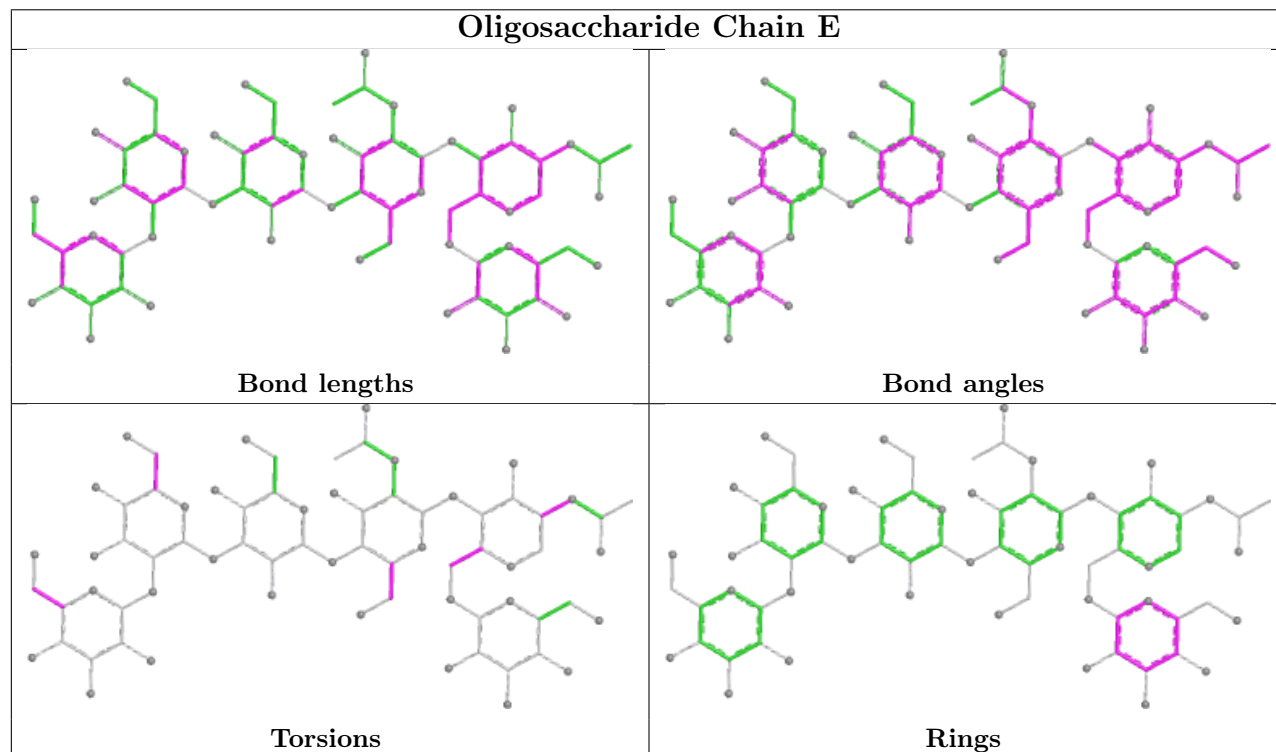
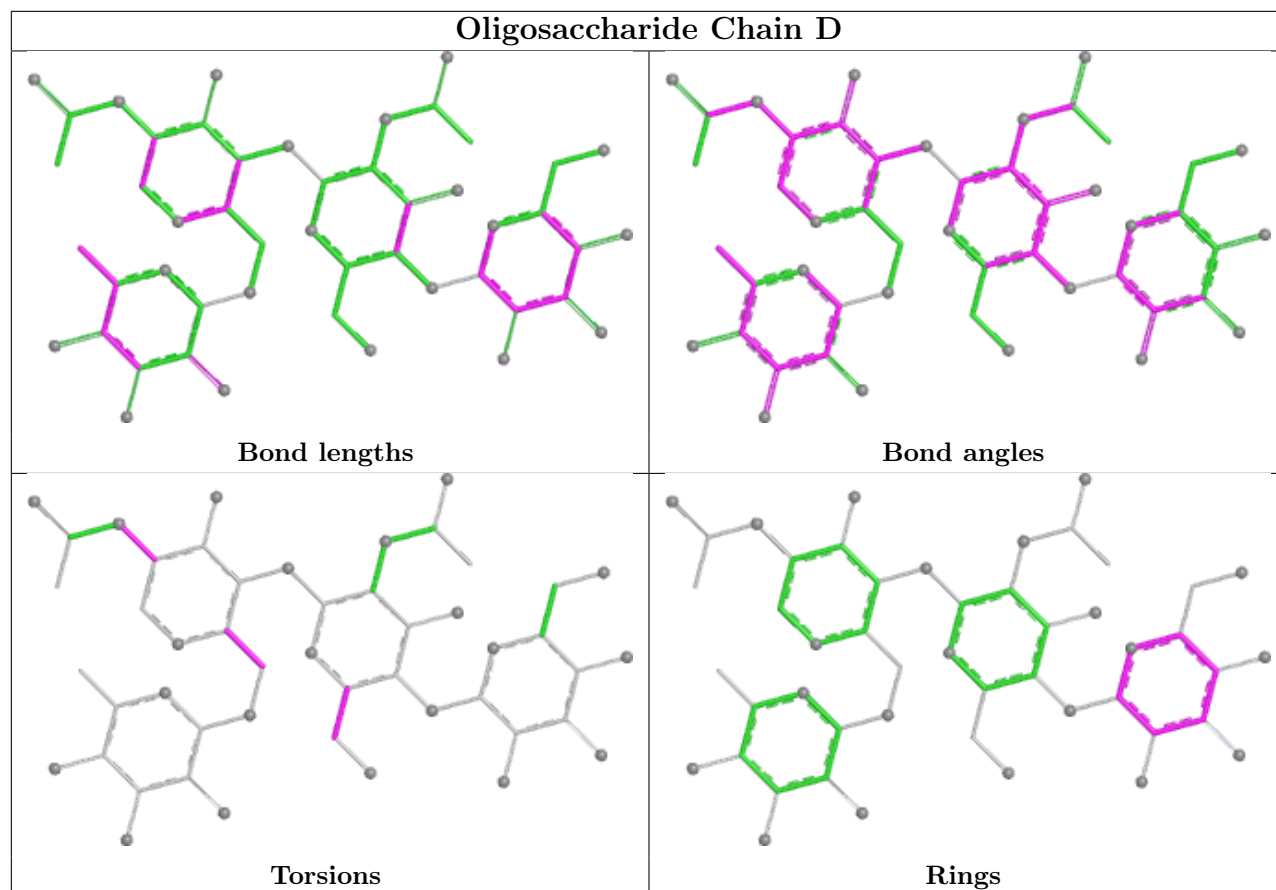
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

