



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:37 PM UTC

PDB ID : 8FZ1 / pdb_00008fz1
Title : Crystal structure of human PARP1 ART domain bound to inhibitor UKTT22 (compound 14)
Authors : Rouleau-Turcotte, E.; Pascal, J.M.
Deposited on : 2023-01-27
Resolution : 2.70 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

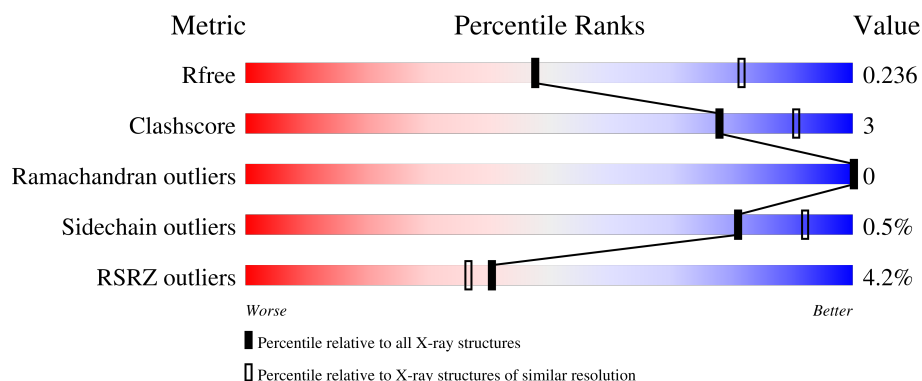
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	271	3% 79% 7% 14%
1	B	271	4% 82% 6% 12%
2	D	2	100%
2	E	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3919 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	234	Total	C	N	O	S	0	0	0
			1842	1183	312	341	6			
1	B	239	Total	C	N	O	S	0	0	0
			1881	1206	319	350	6			

There are 58 discrepancies between the modelled and reference sequences:

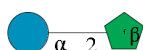
Chain	Residue	Modelled	Actual	Comment	Reference
A	742	MET	-	initiating methionine	UNP P09874
A	743	GLY	-	expression tag	UNP P09874
A	744	SER	-	expression tag	UNP P09874
A	745	SER	-	expression tag	UNP P09874
A	746	HIS	-	expression tag	UNP P09874
A	747	HIS	-	expression tag	UNP P09874
A	748	HIS	-	expression 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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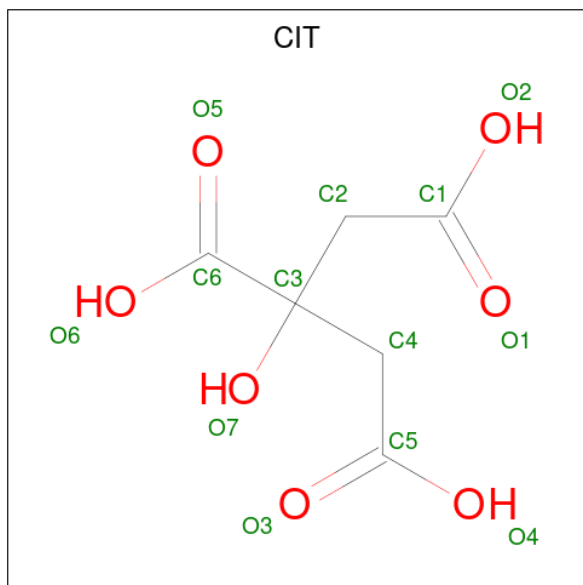
Chain	Residue	Modelled	Actual	Comment	Reference
A	784	GLY	-	linker	UNP P09874
A	785	SER	-	linker	UNP P09874
A	786	GLY	-	linker	UNP P09874
A	787	GLY	-	linker	UNP P09874
B	742	MET	-	initiating methionine	UNP P09874
B	743	GLY	-	expression tag	UNP P09874
B	744	SER	-	expression tag	UNP P09874
B	745	SER	-	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.



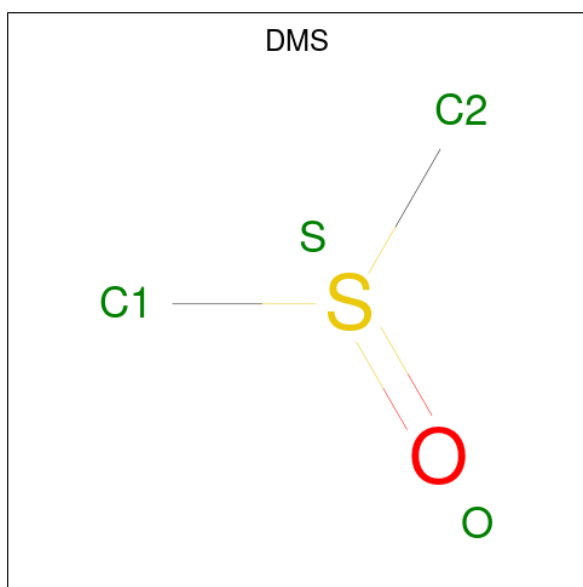
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



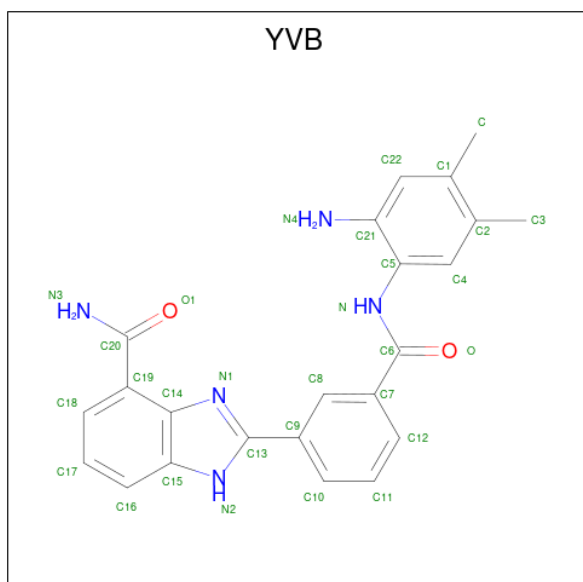
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



