WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2022 – 05:37 PM EST

PDB ID	:	1FI1
Title	:	FhuA in complex with lipopolysaccharide and rifamycin CGP4832
Authors	:	Ferguson, A.D.; Koedding, J.; Boes, C.; Walker, G.; Coulton, J.W.; Diederichs, K.; Braun, V.; Welte, W.
Deposited on	:	2000-08-03
Resolution	:	2.90 Å(reported)

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

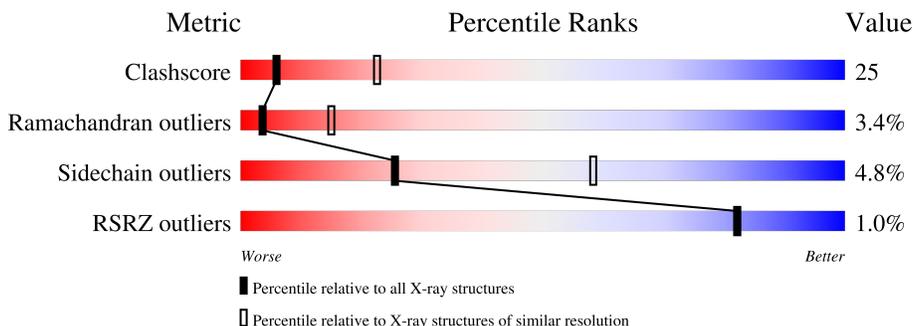|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.90 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	Percentile Ranks	Value
Clashscore		25
Ramachandran outliers		3.4%
Sidechain outliers		4.8%
RSRZ outliers		1.0%

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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	707	56% 39% 5%
2	B	11	27% 45% 27%

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
2	GMH	B	10	X	-	-	-
2	GCN	B	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GMH	B	5	X	-	-	-
3	FTT	A	1002	X	-	-	-
3	FTT	A	1006	X	-	-	-
9	RIF	A	1022	X	-	-	-

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 6030 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 FERRICHROME-IRON RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total 5523	C 3475	N 944	O 1090	S 14	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	expression tag	UNP P06971
A	407	SER	-	expression tag	UNP P06971
A	408	HIS	-	expression tag	UNP P06971
A	409	HIS	-	expression tag	UNP P06971
A	410	HIS	-	expression tag	UNP P06971
A	411	HIS	-	expression tag	UNP P06971
A	412	HIS	-	expression tag	UNP P06971
A	413	HIS	-	expression tag	UNP P06971
A	414	GLY	-	expression tag	UNP P06971
A	415	SER	-	expression tag	UNP P06971
A	416	SER	-	expression tag	UNP P06971

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-mann o-heptopyranose-(1-7)]L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-ma nno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucoyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.
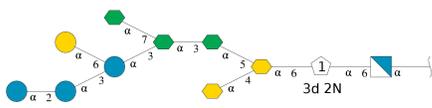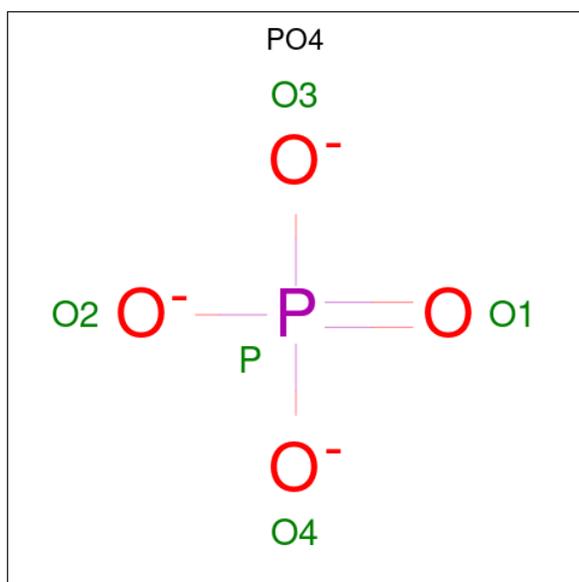

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total 134	C 73	N 2	O 59	0	0	0

- Molecule 3 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).
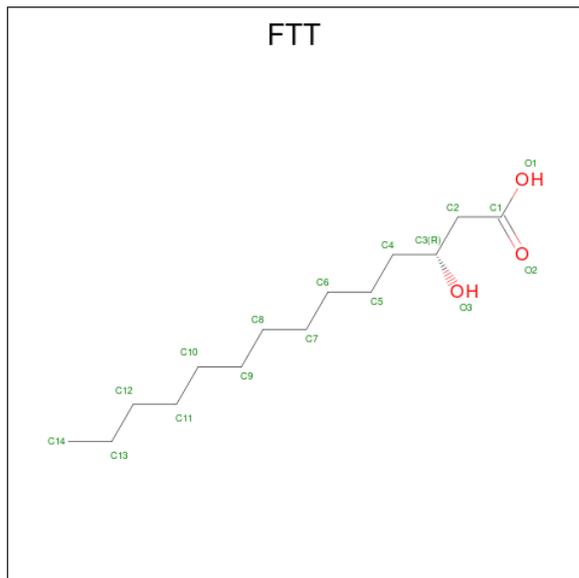
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 16	C 14	O 2	0	0
3	A	1	Total 16	C 14	O 2	0	0
3	A	1	Total 9	C 6	O 3	0	0
3	A	1	Total 13	C 12	O 1	0	0
3	A	1	Total 17	C 14	O 3	0	0
3	A	1	Total 15	C 14	O 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O2 — P = O O1

