W O R L D W I D E

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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2024 – 10:21 PM EDT

PDB ID	:	2PMV
Title	:	Crystal Structure of Human Intrinsic Factor- Cobalamin Complex at 2.6 A Resolution
Authors	:	Mathews, F.S.; Gordon, M.M.; Chen, Z.; Rajashankar, K.R.; Ealick, S.E.; Alpers, D.H.; Sukumar, N.
Deposited on	:	2007-04-23
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

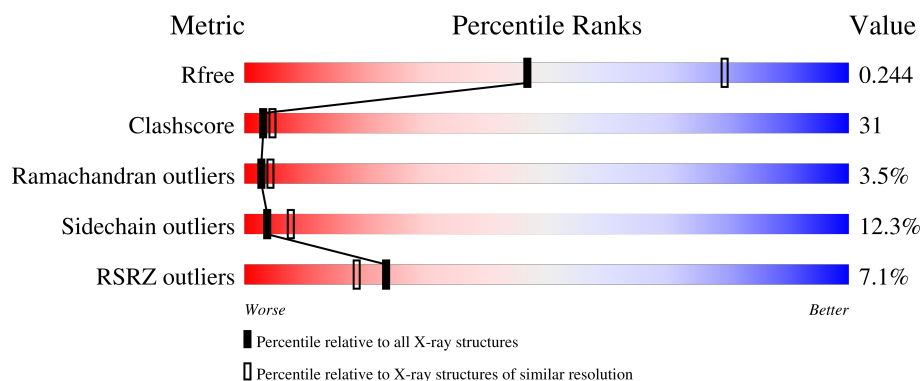|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.60 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		0.244
Clashscore		31
Ramachandran outliers		3.5%
Sidechain outliers		12.3%
RSRZ outliers		7.1%

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$_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	399	7% · 52% 31% 11% · 5%
1	B	399	2% · 41% 21% 5% · 33%
1	C	399	11% · 49% 34% 10% · 5%
1	D	399	3% · 41% 21% 5% · 33%

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Mol	Chain	Length	Quality of chain
2	E	2	100%
2	F	2	100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10457 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 Gastric intrinsic factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total 2871	C 1820	N 475	O 557	S 19	3	0	0
1	B	267	Total 2009	C 1268	N 332	O 392	S 17	0	0	0
1	C	378	Total 2871	C 1820	N 475	O 557	S 19	5	0	0
1	D	267	Total 2009	C 1268	N 332	O 392	S 17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIS	GLN	conflict	UNP P27352
B	73	HIS	GLN	conflict	UNP P27352
C	73	HIS	GLN	conflict	UNP P27352
D	73	HIS	GLN	conflict	UNP P27352

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).

B12
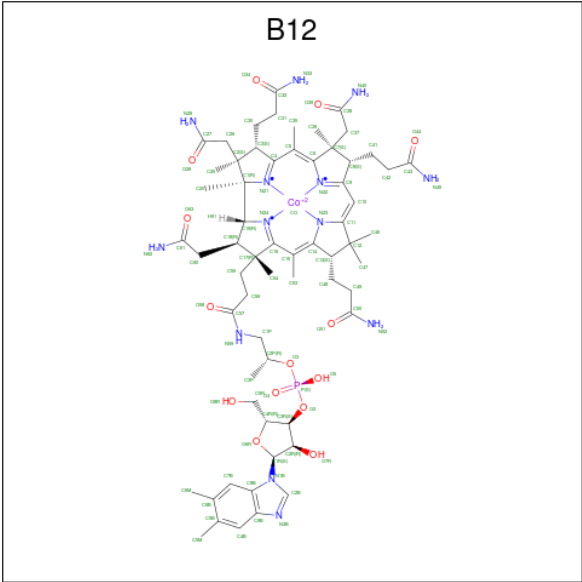
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	100	Total	O	0	0
			100	100		
4	C	129	Total	O	0	0
			129	129		
4	D	95	Total	O	0	0
			95	95		

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: Gastric intrinsic factor

- Molecule 1: Gastric intrinsic factor

PHE LYS PHE GLU THR THR MET THR SER TRP GLY LEU VAL VAL SER SER ILE ASN ASN ILE ALA GLU ASN VAL HIS LYS THR TYR TRP GLN PHE LEU SER GLY VAL THR PRO LEU ASN GLU GLY VAL ALA ASP TYR ILE PRO PHE ASN HIS GLU HIS ILE THR ALA ASN PHE THR GLN

TYR

• Molecule 1: Gastric intrinsic factor

Chain C:

• Molecule 1: Gastric intrinsic factor

Chain D:

THR LEU PRO SER ASN PRO GLY PRO GLY THR SER GLY LEU VAL VAL SER ILE ASN ILE ALA GLU ASN VAL ASN HIS LYS THR TYR TRP GLN PHE LEU SER GLY VAL THR PRO LEU ASN GLU GLY VAL ALA ASP TYR ILE PRO PHE ASN HIS GLU HIS ILE THR ALA ASN PHE THR GLN

PHE LYS PHE GLU THR THR MET THR SER TRP GLY LEU VAL VAL SER SER ILE ASN ILE ALA GLU ASN VAL ASN HIS LYS THR TYR TRP GLN PHE LEU SER GLY VAL THR PRO LEU ASN GLU GLY VAL ALA ASP TYR ILE PRO PHE ASN HIS GLU HIS ILE THR ALA ASN PHE THR GLN

