



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2023 – 04:46 AM EDT

PDB ID : 8SSE
Title : Methionine synthase, C-terminal fragment, Cobalamin and Reactivation Domains from *Thermus thermophilus* HB8
Authors : Yamada, K.; Mendoza, J.; Koutmos, M.
Deposited on : 2023-05-08
Resolution : 3.15 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 ⓘ 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)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

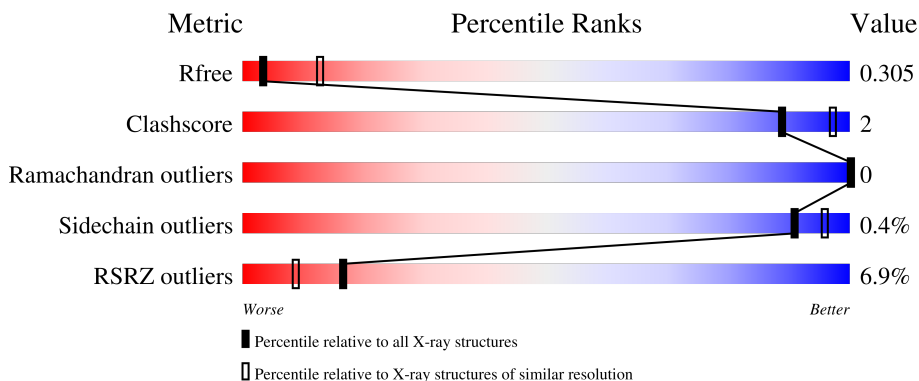
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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.



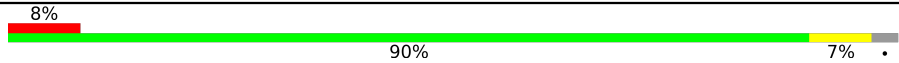
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	523	 7% 89% 7% . .
1	B	523	 10% 90% 7% .
1	C	523	 6% 91% 6% .
1	D	523	 7% 92% 5% .
1	E	523	 3% 91% 6% .

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Mol	Chain	Length	Quality of chain
1	F	523	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a red segment on the left labeled '8%', a large green segment in the middle labeled '90%', and a yellow segment on the right labeled '7%'. A small grey dot is visible at the end of the bar.</p>

2 Entry composition [i](#)

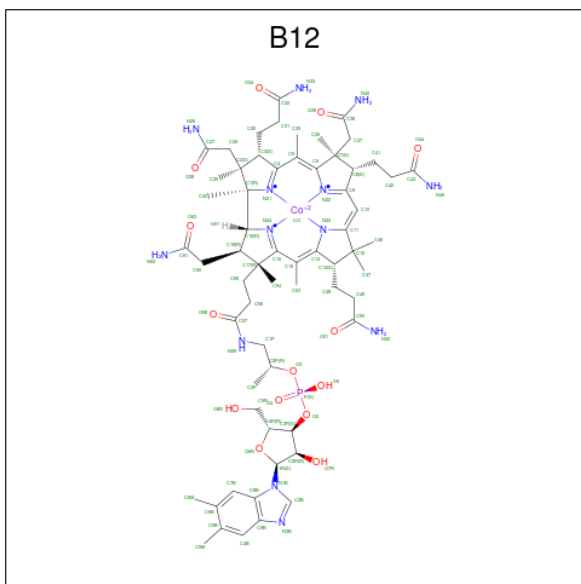
There are 3 unique types of molecules in this entry. The entry contains 24880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	Total 4012	C 2572	N 705	O 719	S 16	0	0	0
1	B	506	Total 4005	C 2567	N 704	O 718	S 16	0	0	0
1	C	507	Total 4012	C 2572	N 705	O 719	S 16	0	0	0
1	D	506	Total 4005	C 2567	N 704	O 718	S 16	0	0	0
1	E	507	Total 4012	C 2572	N 705	O 719	S 16	0	0	0
1	F	505	Total 3994	C 2561	N 700	O 717	S 16	0	0	0

- 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		
2	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	D	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	F	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

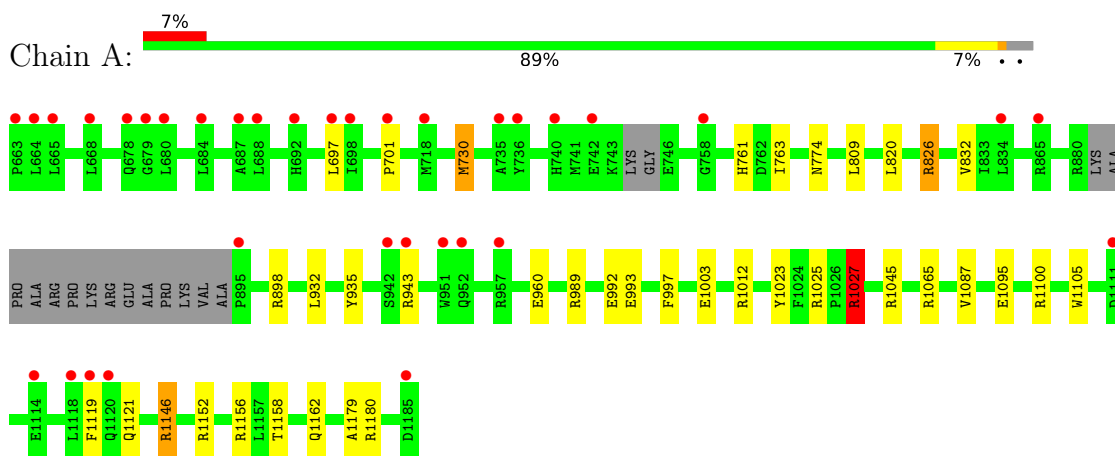
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	40	Total	O	0	0
			40	40		
3	C	62	Total	O	0	0
			62	62		
3	D	40	Total	O	0	0
			40	40		
3	E	55	Total	O	0	0
			55	55		
3	F	50	Total	O	0	0
			50	50		

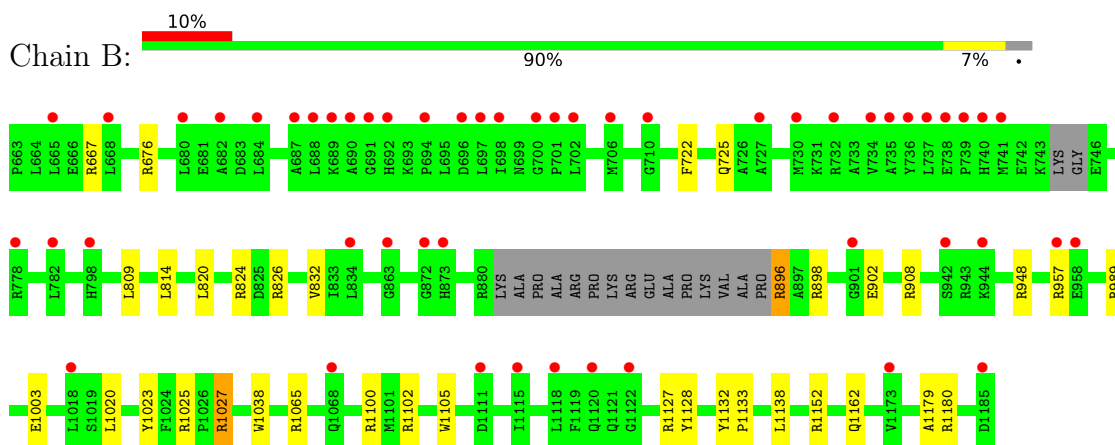
3 Residue-property plots

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.

