WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2023 – 12:49 PM EDT

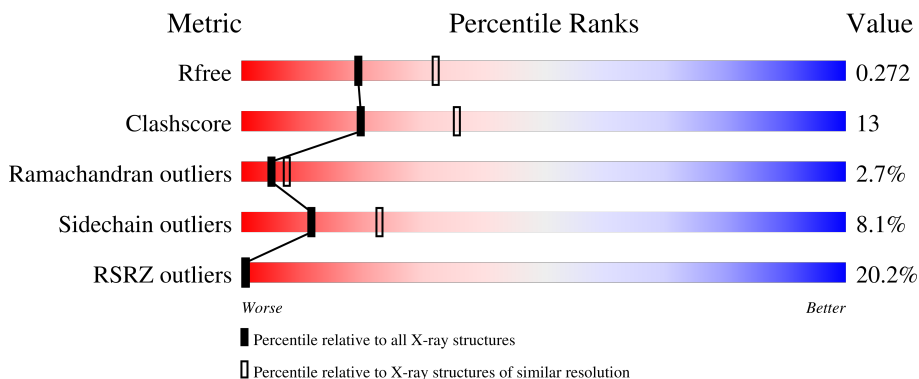|		
PDB ID	:	3BT2
Title	:	Structure of urokinase receptor, urokinase and vitronectin complex
Authors	:	Huang, M.
Deposited on	:	2007-12-27
Resolution	:	2.50 Å(reported)

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
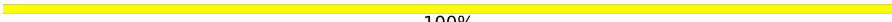
Metric	Percentile Ranks	Value
Rfree		0.272
Clashscore		13
Ramachandran outliers		2.7%
Sidechain outliers		8.1%
RSRZ outliers		20.2%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	135	34% / 65% 23% • 8%
2	B	40	98% / 70% 25% 5%
3	L	212	5% / 77% 19% •
4	H	214	6% / 86% 11% ••
5	U	283	22% / 64% 21% 6% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	C	2	100%
6	D	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	D	1	-	-	X	-
6	NAG	D	2	-	-	X	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6654 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			980	603	186	177	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP P00749
A	0	SER	-	expression tag	UNP P00749

- Molecule 2 is a protein called Vitronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	S	0	0	0
			312	185	51	68	8			

- Molecule 3 is a protein called anti-uPAR antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1628	1020	268	333	7			

- Molecule 4 is a protein called anti-uPAR antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	212	Total	C	N	O	S	0	0	0
			1617	1035	262	314	6			

- Molecule 5 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	259	Total	C	N	O	S	0	0	0
			1990	1192	366	398	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	0	ARG	-	expression tag	UNP Q03405
U	1A	SER	-	expression tag	UNP Q03405

- Molecule 6 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
6	C	2	Total 28	C 16	N 2	O 10	0	0	0
6	D	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
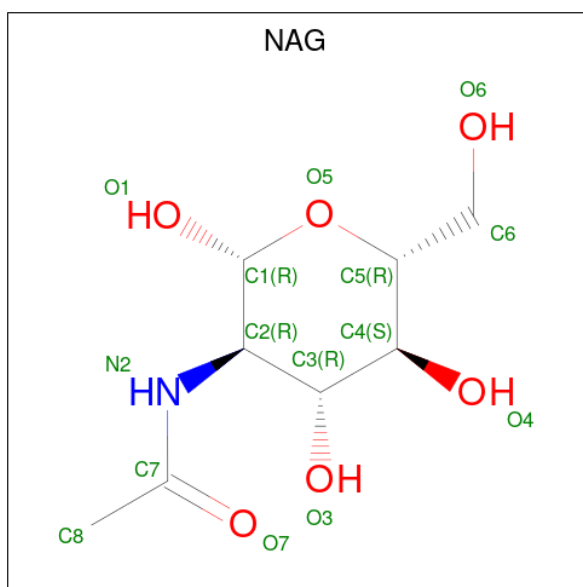
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	U	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	O 4	0	0
8	L	20	Total 20	O 20	0	0
8	H	26	Total 26	O 26	0	0
8	U	7	Total 7	O 7	0	0