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	O 3	P 1	0	0
4	A	1	Total 4	O 3	P 1	0	0

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ni 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Mg 1	0	0

- Molecule 8 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).

DPO
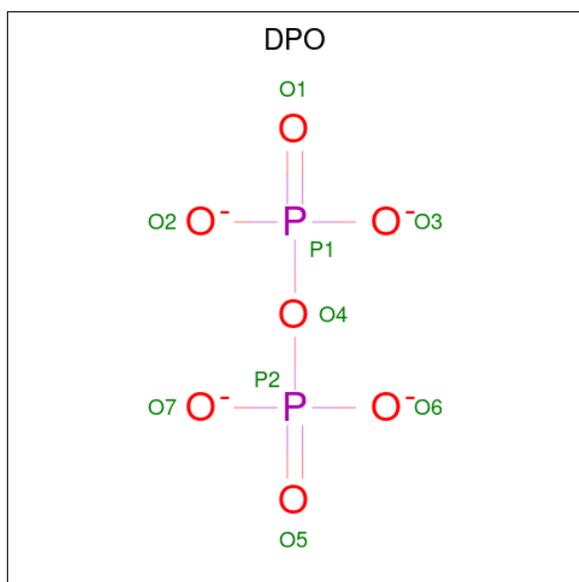
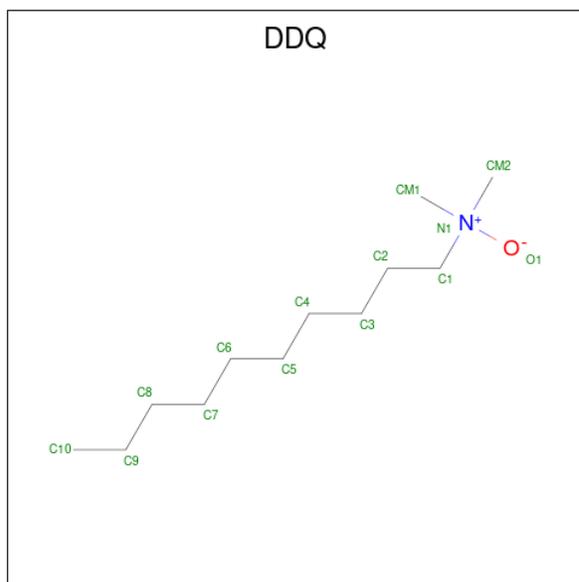| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 8	O 6	P 2	0	0
8	A	1	Total 8	O 6	P 2	0	0

• Molecule 9 is RIFAMYCIN CGP 4832 (three-letter code: RIF) (formula: $C_{49}H_{65}N_3O_{15}$).

RIF
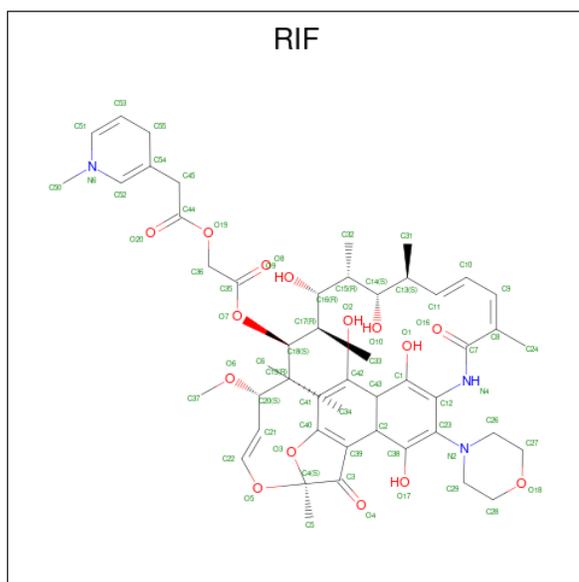
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 67	C 49	N 3	O 15	0	0

• Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ)

