Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 06:36 PM EST

PDB ID : 8FYZ
Title : Crystal structure of human PARP1 ART domain bound to inhibitor UKTT10 (compound 13)
Authors : Rouleau-Turcotte, E.; Pascal, J.M.
Deposited on : 2023-01-27
Resolution : 3.40 Å(reported)

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

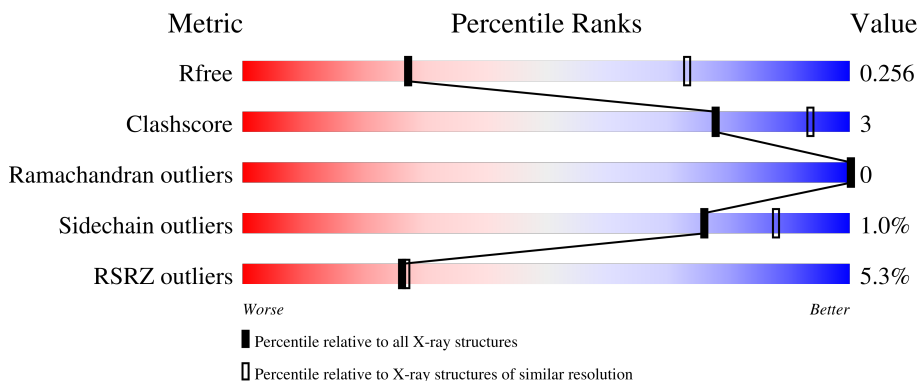|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		5.3%

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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	271	5% 79% 9% 13%
1	B	271	4% 80% 8% 12%
2	D	2	50% 50%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3857 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 Poly [ADP-ribose] polymerase 1, processed C-terminus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1861	1194	316	345	6			
1	B	238	Total	C	N	O	S	0	0	0
			1870	1200	318	346	6			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	742	MET	-	initiating methionine	UNP P09874
A	743	GLY	-	expression tag	UNP P09874
A	744	SER	-	expression tag	UNP P09874
A	745	SER	-	expression tag	UNP P09874
A	746	HIS	-	expression tag	UNP P09874
A	747	HIS	-	expression tag	UNP P09874
A	748	HIS	-	expression tag	UNP P09874
A	749	HIS	-	expression tag	UNP P09874
A	750	HIS	-	expression tag	UNP P09874
A	751	HIS	-	expression tag	UNP P09874
A	752	SER	-	expression tag	UNP P09874
A	753	SER	-	expression tag	UNP P09874
A	754	GLY	-	expression tag	UNP P09874
A	755	LEU	-	expression tag	UNP P09874
A	756	VAL	-	expression tag	UNP P09874
A	757	PRO	-	expression tag	UNP P09874
A	758	ARG	-	expression tag	UNP P09874
A	759	GLY	-	expression tag	UNP P09874
A	760	SER	-	expression tag	UNP P09874
A	761	HIS	-	expression tag	UNP P09874
A	762	MET	-	expression tag	UNP P09874
A	780	GLY	-	linker	UNP P09874
A	781	SER	-	linker	UNP P09874
A	782	GLY	-	linker	UNP P09874
A	783	SER	-	linker	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
A	784	GLY	-	linker	UNP P09874
A	785	SER	-	linker	UNP P09874
A	786	GLY	-	linker	UNP P09874
A	787	GLY	-	linker	UNP P09874
B	742	MET	-	initiating methionine	UNP P09874
B	743	GLY	-	expression tag	UNP P09874
B	744	SER	-	expression tag	UNP P09874
B	745	SER	-	expression tag	UNP P09874
B	746	HIS	-	expression tag	UNP P09874
B	747	HIS	-	expression tag	UNP P09874
B	748	HIS	-	expression tag	UNP P09874
B	749	HIS	-	expression tag	UNP P09874
B	750	HIS	-	expression tag	UNP P09874
B	751	HIS	-	expression tag	UNP P09874
B	752	SER	-	expression tag	UNP P09874
B	753	SER	-	expression tag	UNP P09874
B	754	GLY	-	expression tag	UNP P09874
B	755	LEU	-	expression tag	UNP P09874
B	756	VAL	-	expression tag	UNP P09874
B	757	PRO	-	expression tag	UNP P09874
B	758	ARG	-	expression tag	UNP P09874
B	759	GLY	-	expression tag	UNP P09874
B	760	SER	-	expression tag	UNP P09874
B	761	HIS	-	expression tag	UNP P09874
B	762	MET	-	expression tag	UNP P09874
B	780	GLY	-	linker	UNP P09874
B	781	SER	-	linker	UNP P09874
B	782	GLY	-	linker	UNP P09874
B	783	SER	-	linker	UNP P09874
B	784	GLY	-	linker	UNP P09874
B	785	SER	-	linker	UNP P09874
B	786	GLY	-	linker	UNP P09874
B	787	GLY	-	linker	UNP P09874