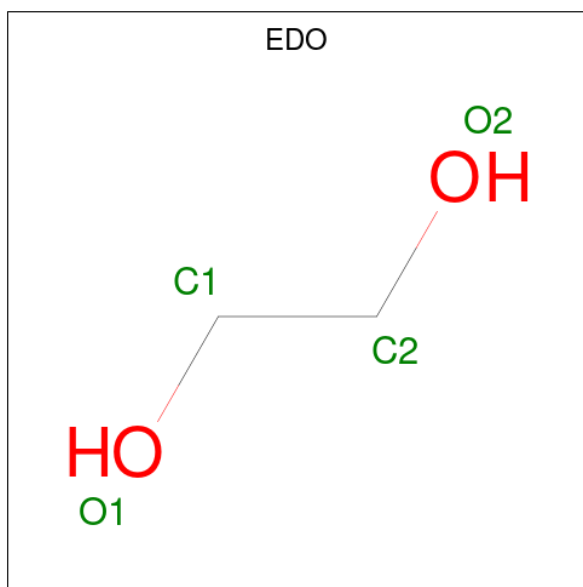
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is (2P)-2-{3-[(2-amino-4,5-dimethylphenyl)carbamoyl]phenyl}-1H-benzimidazole-4-carboxamide (CCD ID: YVB) (formula: $C_{23}H_{21}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			30	23	5	2		
5	B	1	Total	C	N	O	0	0
			30	23	5	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

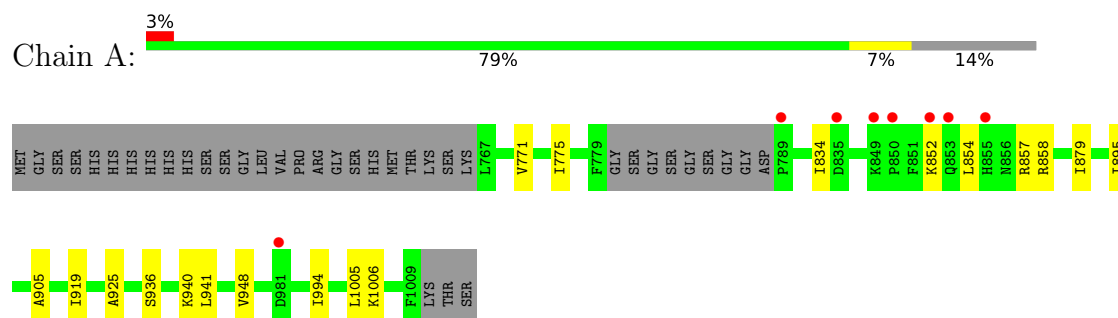
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	9	Total	O	0	0
			9	9		

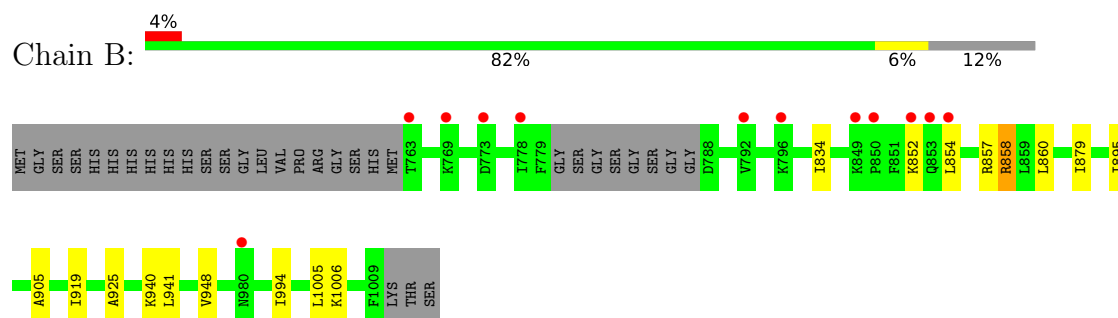
3 Residue-property plots [i](#)

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



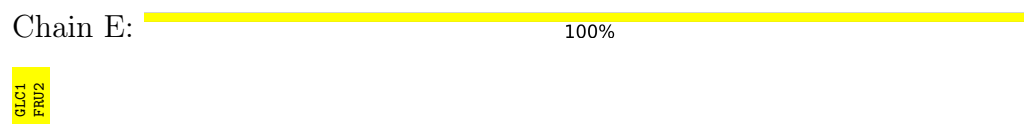
- Molecule 1: Poly [ADP-ribose] polymerase 1, processed C-terminus



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	95.60Å 95.60Å 128.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.80 – 2.70 47.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.80-2.70) 99.9 (47.80-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.191 , 0.231 0.195 , 0.236	Depositor DCC
R_{free} test set	911 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3919	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: EDO, FRU, GLC, DMS, CIT, YVB

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	0.30	0/1882	0.45	0/2545
1	B	0.30	0/1921	0.45	0/2597
All	All	0.30	0/3803	0.45	0/5142