TYR

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

Chain E:

100%

NAG1
NAG2

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

Chain F:

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	90.10Å 67.30Å 147.70Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	37.53 – 2.60 37.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.4 (37.53-2.60) 93.3 (37.53-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.249 0.205 , 0.244	Depositor DCC
R_{free} test set	1564 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	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	0.94	EDS
Total number of atoms	10457	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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   ⓘ

5.1   Standard geometry   ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B12, 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	0.63	2/2925 (0.1%)	0.97	13/3978 (0.3%)
1	B	0.56	0/2044	0.76	1/2775 (0.0%)
1	C	0.64	5/2925 (0.2%)	0.94	12/3978 (0.3%)
1	D	0.55	0/2044	0.76	2/2775 (0.1%)
All	All	0.60	7/9938 (0.1%)	0.88	28/13506 (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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	GLU	CB-CG	-8.85	1.35	1.52
1	C	52	LYS	CB-CG	-8.64	1.29	1.52
1	A	308	GLU	CD-OE1	-6.67	1.18	1.25
1	C	308	GLU	CD-OE1	-6.52	1.18	1.25
1	C	52	LYS	CG-CD	-6.31	1.30	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLU	N-CA-CB	-13.05	87.12	110.60
1	C	52	LYS	CD-CE-NZ	-12.87	82.11	111.70
1	A	52	LYS	CD-CE-NZ	-12.63	82.66	111.70
1	A	321	SER	N-CA-C	-11.86	78.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	304	LEU	N-CA-C	11.50	142.05	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLU	Mainchain

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	2871	0	2861	214	1
1	B	2009	0	2043	99	0
1	C	2871	0	2861	223	1
1	D	2009	0	2043	84	0
2	E	28	0	25	1	0
2	F	28	0	25	2	0
3	A	91	0	87	10	0
3	C	91	0	87	2	0
4	A	135	0	0	8	0
4	B	100	0	0	15	0
4	C	129	0	0	12	0
4	D	95	0	0	8	0
All	All	10457	0	10032	617	1

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 31.

The worst 5 of 617 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:175:GLU:OE1	1:A:177:TYR:CE1	1.89	1.24
1:C:305:ARG:O	1:C:307:VAL:N	1.80	1.14
1:A:333:GLN:HE21	1:A:340:LYS:HB2	1.09	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:CD1	1:C:305:ARG:HG3	1.77	1.13
1:C:302:ASN:HD22	1:C:303:GLN:N	1.46	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:O	1:C:52:LYS:NZ[1_655]	1.87	0.33

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	374/399 (94%)	333 (89%)	24 (6%)	17 (4%)	2	2
1	B	265/399 (66%)	240 (91%)	20 (8%)	5 (2%)	6	13
1	C	374/399 (94%)	334 (89%)	22 (6%)	18 (5%)	2	2
1	D	265/399 (66%)	243 (92%)	17 (6%)	5 (2%)	6	13
All	All	1278/1596 (80%)	1150 (90%)	83 (6%)	45 (4%)	3	4

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ALA
1	A	291	ALA
1	A	306	GLY
1	A	311	PHE
1	A	320	LYS

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	322/349 (92%)	281 (87%)	41 (13%)	3	7
1	B	229/349 (66%)	203 (89%)	26 (11%)	4	9
1	C	322/349 (92%)	280 (87%)	42 (13%)	3	6
1	D	229/349 (66%)	203 (89%)	26 (11%)	4	9
All	All	1102/1396 (79%)	967 (88%)	135 (12%)	4	8

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	LEU
1	D	124	LEU
1	D	232	THR
1	B	74	LEU
1	B	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	108	ASN
1	D	128	ASN
1	B	67	ASN
1	B	54	GLN
1	D	146	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 (i)

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	NAG	E	1	1,2	14,14,15	1.38	2 (14%)	17,19,21	1.93	4 (23%)
2	NAG	E	2	2	14,14,15	1.40	2 (14%)	17,19,21	1.40	3 (17%)
2	NAG	F	1	1,2	14,14,15	1.77	4 (28%)	17,19,21	2.05	4 (23%)
2	NAG	F	2	2	14,14,15	1.22	2 (14%)	17,19,21	1.33	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
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	4.10	1.57	1.52
2	E	1	NAG	C1-C2	3.13	1.56	1.52
2	E	2	NAG	C4-C5	2.84	1.59	1.53
2	F	1	NAG	C4-C5	2.82	1.59	1.53
2	F	2	NAG	C4-C5	2.47	1.58	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C2-N2-C7	5.08	129.71	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C2-N2-C7	4.66	129.14	122.90
2	F	1	NAG	C8-C7-N2	4.29	123.23	116.12
2	E	1	NAG	C8-C7-N2	4.18	123.05	116.12
2	F	1	NAG	O7-C7-C8	-3.74	115.40	122.05

