Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 06:33 PM JST

PDB ID	:	8JBT
Title	:	B12-binding domain from Chloracidobacterium thermophilum MerR family protein, anaerobic light state
Authors	:	Zhang, S.; Yu, Y.
Deposited on	:	2023-05-09
Resolution	:	2.30 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:

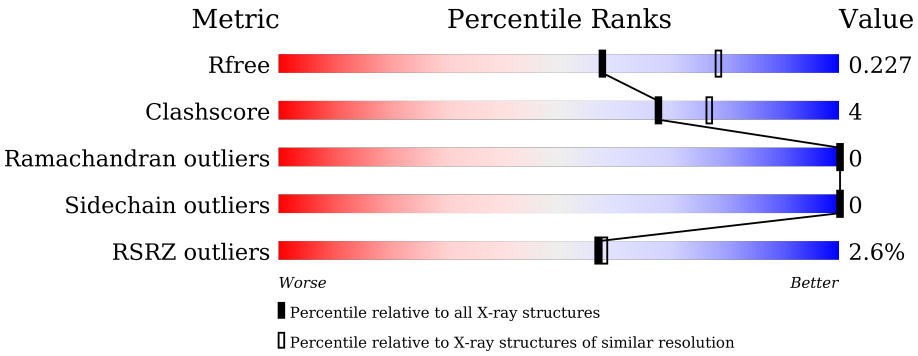
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	327	2% 67% 30%
1	B	327	2% 63% 6% 31%

2 Entry composition

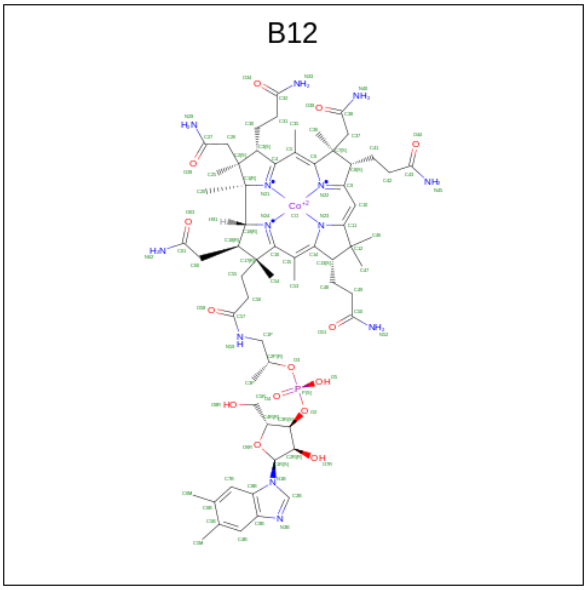
There are 7 unique types of molecules in this entry. The entry contains 3903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative cobalamin binding protein.

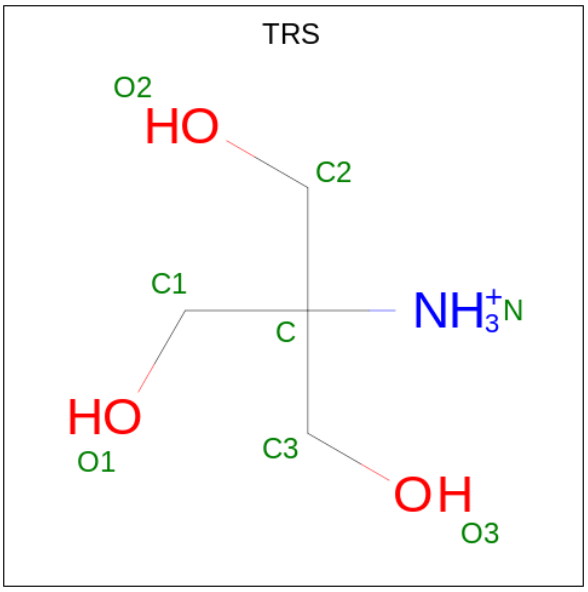
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1805	1152	329	320	4			
1	B	225	Total	C	N	O	S	0	1	0
			1796	1146	329	317	4			

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



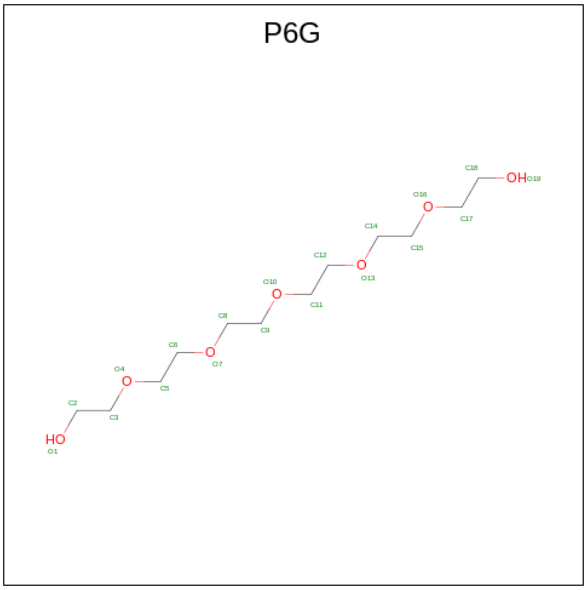
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