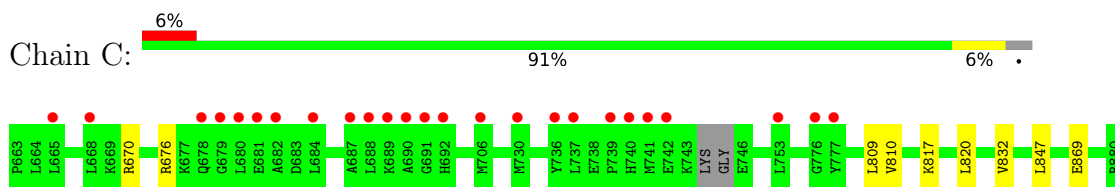
- Molecule 1: Methionine synthase

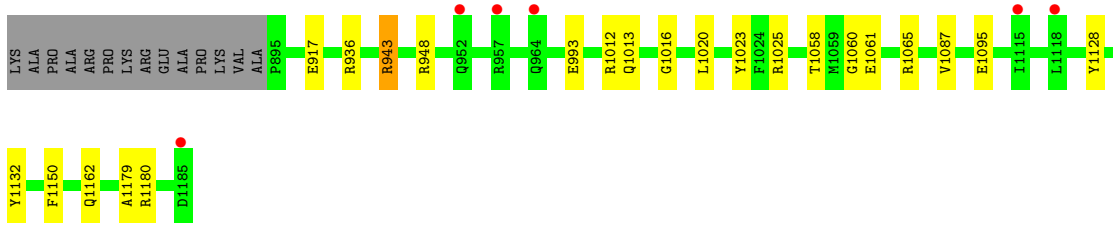


- Molecule 1: Methionine synthase

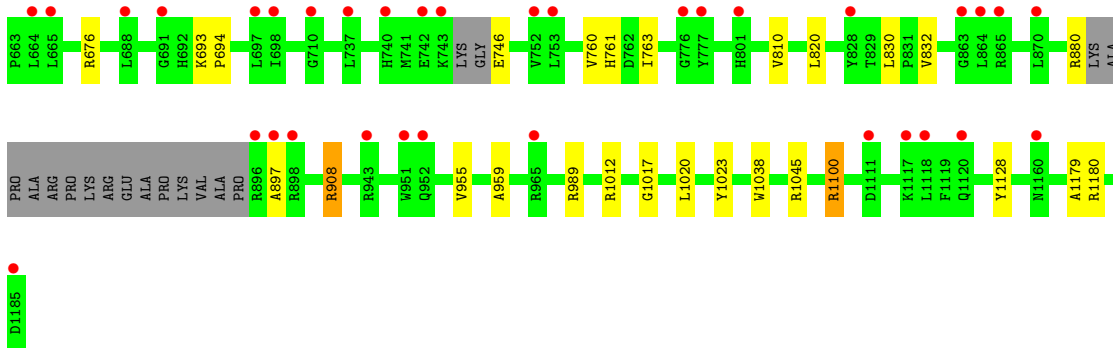
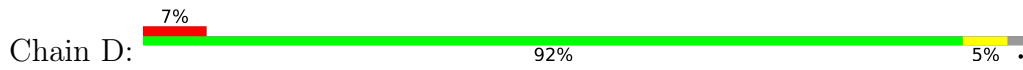


- Molecule 1: Methionine synthase

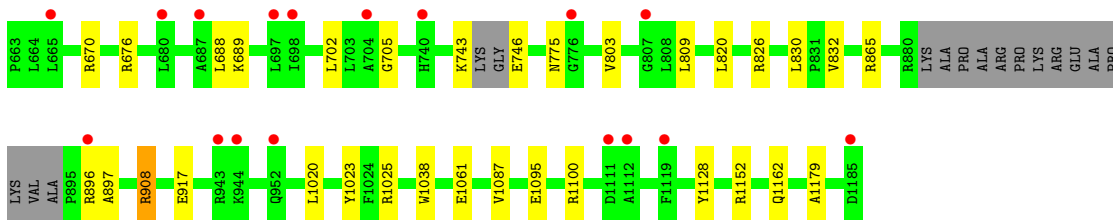
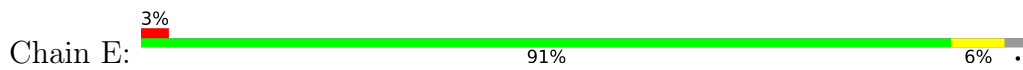




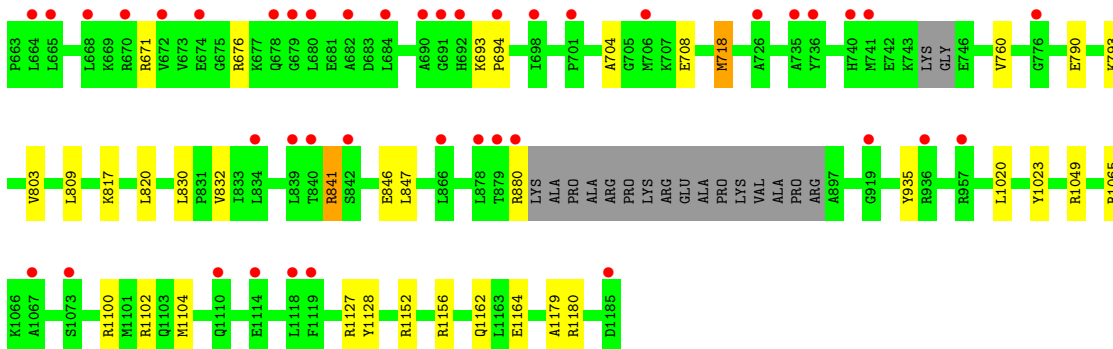
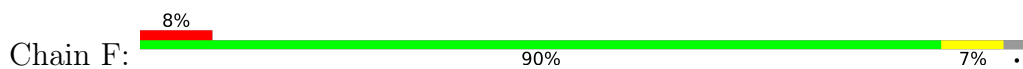
- Molecule 1: Methionine synthase



- Molecule 1: Methionine synthase



- Molecule 1: Methionine synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.13Å 95.84Å 238.75Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	49.30 – 3.15 49.25 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.30-3.15) 98.7 (49.25-3.15)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.245 , 0.307 0.246 , 0.305	Depositor DCC
R_{free} test set	3279 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtrriage
Anisotropy	0.452	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.006 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.023 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24880	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9241e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: B12