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: Urokinase-type plasminogen activator
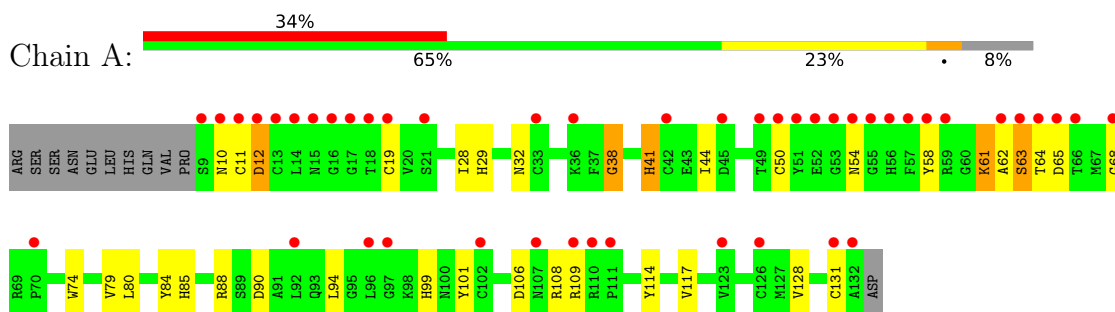
- Molecule 2: Vitronectin
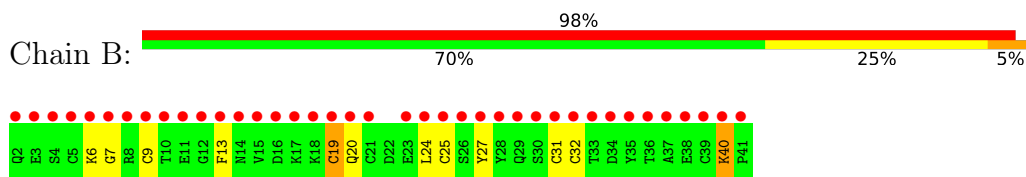
- Molecule 3: anti-uPAR antibody, light chain

- Molecule 4: anti-uPAR antibody, heavy chain

S198 T199 A208 GLY

• Molecule 5: Urokinase plasminogen activator surface receptor
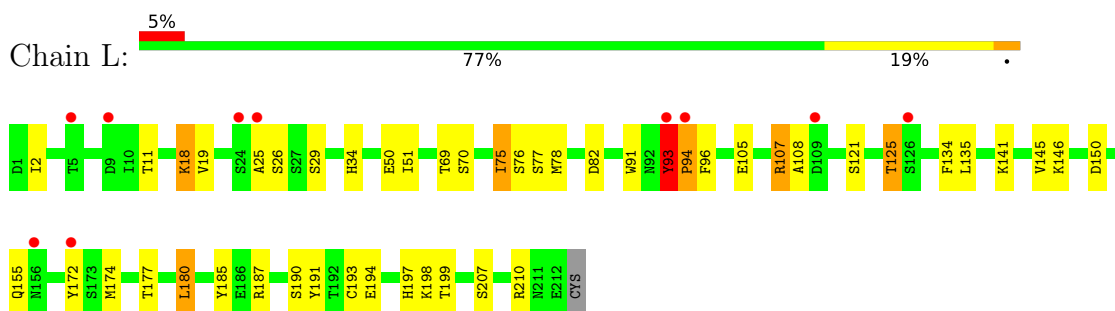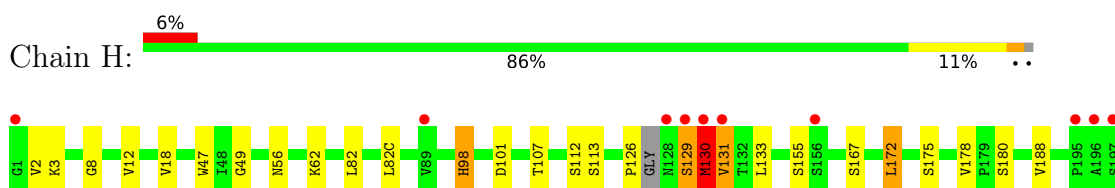
Chain U:

ARG S1A L1 R2 C3 M4 Q5 C6 K7 G10 D11 C12 R13 V14 L23 C24 T27 I28 V29 R30 L31 W32 E33 E34 G35 E36 L40 K43 S44 H47 S48 T54 L55 R58 T59 K62 I63 T64 S65 L66 T67 E68 V69 V70 C71 G72 L73 D74 L75 N80

SER GLY ARG ALA VAL THR Y87 S88 R89 S90 R91 Y92 L93 S100 S101 D102 M103 S104 C105 L113 Q114 C115 R116 L123 D124 V125 V126 T127 H128 W129 I130 GLN GLU GLY GLU GLY ARG PRO K139 H143 L144 Y149 L150 P151 G152 C153 P154 G155 N161 C170 C171

E183 Q189 R192 Y195 G199 G204 C205 S206 S207 E208 L212 I213 D214 C215 M219 C222 L223 V224 G227 T228 H229 E230 P231 K232 N233 Q234 S235 Y236 R239 M246 C247 Q248 HIS ALA HIS L252 G253 F256 S257 M258 N259 H260 I261 D262 V263 C266

C271 N272 H273 P274 D275 LEU ASP VAL GLN TYR ARG

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.10Å 87.20Å 124.27Å 90.00° 94.31° 90.00°	Depositor
Resolution (Å)	42.88 – 2.50 42.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.88-2.50) 99.2 (42.88-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.229 , 0.272 0.232 , 0.272	Depositor DCC
R_{free} test set	1191 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 64.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.77	2/1007 (0.2%)	0.77	3/1361 (0.2%)
2	B	0.41	0/316	0.68	1/421 (0.2%)
3	L	0.92	1/1668 (0.1%)	0.96	5/2267 (0.2%)
4	H	0.93	0/1667	0.82	2/2282 (0.1%)
5	U	0.90	6/2019 (0.3%)	0.86	4/2715 (0.1%)
All	All	0.88	9/6677 (0.1%)	0.86	15/9046 (0.2%)

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
2	B	1	0
4	H	0	1
5	U	0	1
All	All	1	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	183	GLU	CB-CG	13.87	1.78	1.52
5	U	7	LYS	C-O	10.18	1.42	1.23
1	A	38	GLY	C-O	8.25	1.36	1.23
3	L	193	CYS	CB-SG	-7.85	1.68	1.82
5	U	183	GLU	CD-OE2	6.97	1.33	1.25

The worst 5 of 15 bond angle outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	192	ARG	NE-CZ-NH2	-10.53	115.04	120.30
3	L	187	ARG	NE-CZ-NH2	-9.25	115.67	120.30
3	L	93	TYR	CB-CG-CD1	-7.71	116.37	121.00
3	L	187	ARG	NE-CZ-NH1	6.95	123.77	120.30
3	L	93	TYR	CB-CG-CD2	6.73	125.04	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	40	LYS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	LYS	Peptide
4	H	130	MET	Peptide
5	U	271	CYS	Peptide

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	980	0	911	28	0
2	B	312	0	272	5	0
3	L	1628	0	1554	32	0
4	H	1617	0	1558	20	0
5	U	1990	0	1856	74	0
6	C	28	0	25	0	0
6	D	28	0	25	12	0
7	U	14	0	13	0	0
8	A	4	0	0	0	0
8	H	26	0	0	0	0
8	L	20	0	0	1	0
8	U	7	0	0	0	0
All	All	6654	0	6214	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

The worst 5 of 162 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)
5:U:183:GLU:CB	5:U:183:GLU:CG	1.78	1.57
6:D:1:NAG:C3	6:D:2:NAG:H82	1.85	1.07
5:U:128:HIS:NE2	5:U:183:GLU:OE2	1.92	1.02
5:U:116:ARG:CZ	5:U:116:ARG:HB2	1.86	1.02
4:H:131:VAL:CG1	4:H:178:VAL:O	2.12	0.98

There are no symmetry-related clashes.