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

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	1842	0	1858	12	0
1	B	1881	0	1899	10	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
3	A	26	0	10	0	0
3	B	13	0	5	0	0
4	A	8	0	12	3	0
4	B	8	0	12	1	0
5	A	30	0	0	0	0
5	B	30	0	0	0	0
6	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	18	0	0
7	A	6	0	0	0	0
7	B	9	0	0	0	0
All	All	3919	0	3868	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:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.74	0.69
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.76	0.66
1:B:895:ILE:HD11	1:B:994:ILE:HG22	1.77	0.66
1:A:854:LEU:HD23	1:A:925:ALA:HB1	1.78	0.66
1:B:854:LEU:HD23	1:B:925:ALA:HB1	1.76	0.66
1:A:895:ILE:HD11	1:A:994:ILE:HG22	1.76	0.65
1:A:940:LYS:O	4:A:1402:DMS:H12	1.98	0.64
1:A:936:SER:OG	4:A:1402:DMS:H23	1.98	0.63
1:A:940:LYS:C	4:A:1402:DMS:H12	2.33	0.53
1:B:858:ARG:HG2	1:B:860:LEU:HD21	1.91	0.52
1:B:941:LEU:HD21	1:B:948:VAL:HG23	1.95	0.49
1:B:852:LYS:O	1:B:857:ARG:NH1	2.47	0.48
1:A:941:LEU:HD21	1:A:948:VAL:HG23	1.96	0.48
1:A:879:ILE:HD13	1:A:895:ILE:HG13	1.97	0.47
1:A:852:LYS:O	1:A:857:ARG:NH1	2.48	0.46
1:B:919:ILE:HG13	1:B:1005:LEU:HD12	1.96	0.46
1:B:879:ILE:HD13	1:B:895:ILE:HG13	1.98	0.46
1:A:919:ILE:HG13	1:A:1005:LEU:HD12	1.98	0.44
1:A:905:ALA:HB2	1:A:919:ILE:HD11	2.00	0.43
1:B:905:ALA:HB2	1:B:919:ILE:HD11	2.00	0.43
1:B:940:LYS:O	4:B:1601:DMS:H11	2.20	0.42
1:A:771:VAL:O	1:A:775:ILE:HG12	2.21	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	230/271 (85%)	222 (96%)	8 (4%)	0	100	100
1	B	235/271 (87%)	227 (97%)	8 (3%)	0	100	100
All	All	465/542 (86%)	449 (97%)	16 (3%)	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	202/233 (87%)	201 (100%)	1 (0%)	81	92
1	B	207/233 (89%)	206 (100%)	1 (0%)	81	92
All	All	409/466 (88%)	407 (100%)	2 (0%)	81	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	858	ARG
1	B	858	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	793	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 ⓘ

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	$\# Z > 2$
2	GLC	D	1	2	11,11,12	0.55	0	15,15,17	0.87	0
2	FRU	D	2	2	11,12,12	0.52	0	10,18,18	0.67	0
2	GLC	E	1	2	11,11,12	0.60	0	15,15,17	1.66	3 (20%)
2	FRU	E	2	2	11,12,12	0.63	0	10,18,18	0.89	1 (10%)

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	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	4/5/24/24	0/1/1/1
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	FRU	E	2	2	-	1/5/24/24	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	C3-C4-C5	4.11	117.68	110.23
2	E	1	GLC	C1-O5-C5	2.90	116.08	112.19
2	E	2	FRU	C6-C5-C4	-2.25	109.79	115.10
2	E	1	GLC	C1-C2-C3	-2.08	106.61	109.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

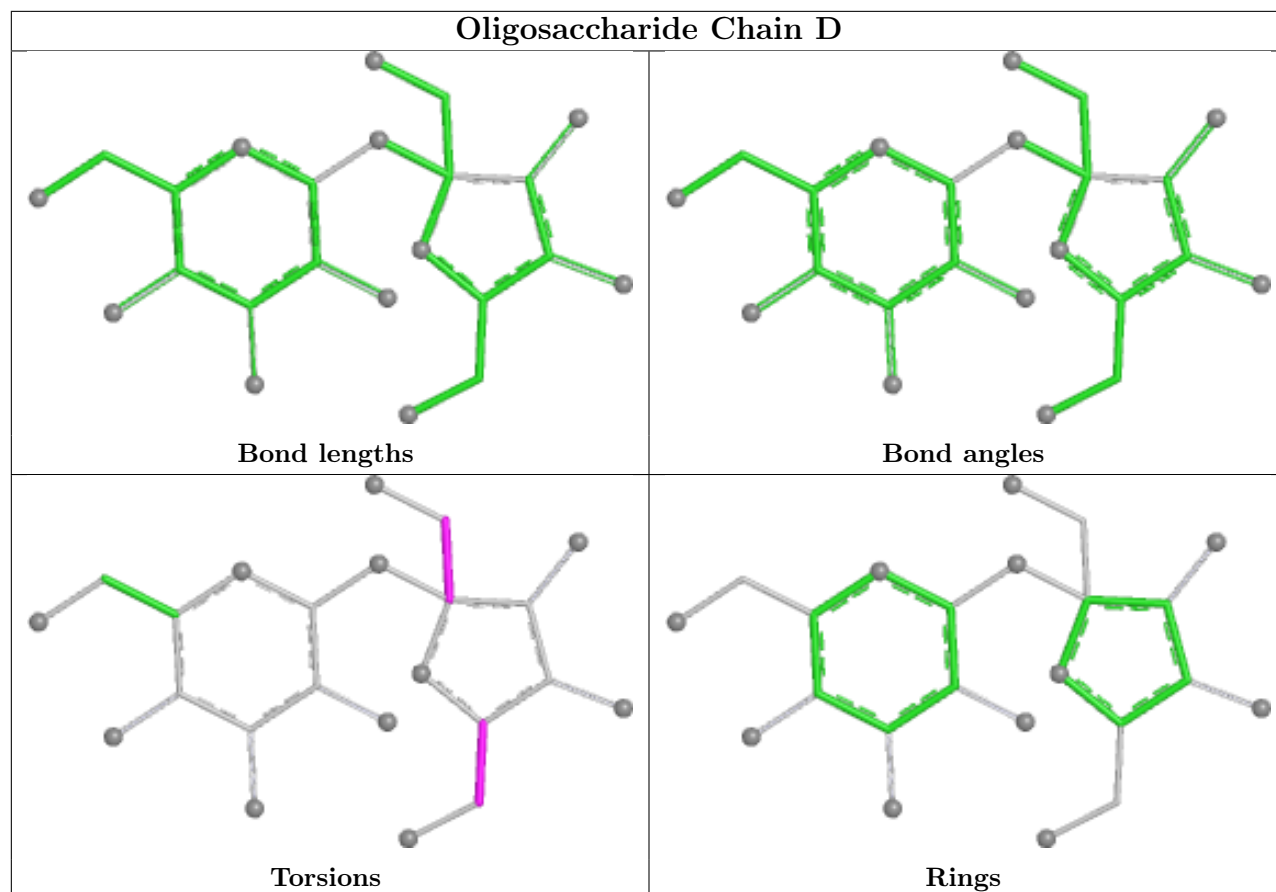
Mol	Chain	Res	Type	Atoms
2	D	2	FRU	O1-C1-C2-O2
2	E	1	GLC	O5-C5-C6-O6
2	D	2	FRU	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	D	2	FRU	O1-C1-C2-O5
2	E	2	FRU	O5-C5-C6-O6