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	0.66	5/4107 (0.1%)	1.00	11/5548 (0.2%)
1	B	0.57	1/4099 (0.0%)	0.97	10/5537 (0.2%)
1	C	0.66	5/4107 (0.1%)	0.99	4/5548 (0.1%)
1	D	0.57	0/4099	0.96	2/5537 (0.0%)
1	E	0.64	3/4107 (0.1%)	0.98	3/5548 (0.1%)
1	F	0.55	0/4088	0.96	8/5523 (0.1%)
All	All	0.61	14/24607 (0.1%)	0.98	38/33241 (0.1%)

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	9
1	B	0	9
1	C	0	6
1	D	0	7
1	E	0	8
1	F	0	3
All	All	0	42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1095	GLU	CD-OE2	8.50	1.34	1.25
1	A	1095	GLU	CD-OE2	8.27	1.34	1.25
1	E	1095	GLU	CD-OE2	7.57	1.33	1.25
1	A	993	GLU	CD-OE1	7.27	1.33	1.25
1	C	869	GLU	CD-OE2	6.33	1.32	1.25

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1027	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	B	1025	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	1158	THR	OG1-CB-CG2	-7.33	93.13	110.00
1	B	1027	ARG	CG-CD-NE	7.24	127.01	111.80
1	A	1146	ARG	CG-CD-NE	6.70	125.87	111.80

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1012	ARG	Sidechain
1	A	1025	ARG	Sidechain
1	A	1027	ARG	Sidechain
1	A	826	ARG	Sidechain
1	A	989	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	4012	0	4013	13	0
1	B	4005	0	4005	9	0
1	C	4012	0	4013	12	0
1	D	4005	0	4005	11	0
1	E	4012	0	4013	14	0
1	F	3994	0	3992	15	0
2	A	91	0	88	6	0
2	B	91	0	88	2	0
2	C	91	0	88	7	0
2	D	91	0	88	5	0
2	E	91	0	88	4	0
2	F	91	0	88	3	0
3	A	47	0	0	1	0
3	B	40	0	0	0	0
3	C	62	0	0	1	0
3	D	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	55	0	0	1	0
3	F	50	0	0	1	0
All	All	24880	0	24569	94	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 2.

The worst 5 of 94 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:E:688:LEU:HD11	1:E:689:LYS:NZ	2.03	0.74
1:F:760:VAL:HG22	3:F:1301:HOH:O	1.88	0.74
1:A:697:LEU:HA	1:A:701:PRO:HD2	1.75	0.68
1:C:1058:THR:HG22	1:C:1060:GLY:H	1.59	0.66
1:F:841:ARG:HD2	1:F:880:ARG:HB3	1.82	0.62

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	501/523 (96%)	489 (98%)	12 (2%)	0	100	100
1	B	500/523 (96%)	488 (98%)	12 (2%)	0	100	100
1	C	501/523 (96%)	490 (98%)	11 (2%)	0	100	100
1	D	500/523 (96%)	490 (98%)	10 (2%)	0	100	100
1	E	501/523 (96%)	491 (98%)	10 (2%)	0	100	100
1	F	499/523 (95%)	491 (98%)	8 (2%)	0	100	100
All	All	3002/3138 (96%)	2939 (98%)	63 (2%)	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	408/419 (97%)	406 (100%)	2 (0%)	88	95
1	B	407/419 (97%)	404 (99%)	3 (1%)	84	93
1	C	408/419 (97%)	407 (100%)	1 (0%)	93	98
1	D	407/419 (97%)	405 (100%)	2 (0%)	88	95
1	E	408/419 (97%)	407 (100%)	1 (0%)	93	98
1	F	406/419 (97%)	405 (100%)	1 (0%)	93	98
All	All	2444/2514 (97%)	2434 (100%)	10 (0%)	91	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	830	LEU
1	E	775	ASN
1	F	718	MET
1	B	1003	GLU
1	B	1105	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	692	HIS
1	F	1160	ASN
1	F	1162	GLN
1	C	1160	ASN
1	C	1162	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	B	1201	-	90,101,101	1.12	7 (7%)	137,166,166	1.57	26 (18%)
2	B12	D	1201	-	90,101,101	1.11	6 (6%)	137,166,166	1.69	36 (26%)
2	B12	C	1201	-	90,101,101	1.12	7 (7%)	137,166,166	1.65	33 (24%)
2	B12	A	1201	-	90,101,101	1.05	7 (7%)	137,166,166	1.79	32 (23%)
2	B12	F	1201	-	90,101,101	1.16	8 (8%)	137,166,166	1.47	27 (19%)
2	B12	E	1201	-	90,101,101	1.14	8 (8%)	137,166,166	1.61	26 (18%)

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	B	1201	-	-	21/52/223/223	0/3/11/11
2	B12	D	1201	-	-	18/52/223/223	0/3/11/11
2	B12	C	1201	-	-	22/52/223/223	0/3/11/11
2	B12	A	1201	-	-	21/52/223/223	0/3/11/11
2	B12	F	1201	-	-	22/52/223/223	0/3/11/11
2	B12	E	1201	-	-	23/52/223/223	0/3/11/11

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	B12	C20-C1	3.43	1.60	1.53
2	C	1201	B12	O51-C50	3.33	1.33	1.24
2	D	1201	B12	C19-N24	-3.31	1.42	1.48
2	F	1201	B12	C19-N24	-3.26	1.42	1.48
2	E	1201	B12	C19-N24	-3.24	1.42	1.48

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	B12	C41-C8-C9	-7.30	98.32	111.19
2	E	1201	B12	O34-C32-N33	-5.67	107.03	122.50
2	B	1201	B12	O58-C57-C56	-5.55	111.87	122.02
2	C	1201	B12	C35-C5-C6	-5.00	114.47	122.43
2	A	1201	B12	O58-C57-C56	-4.99	112.88	122.02

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	B12	C4-C3-C30-C31
2	A	1201	B12	C38-C37-C7-C36
2	A	1201	B12	C38-C37-C7-C8
2	A	1201	B12	C12-C13-C48-C49
2	A	1201	B12	C18-C60-C61-O63