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	2	0
2	F	2	NAG	1	0
2	E	1	NAG	1	0
2	E	2	NAG	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 E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
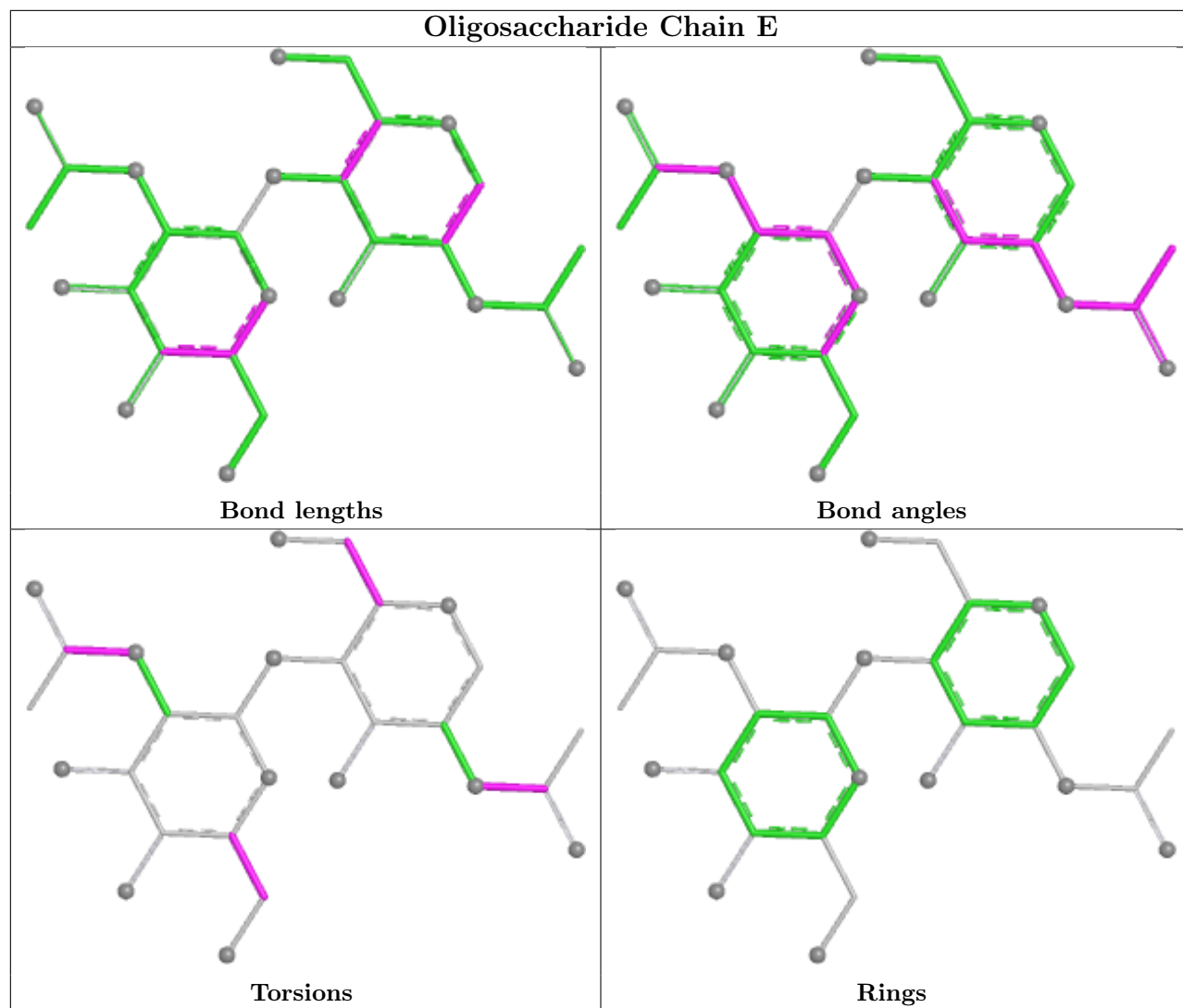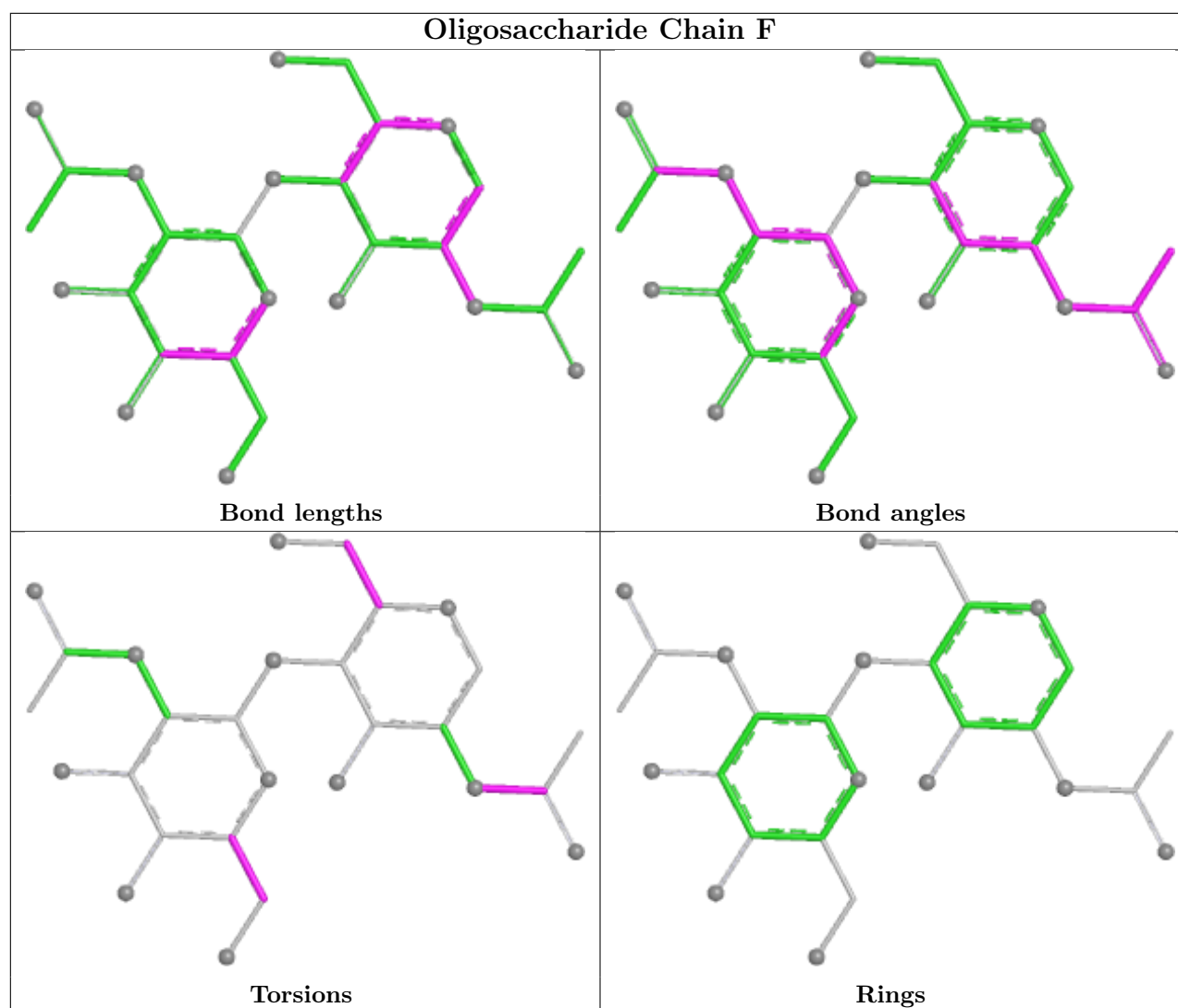
5.6   Ligand geometry (i)