There are no ring outliers.

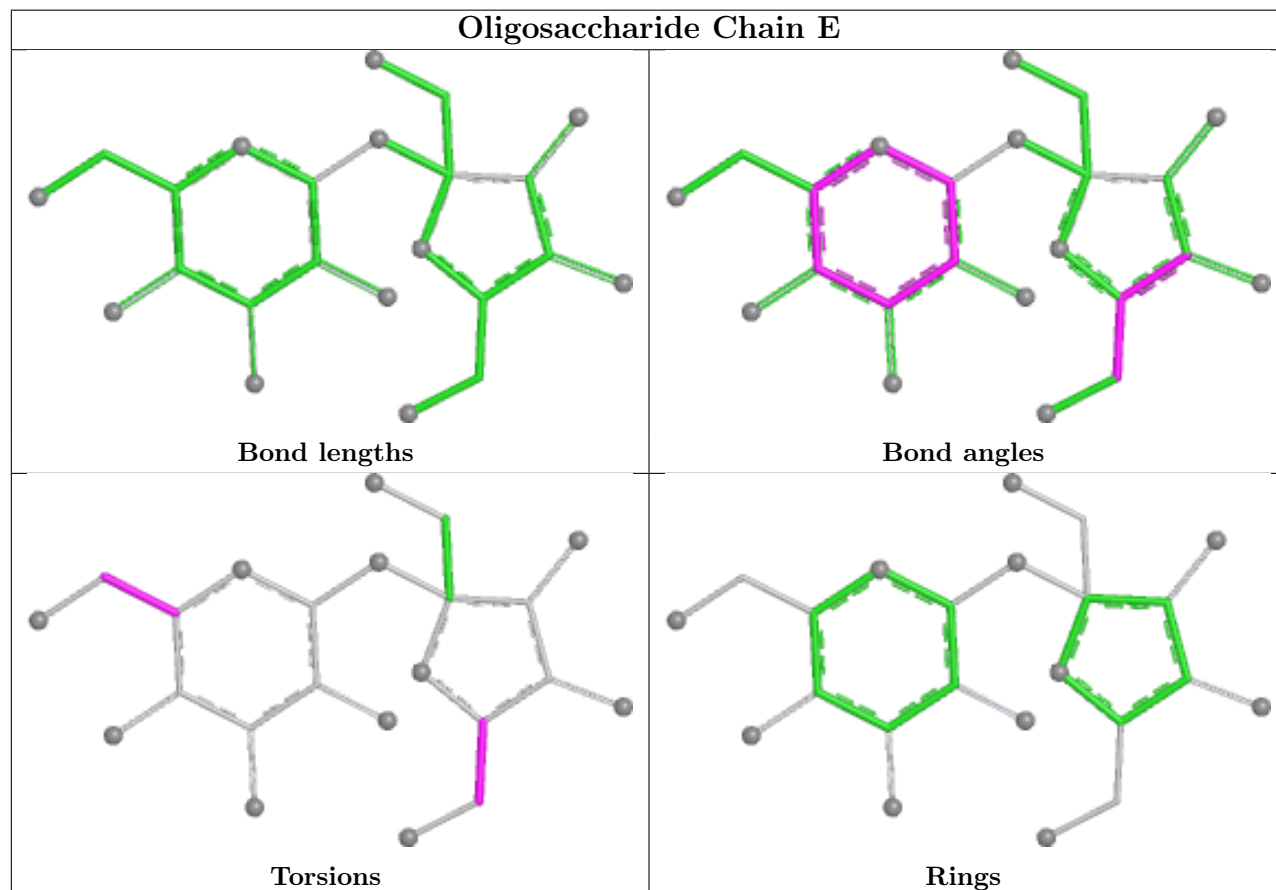
No monomer is involved in short contacts.