(formula: $C_{12}H_{27}NO$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	14	12	1	1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	179	179	179	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 d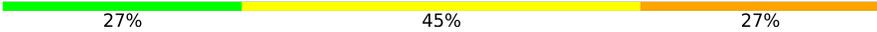ot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FERRICHROME-IRON RECEPTOR
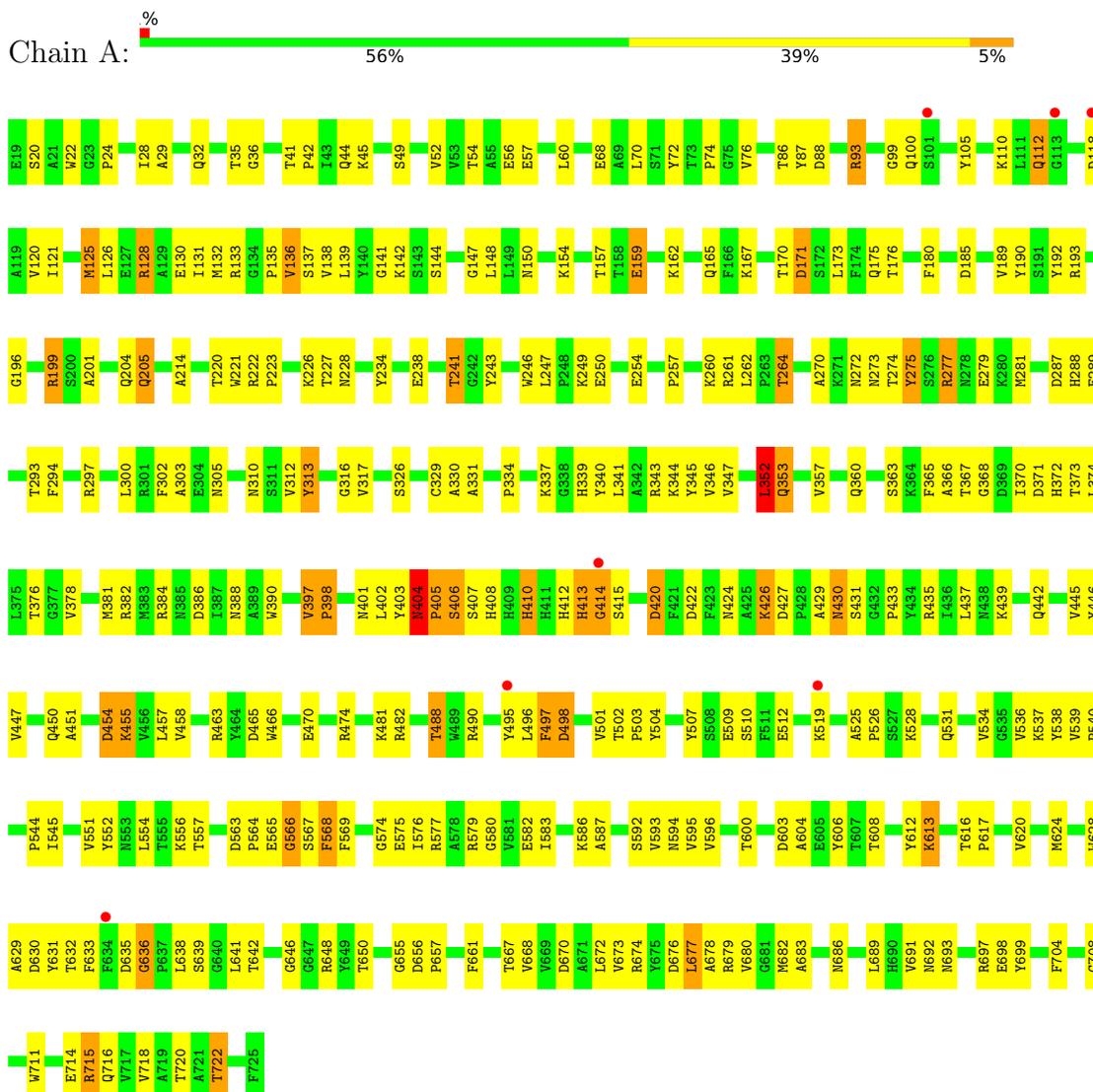
• Molecule 2: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-heptopyranose-(1-7)]L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucoyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	172.82Å 172.82Å 87.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 41.51 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.90) 97.9 (41.51-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.71 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.275 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.2	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6030	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 2.94% 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: DPO, MG, GCN, FTT, DDQ, KDO, GMH, PO4, PA1, NI, GLC, GLA, RIF, NA

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	0.39	0/5663	0.65	1/7696 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	LEU	CA-CB-CG	5.04	126.89	115.30

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	5523	0	5223	273	0
2	B	134	0	103	2	0
3	A	86	0	130	15	0
4	A	8	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	16	0	0	1	0
9	A	67	0	61	4	0
10	A	14	0	27	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	179	0	0	8	0
All	All	6030	0	5544	285	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 25.