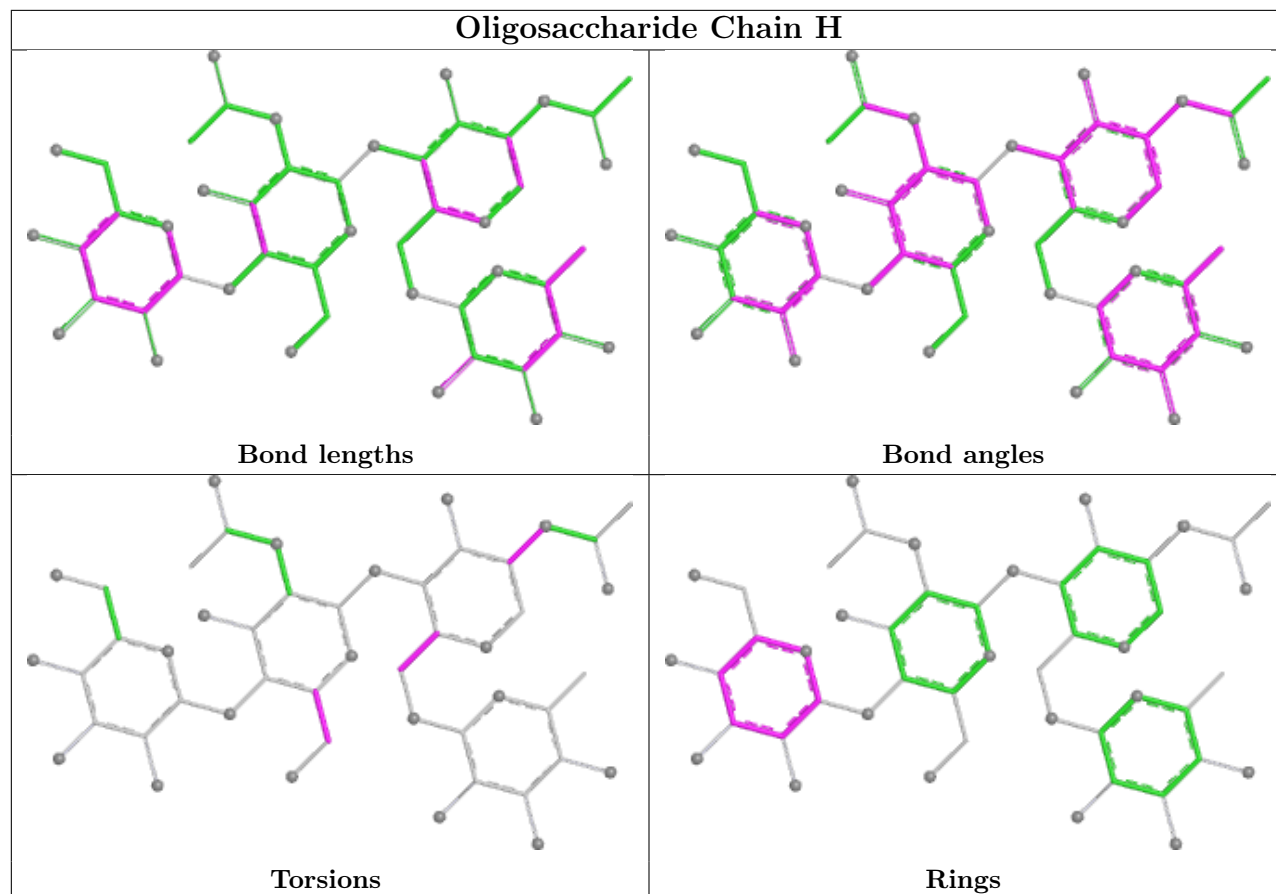
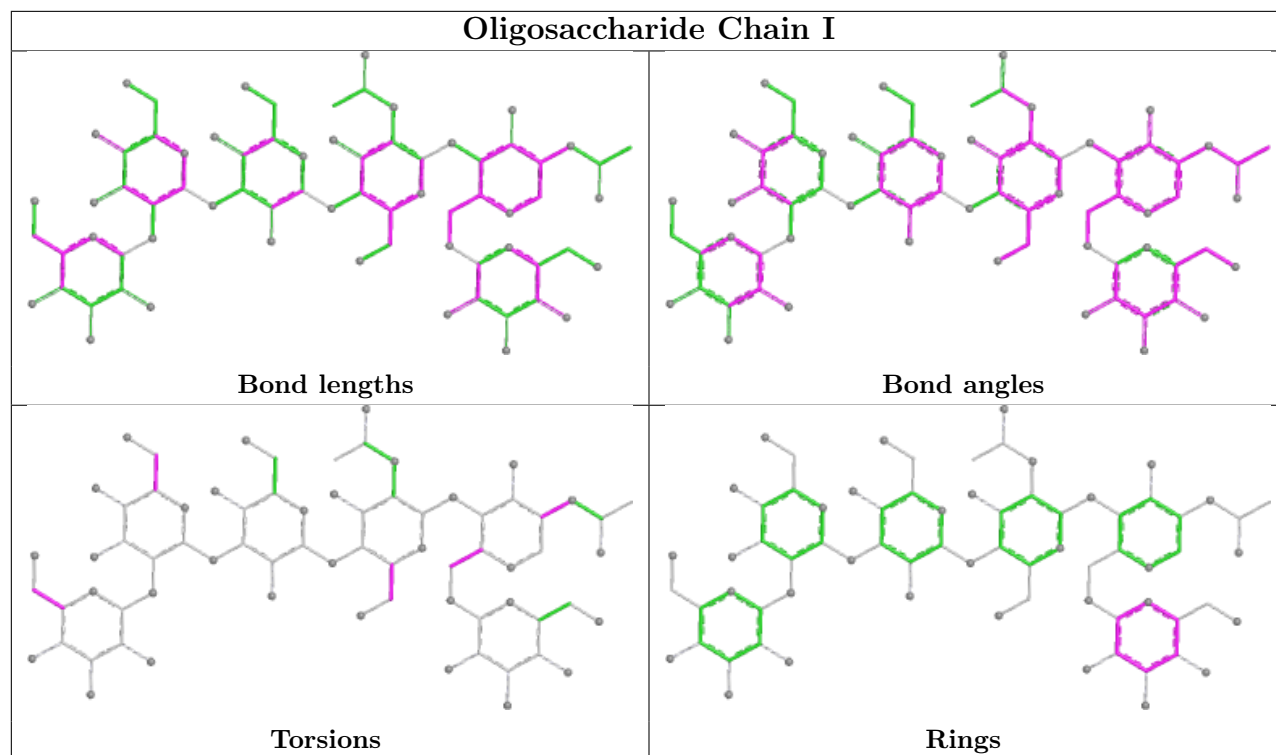