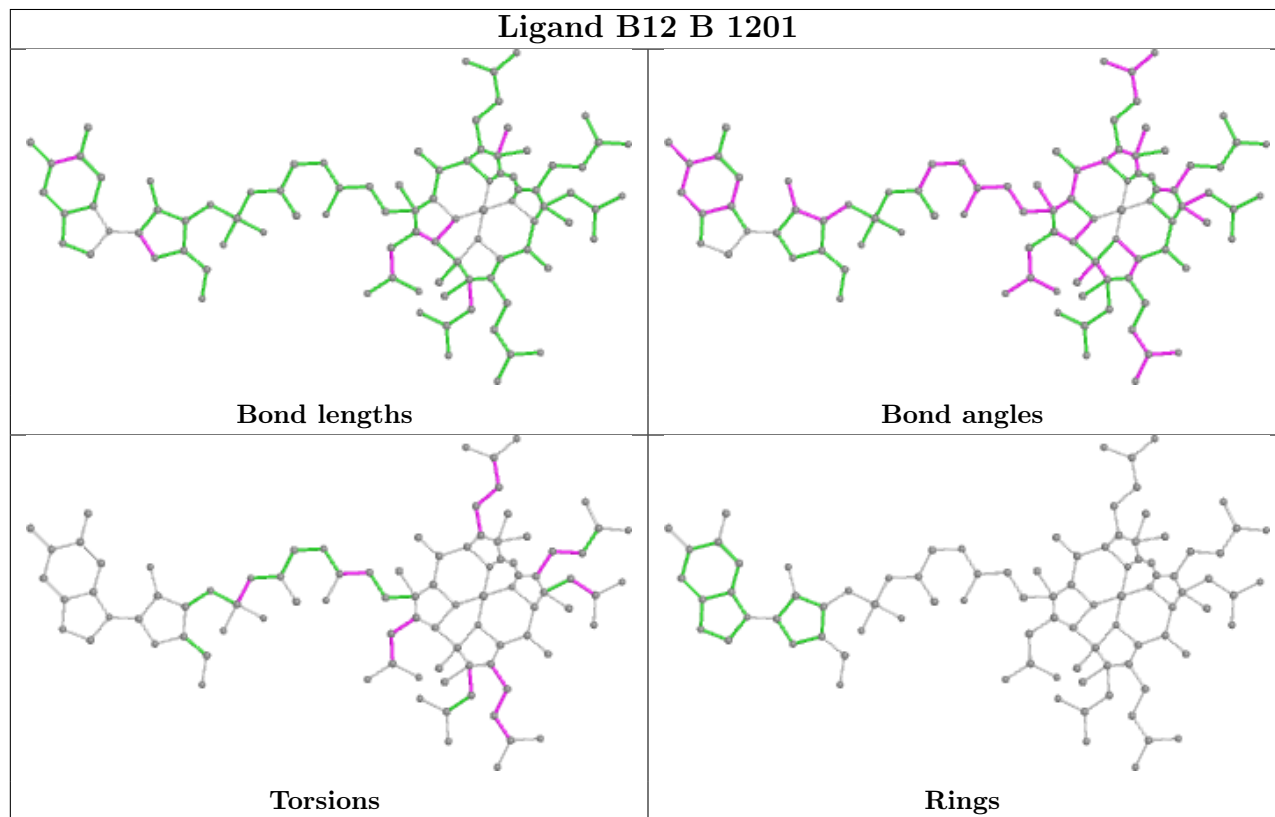
There are no ring outliers.

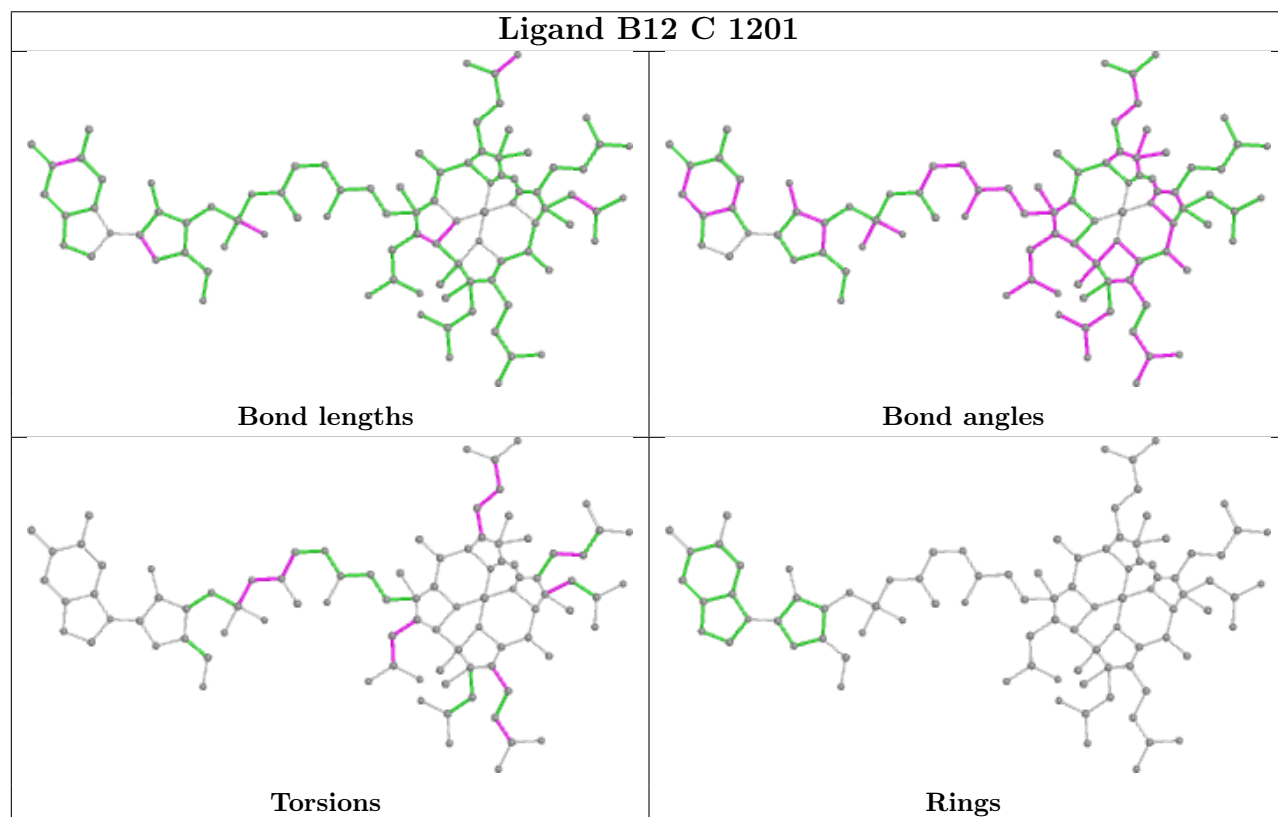
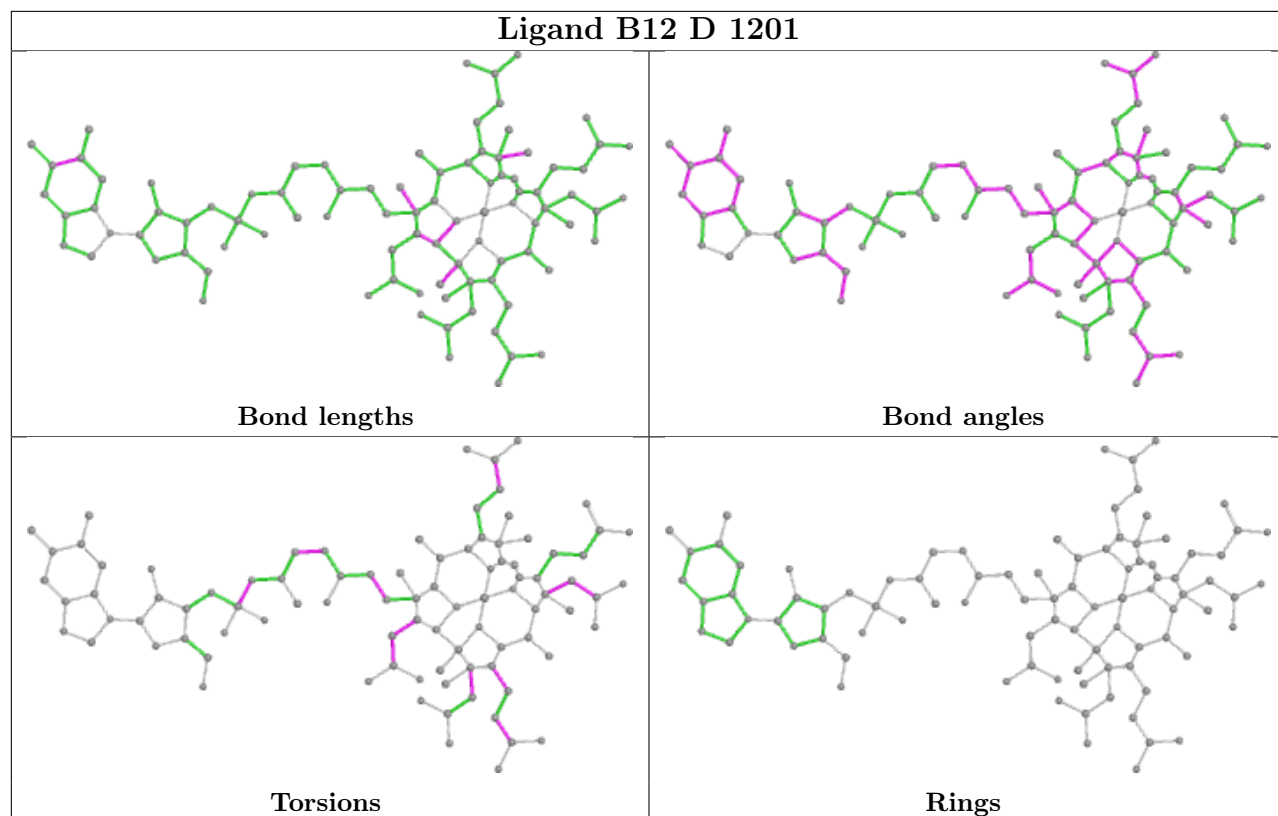
6 monomers are involved in 27 short contacts:

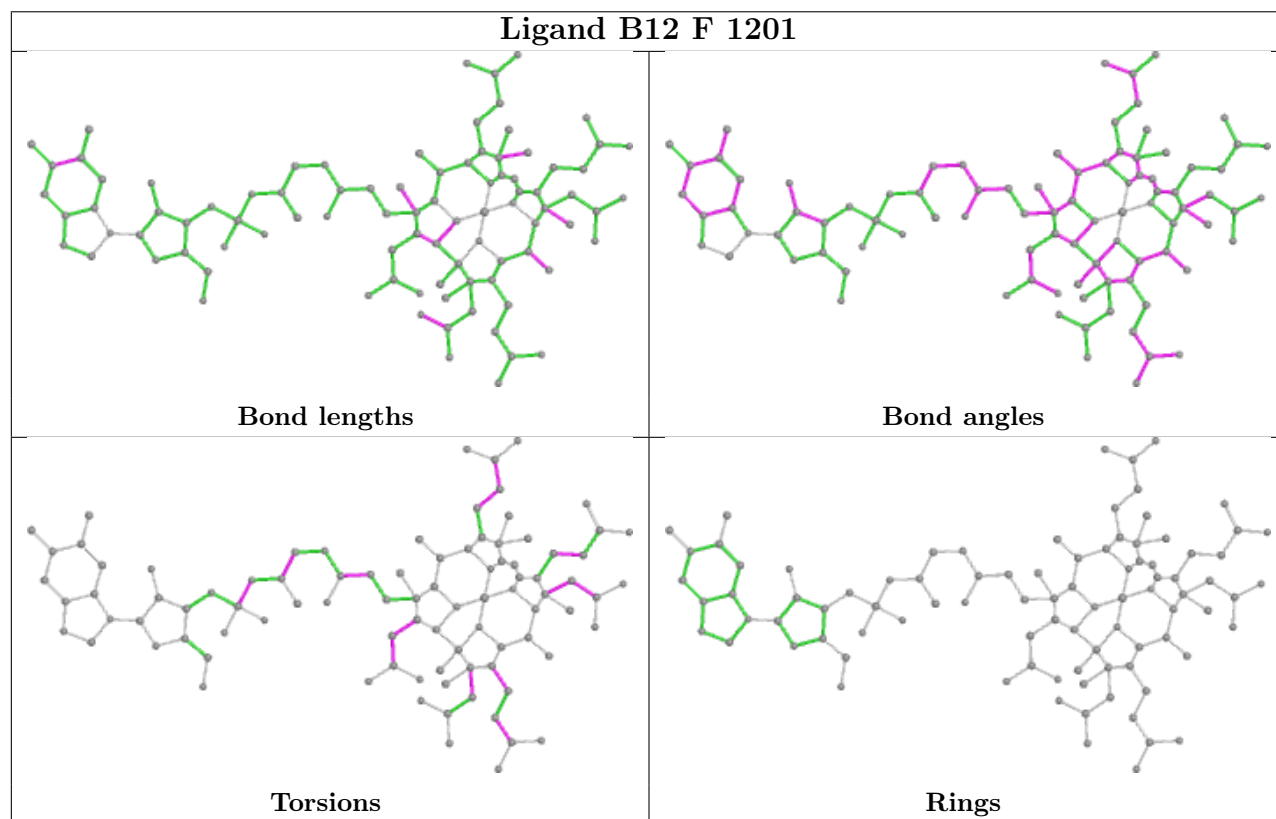
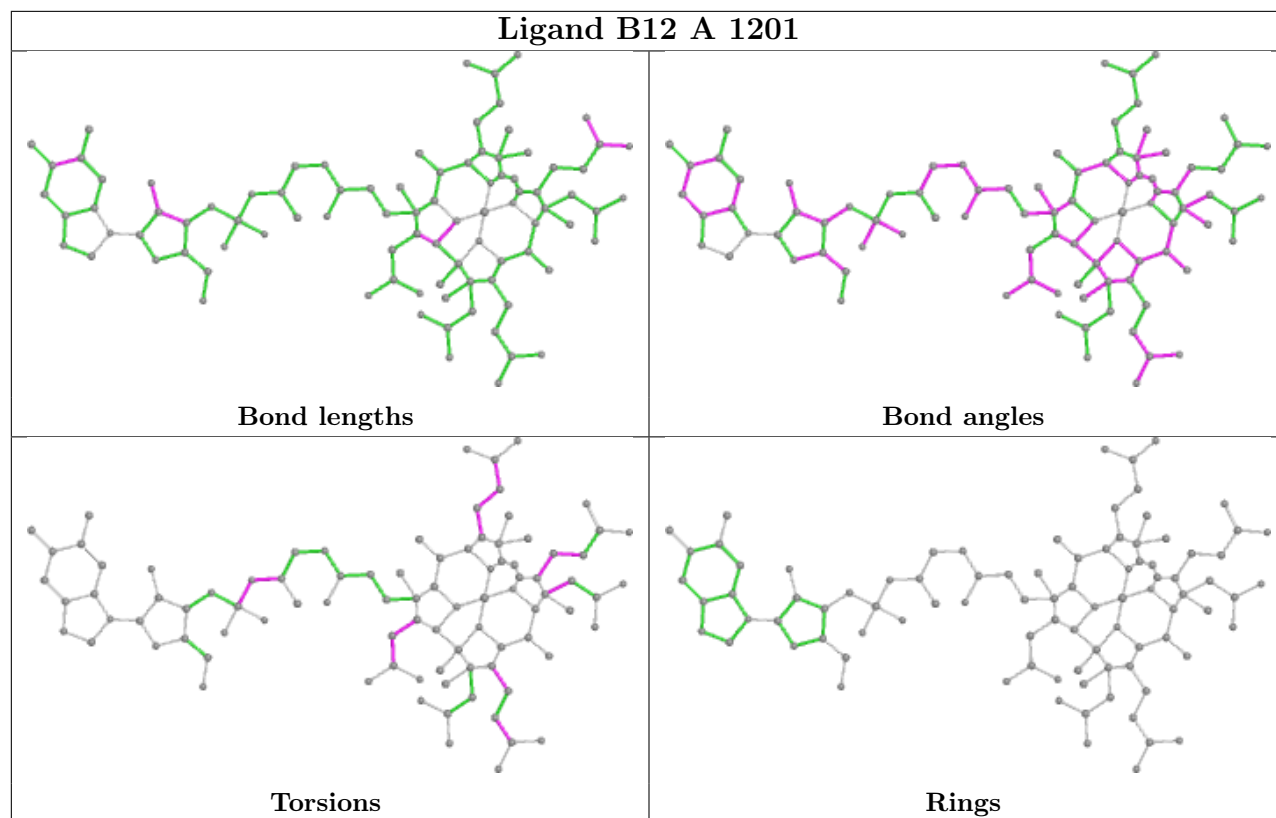
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	B12	2	0
2	D	1201	B12	5	0
2	C	1201	B12	7	0
2	A	1201	B12	6	0
2	F	1201	B12	3	0
2	E	1201	B12	4	0