The worst 5 of 285 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:274:THR:HG22	1:A:310:ASN:HB2	1.41	1.00
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.34	0.91
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.51	0.91
1:A:624:MET:HA	11:A:1179:HOH:O	1.71	0.89
1:A:74:PRO:HG2	1:A:133:ARG:HH12	1.37	0.88

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	705/707 (100%)	621 (88%)	60 (8%)	24 (3%)	3	15

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	PRO
1	A	406	SER
1	A	413	HIS
1	A	613	LYS
1	A	20	SER

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	587/587 (100%)	559 (95%)	28 (5%)	25	58

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	LEU
1	A	722	THR
1	A	404	ASN
1	A	534	VAL
1	A	397	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	A	522	ASN
1	A	692	ASN
1	A	553	ASN
1	A	430	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 ⓘ

11 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	PA1	B	1	3,8,2	11,11,12	2.50	5 (45%)	14,15,17	2.66	8 (57%)
2	GMH	B	10	2	13,13,14	0.50	0	17,18,20	0.81	1 (5%)
2	KDO	B	11	2	15,15,16	0.78	0	19,21,24	1.02	0
2	GCN	B	2	3,4,2	10,10,11	1.86	3 (30%)	13,13,15	4.22	5 (38%)
2	KDO	B	3	2	15,15,16	1.05	0	19,21,24	1.02	1 (5%)
2	GMH	B	4	8,2	13,13,14	0.80	0	17,18,20	1.25	3 (17%)
2	GMH	B	5	4,2	13,13,14	0.98	1 (7%)	17,18,20	1.11	2 (11%)
2	GLC	B	6	2	11,11,12	0.57	0	15,15,17	0.99	2 (13%)
2	GLC	B	7	2	11,11,12	0.54	0	15,15,17	0.54	0
2	GLC	B	8	2	11,11,12	0.54	0	15,15,17	0.59	0
2	GLA	B	9	2	11,11,12	0.47	0	15,15,17	0.53	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	PA1	B	1	3,8,2	-	0/2/18/22	0/1/1/1
2	GMH	B	10	2	2/2/5/6	4/6/23/26	0/1/1/1
2	KDO	B	11	2	-	3/10/26/30	0/1/1/1
2	GCN	B	2	3,4,2	1/1/3/4	1/2/15/18	0/1/1/1
2	KDO	B	3	2	-	1/10/26/30	0/1/1/1
2	GMH	B	4	8,2	-	0/6/23/26	0/1/1/1
2	GMH	B	5	4,2	2/2/5/6	5/6/23/26	0/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1
2	GLC	B	7	2	-	2/2/19/22	0/1/1/1
2	GLC	B	8	2	-	2/2/19/22	0/1/1/1
2	GLA	B	9	2	-	1/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	PA1	C1-C2	5.32	1.59	1.52
2	B	1	PA1	C3-C4	-3.93	1.46	1.52
2	B	2	GCN	C4-C5	3.93	1.59	1.52
2	B	1	PA1	O5-C1	3.17	1.50	1.42
2	B	2	GCN	C1-C2	-2.75	1.48	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GCN	C4-C3-C2	-11.92	98.42	112.39
2	B	2	GCN	C3-C2-C1	7.63	116.02	109.82
2	B	1	PA1	C3-C4-C5	-4.96	104.34	110.77
2	B	1	PA1	C3-C2-C1	-4.42	98.77	109.59
2	B	1	PA1	C6-C5-C4	-4.01	107.95	113.54

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	GCN	C1
2	B	5	GMH	C1
2	B	5	GMH	C6
2	B	10	GMH	C1
2	B	10	GMH	C6

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	GMH	O5-C5-C6-O6
2	B	5	GMH	C5-C6-C7-O7
2	B	5	GMH	O6-C6-C7-O7
2	B	10	GMH	C4-C5-C6-C7
2	B	10	GMH	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	11	KDO	1	0
2	B	4	GMH	1	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 B