2 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	B12	A	1001	-	91,101,101	1.74	23 (25%)	140,166,166	1.35	20 (14%)
3	B12	C	1002	-	91,101,101	1.71	18 (19%)	140,166,166	1.32	17 (12%)

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
3	B12	A	1001	-	-	10/52/223/223	0/3/11/11
3	B12	C	1002	-	-	5/52/223/223	0/3/11/11

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	B12	C14-N23	5.08	1.41	1.35
3	A	1001	B12	C14-N23	4.42	1.41	1.35
3	A	1001	B12	C11-N23	4.24	1.44	1.36
3	C	1002	B12	C41-C8	4.22	1.64	1.54
3	A	1001	B12	C6B-C5B	3.99	1.50	1.40

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	B12	C60-C18-C17	4.05	126.91	115.82
3	A	1001	B12	C12-C13-C14	3.86	108.60	102.26
3	C	1002	B12	C12-C13-C14	3.75	108.43	102.26
3	A	1001	B12	C60-C18-C17	3.72	125.99	115.82
3	A	1001	B12	C41-C8-C9	3.65	117.56	111.19

There are no chirality outliers.

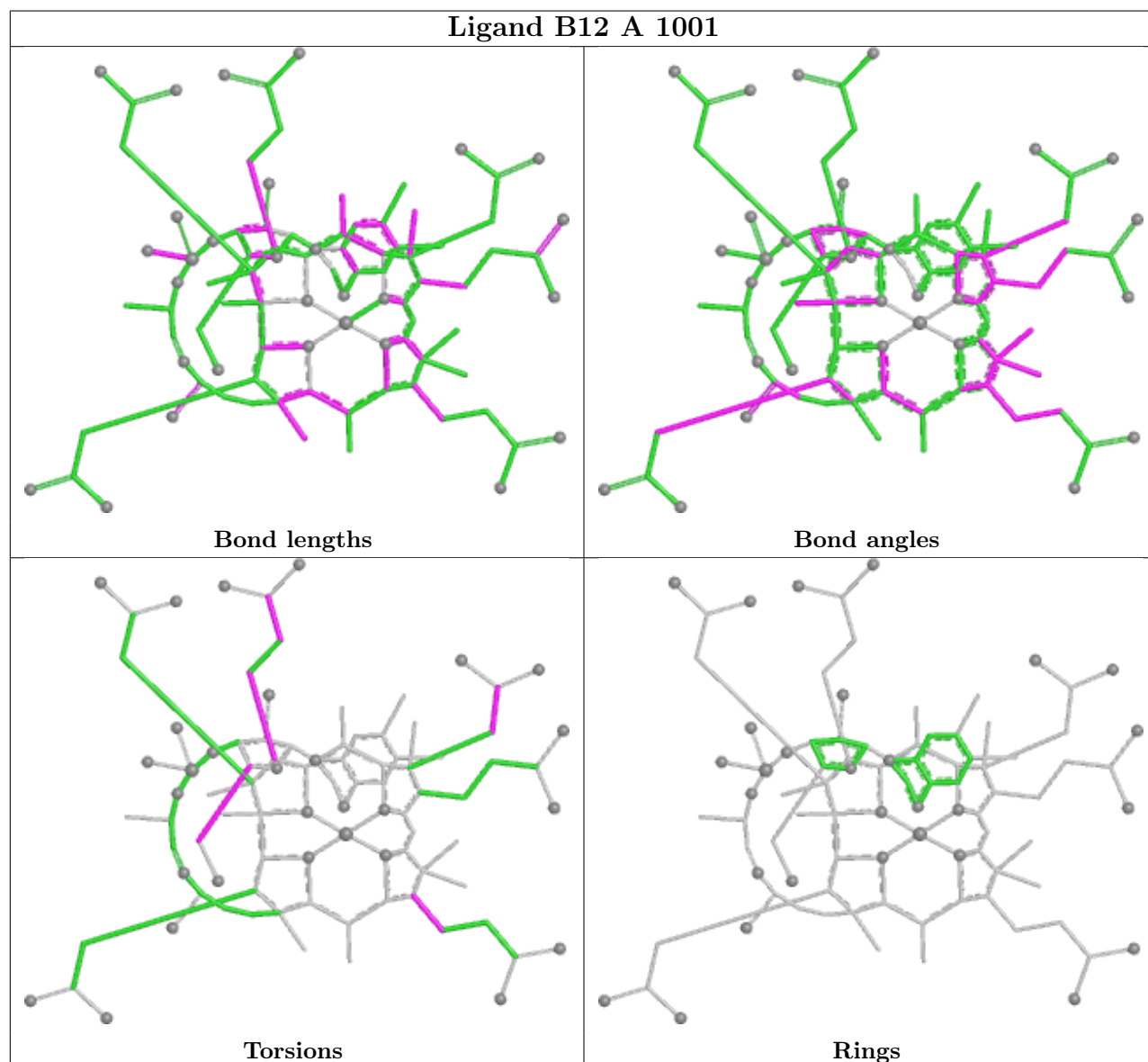5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	B12	C3R-C4R-C5R-O8R
3	A	1001	B12	O6R-C4R-C5R-O8R
3	C	1002	B12	C3R-C4R-C5R-O8R
3	C	1002	B12	O6R-C4R-C5R-O8R
3	A	1001	B12	C7-C37-C38-N40

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	B12	10	0
3	C	1002	B12	2	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 B12 A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 C 1002