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.
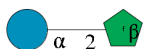
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total 23	C 12	O 11	0	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	B	1	Total 4	C 2	O 1	S 1	0	0
3	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0

- Molecule 5 is (2P)-2-{3-[(4R)-3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[4,3-a]pyrazine-7(8H)-carbonyl]phenyl}-1H-benzimidazole-4-carboxamide (three-letter code: YNQ) (formula: $C_{21}H_{16}F_3N_7O_2$) (labeled as "Ligand of Interest" by depositor).
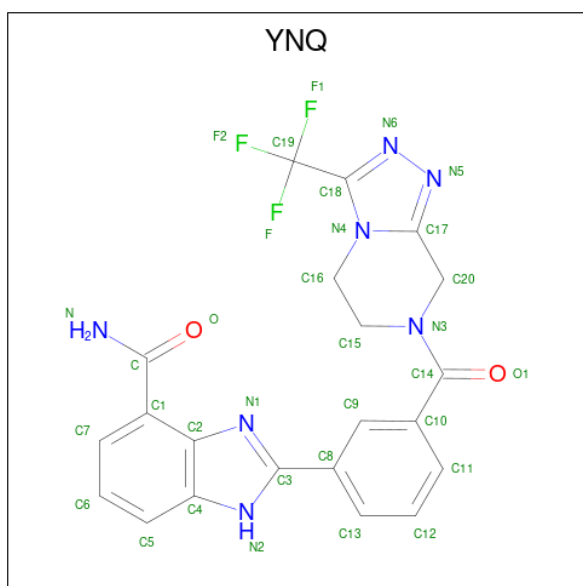
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 33	C 21	F 3	N 7	O 2	0	0
5	B	1	Total 33	C 21	F 3	N 7	O 2	0	0

• Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	O 4	0	0
6	B	4	Total 4	O 4	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: Poly [ADP-ribose] polymerase 1, processed C-terminus

Chain A:

- Molecule 1: Poly [ADP-ribose] polymerase 1, processed C-terminus

Chain B:
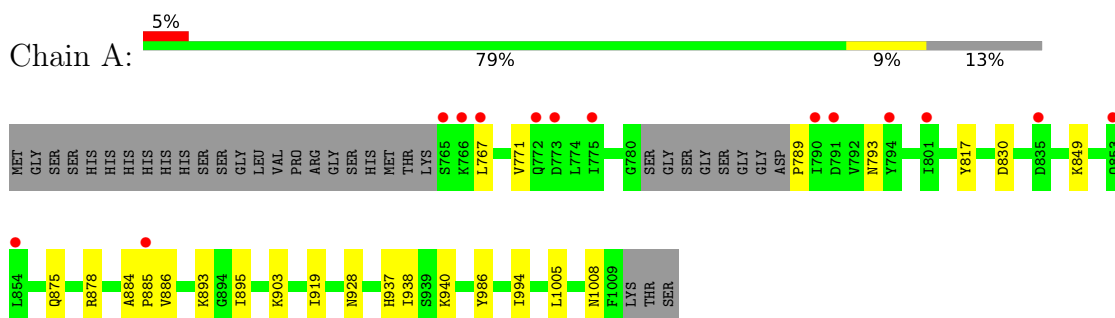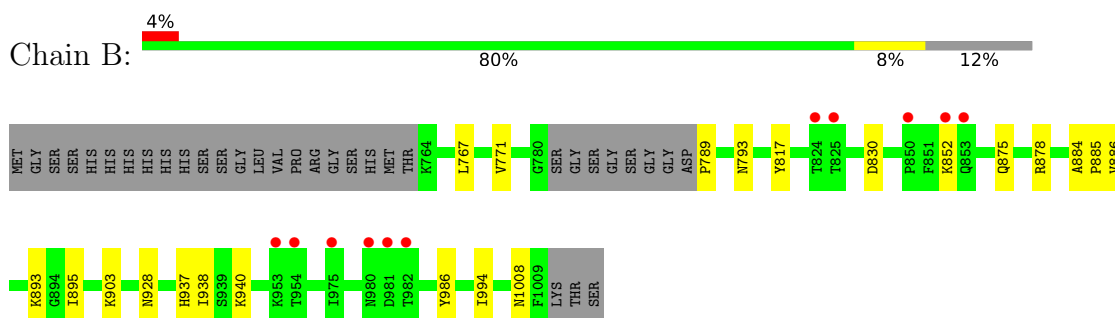
- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	95.88Å 95.88Å 130.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.94 – 3.40 47.94 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.94-3.40) 99.0 (47.94-3.40)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.267 0.218 , 0.256	Depositor DCC
R_{free} test set	457 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	71.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 98.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3857	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, DMS, GLC, YNQ, FRU

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	0.25	0/1901	0.47	0/2569
1	B	0.25	0/1910	0.47	0/2580
All	All	0.25	0/3811	0.47	0/5149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1861	0	1879	12	0
1	B	1870	0	1892	11	0
2	D	23	0	21	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	13	0	5	0	0
5	A	33	0	0	0	0
5	B	33	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	3857	0	3821	22	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 3.