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	122/135 (90%)	104 (85%)	15 (12%)	3 (2%)	5	8
2	B	38/40 (95%)	28 (74%)	6 (16%)	4 (10%)	0	0
3	L	209/212 (99%)	195 (93%)	9 (4%)	5 (2%)	6	9
4	H	208/214 (97%)	200 (96%)	5 (2%)	3 (1%)	11	20
5	U	251/283 (89%)	229 (91%)	15 (6%)	7 (3%)	5	7
All	All	828/884 (94%)	756 (91%)	50 (6%)	22 (3%)	5	7

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	40	LYS
3	L	2	ILE
3	L	93	TYR
4	H	129	SER

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	108/119 (91%)	99 (92%)	9 (8%)	11	22
2	B	37/37 (100%)	33 (89%)	4 (11%)	6	12
3	L	185/186 (100%)	173 (94%)	12 (6%)	17	33
4	H	182/182 (100%)	169 (93%)	13 (7%)	14	28
5	U	232/251 (92%)	210 (90%)	22 (10%)	8	17
All	All	744/775 (96%)	684 (92%)	60 (8%)	11	23

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	62	LYS
5	U	189	GLN
4	H	167	SER
5	U	153	CYS
5	U	246	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
5	U	189	GLN
5	U	272	ASN
5	U	229	HIS
4	H	52(A)	HIS
5	U	166	HIS

5.3.3 RNA (i)

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 ⓘ

4 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	$\#|Z| > 2$
6	NAG	C	1	5,6	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
6	NAG	C	2	6	14,14,15	0.47	0	17,19,21	1.75	5 (29%)
6	NAG	D	1	5,6	14,14,15	0.57	0	17,19,21	3.08	7 (41%)
6	NAG	D	2	6	14,14,15	0.57	0	17,19,21	3.08	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	4/6/23/26	0/1/1/1
6	NAG	D	1	5,6	-	4/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1	NAG	C4-C3-C2	-6.59	101.36	111.02
6	D	2	NAG	C4-C3-C2	-6.58	101.38	111.02
6	D	1	NAG	C1-O5-C5	6.54	121.05	112.19
6	D	2	NAG	C1-O5-C5	6.54	121.05	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	2	NAG	O4-C4-C5	4.59	120.69	109.30

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
6	C	1	NAG	C4-C5-C6-O6
6	C	1	NAG	O5-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	C	2	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2	NAG	12	0
6	D	1	NAG	12	0