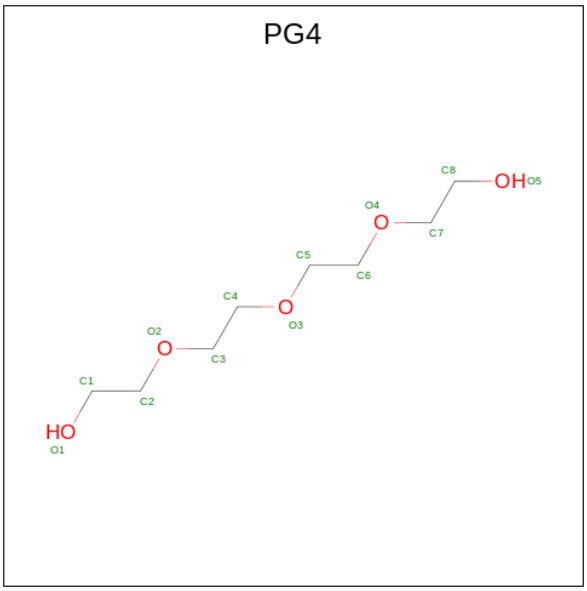
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 1 3	0	0
3	B	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



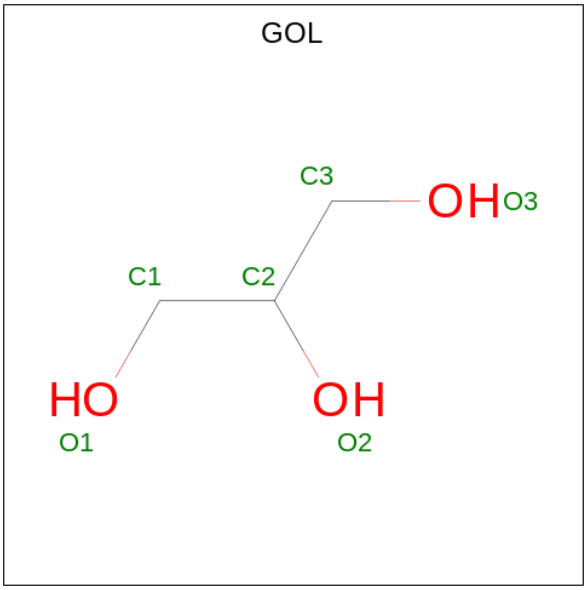
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 19 12 7	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 8 5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

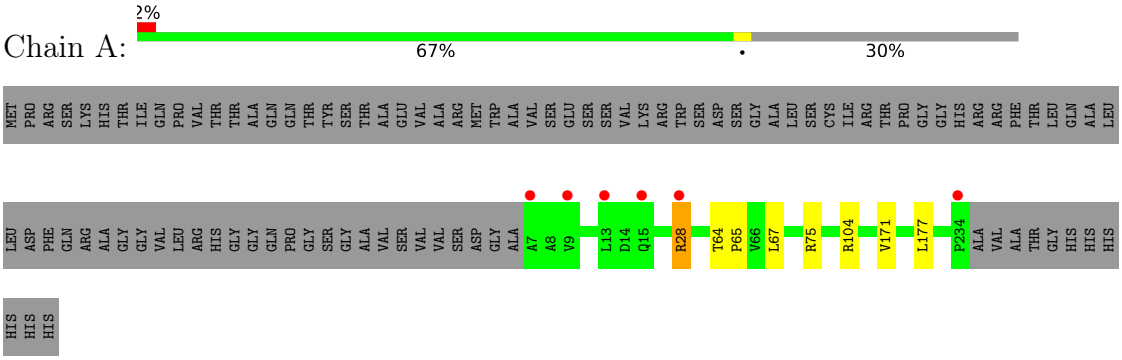
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	26	Total O 26 26	0	0
7	B	40	Total O 40 40	0	0

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.