All (22) 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:884:ALA:HB3	1:B:893:LYS:HE2	1.82	0.61
1:A:938:ILE:HG22	1:A:940:LYS:H	1.68	0.59
1:B:938:ILE:HG22	1:B:940:LYS:H	1.68	0.59
1:A:875:GLN:HB3	1:A:878:ARG:HE	1.70	0.56
1:A:884:ALA:HB3	1:A:893:LYS:HE2	1.86	0.56
1:B:875:GLN:HB3	1:B:878:ARG:HE	1.71	0.55
1:A:884:ALA:HB1	1:A:885:PRO:HD2	1.89	0.55
1:B:884:ALA:HB1	1:B:885:PRO:HD2	1.90	0.54
1:A:903:LYS:NZ	1:A:986:TYR:O	2.41	0.54
1:B:830:ASP:N	1:B:1008:ASN:O	2.41	0.53
1:B:903:LYS:NZ	1:B:986:TYR:O	2.42	0.53
1:A:830:ASP:N	1:A:1008:ASN:O	2.41	0.52
1:A:895:ILE:HD11	1:A:994:ILE:HG22	1.95	0.49
1:A:886:VAL:HG11	1:A:937:HIS:O	2.14	0.48
1:B:886:VAL:HG11	1:B:937:HIS:O	2.14	0.48
1:B:895:ILE:HD11	1:B:994:ILE:HG22	1.95	0.47
1:A:767:LEU:HD22	1:A:771:VAL:HG11	1.96	0.47
1:B:767:LEU:HD22	1:B:771:VAL:HG11	1.97	0.47
1:A:849:LYS:O	1:B:852:LYS:CB	2.67	0.42
1:A:789:PRO:O	1:A:793:ASN:ND2	2.54	0.41
1:B:789:PRO:O	1:B:793:ASN:ND2	2.55	0.40
1:A:919:ILE:HG21	1:A:1005:LEU:HD11	2.03	0.40