Bond lengths

Bond angles

Torsions

Rings
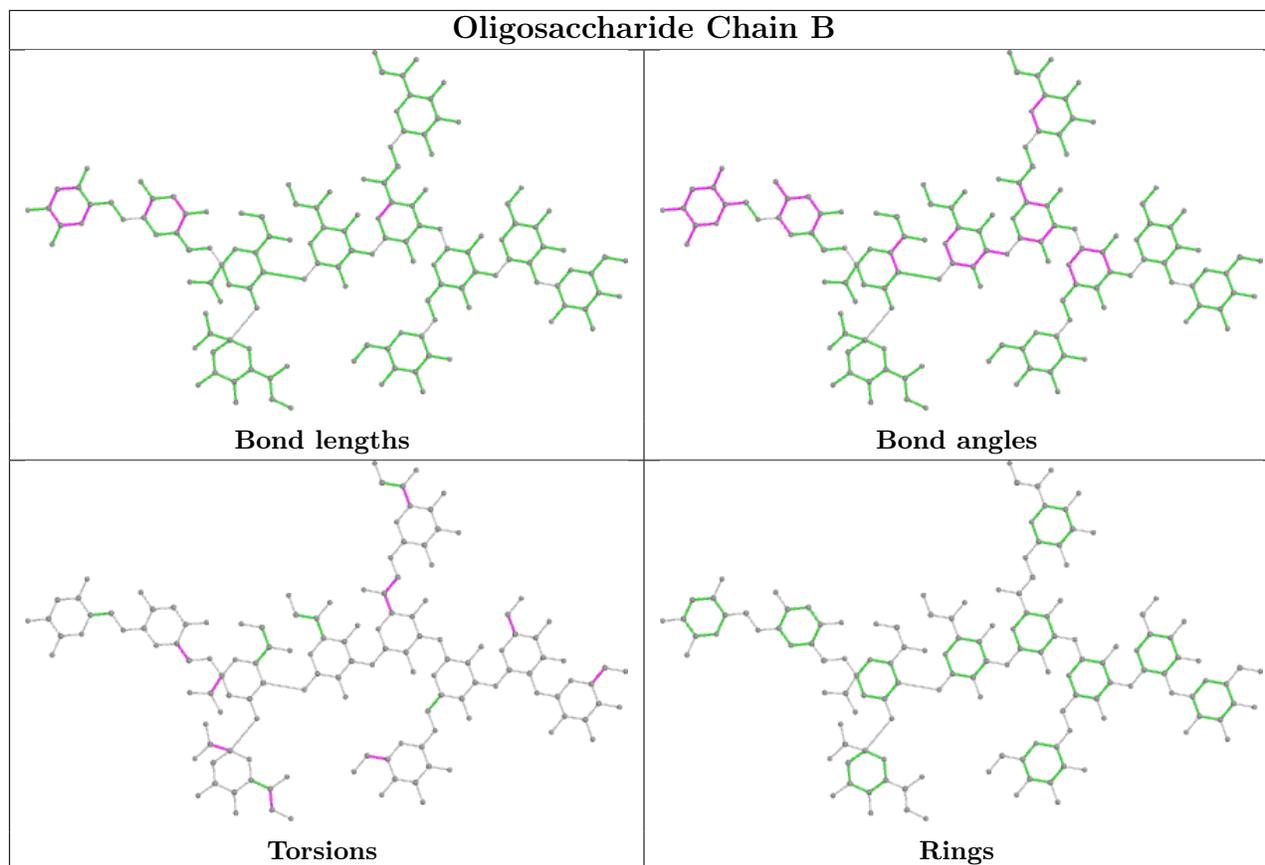
5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\#|Z| > 2$
8	DPO	A	1013	2	4,7,8	2.25	1 (25%)	5,10,13	1.00	0
3	FTT	A	1005	3	12,12,16	0.44	0	11,11,17	0.66	0
9	RIF	A	1022	-	68,72,72	3.02	23 (33%)	81,106,106	2.70	25 (30%)
4	PO4	A	1016	5,2	0,3,4	-	-	0,3,6	-	-
10	DDQ	A	1023	-	10,13,13	0.51	0	12,15,15	0.54	0
8	DPO	A	1015	2	4,7,8	2.52	1 (25%)	5,10,13	0.95	0
3	FTT	A	1004	3,2	15,15,16	0.84	1 (6%)	15,15,17	2.55	2 (13%)
3	FTT	A	1007	3	14,14,16	0.37	0	13,13,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	FTT	A	1003	2	8,8,16	1.68	1 (12%)	8,9,17	1.28	1 (12%)
4	PO4	A	1014	2	0,3,4	-	-	0,3,6	-	-
3	FTT	A	1002	2	15,15,16	1.47	2 (13%)	15,15,17	2.93	2 (13%)
3	FTT	A	1006	3,2	16,16,16	1.08	1 (6%)	17,17,17	1.09	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
9	RIF	A	1022	-	2/2/27/36	15/68/145/145	0/5/6/6
3	FTT	A	1005	3	-	0/9/10/15	-
8	DPO	A	1013	2	-	0/2/5/6	-
10	DDQ	A	1023	-	-	7/11/11/11	-
8	DPO	A	1015	2	-	0/2/5/6	-
3	FTT	A	1004	3,2	-	2/14/14/15	-
3	FTT	A	1007	3	-	0/11/12/15	-
3	FTT	A	1003	2	-	0/7/7/15	-
3	FTT	A	1002	2	1/1/1/2	4/14/14/15	-
3	FTT	A	1006	3,2	1/1/2/2	2/15/15/15	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1022	RIF	C41-C42	10.70	1.49	1.34
9	A	1022	RIF	C2-C38	-10.39	1.44	1.51
9	A	1022	RIF	C40-C39	8.25	1.45	1.34
9	A	1022	RIF	C52-C54	6.66	1.41	1.33
9	A	1022	RIF	C43-C42	5.65	1.55	1.51