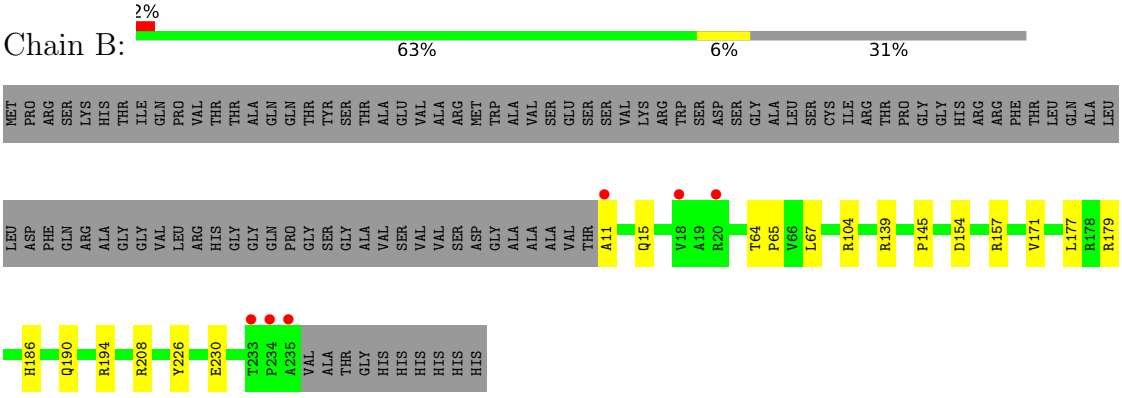
• Molecule 1: Putative cobalamin binding protein

Chain A:



• Molecule 1: Putative cobalamin binding protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.48Å 123.48Å 73.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	106.94 – 2.30 106.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (106.94-2.30) 100.0 (106.94-2.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.206 , 0.225 0.207 , 0.227	Depositor DCC
R_{free} test set	1425 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 19.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3903	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: P6G, GOL, B12, TRS, PG4

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	0.23	0/1850	0.53	0/2521
1	B	0.22	0/1842	0.54	0/2509
All	All	0.23	0/3692	0.54	0/5030

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	3
1	B	0	5
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	75	ARG	Sidechain
1	B	104	ARG	Sidechain
1	B	139	ARG	Sidechain
1	B	179	ARG	Sidechain
1	B	194	ARG	Sidechain
1	B	208	ARG	Sidechain

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	1805	0	1783	5	0
1	B	1796	0	1768	8	0
2	A	91	0	88	7	0
2	B	91	0	88	10	0
3	A	8	0	12	0	0
3	B	8	0	12	1	0
4	A	19	0	26	0	0
5	B	13	0	18	0	0
6	B	6	0	8	0	0
7	A	26	0	0	0	0
7	B	40	0	0	0	0
All	All	3903	0	3803	27	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 4.