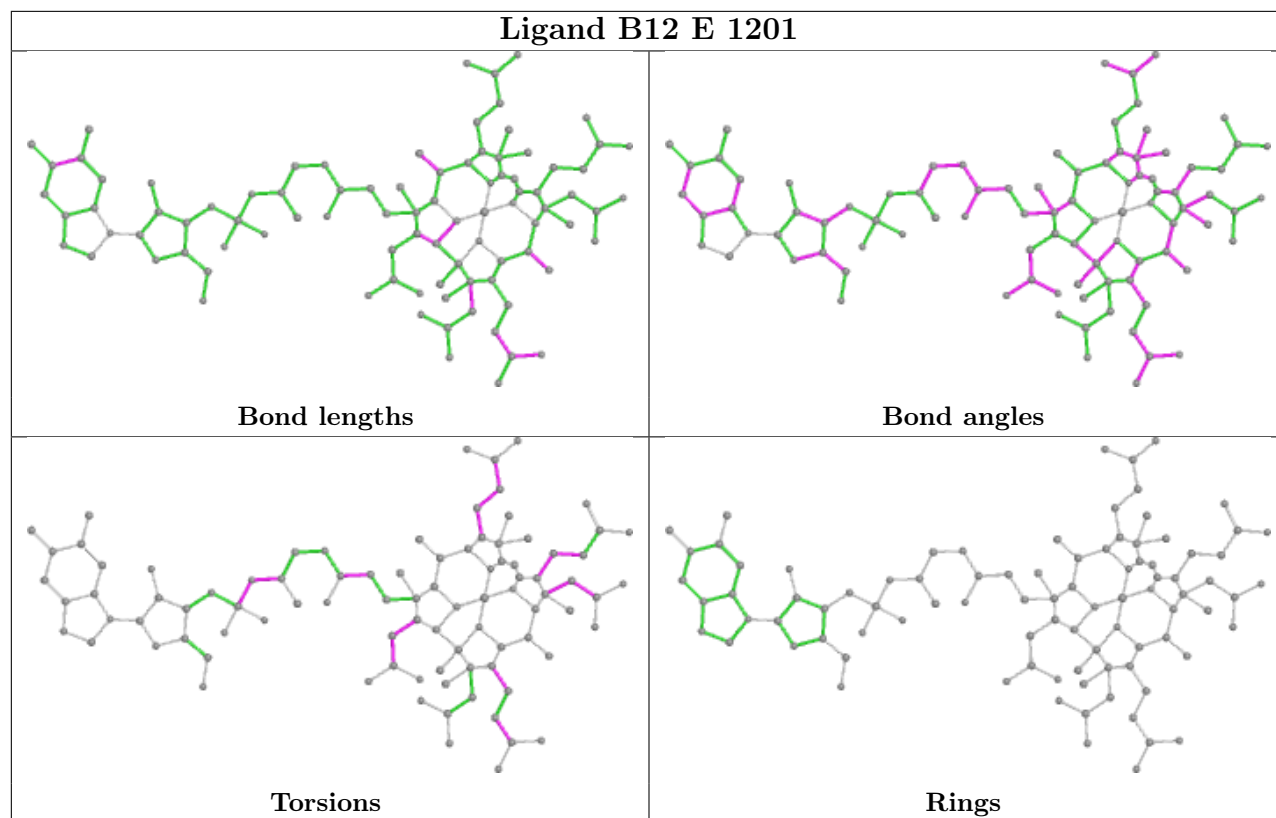
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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	507/523 (96%)	0.25	34 (6%) 17 9	30, 65, 160, 219	0
1	B	506/523 (96%)	0.56	52 (10%) 6 3	49, 86, 163, 226	0
1	C	507/523 (96%)	0.21	31 (6%) 21 11	30, 65, 151, 220	0
1	D	506/523 (96%)	0.40	34 (6%) 17 9	45, 86, 147, 211	0
1	E	507/523 (96%)	0.13	17 (3%) 45 28	30, 63, 133, 176	0
1	F	505/523 (96%)	0.60	42 (8%) 11 6	46, 86, 156, 271	0
All	All	3038/3138 (96%)	0.36	210 (6%) 16 9	30, 77, 154, 271	0

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	879	THR	37.0
1	F	880	ARG	8.1
1	D	896	ARG	7.8
1	D	1185	ASP	7.8
1	A	665	LEU	7.4

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](#)