Bond lengths

Bond angles

Torsions

Rings
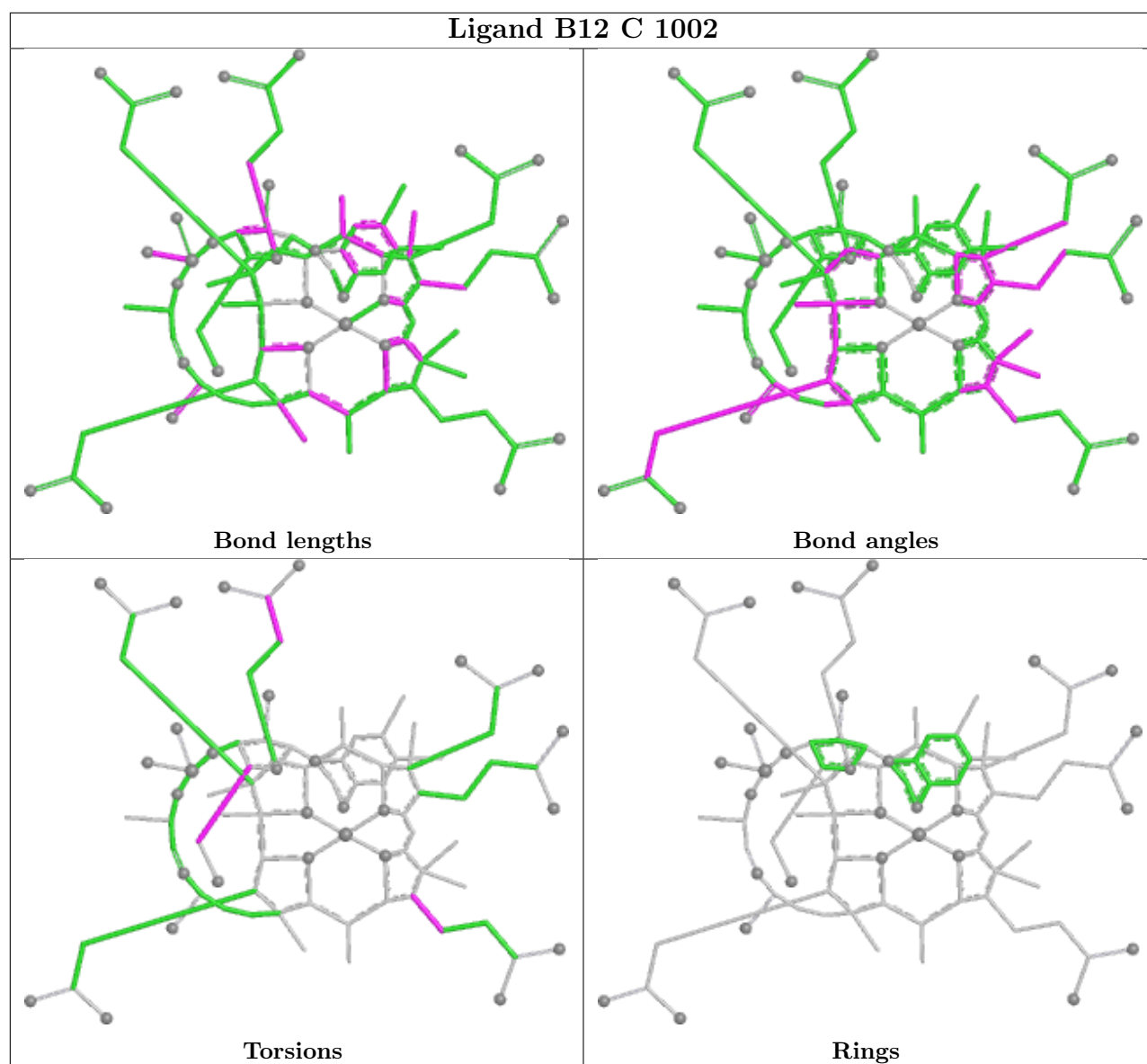
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	378/399 (94%)	0.14	29 (7%)	21	17	29, 49, 97, 99	1 (0%)
1	B	267/399 (66%)	-0.06	9 (3%)	48	42	31, 48, 85, 99	0
1	C	378/399 (94%)	0.40	43 (11%)	11	8	30, 52, 99, 99	2 (0%)
1	D	267/399 (66%)	-0.12	10 (3%)	45	39	30, 46, 81, 99	0
All	All	1290/1596 (80%)	0.12	91 (7%)	23	18	29, 49, 97, 99	3 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	ALA	5.8
1	A	304	LEU	5.6
1	C	321	SER	5.4