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

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry

14 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
5	YVB	A	1403	-	33,33,33	0.19	0	47,48,48	0.53	1 (2%)
5	YVB	B	1603	-	33,33,33	0.19	0	47,48,48	0.53	1 (2%)
6	EDO	B	1606	-	3,3,3	0.36	0	2,2,2	0.20	0
6	EDO	B	1605	-	3,3,3	0.25	0	2,2,2	0.52	0
3	CIT	A	1401	-	12,12,12	1.08	0	17,17,17	1.64	3 (17%)
4	DMS	B	1601	-	3,3,3	0.65	0	3,3,3	0.74	0
6	EDO	A	1407	-	3,3,3	0.34	0	2,2,2	0.39	0
4	DMS	A	1402	-	3,3,3	0.64	0	3,3,3	0.91	0
4	DMS	B	1604	-	3,3,3	0.69	0	3,3,3	0.87	0
4	DMS	A	1405	-	3,3,3	0.72	0	3,3,3	0.48	0
3	CIT	B	1602	-	12,12,12	1.04	0	17,17,17	1.69	4 (23%)
3	CIT	A	1404	-	12,12,12	1.14	0	17,17,17	1.56	4 (23%)
6	EDO	A	1406	-	3,3,3	0.33	0	2,2,2	0.66	0
6	EDO	B	1607	-	3,3,3	0.29	0	2,2,2	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	YVB	A	1403	-	-	6/16/16/16	0/4/4/4
5	YVB	B	1603	-	-	6/16/16/16	0/4/4/4
6	EDO	B	1606	-	-	0/1/1/1	-
6	EDO	B	1605	-	-	1/1/1/1	-
3	CIT	A	1401	-	-	13/16/16/16	-
6	EDO	A	1407	-	-	1/1/1/1	-
3	CIT	B	1602	-	-	3/16/16/16	-
3	CIT	A	1404	-	-	12/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1406	-	-	0/1/1/1	-
6	EDO	B	1607	-	-	0/1/1/1	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1602	CIT	O6-C6-C3	4.25	121.30	113.14
3	A	1401	CIT	O6-C6-C3	3.88	120.58	113.14
3	A	1404	CIT	O6-C6-C3	3.44	119.74	113.14
3	A	1401	CIT	O4-C5-C4	2.71	122.94	114.35
3	B	1602	CIT	O2-C1-C2	2.42	122.00	114.35
3	A	1401	CIT	O4-C5-O3	-2.39	117.18	123.33
5	A	1403	YVB	C21-C22-C1	-2.28	121.19	122.68
5	B	1603	YVB	C21-C22-C1	-2.20	121.25	122.68
3	A	1404	CIT	O2-C1-C2	2.18	121.24	114.35
3	B	1602	CIT	O6-C6-O5	-2.15	116.98	123.86
3	A	1404	CIT	O2-C1-O1	-2.14	117.84	123.33
3	A	1404	CIT	O4-C5-C4	2.07	120.90	114.35
3	B	1602	CIT	O4-C5-C4	2.07	120.89	114.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	CIT	C2-C3-C4-C5
3	A	1401	CIT	O7-C3-C4-C5
3	A	1401	CIT	C6-C3-C4-C5
3	A	1401	CIT	O7-C3-C6-O5
3	A	1401	CIT	O7-C3-C6-O6
3	A	1404	CIT	C2-C3-C4-C5
3	A	1404	CIT	O7-C3-C4-C5
3	A	1404	CIT	C6-C3-C4-C5
3	A	1404	CIT	O7-C3-C6-O5
3	A	1404	CIT	O7-C3-C6-O6
3	A	1404	CIT	C4-C3-C6-O5
3	A	1404	CIT	C4-C3-C6-O6
5	A	1403	YVB	O-C6-C7-C12
5	B	1603	YVB	O-C6-C7-C12
5	A	1403	YVB	O-C6-C7-C8
5	B	1603	YVB	O-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	A	1403	YVB	N-C6-C7-C8
5	A	1403	YVB	N-C6-C7-C12
5	B	1603	YVB	N-C6-C7-C12
5	B	1603	YVB	N-C6-C7-C8
3	A	1401	CIT	C1-C2-C3-O7
3	A	1401	CIT	C1-C2-C3-C6
6	A	1407	EDO	O1-C1-C2-O2
5	A	1403	YVB	C4-C5-N-C6
5	A	1403	YVB	C21-C5-N-C6
5	B	1603	YVB	C21-C5-N-C6
5	B	1603	YVB	C4-C5-N-C6
3	A	1401	CIT	C2-C3-C6-O5
3	A	1404	CIT	C1-C2-C3-O7
3	A	1401	CIT	C2-C3-C6-O6
3	A	1401	CIT	C4-C3-C6-O6
3	A	1401	CIT	C1-C2-C3-C4
3	A	1404	CIT	O2-C1-C2-C3
3	A	1401	CIT	C4-C3-C6-O5
3	A	1404	CIT	C2-C3-C6-O6
3	A	1404	CIT	O1-C1-C2-C3
3	A	1404	CIT	C2-C3-C6-O5
3	B	1602	CIT	C2-C3-C6-O6
3	B	1602	CIT	C1-C2-C3-C6
3	B	1602	CIT	O7-C3-C4-C5
3	A	1401	CIT	C3-C4-C5-O3
6	B	1605	EDO	O1-C1-C2-O2