All (27) 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)
2:B:302:B12:H362	2:B:302:B12:H351	1.38	1.06
2:A:301:B12:H362	2:A:301:B12:H351	1.35	1.02
2:A:301:B12:H531	2:A:301:B12:H543	1.64	0.80
2:B:302:B12:H351	2:B:302:B12:C36	2.16	0.74
2:A:301:B12:H351	2:A:301:B12:C36	2.14	0.73
2:B:302:B12:H552	2:B:302:B12:H531	1.71	0.73
1:B:11:ALA:O	1:B:15:GLN:HG3	2.00	0.60
1:B:226:TYR:CE1	1:B:230:GLU:HG3	2.40	0.56
2:A:301:B12:H4R	2:A:301:B12:H3P1	1.88	0.55
2:B:302:B12:H562	2:B:302:B12:H621	1.74	0.52
1:B:64:THR:HB	1:B:65:PRO:HD3	1.91	0.51
1:B:145:PRO:O	3:B:303:TRS:H12	2.10	0.51
1:A:64:THR:HB	1:A:65:PRO:HD3	1.92	0.51
2:B:302:B12:H531	2:B:302:B12:C55	2.39	0.49
1:B:186:HIS:NE2	1:B:190:GLN:NE2	2.64	0.45
2:B:302:B12:C36	2:B:302:B12:C35	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG13	1:A:177:LEU:HD12	1.99	0.44
2:B:302:B12:H362	2:B:302:B12:C35	2.27	0.43
1:A:67:LEU:HB3	2:A:301:B12:C56	2.48	0.43
1:A:67:LEU:HB3	2:A:301:B12:H562	2.01	0.43
2:A:301:B12:H362	2:A:301:B12:C35	2.25	0.42
1:B:154:ASP:OD1	1:B:157:ARG:NH2	2.49	0.42
1:B:171:VAL:HG13	1:B:177:LEU:HD12	2.01	0.42
2:B:302:B12:H262	2:B:302:B12:H91	1.97	0.41
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.86	0.41
2:B:302:B12:H203	2:B:302:B12:H301	2.02	0.40
1:B:67:LEU:O	2:B:302:B12:H541	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	226/327 (69%)	225 (100%)	1 (0%)	0	100	100
1	B	224/327 (68%)	222 (99%)	2 (1%)	0	100	100
All	All	450/654 (69%)	447 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/260 (70%)	183 (100%)	0	100	100
1	B	182/260 (70%)	182 (100%)	0	100	100
All	All	365/520 (70%)	365 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	B	190	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	B12	A	301	1,7	90,101,101	0.65	3 (3%)	137,166,166	0.99	8 (5%)
2	B12	B	302	1,7	90,101,101	0.66	3 (3%)	137,166,166	0.95	7 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	P6G	A	303	-	18,18,18	0.21	0	17,17,17	0.10	0
6	GOL	B	304	-	5,5,5	0.11	0	5,5,5	0.32	0
3	TRS	B	303	-	7,7,7	0.15	0	9,9,9	0.26	0
5	PG4	B	301	-	12,12,12	0.21	0	11,11,11	0.08	0
3	TRS	A	302	-	7,7,7	0.15	0	9,9,9	0.25	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	B12	A	301	1,7	-	13/52/223/223	0/3/11/11
2	B12	B	302	1,7	-	11/52/223/223	0/3/11/11
4	P6G	A	303	-	-	7/16/16/16	-
6	GOL	B	304	-	-	4/4/4/4	-
3	TRS	B	303	-	-	3/9/9/9	-
5	PG4	B	301	-	-	3/10/10/10	-
3	TRS	A	302	-	-	3/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	B12	C14-N23	2.68	1.38	1.35
2	A	301	B12	C16-C15	-2.65	1.37	1.44
2	B	302	B12	C16-C15	-2.59	1.37	1.44
2	A	301	B12	C14-N23	2.21	1.37	1.35
2	A	301	B12	C9-N22	2.20	1.36	1.30
2	B	302	B12	C9-N22	2.07	1.35	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	B12	C55-C17-C16	-4.33	108.09	116.65
2	B	302	B12	C1P-N59-C57	3.66	130.65	122.69
2	A	301	B12	C18-C17-C16	3.33	104.72	100.67
2	B	302	B12	C19-C1-N21	3.15	105.39	102.16
2	A	301	B12	C1-C19-C18	-3.13	116.75	121.88
2	B	302	B12	C20-C1-N21	-2.92	105.48	110.27
2	B	302	B12	C26-C2-C1	2.71	114.22	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	302	B12	C56-C57-N59	2.53	120.67	116.42
2	A	301	B12	C20-C1-N21	-2.36	106.39	110.27
2	A	301	B12	C3P-C2P-C1P	-2.32	106.89	111.39
2	B	302	B12	C7-C8-C9	-2.21	98.08	100.90
2	A	301	B12	O3-C2P-C1P	2.16	111.23	106.92
2	A	301	B12	C7-C8-C9	-2.15	98.16	100.90
2	A	301	B12	C35-C5-C6	-2.10	119.08	122.43
2	B	302	B12	C1-C19-N24	2.01	108.50	106.24

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	B12	C16-C17-C55-C56
2	A	301	B12	C54-C17-C55-C56
2	A	301	B12	C18-C17-C55-C56
2	B	302	B12	N59-C1P-C2P-O3
3	A	302	TRS	C2-C-C3-O3
3	B	303	TRS	C2-C-C1-O1
3	B	303	TRS	C3-C-C1-O1
3	B	303	TRS	N-C-C1-O1
6	B	304	GOL	O1-C1-C2-C3
2	B	302	B12	C56-C57-N59-C1P
2	B	302	B12	O58-C57-N59-C1P
4	A	303	P6G	O13-C14-C15-O16
4	A	303	P6G	O10-C11-C12-O13
5	B	301	PG4	O2-C3-C4-O3
5	B	301	PG4	O3-C5-C6-O4
2	A	301	B12	C18-C60-C61-N62
2	B	302	B12	C18-C60-C61-O63
2	B	302	B12	C18-C60-C61-N62
6	B	304	GOL	C1-C2-C3-O3
3	A	302	TRS	C1-C-C3-O3
4	A	303	P6G	O16-C17-C18-O19
5	B	301	PG4	O4-C7-C8-O5
2	A	301	B12	C18-C60-C61-O63
6	B	304	GOL	O1-C1-C2-O2
2	A	301	B12	C48-C49-C50-O51
4	A	303	P6G	C8-C9-O10-C11
4	A	303	P6G	C18-C17-O16-C15
2	A	301	B12	C48-C49-C50-N52
2	B	302	B12	N59-C1P-C2P-C3P