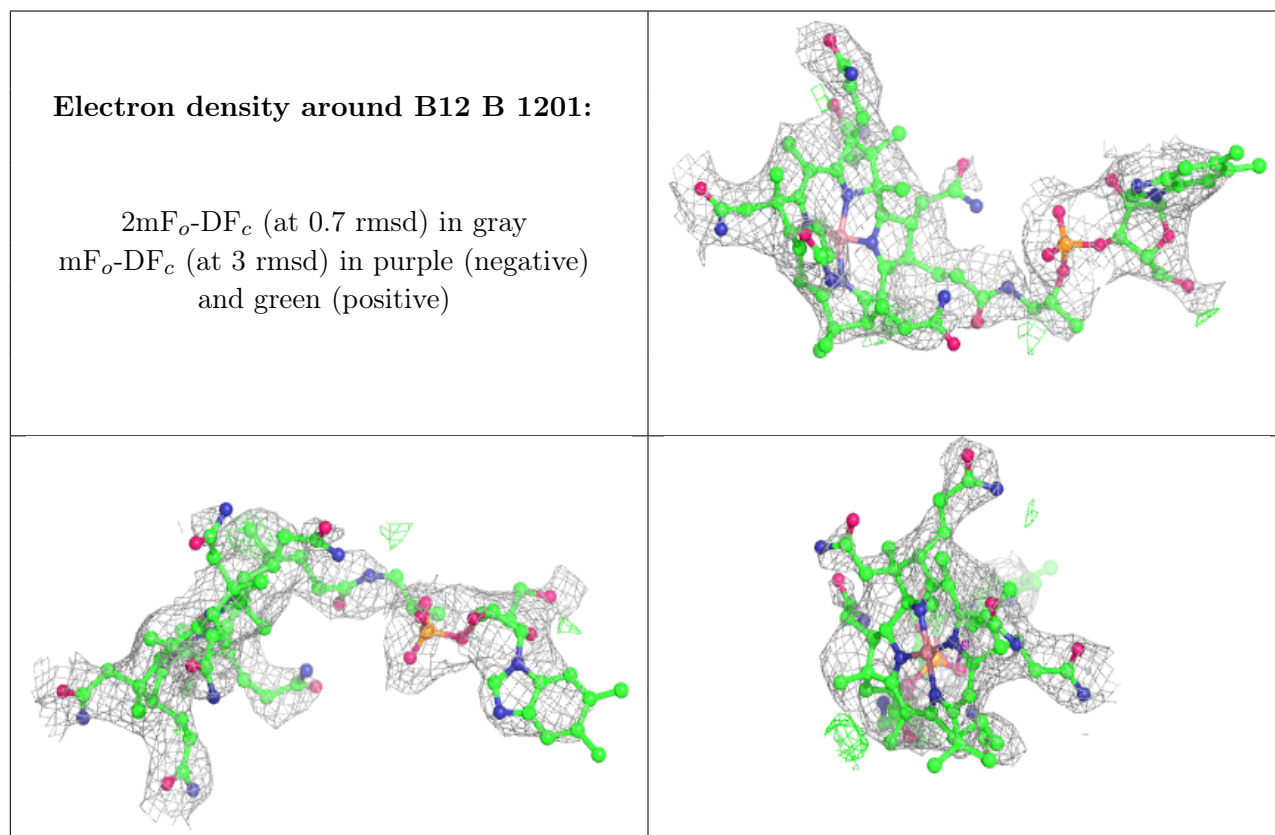
There are no monosaccharides in this entry.

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.

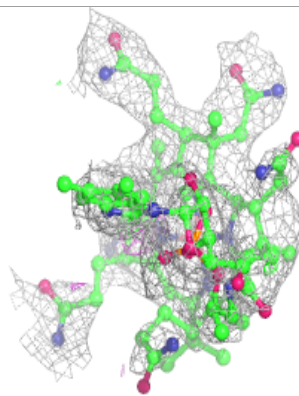
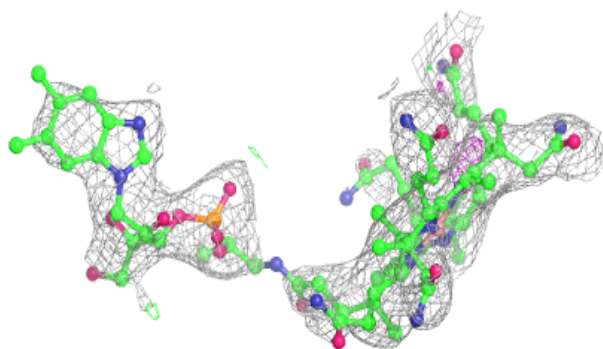
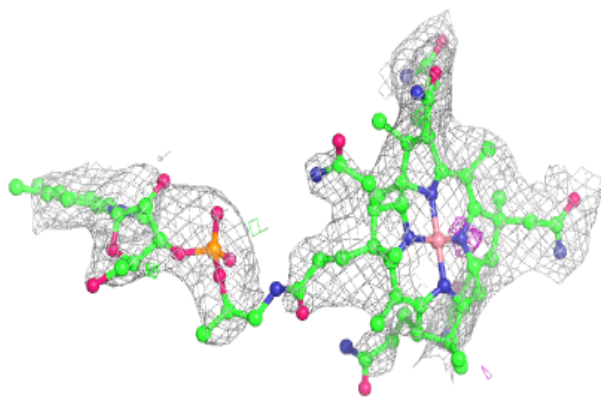
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	B12	B	1201	91/91	0.92	0.27	56,80,101,115	0
2	B12	D	1201	91/91	0.92	0.29	53,78,104,119	0
2	B12	F	1201	91/91	0.93	0.30	49,83,119,134	0
2	B12	A	1201	91/91	0.95	0.25	34,54,86,103	0
2	B12	C	1201	91/91	0.95	0.22	41,56,79,94	0
2	B12	E	1201	91/91	0.96	0.24	36,52,80,93	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.

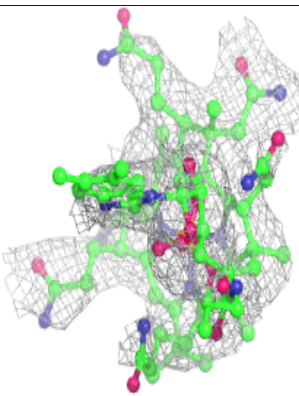
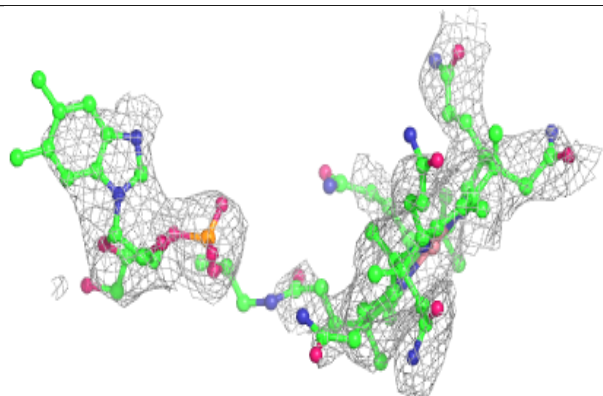
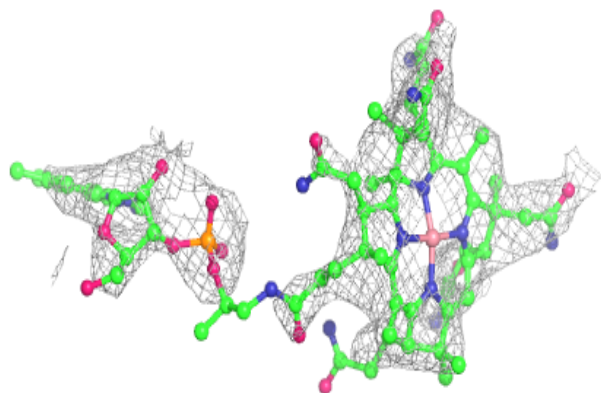


Electron density around B12 D 1201:

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

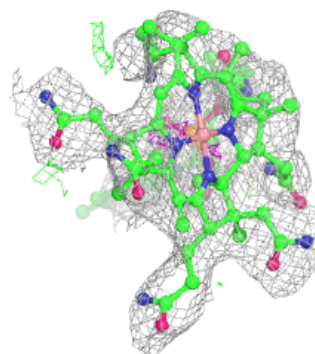
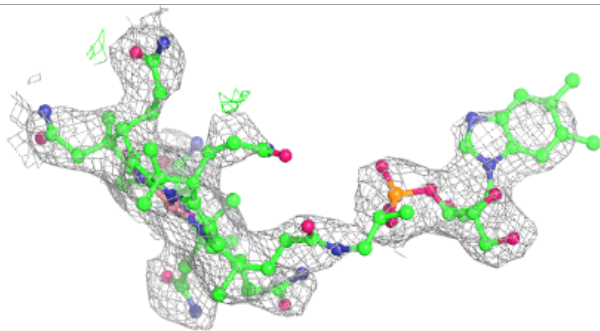
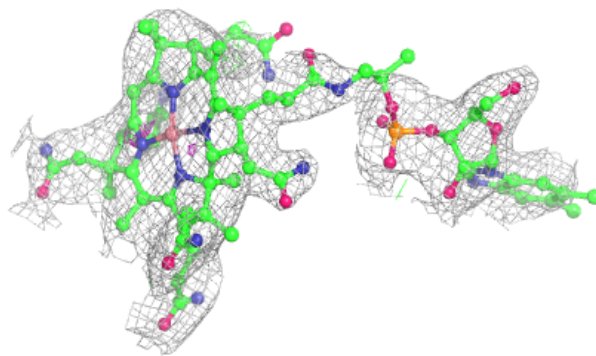
**Electron density around B12 F 1201:**

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

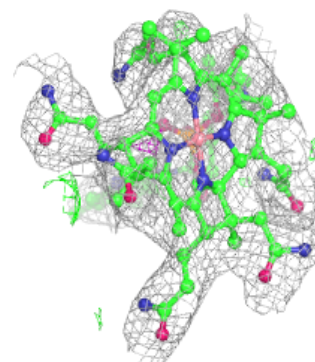
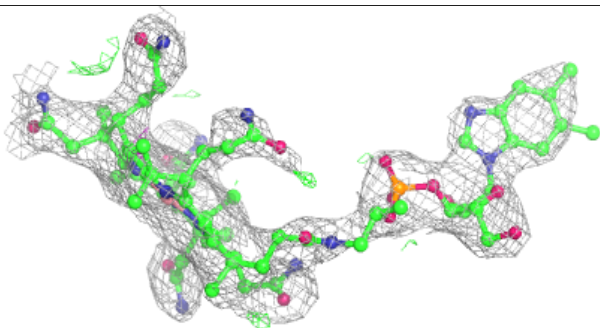
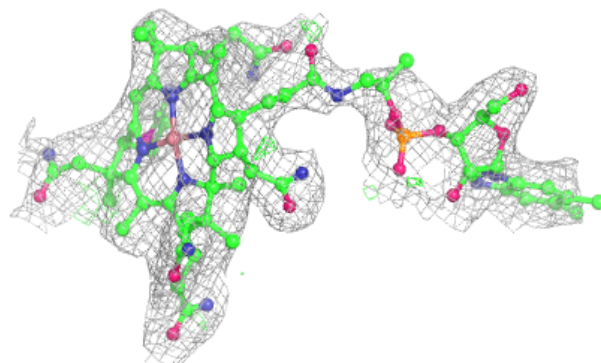


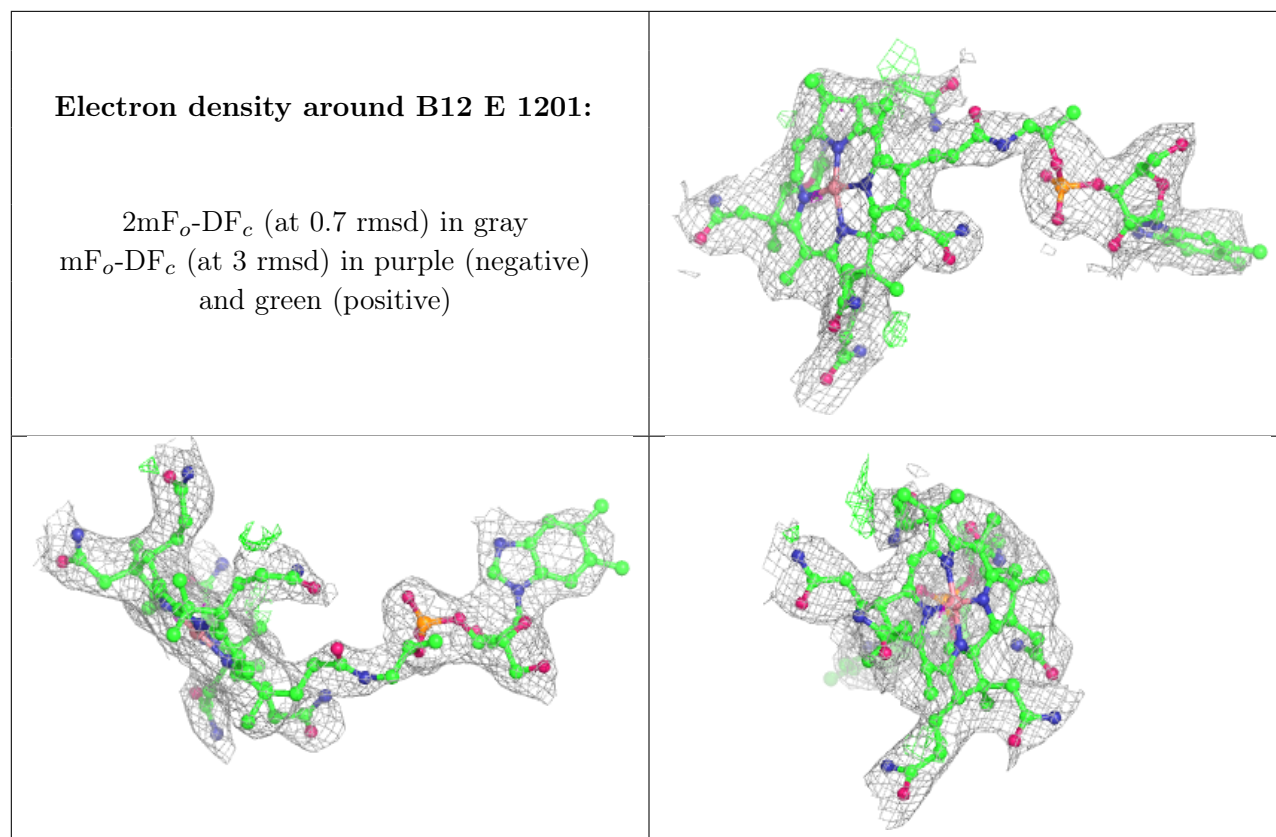
Electron density around B12 A 1201:

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

**Electron density around B12 C 1201:**

$2mF_o-DF_c$ (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.