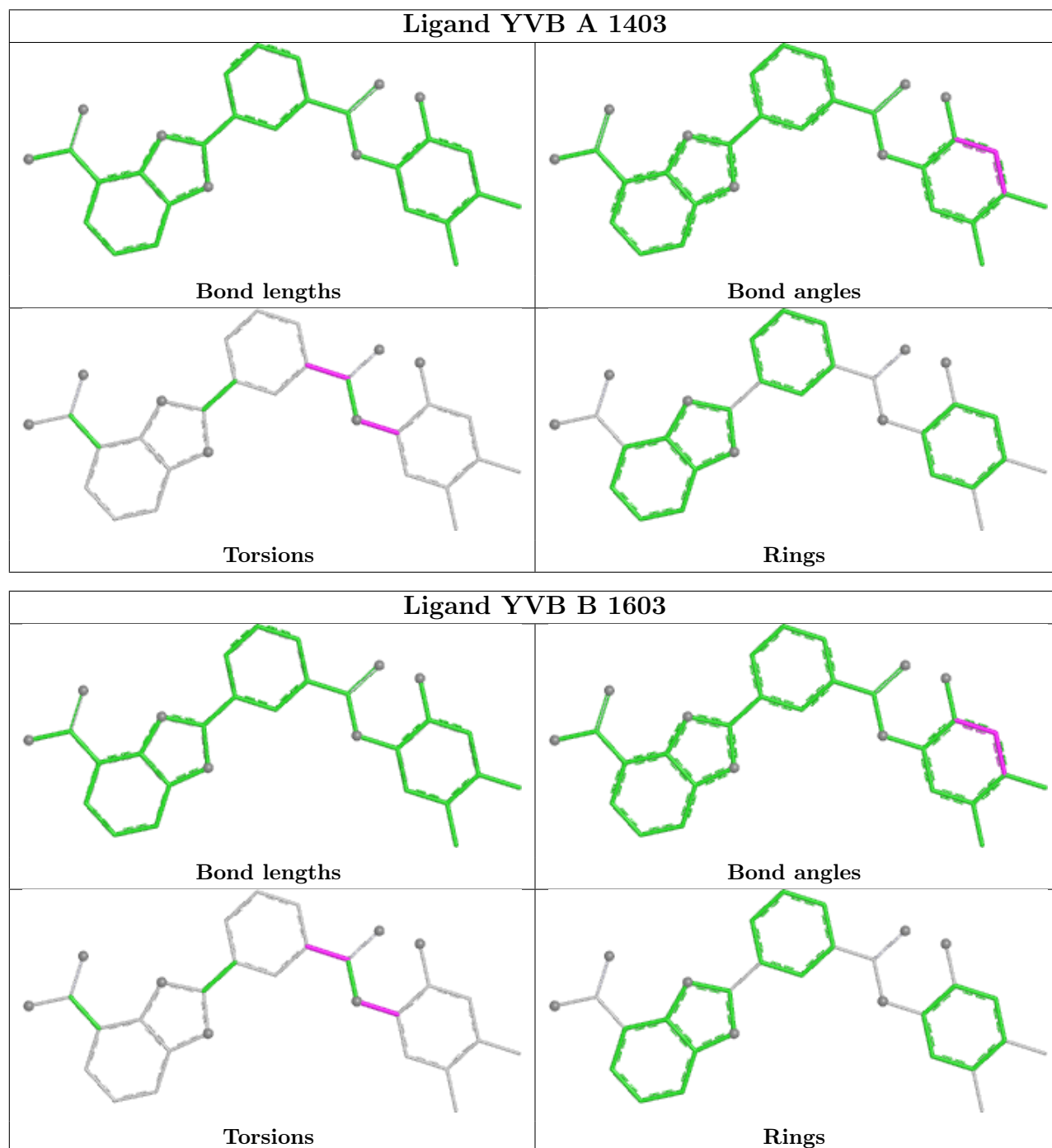
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1601	DMS	1	0
4	A	1402	DMS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



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	234/271 (86%)	0.27	8 (3%)	48 44	43, 64, 99, 116	0
1	B	239/271 (88%)	0.39	12 (5%)	34 30	44, 65, 95, 123	0
All	All	473/542 (87%)	0.33	20 (4%)	40 37	43, 65, 97, 123	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	853	GLN	4.9
1	B	850	PRO	3.8
1	B	849	LYS	3.6
1	A	853	GLN	3.4
1	B	980	ASN	3.1
1	B	852	LYS	2.8
1	A	981	ASP	2.6
1	B	796	LYS	2.6
1	A	852	LYS	2.5
1	B	763	THR	2.5
1	B	792	VAL	2.4
1	B	854	LEU	2.4
1	A	849	LYS	2.3
1	B	769	LYS	2.3
1	A	850	PRO	2.2
1	A	835	ASP	2.2
1	A	855	HIS	2.2
1	B	778	ILE	2.2
1	A	789	PRO	2.1
1	B	773	ASP	2.1

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

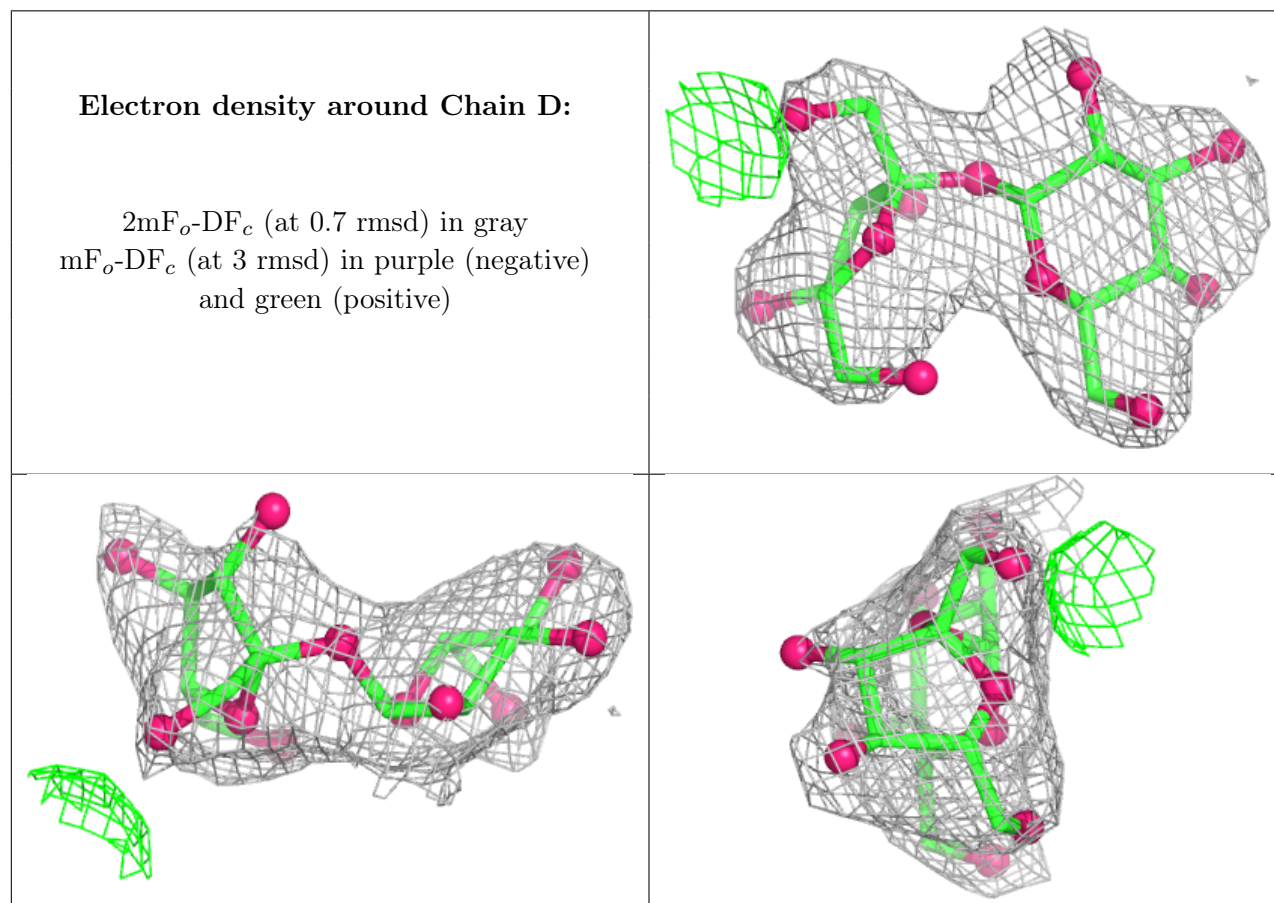
There are no non-standard protein/DNA/RNA residues in this entry.