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	233/271 (86%)	223 (96%)	10 (4%)	0	100	100
1	B	234/271 (86%)	224 (96%)	10 (4%)	0	100	100
All	All	467/542 (86%)	447 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	204/233 (88%)	202 (99%)	2 (1%)	76	88
1	B	205/233 (88%)	203 (99%)	2 (1%)	76	88
All	All	409/466 (88%)	405 (99%)	4 (1%)	76	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	817	TYR
1	A	928	ASN
1	B	817	TYR
1	B	928	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 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	GLC	D	1	2	11,11,12	0.50	0	15,15,17	1.95	2 (13%)
2	FRU	D	2	2	11,12,12	0.57	0	10,18,18	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	1/2/19/22	0/1/1/1
2	FRU	D	2	2	-	2/5/24/24	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	GLC	C1-O5-C5	6.55	121.07	112.19
2	D	1	GLC	C2-C3-C4	-2.24	107.01	110.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	FRU	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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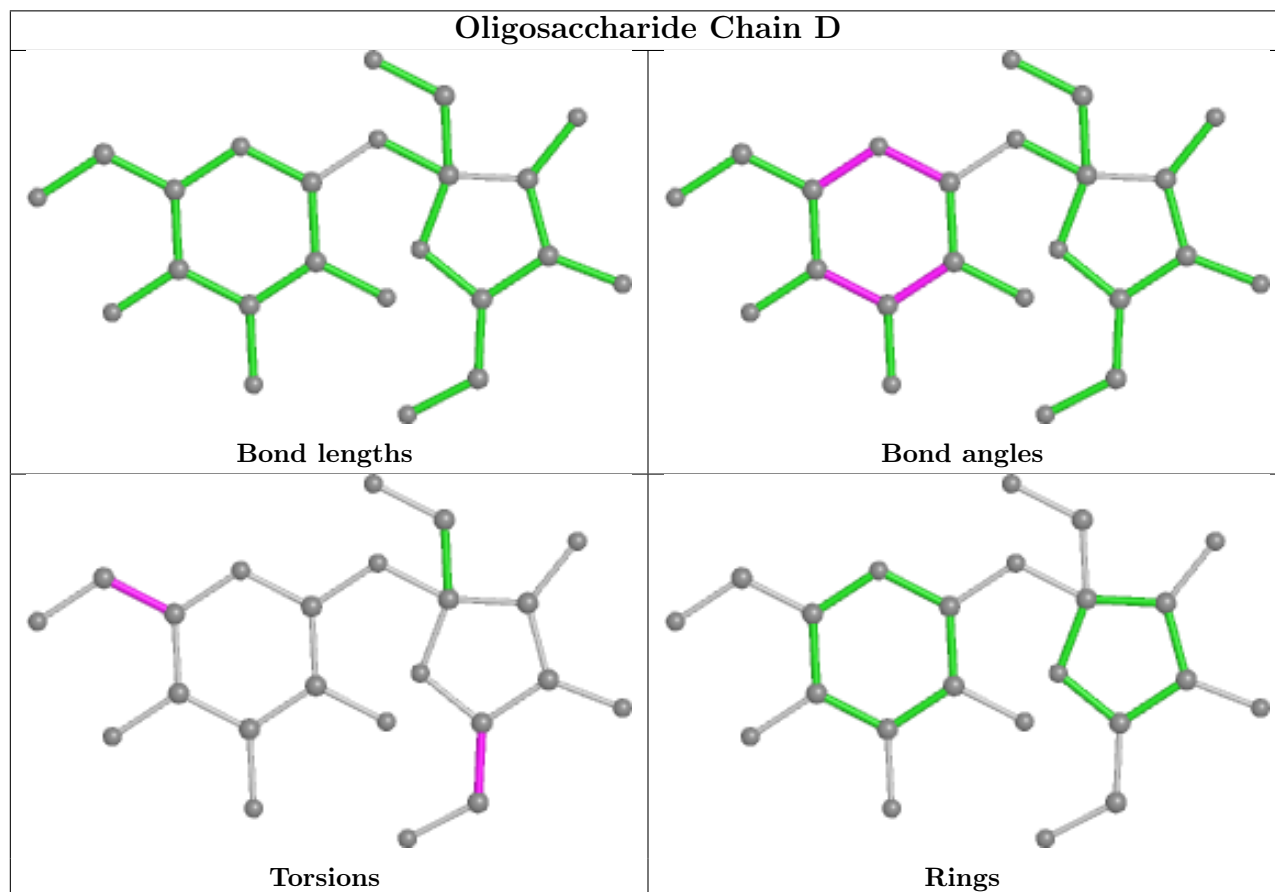
5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	DMS	A	1101	-	3,3,3	0.66	0	3,3,3	0.48	0
3	DMS	A	1102	-	3,3,3	0.65	0	3,3,3	0.43	0
3	DMS	B	1202	-	3,3,3	0.65	0	3,3,3	0.46	0
5	YNQ	A	1104	-	33,37,37	0.81	0	40,56,56	0.91	1 (2%)
3	DMS	B	1201	-	3,3,3	0.66	0	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	YNQ	B	1203	-	33,37,37	0.81	1 (3%)	40,56,56	0.89	1 (2%)
4	CIT	A	1103	-	12,12,12	1.01	0	17,17,17	1.53	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	YNQ	B	1203	-	-	5/22/31/31	0/4/5/5
5	YNQ	A	1104	-	-	7/22/31/31	0/4/5/5
4	CIT	A	1103	-	-	9/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1203	YNQ	C1-C2	-2.03	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	CIT	O6-C6-C3	3.91	119.85	113.05
5	A	1104	YNQ	C16-N4-C18	3.71	132.90	125.38
5	B	1203	YNQ	C16-N4-C18	3.53	132.54	125.38
4	A	1103	CIT	O2-C1-C2	2.18	121.36	114.35
4	A	1103	CIT	O4-C5-C4	2.02	120.83	114.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1103	CIT	C1-C2-C3-O7
4	A	1103	CIT	C1-C2-C3-C4
4	A	1103	CIT	C1-C2-C3-C6
4	A	1103	CIT	O7-C3-C6-O5
4	A	1103	CIT	O7-C3-C6-O6
4	A	1103	CIT	C4-C3-C6-O5
4	A	1103	CIT	C4-C3-C6-O6
5	A	1104	YNQ	O1-C14-N3-C15
5	A	1104	YNQ	C10-C14-N3-C15

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Mol	Chain	Res	Type	Atoms
5	A	1104	YNQ	O1-C14-N3-C20
5	A	1104	YNQ	C10-C14-N3-C20
5	B	1203	YNQ	C10-C14-N3-C15
5	B	1203	YNQ	O1-C14-N3-C20
5	B	1203	YNQ	O1-C14-N3-C15
5	B	1203	YNQ	C10-C14-N3-C20
4	A	1103	CIT	C2-C3-C6-O6
4	A	1103	CIT	C2-C3-C6-O5
5	A	1104	YNQ	N-C-C1-C2
5	A	1104	YNQ	O-C-C1-C2
5	B	1203	YNQ	N1-C3-C8-C13
5	A	1104	YNQ	N-C-C1-C7