5.6 Ligand geometry

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	ST1	A	471	-	17,17,17	1.99	5 (29%)	19,24,24	2.32	4 (21%)
7	ST1	B	471	-	17,17,17	1.99	5 (29%)	19,24,24	2.32	4 (21%)

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	ST1	A	471	-	-	4/10/12/12	0/1/1/1
7	ST1	B	471	-	-	4/10/12/12	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	471	ST1	C5-N5	-5.28	1.36	1.45
7	B	471	ST1	C5-N5	-5.28	1.36	1.45
7	A	471	ST1	C1-C'	-4.05	1.40	1.49
7	B	471	ST1	C1-C'	-4.05	1.40	1.49
7	A	471	ST1	ON2-N5	-2.22	1.20	1.35
7	B	471	ST1	ON2-N5	-2.22	1.20	1.35
7	A	471	ST1	C4-N4	-2.14	1.39	1.43
7	B	471	ST1	C4-N4	-2.14	1.39	1.43
7	A	471	ST1	C4-C5	-2.07	1.38	1.42
7	B	471	ST1	C4-C5	-2.07	1.38	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	471	ST1	C4-N4-C4'	-7.19	110.54	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	471	ST1	C4-N4-C4'	-7.19	110.54	122.82
7	A	471	ST1	ON1-N5-C5	-4.49	111.35	119.03
7	B	471	ST1	ON1-N5-C5	-4.49	111.35	119.03
7	A	471	ST1	CM4-C4'-N4	3.07	119.56	114.95
7	B	471	ST1	CM4-C4'-N4	3.07	119.56	114.95
7	A	471	ST1	C5-C4-N4	-2.37	119.07	123.20
7	B	471	ST1	C5-C4-N4	-2.37	119.07	123.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	471	ST1	O4'-C4'-N4-C4
7	A	471	ST1	CM4-C4'-N4-C4
7	B	471	ST1	O4'-C4'-N4-C4
7	B	471	ST1	CM4-C4'-N4-C4
7	A	471	ST1	C6-C5-N5-ON1
7	B	471	ST1	C6-C5-N5-ON1
7	A	471	ST1	C4-C5-N5-ON1
7	B	471	ST1	C4-C5-N5-ON1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	471	ST1	1	0
7	B	471	ST1	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/388 (100%)	0.74	30 (7%) 19 21	2, 7, 17, 33	0
1	B	388/388 (100%)	0.79	33 (8%) 16 17	2, 7, 17, 33	0
All	All	776/776 (100%)	0.77	63 (8%) 18 19	2, 7, 17, 33	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	VAL	4.6
1	A	346	THR	4.2
1	B	326	PRO	3.9
1	A	270	GLY	3.7
1	A	345	GLY	3.3
1	B	436	VAL	3.2
1	B	434	THR	3.2
1	A	385	THR	3.2
1	B	217	SER	3.1
1	A	186	GLY	3.1
1	A	336	ASN	3.0
1	A	464	ILE	3.0
1	B	346	THR	2.9
1	A	317	VAL	2.8
1	A	404	SER	2.8
1	A	458	TRP	2.8
1	B	87	TRP	2.8
1	A	331	ARG	2.8
1	B	416	SER	2.7
1	B	412	VAL	2.7
1	B	245	SER	2.7
1	A	384	SER	2.6
1	A	469	ILE	2.6
1	B	124	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	2.6
1	B	86	ASN	2.6
1	A	446	PHE	2.5
1	B	246	ALA	2.5
1	B	345	GLY	2.5
1	A	245	SER	2.5
1	A	418	ILE	2.5
1	A	326	PRO	2.5
1	B	468	PRO	2.5
1	B	320	GLY	2.4
1	A	87	TRP	2.4
1	B	414	GLY	2.4
1	B	193	CYS	2.4
1	A	434	THR	2.4
1	A	332	SER	2.4
1	B	409	ILE	2.3
1	B	383	TRP	2.3
1	A	433	GLU	2.3
1	A	436	VAL	2.3
1	A	297	GLY	2.2
1	B	405	GLY	2.2
1	B	133	ALA	2.2
1	B	151	ASP	2.2
1	B	433	GLU	2.2
1	B	134	LEU	2.2
1	B	322	VAL	2.2
1	A	244	GLY	2.2
1	B	83	GLU	2.1
1	B	349	VAL	2.1
1	A	117	THR	2.1
1	B	126	PRO	2.1
1	B	391	GLN	2.1
1	B	106	ILE	2.0
1	A	423	TYR	2.0
1	A	139	THR	2.0
1	A	383	TRP	2.0
1	A	437	TRP	2.0
1	A	200	ASN	2.0
1	B	445	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