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

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths | Bond angles
Torsions | Rings
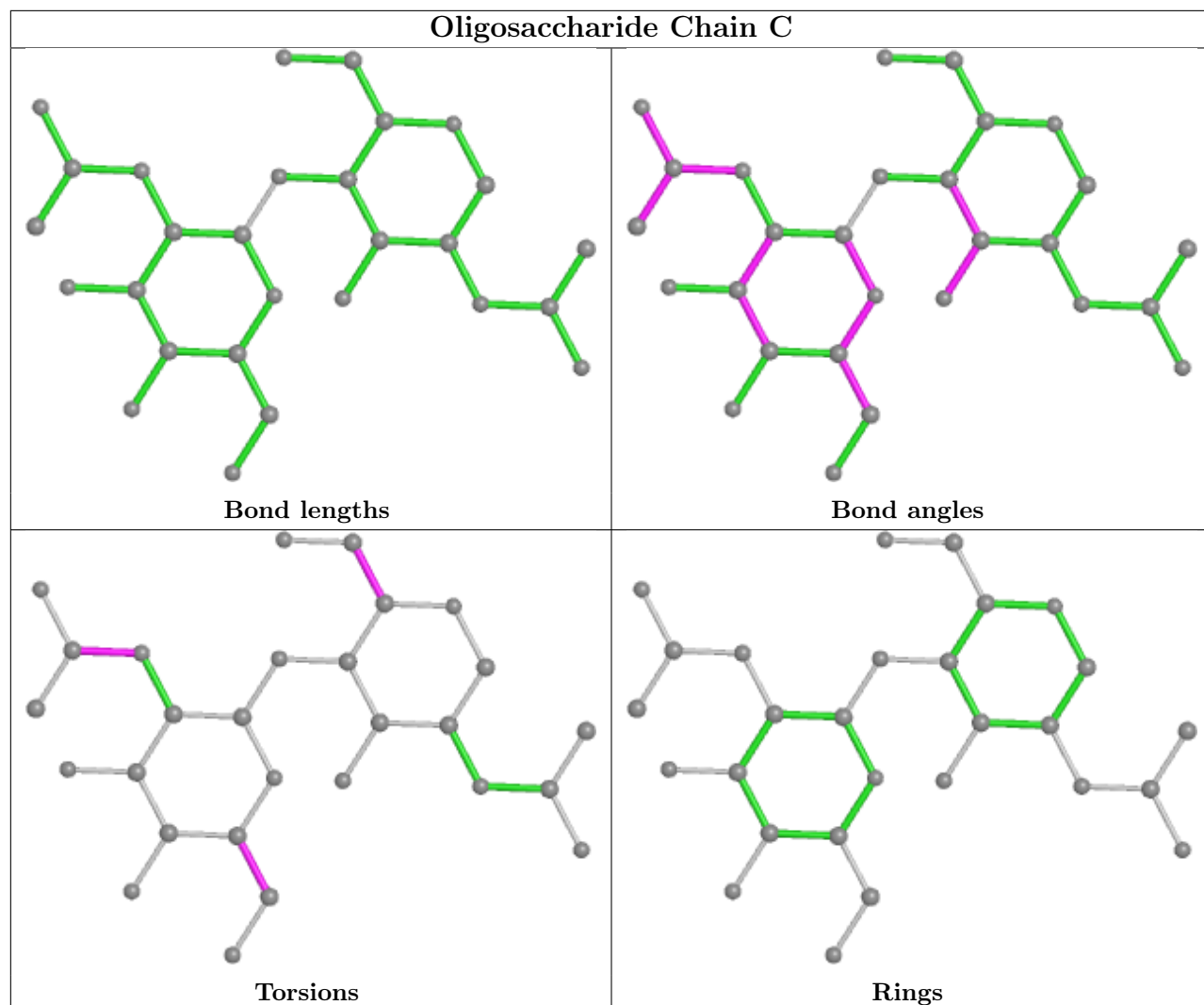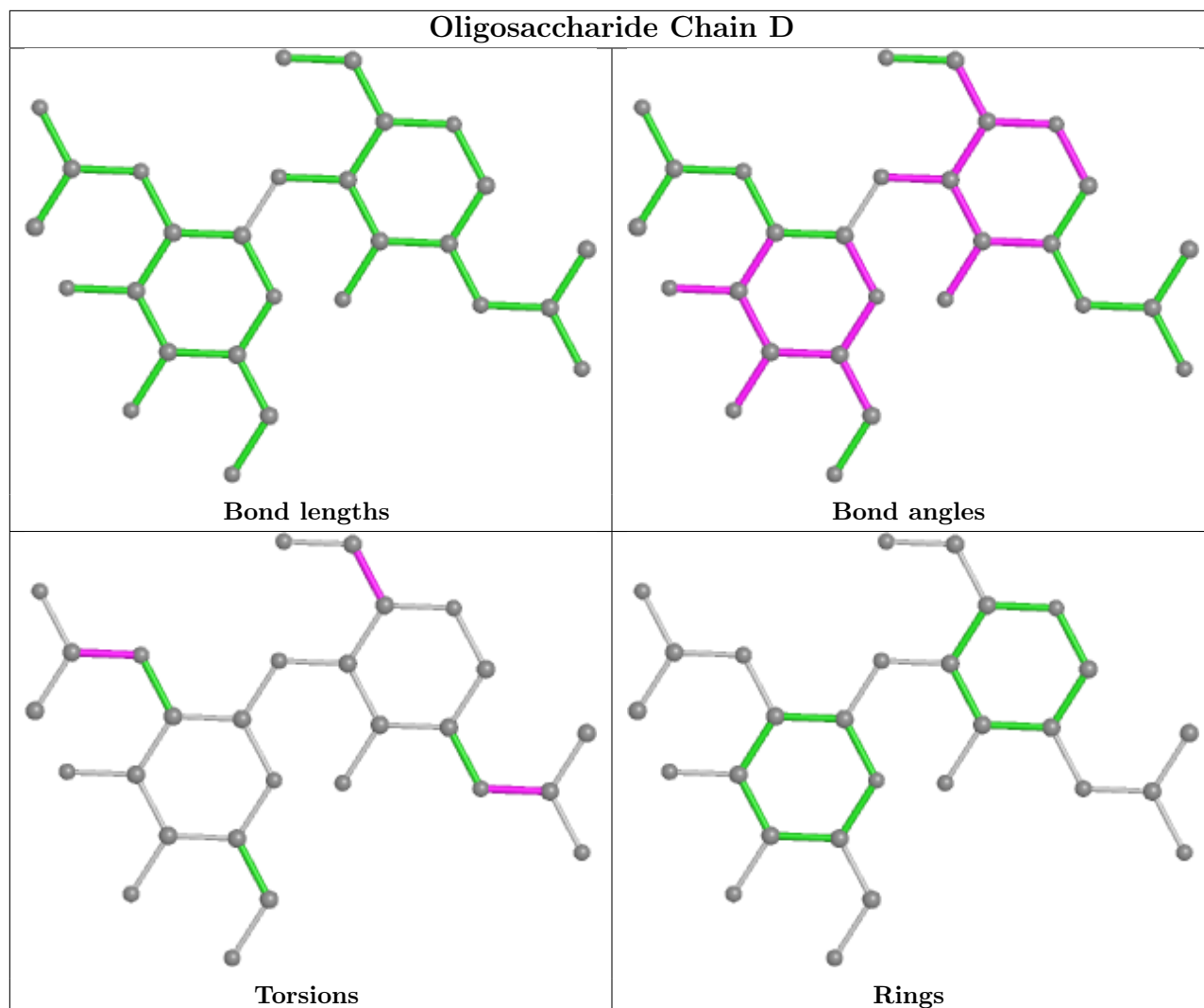
5.6 Ligand geometry (i)