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand YNQ A 1104

Bond lengths

Bond angles

Torsions

Rings

Ligand YNQ B 1203

Bond lengths

Bond angles

Torsions

Rings
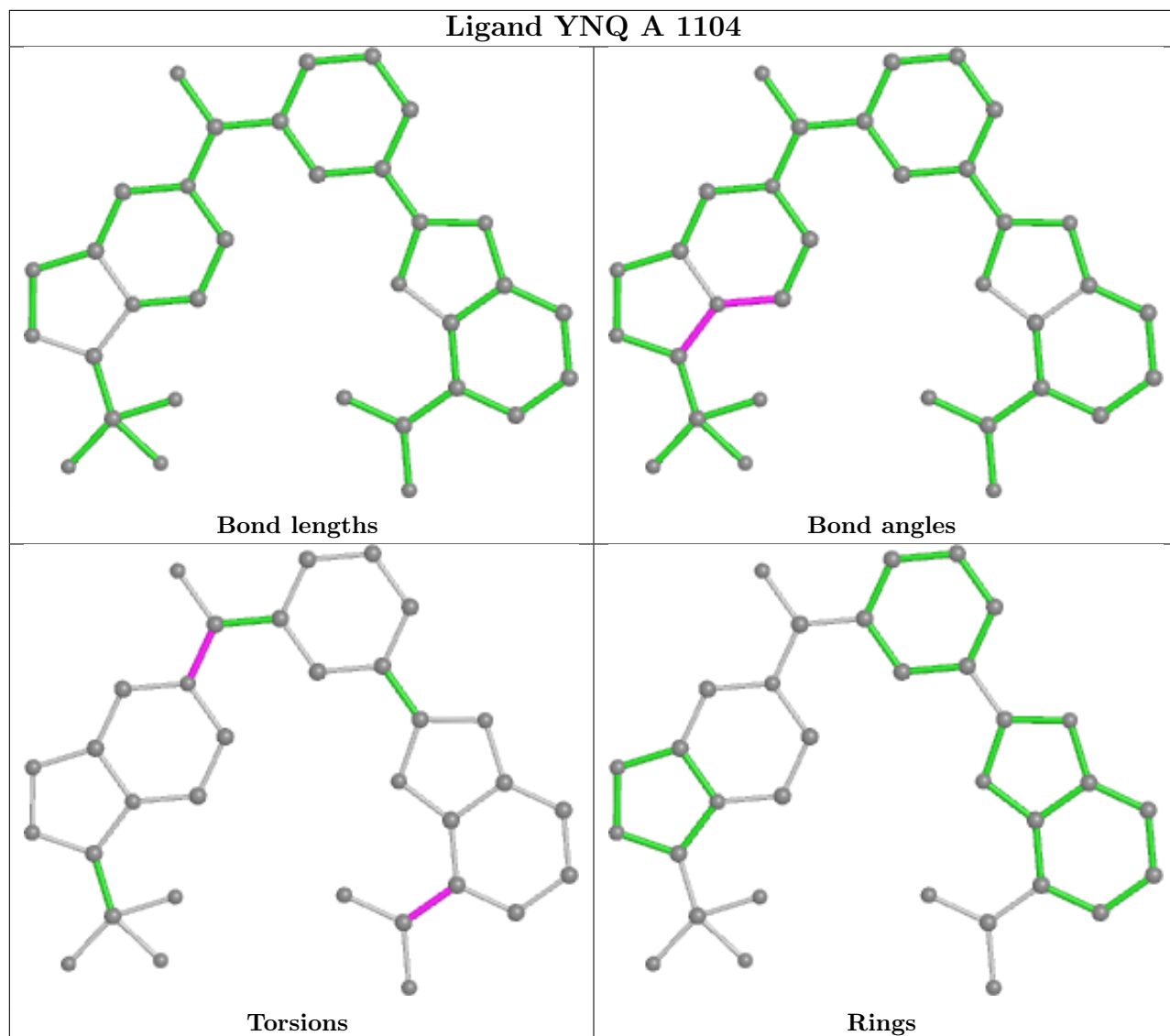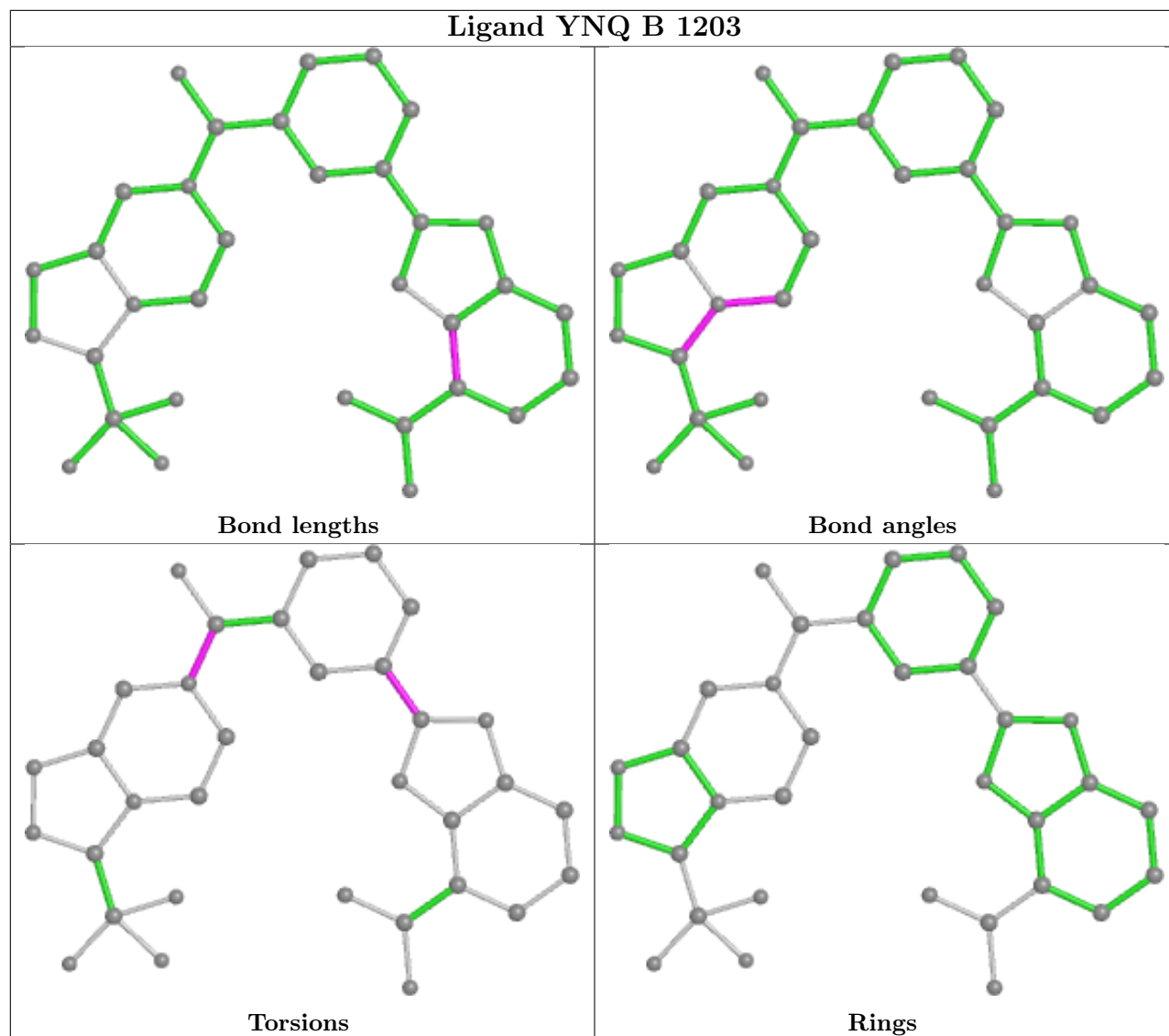
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	237/271 (87%)	0.58	14 (5%)	22	23	48, 73, 115, 159	0
1	B	238/271 (87%)	0.52	11 (4%)	32	32	51, 75, 114, 174	0
All	All	475/542 (87%)	0.55	25 (5%)	26	27	48, 74, 115, 174	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	853	GLN	6.2
1	B	852	LYS	4.6
1	B	980	ASN	4.1
1	A	853	GLN	3.8