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1022	RIF	O17-C38-C2	11.19	122.61	112.25
3	A	1002	FTT	O2-C1-C2	-10.78	94.01	125.43
3	A	1004	FTT	O2-C1-C2	-9.20	98.61	125.43
9	A	1022	RIF	O2-C42-C43	8.51	120.13	112.25
9	A	1022	RIF	O1-C1-C43	8.16	119.81	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1002	FTT	C3
3	A	1006	FTT	C3
9	A	1022	RIF	C2
9	A	1022	RIF	C43

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	FTT	C1-C2-C3-C4
3	A	1004	FTT	C1-C2-C3-O3
10	A	1023	DDQ	C2-C1-N1-CM1
9	A	1022	RIF	C45-C44-O19-C36
9	A	1022	RIF	O20-C44-O19-C36

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	FTT	2	0
9	A	1022	RIF	4	0
8	A	1015	DPO	1	0
3	A	1007	FTT	5	0
3	A	1002	FTT	8	0
3	A	1006	FTT	7	0

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

Ligand RIF A 1022

Bond lengths

Bond angles

Torsions

Rings
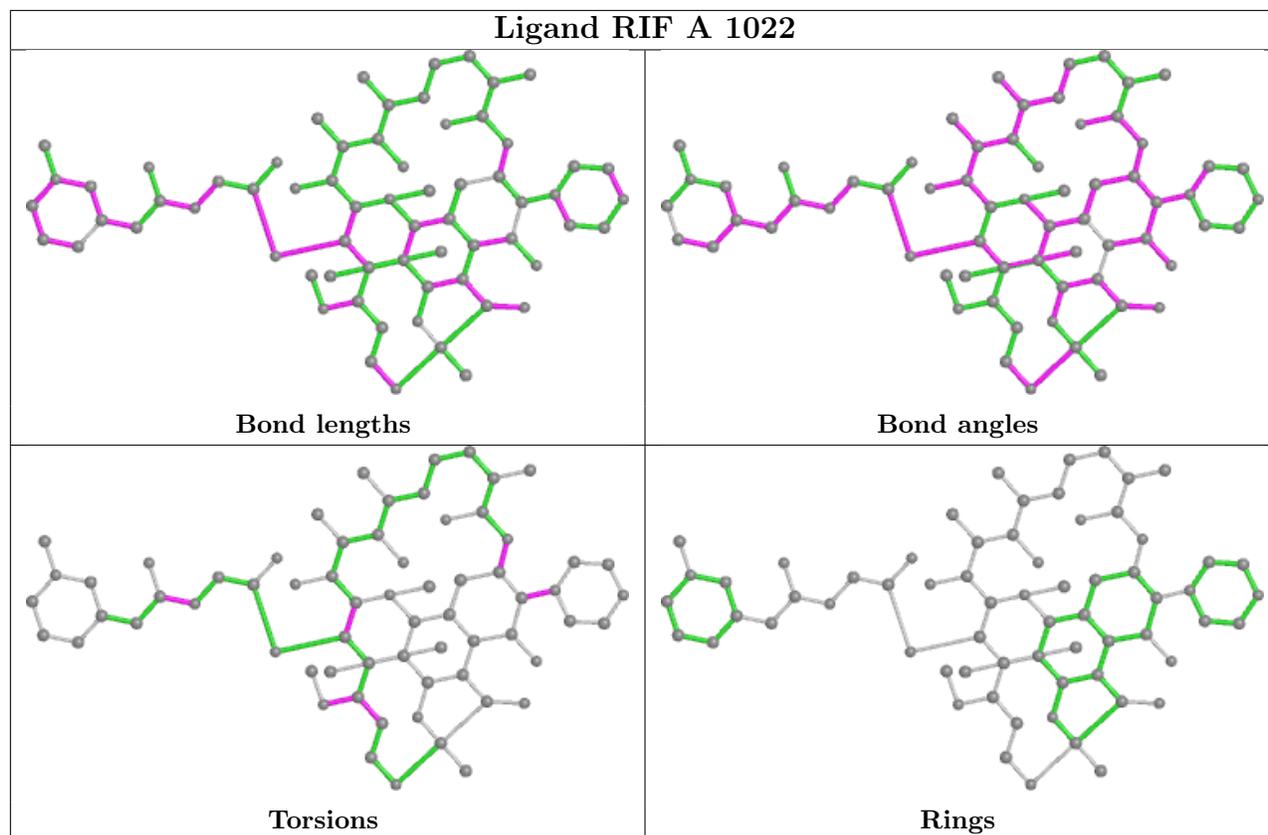
5.7 Other polymers ⓘ

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	707/707 (100%)	-0.10	7 (0%)	82	82	28, 64, 106, 122	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	GLY	4.5
1	A	101	SER	2.7
1	A	495	TYR	2.3
1	A	113	GLY	2.3
1	A	519	LYS	2.3