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Mol	Chain	Res	Type	Atoms
2	A	301	B12	C17-C18-C60-C61
2	A	301	B12	C3R-O2-P-O5
2	A	301	B12	C19-C18-C60-C61
2	B	302	B12	C19-C18-C60-C61
4	A	303	P6G	C6-C5-O4-C3
2	A	301	B12	C4-C3-C30-C31
2	A	301	B12	C1P-C2P-O3-P
6	B	304	GOL	O2-C2-C3-O3
2	B	302	B12	C48-C49-C50-N52
3	A	302	TRS	N-C-C3-O3
2	A	301	B12	C3R-O2-P-O3
2	B	302	B12	C3R-O2-P-O3
2	B	302	B12	C48-C49-C50-O51
2	B	302	B12	C17-C18-C60-C61
4	A	303	P6G	C2-C3-O4-C5

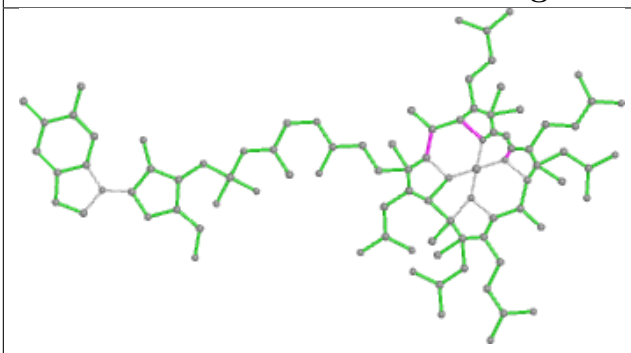
There are no ring outliers.

3 monomers are involved in 18 short contacts:

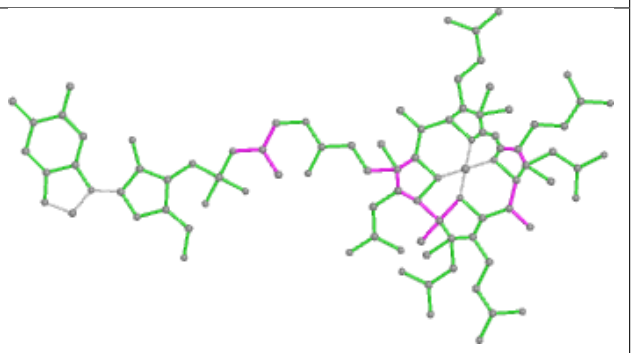
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	B12	7	0
2	B	302	B12	10	0
3	B	303	TRS	1	0