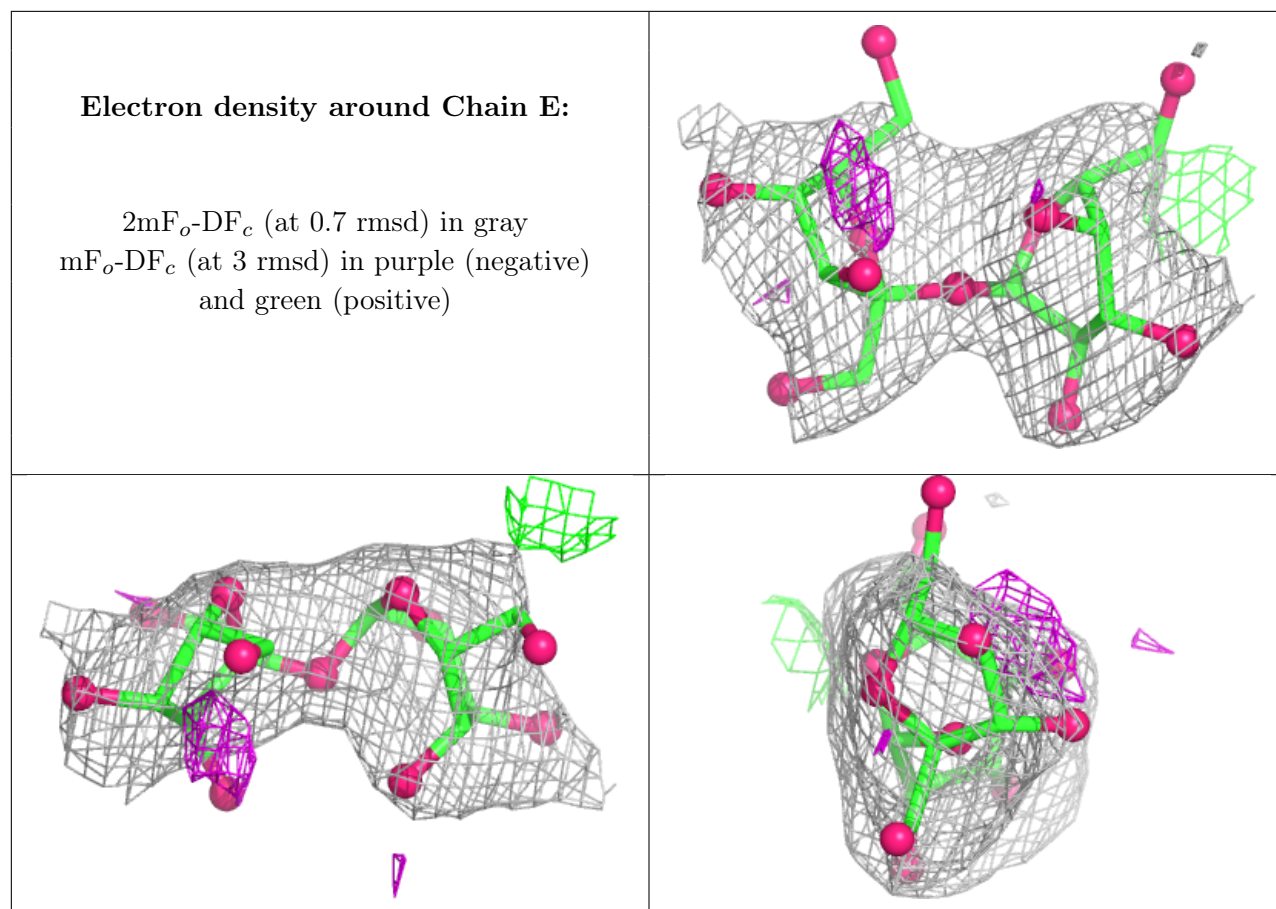
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	FRU	D	2	12/12	0.78	0.14	79,91,107,114	0
2	GLC	D	1	11/12	0.84	0.15	70,81,96,98	0
2	GLC	E	1	11/12	-	-	70,81,99,107	0
2	FRU	E	2	12/12	-	-	85,95,112,118	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.





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.