1	B	981	ASP	3.7
1	A	772	GLN	3.5
1	A	765	SER	3.5
1	A	790	ILE	3.4
1	A	766	LYS	3.3
1	B	850	PRO	3.2
1	A	885	PRO	3.1
1	A	835	ASP	2.9
1	B	825	THR	2.8
1	A	767	LEU	2.6
1	B	954	THR	2.6
1	A	775	ILE	2.6
1	A	794	TYR	2.5
1	B	975	ILE	2.4
1	B	824	THR	2.4
1	B	982	THR	2.4
1	A	791	ASP	2.3
1	A	854	LEU	2.3
1	A	773	ASP	2.2
1	B	953	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	801	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ
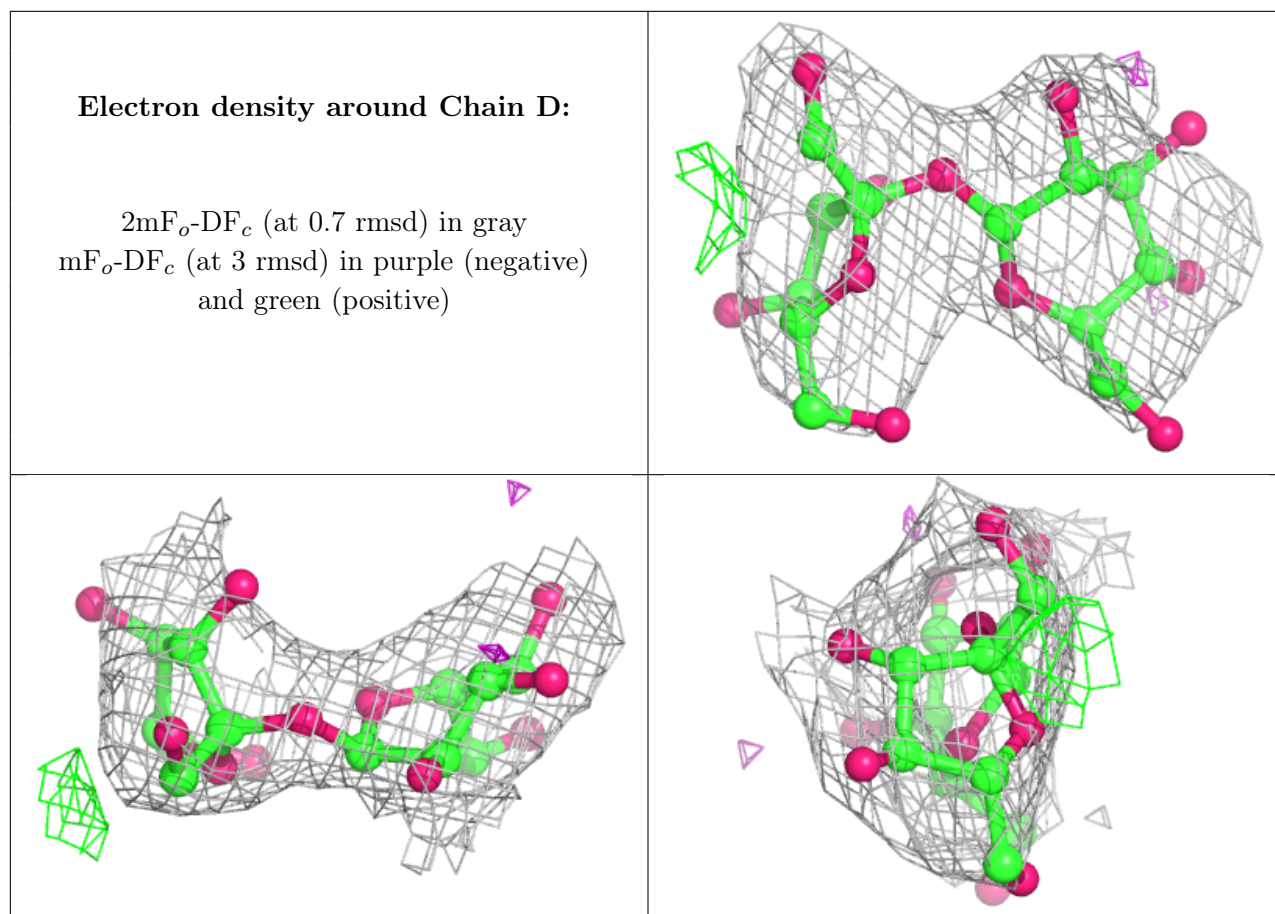
There are no non-standard protein/DNA/RNA residues in this entry.
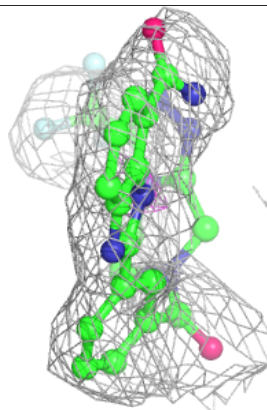
6.3 Carbohydrates ⓘ