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

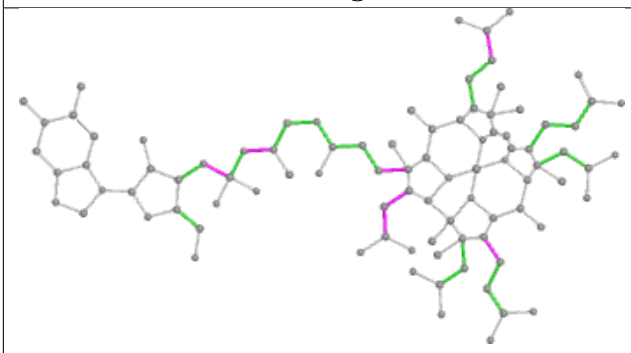
Ligand B12 A 301



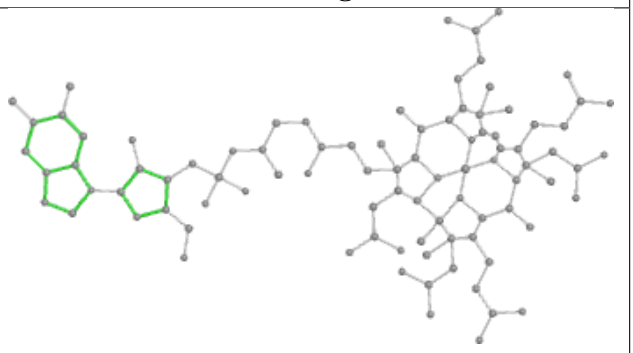
Bond lengths



Bond angles

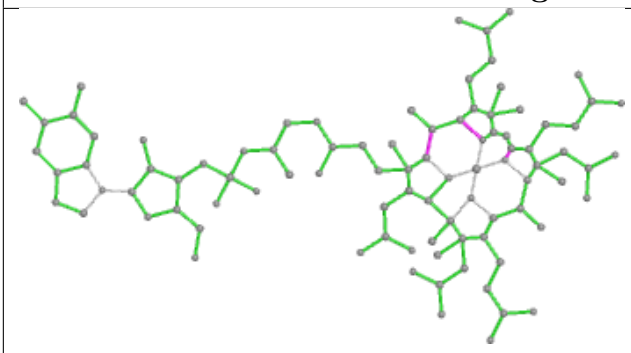


Torsions

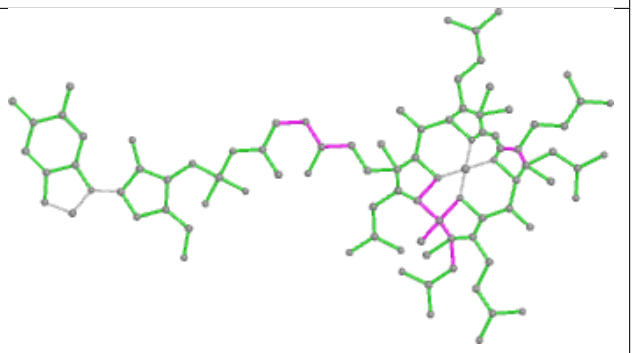


Rings

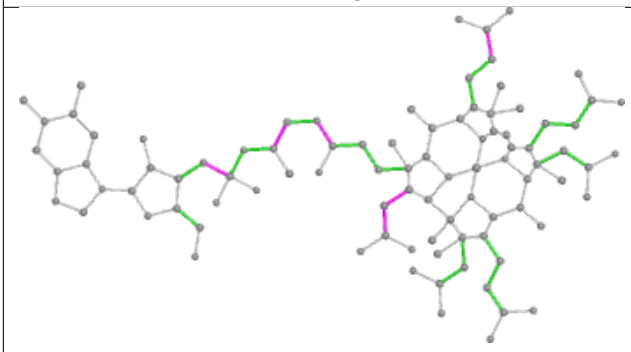
Ligand B12 B 302



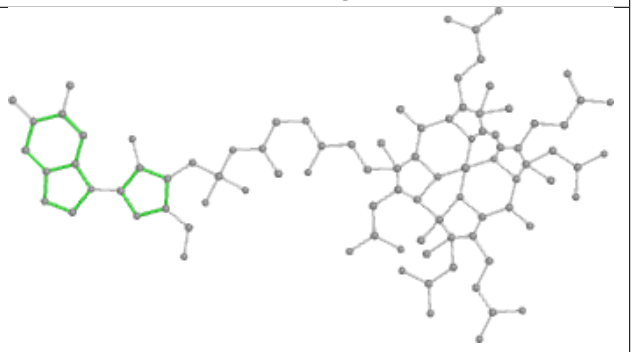
Bond lengths



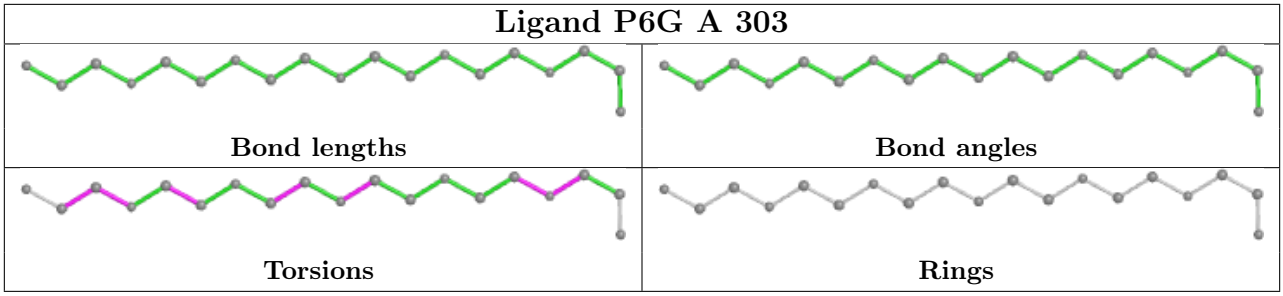
Bond angles



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, 95^{th} 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	228/327 (69%)	0.07	6 (2%) 57 58	32, 46, 73, 90	0
1	B	225/327 (68%)	-0.12	6 (2%) 56 57	17, 39, 69, 101	1 (0%)
All	All	453/654 (69%)	-0.02	12 (2%) 57 58	17, 43, 73, 101	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	6.9
1	A	7	ALA	4.8
1	A	234	PRO	3.8
1	B	234	PRO	3.5
1	B	18	VAL	3.5
1	B	11	ALA	3.3
1	B	233	THR	3.1
1	A	9	VAL	2.8
1	B	20	ARG	2.4
1	A	28	ARG	2.1
1	A	15	GLN	2.1
1	A	13	LEU	2.0

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

There are no monosaccharides in this entry.