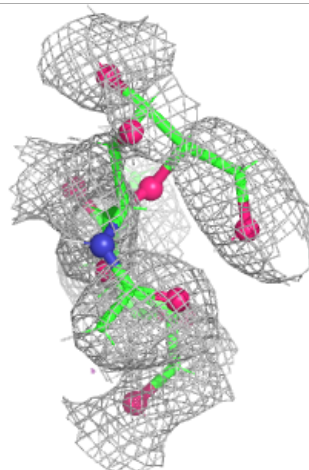
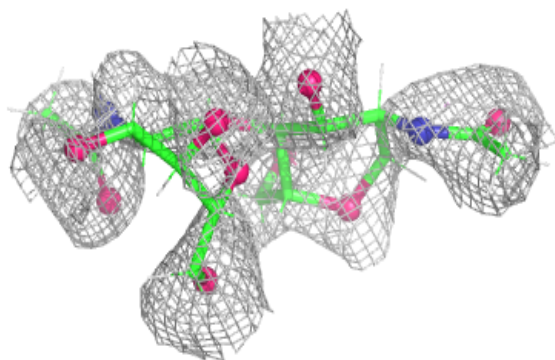
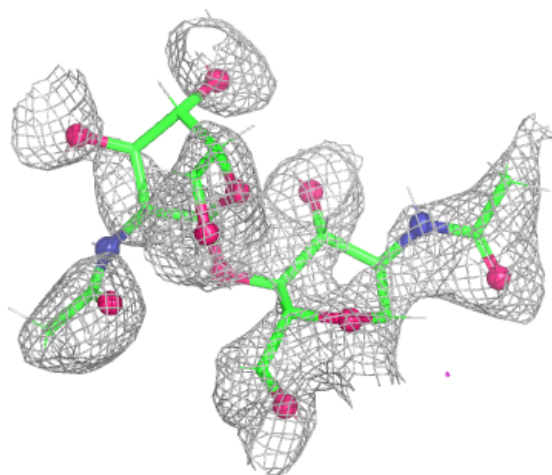
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	H	3	11/12	0.42	0.15	0,0,18,25	0
4	NAG	I	1	14/15	0.50	0.17	0,2,14,17	0
5	NAG	H	1	14/15	0.56	0.14	0,6,19,22	0
3	BMA	D	3	11/12	0.61	0.18	0,0,18,25	0
4	MAN	I	5	11/12	0.65	0.12	0,0,26,30	0
3	NAG	D	2	14/15	0.67	0.15	0,0,35,38	0
3	NAG	D	1	14/15	0.67	0.13	0,6,19,22	0
5	FUC	H	4	10/11	0.68	0.16	0,0,17,21	0
5	NAG	H	2	14/15	0.71	0.14	0,0,35,38	0
4	MAN	E	5	11/12	0.75	0.14	0,0,26,30	0
4	BMA	E	3	11/12	0.77	0.14	0,0,27,29	0
4	MAN	I	4	11/12	0.78	0.10	0,0,22,25	0
2	NAG	G	1	14/15	0.79	0.14	0,0,12,16	0
4	MAN	E	6	11/12	0.79	0.12	0,0,19,20	0
4	MAN	E	4	11/12	0.79	0.16	0,0,22,25	0
2	NAG	C	2	14/15	0.80	0.15	0,0,21,22	0
2	NAG	G	2	14/15	0.81	0.15	0,0,21,22	0
4	NAG	E	1	14/15	0.82	0.11	0,2,14,17	0
4	BMA	I	3	11/12	0.83	0.10	0,0,27,29	0
4	NAG	I	2	14/15	0.84	0.13	0,0,22,23	0
4	NAG	E	2	14/15	0.84	0.17	0,0,22,23	0
2	NAG	F	2	14/15	0.84	0.14	0,0,9,14	0
2	NAG	J	2	14/15	0.84	0.11	0,0,9,14	0
3	FUL	D	4	10/11	0.85	0.11	0,0,17,21	0
2	NAG	F	1	14/15	0.85	0.12	0,0,12,16	0
4	MAN	I	6	11/12	0.86	0.09	0,0,19,20	0
2	NAG	J	1	14/15	0.88	0.13	0,0,12,16	0
2	NAG	C	1	14/15	0.89	0.09	0,0,12,16	0

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

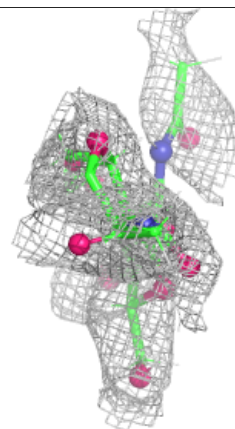
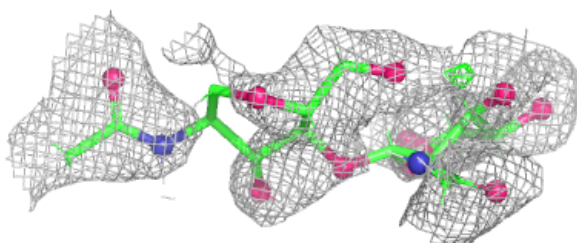
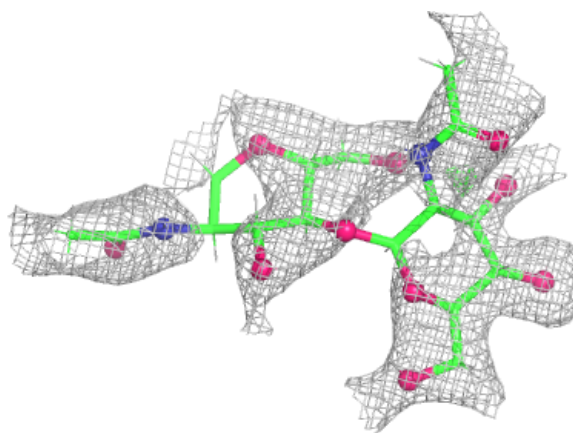
Electron density around Chain C:

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



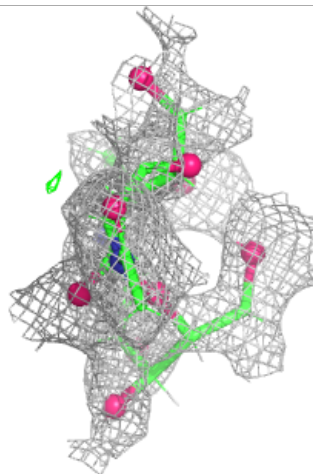
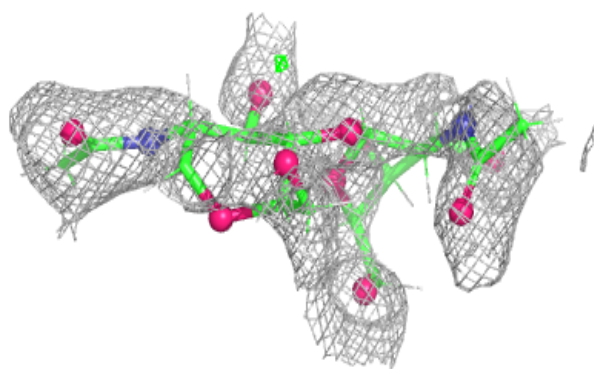
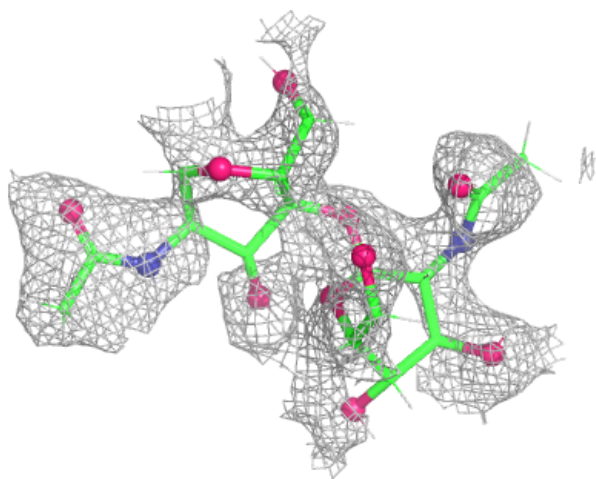
Electron density around Chain F:

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



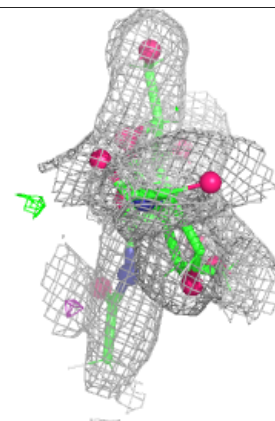
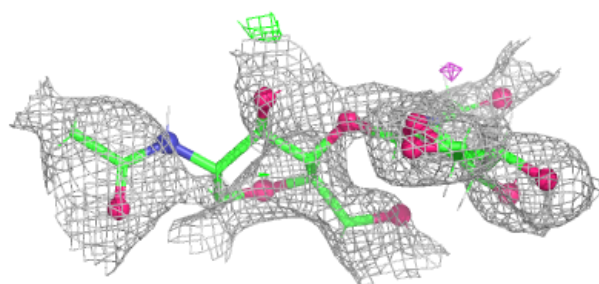
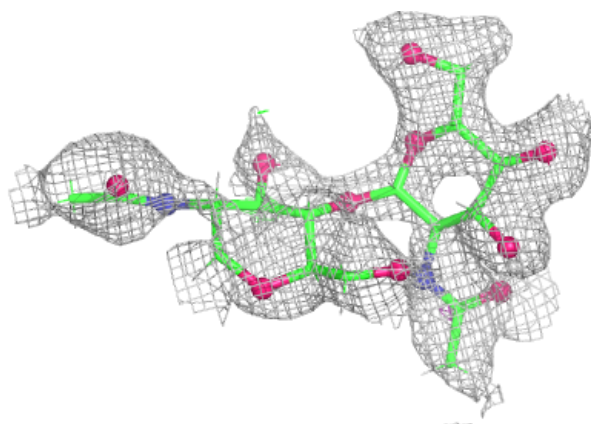
Electron density around Chain G:

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



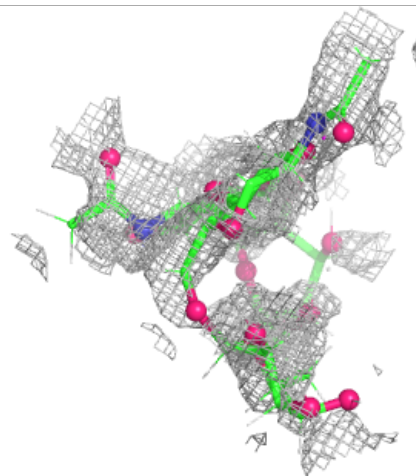
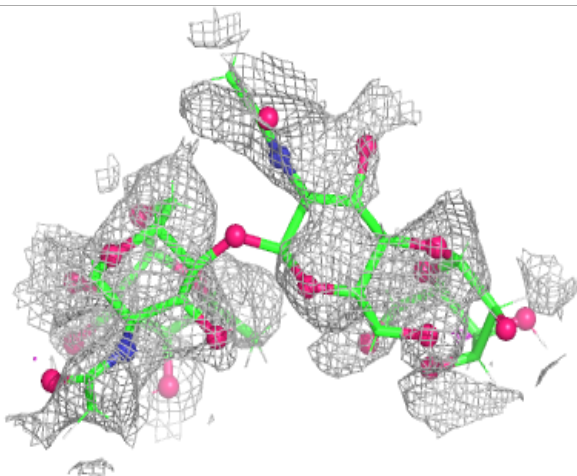
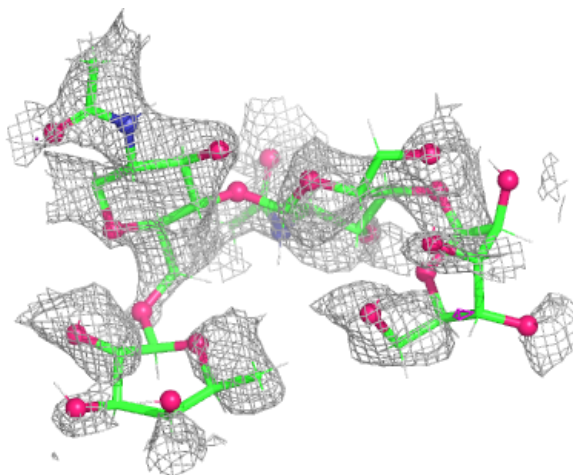
Electron density around Chain J:

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



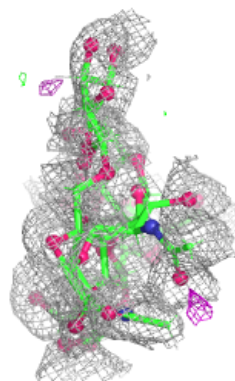
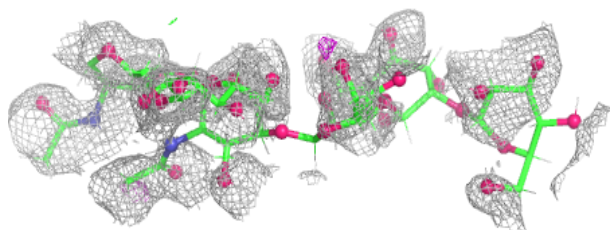
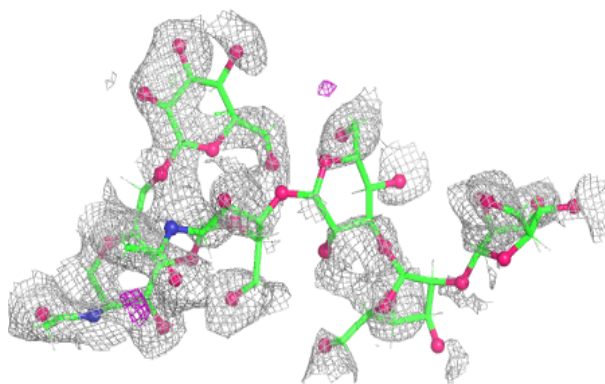
Electron density around Chain D:

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

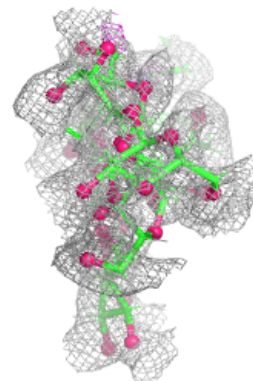
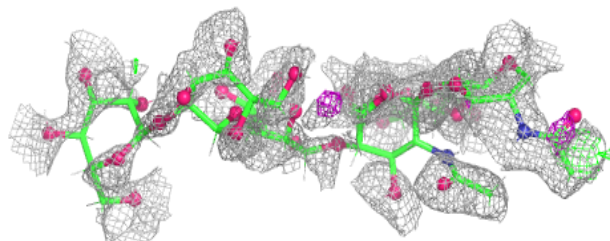
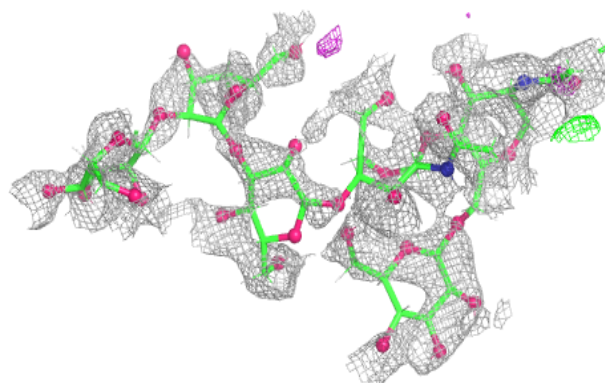