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
2	GLC	D	1	11/12	0.84	0.34	89,93,116,122	0
2	FRU	D	2	12/12	0.86	0.35	79,96,117,131	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 D:

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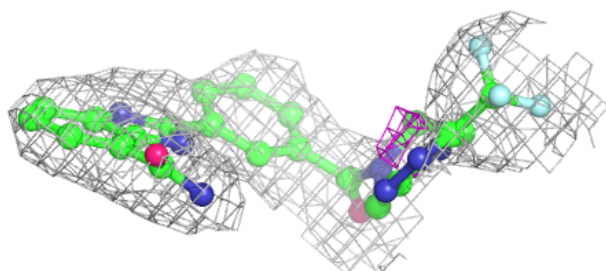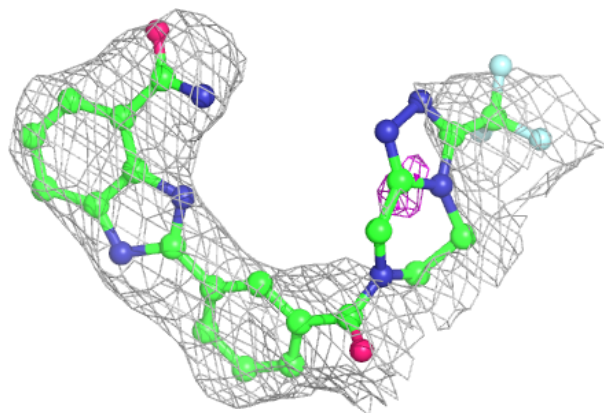and green (positive)