6.4 Ligands

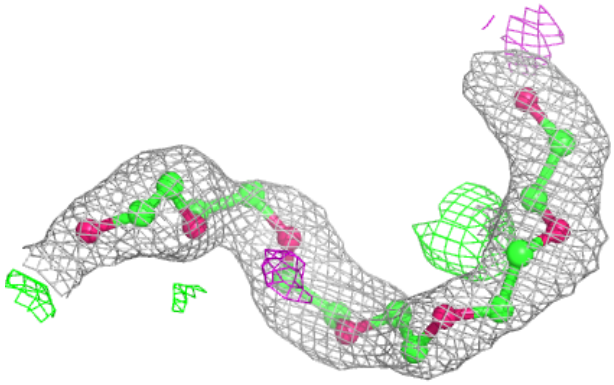
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

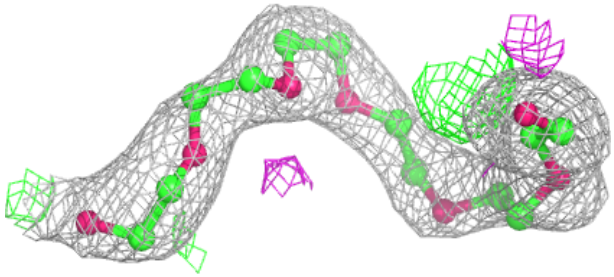
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	304	6/6	0.83	0.19	51,61,68,73	0
3	TRS	B	303	8/8	0.85	0.19	56,63,67,77	0
4	P6G	A	303	19/19	0.88	0.16	42,62,73,77	0
3	TRS	A	302	8/8	0.88	0.14	44,56,60,62	0
5	PG4	B	301	13/13	0.90	0.14	54,59,70,70	0
2	B12	B	302	91/91	0.96	0.08	27,36,42,66	0
2	B12	A	301	91/91	0.97	0.07	30,36,43,50	0

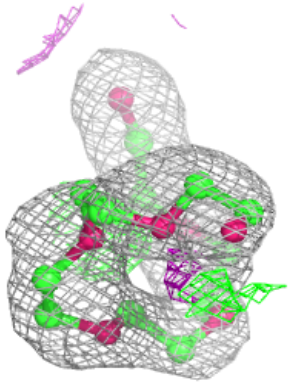
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G A 303:

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

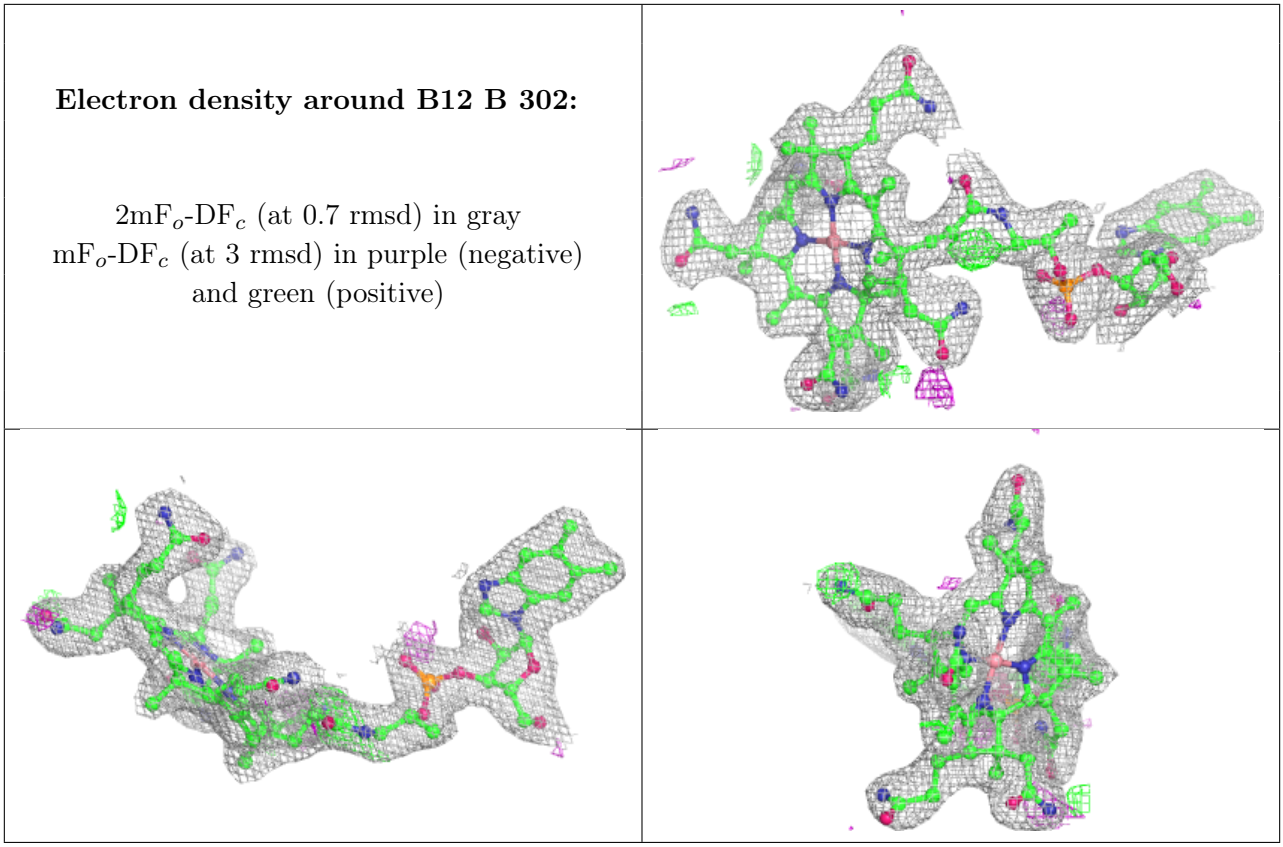






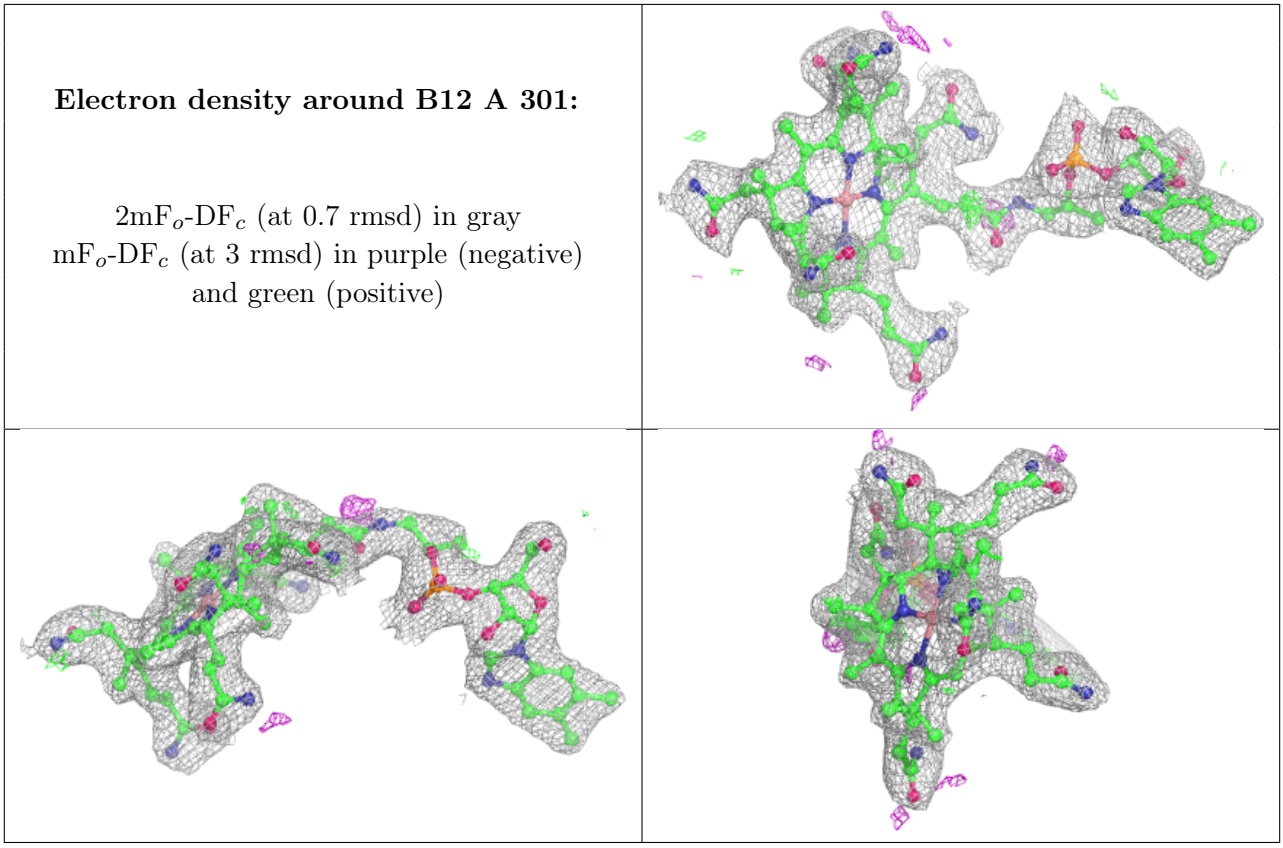
Electron density around B12 B 302:

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



Electron density around B12 A 301:

$2mF_o$-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.