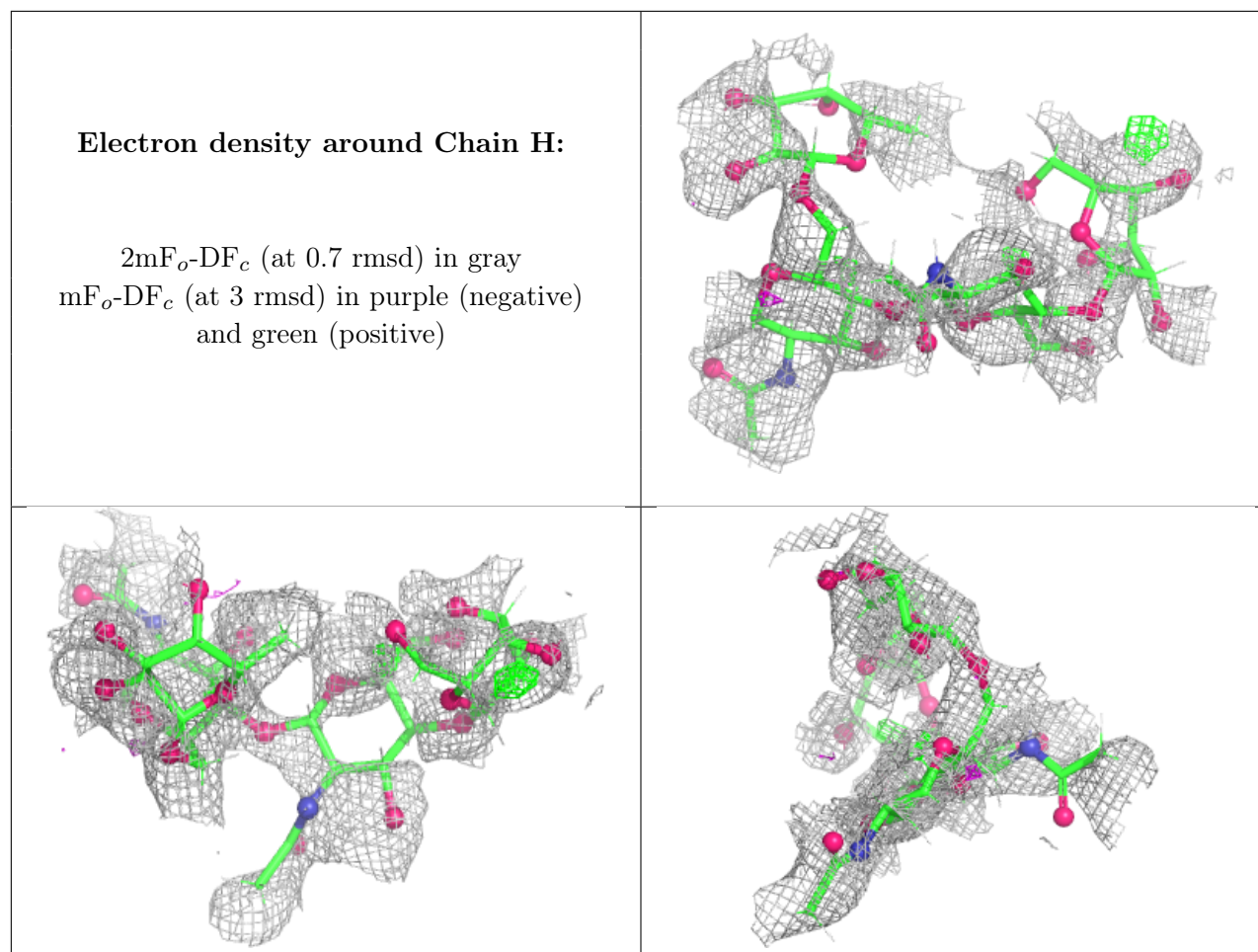
Electron density around Chain E:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CA	B	470	1/1	0.72	0.07	15,15,15,15	0
7	ST1	B	471	17/17	0.85	0.10	0,10,19,22	0
7	ST1	A	471	17/17	0.88	0.12	0,10,19,22	0
6	CA	A	470	1/1	0.92	0.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.