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.
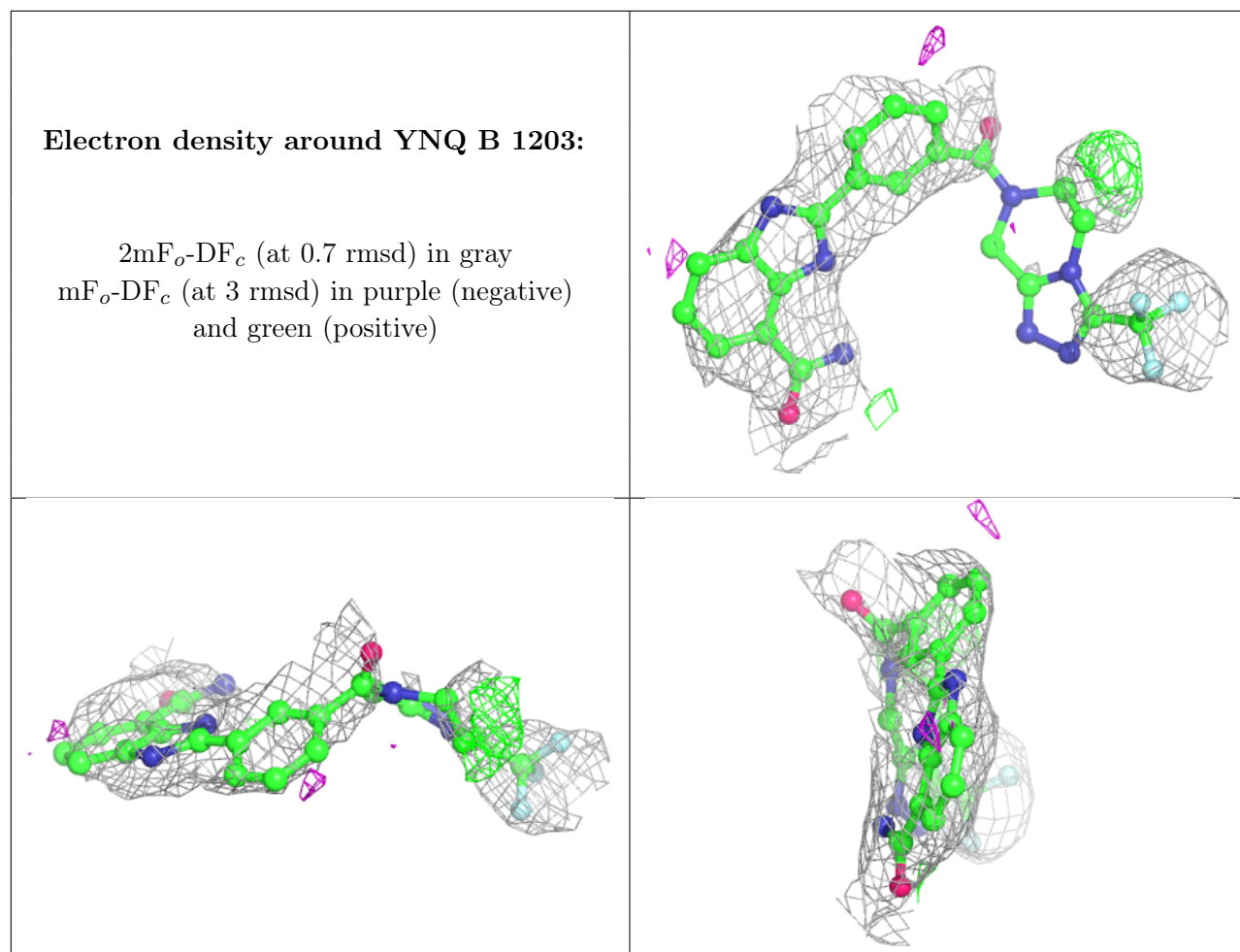
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	YNQ	A	1104	33/33	0.84	0.34	23,74,168,180	0
5	YNQ	B	1203	33/33	0.84	0.45	37,95,170,194	0
3	DMS	B	1202	4/4	0.91	0.65	49,88,89,96	0
4	CIT	A	1103	13/13	0.91	0.27	49,91,124,136	0
3	DMS	B	1201	4/4	0.95	0.32	38,85,104,110	0
3	DMS	A	1101	4/4	0.96	0.32	76,84,89,103	0
3	DMS	A	1102	4/4	0.97	0.52	46,62,84,86	0

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

Electron density around YNQ A 1104:

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

Electron density around YNQ B 1203:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.