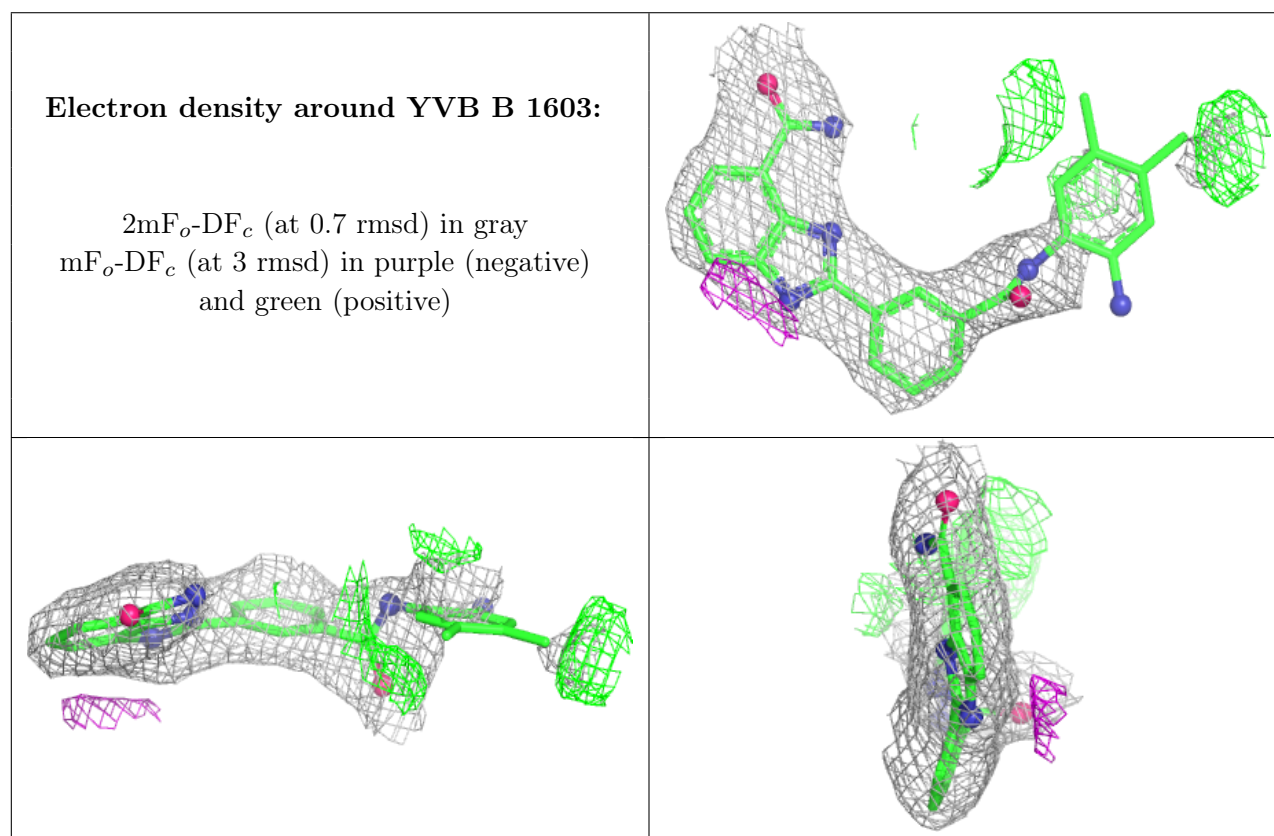
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	1407	4/4	0.75	0.29	63,74,88,91	0
6	EDO	A	1406	4/4	0.76	0.21	63,69,71,78	0
6	EDO	B	1606	4/4	0.76	0.28	64,66,75,83	0
3	CIT	A	1404	13/13	0.78	0.14	67,91,103,104	0
3	CIT	B	1602	13/13	0.83	0.15	74,91,111,114	0
4	DMS	A	1405	4/4	0.84	0.27	66,88,105,112	0
6	EDO	B	1605	4/4	0.84	0.17	60,64,71,79	0
3	CIT	A	1401	13/13	0.84	0.15	61,78,90,100	0
5	YVB	B	1603	30/30	0.86	0.16	42,71,130,140	0
6	EDO	B	1607	4/4	0.86	0.18	50,53,68,82	0
4	DMS	A	1402	4/4	0.90	0.26	51,86,89,100	0
4	DMS	B	1604	4/4	0.90	0.19	50,71,107,108	0
4	DMS	B	1601	4/4	0.92	0.23	62,69,83,100	0

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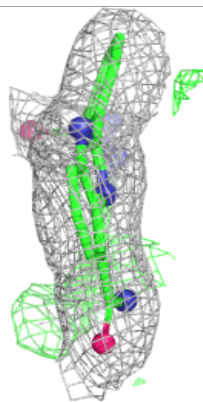
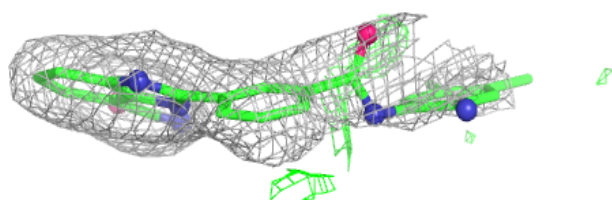
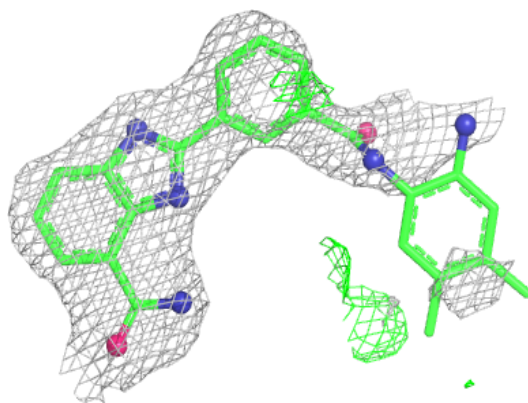
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	YVB	A	1403	30/30	0.92	0.13	42,71,131,138	0

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 YVB A 1403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.