1 ligand is 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	$\#|Z| > 2$
7	NAG	U	1052	5	14,14,15	0.54	0	17,19,21	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	U	1052	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	1052	NAG	C1-O5-C5	3.88	117.45	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	U	1052	NAG	C8-C7-N2-C2
7	U	1052	NAG	O7-C7-N2-C2
7	U	1052	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	124/135 (91%)	2.10	46 (37%)	0	0	63, 74, 81, 83	0
2	B	40/40 (100%)	6.40	39 (97%)	0	0	84, 88, 89, 89	40 (100%)
3	L	211/212 (99%)	0.90	10 (4%)	31	33	51, 68, 80, 86	0
4	H	212/214 (99%)	0.95	13 (6%)	21	22	59, 70, 83, 88	0
5	U	259/283 (91%)	1.51	63 (24%)	0	0	57, 74, 91, 102	0
All	All	846/884 (95%)	1.53	171 (20%)	1	0	51, 72, 87, 102	40 (4%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	9	CYS	15.0
2	B	40	LYS	12.9
2	B	32	CYS	11.6
2	B	11	GLU	10.7
2	B	41	PRO	10.2

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.
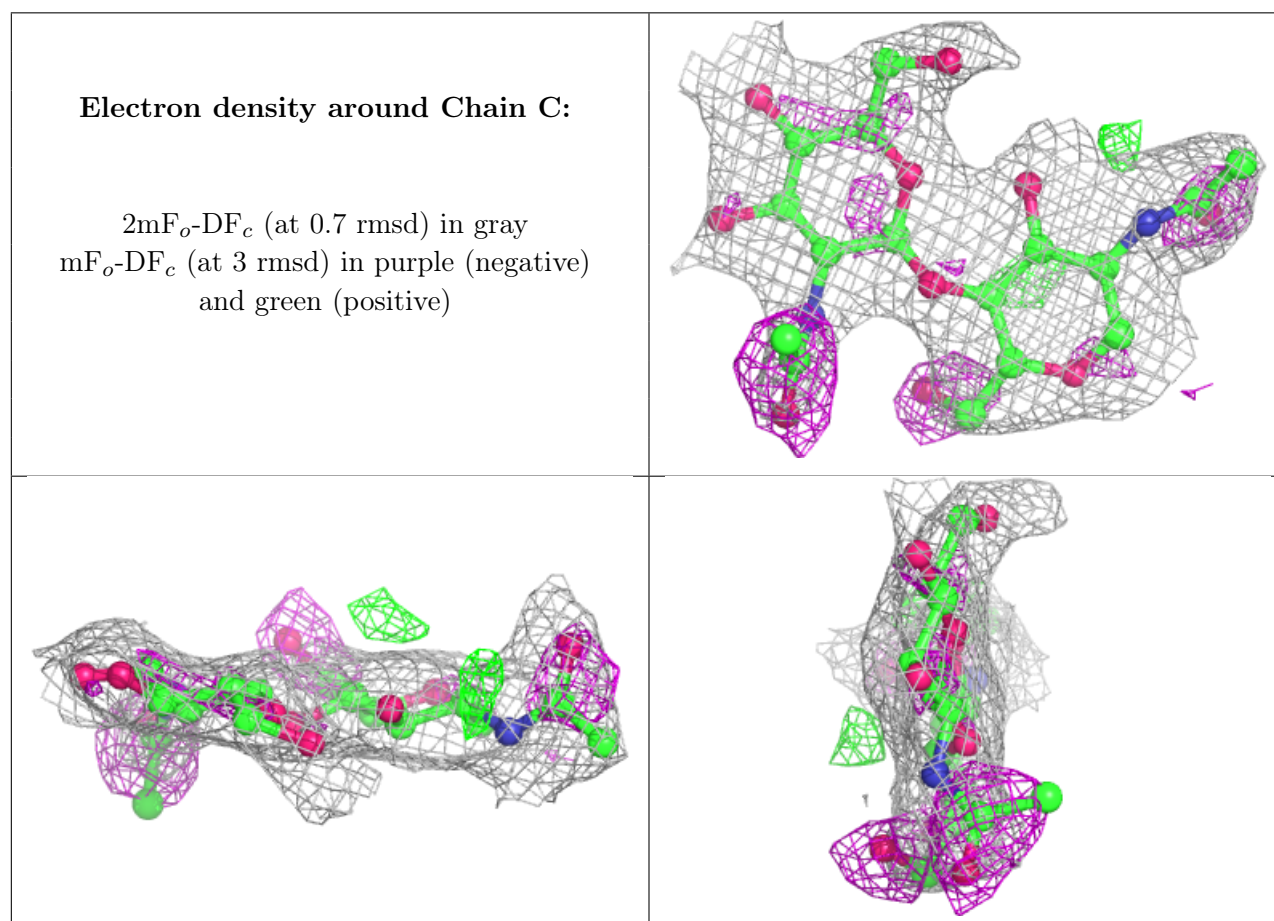
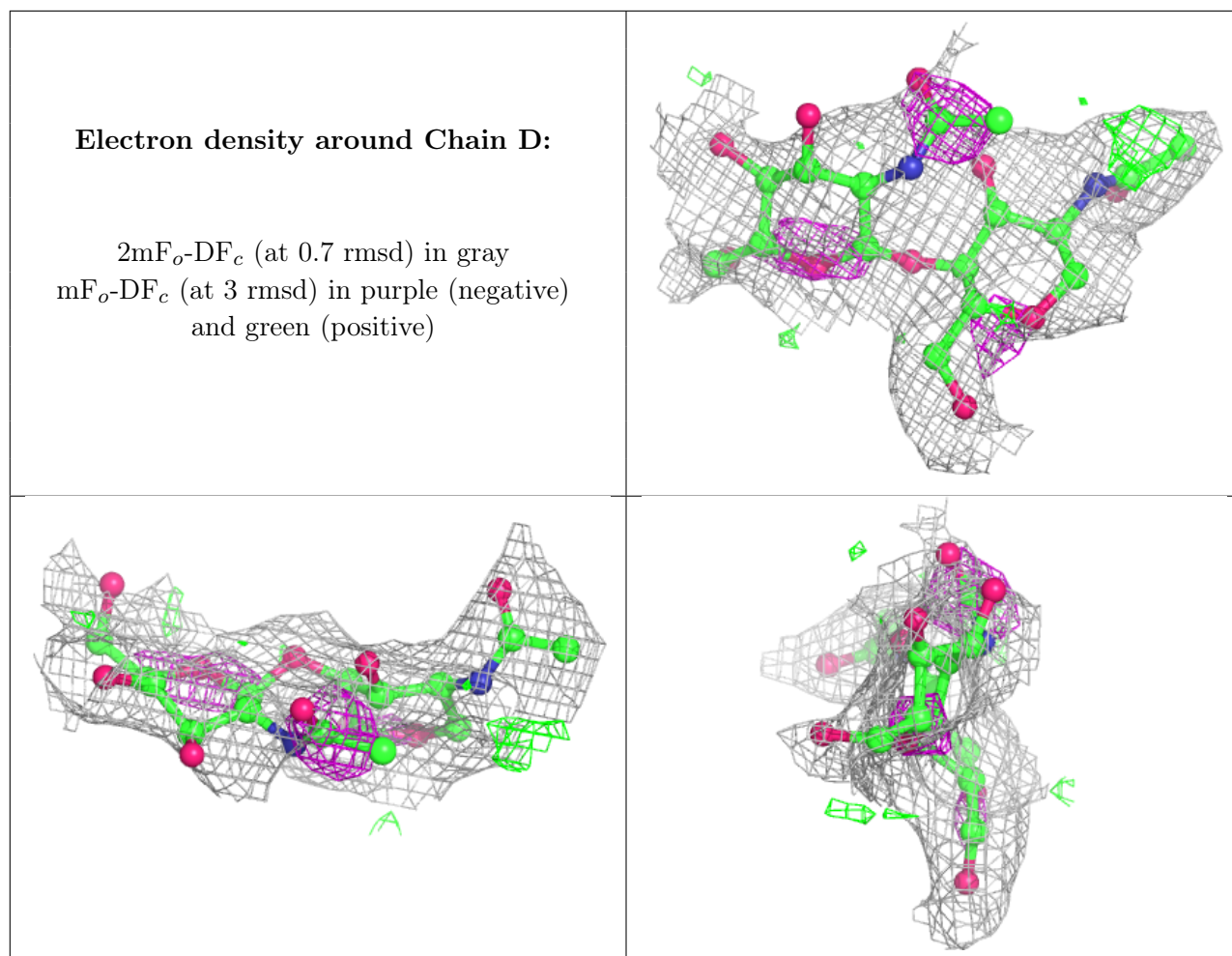| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	D	2	14/15	0.69	0.48	92,96,98,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	D	1	14/15	0.70	0.28	82,86,88,91	0
6	NAG	C	2	14/15	0.84	0.46	74,77,79,80	0
6	NAG	C	1	14/15	0.91	0.30	65,70,72,74	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 D:

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

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	U	1052	14/15	0.66	0.39	83,85,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.