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.
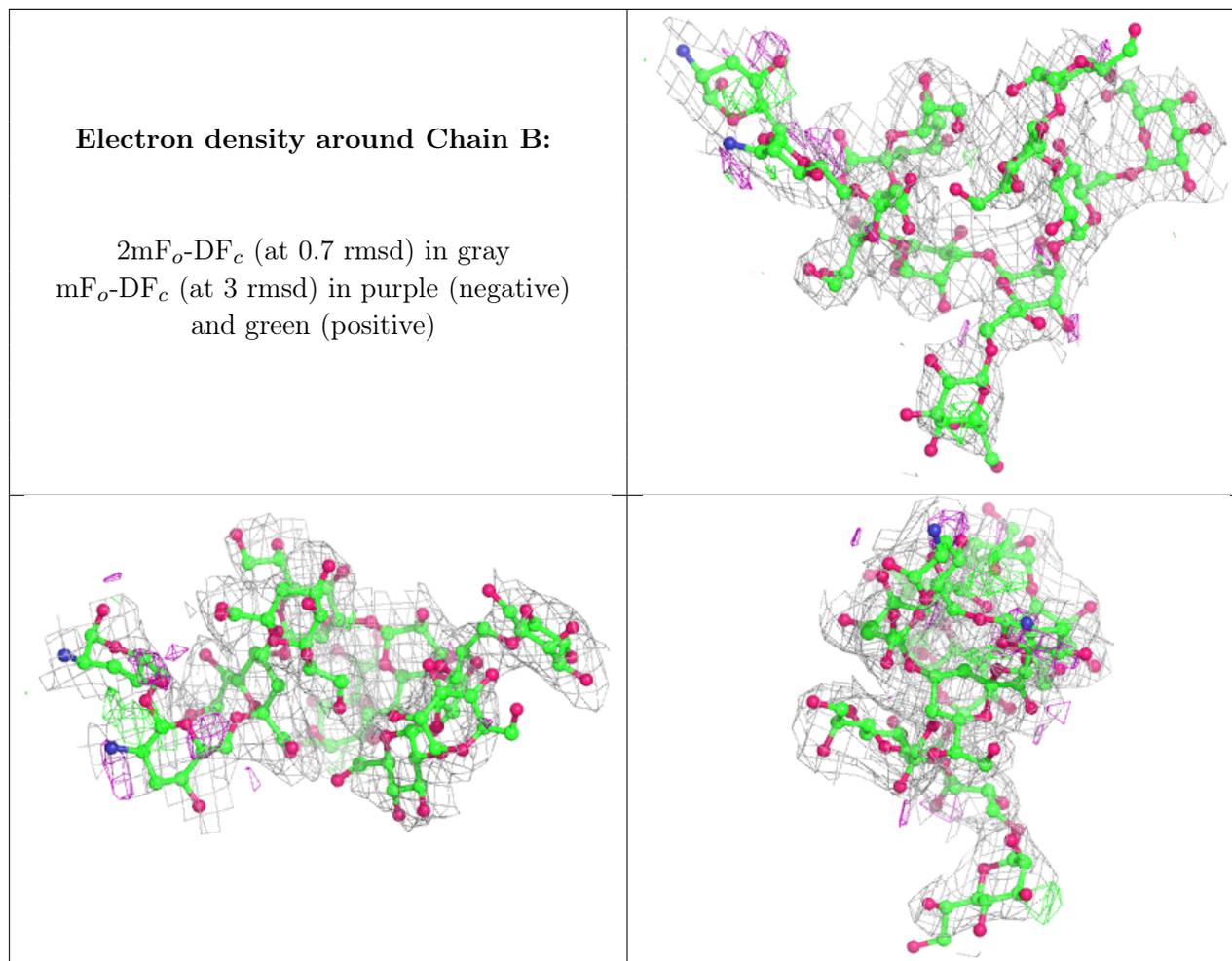
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GMH	B	10	13/14	0.83	0.39	116,119,123,123	0
2	GLC	B	8	11/12	0.87	0.45	122,123,123,123	0
2	GLA	B	9	11/12	0.89	0.28	108,108,111,111	0
2	GLC	B	7	11/12	0.90	0.35	112,116,119,120	0
2	PA1	B	1	11/12	0.90	0.15	51,63,74,80	0
2	KDO	B	11	15/16	0.90	0.16	71,75,82,85	0
2	GMH	B	5	13/14	0.91	0.20	67,87,102,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	B	6	11/12	0.92	0.28	90,93,101,103	0
2	GCN	B	2	10/11	0.93	0.14	35,49,58,61	0
2	GMH	B	4	13/14	0.97	0.12	53,62,72,76	0
2	KDO	B	3	15/16	0.97	0.12	55,62,66,72	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 B:

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.
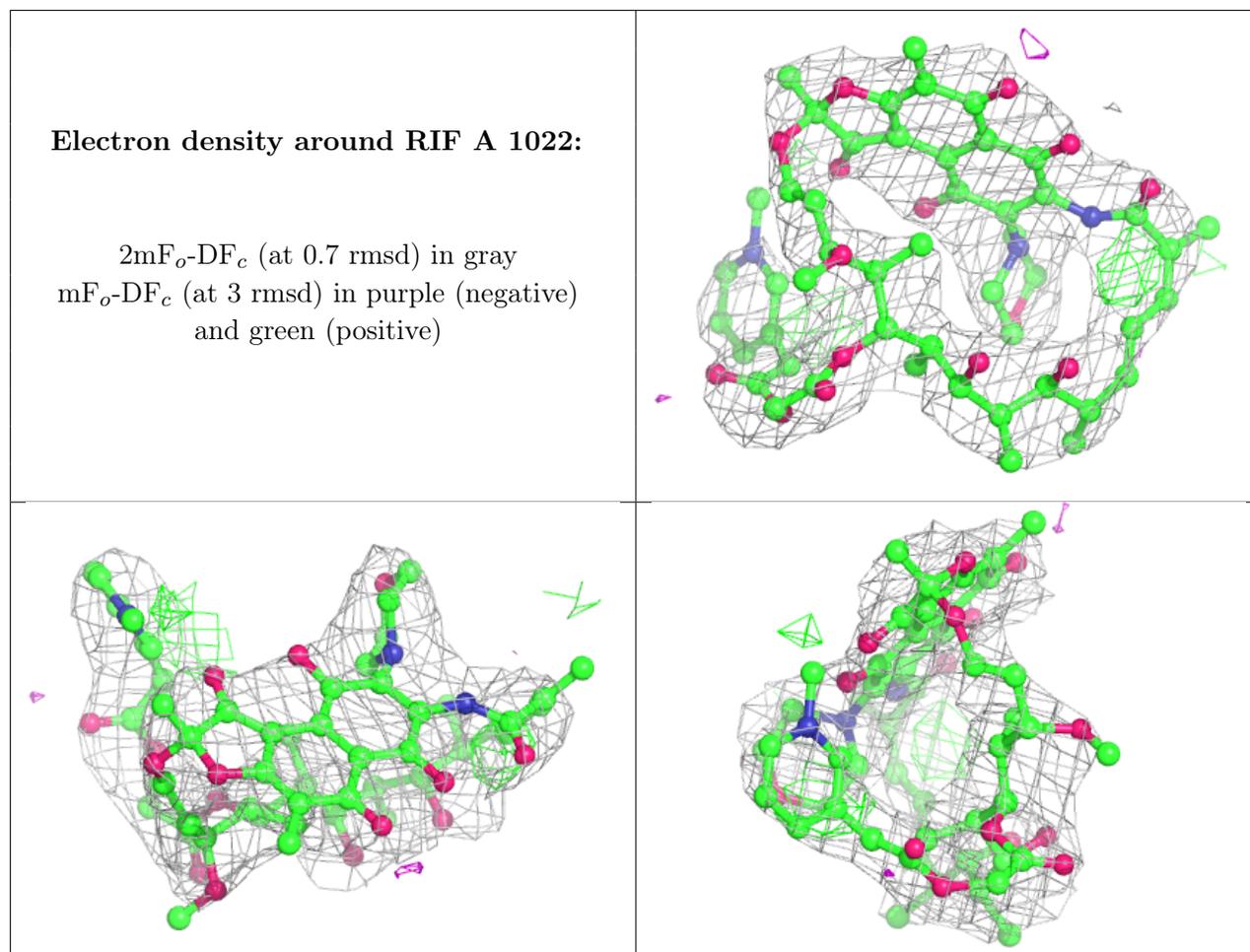
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	1025	1/1	0.79	0.23	90,90,90,90	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
10	DDQ	A	1023	14/14	0.86	0.42	104,110,122,123	0
3	FTT	A	1007	15/17	0.88	0.45	72,84,99,100	0
9	RIF	A	1022	67/67	0.89	0.29	81,98,108,110	0
3	FTT	A	1002	16/17	0.89	0.24	62,67,78,78	0
6	NA	A	1024	1/1	0.90	0.46	102,102,102,102	0
4	PO4	A	1016	4/5	0.90	0.10	91,93,96,98	0
3	FTT	A	1003	9/17	0.92	0.27	81,95,105,105	0
5	NI	A	1021	1/1	0.92	0.08	95,95,95,95	0
3	FTT	A	1004	16/17	0.92	0.28	57,65,69,69	1
3	FTT	A	1006	17/17	0.93	0.32	57,76,87,88	0
4	PO4	A	1014	4/5	0.93	0.15	73,76,80,83	0
3	FTT	A	1005	13/17	0.95	0.21	66,69,72,75	0
8	DPO	A	1013	8/9	0.96	0.10	87,89,92,96	0
8	DPO	A	1015	8/9	0.96	0.10	81,97,108,108	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 RIF A 1022:

$2mF_o$-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 ⓘ

There are no such residues in this entry.