1	C	322	GLY	5.3
1	C	306	GLY	5.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
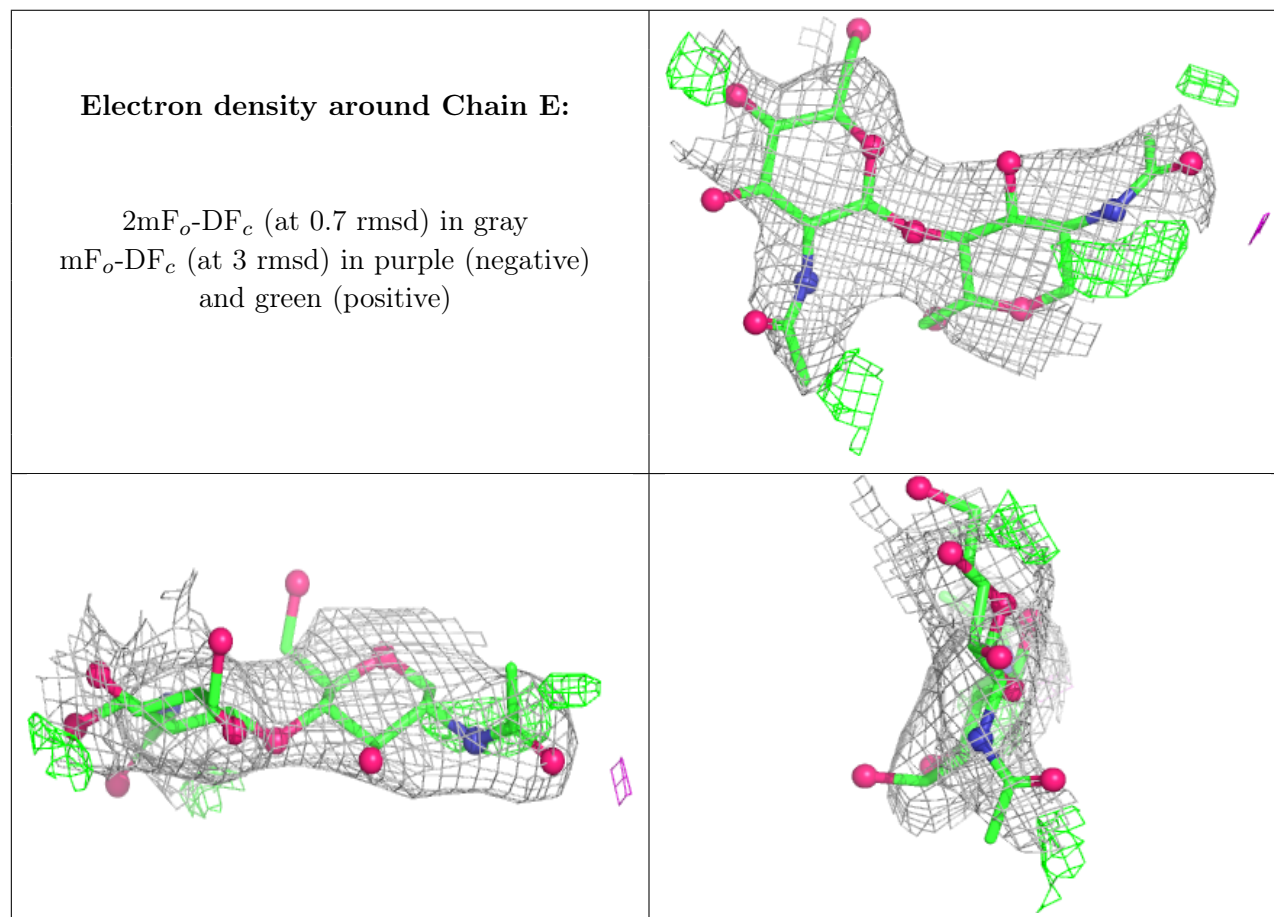
| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NAG	E	2	14/15	0.65	0.18	97,99,99,99	0
2	NAG	F	2	14/15	0.67	0.18	95,98,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	1	14/15	0.82	0.16	86,87,91,94	0
2	NAG	E	1	14/15	0.85	0.18	94,97,99,99	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.
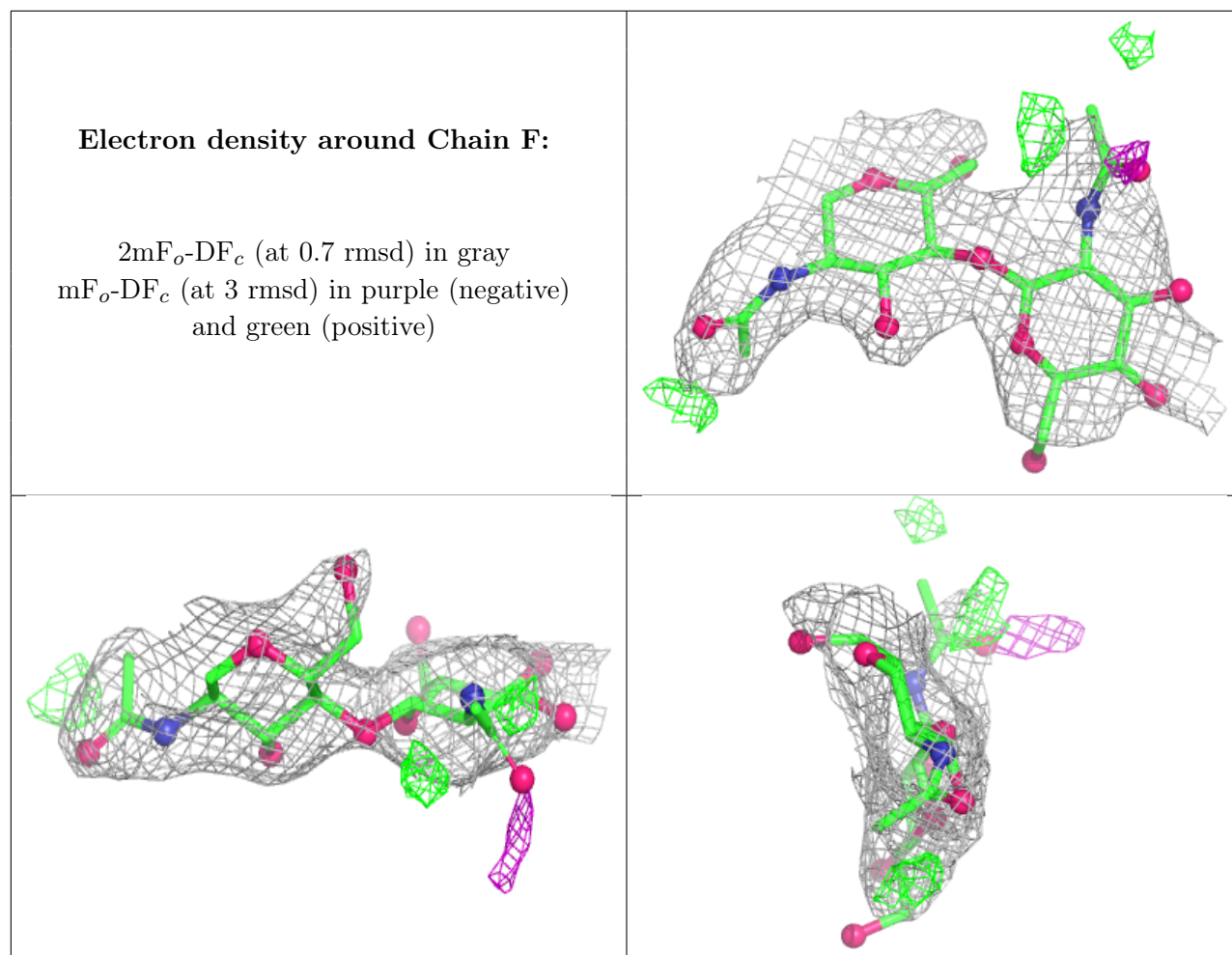
Electron density around Chain E:

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

Electron density around Chain F:

$2mF_o\text{-}DF_c$ (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
3	B12	A	1001	91/91	0.95	0.09	30,41,53,68	0
3	B12	C	1002	91/91	0.95	0.09	37,47,60,66	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.
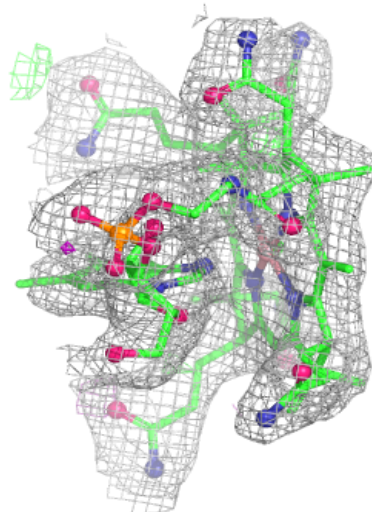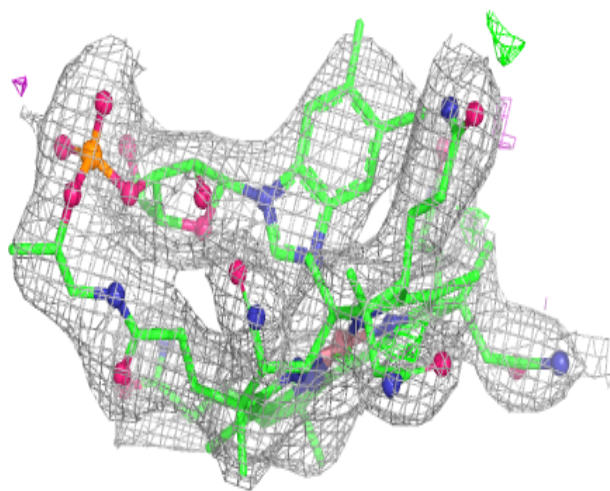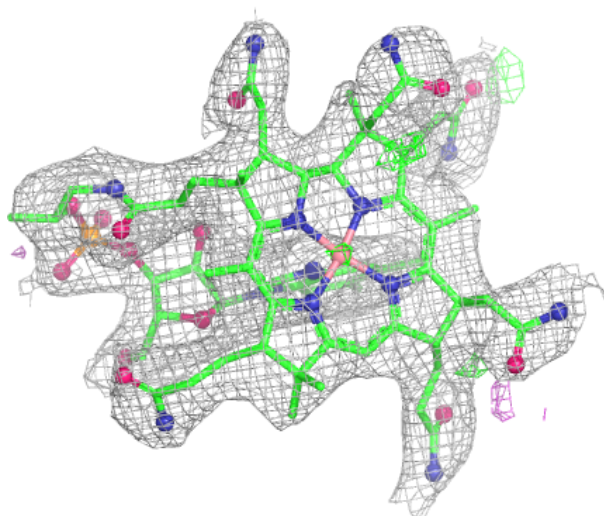
Electron density around B12 A 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
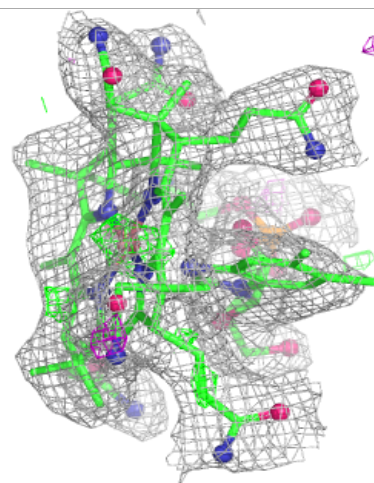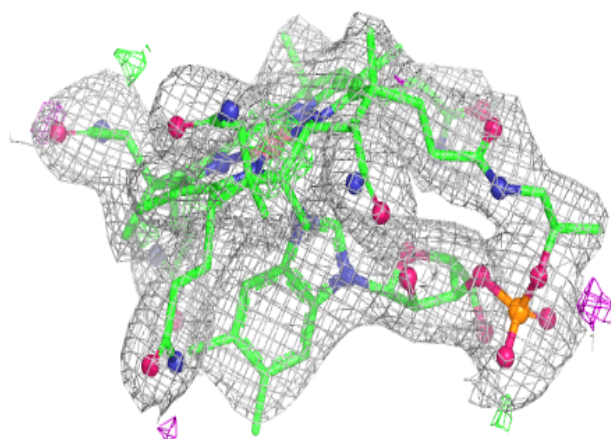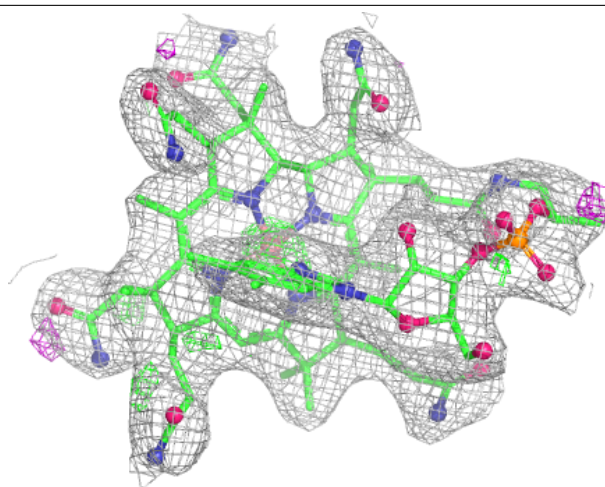
Electron density around B12 C 1002:

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.