

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 11:50 PM EDT

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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 (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 (1)) were used in the production of this report:

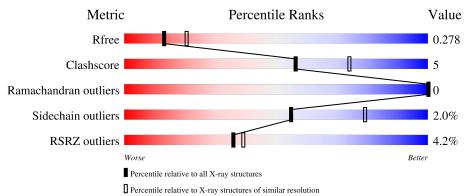
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	А	192	72%	9% •	18%
1	В	192	73%	5%•	22%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5035 atoms, of which 2469 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 Methylmalonic aciduria and homocystinuria type D protein, mitochondrial.

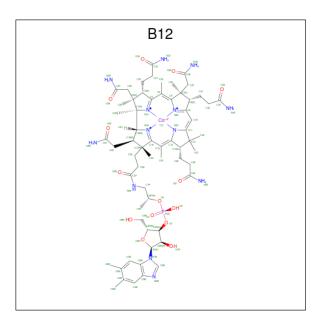
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	158	Total 2372	-	Н 1158	N 204	O 230	S 7	0	0	0
1	В	150	Total 2329	-	Н 1150	N 197	0 221	${f S}{7}$	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	105	GLY	-	expression tag	UNP Q9H3L0
А	106	HIS	-	expression tag	UNP Q9H3L0
А	107	MET	-	expression tag	UNP Q9H3L0
А	262	SER	CYS	engineered mutation	UNP Q9H3L0
В	105	GLY	-	expression tag	UNP Q9H3L0
В	106	HIS	-	expression tag	UNP Q9H3L0
В	107	MET	-	expression tag	UNP Q9H3L0
В	262	SER	CYS	engineered mutation	UNP Q9H3L0

• 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	А	1	Total C Co H N O 140 48 1 72 11 8	0	0
2	В	1	Total C Co H N O P 180 62 1 89 13 14 1	0	0

• Molecule 3 is water.

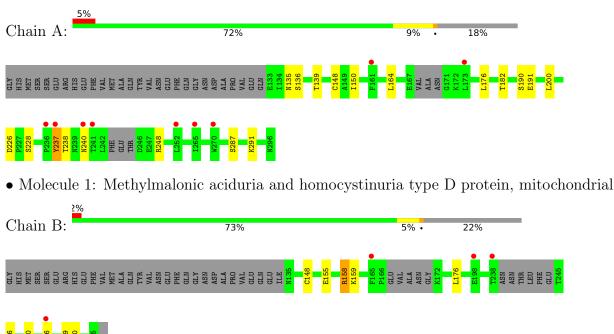
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	9	Total O 9 9	0	0
3	В	5	Total O 5 5	0	0



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: Methylmalonic aciduria and homocystinuria type D protein, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	103.22Å 69.78Å 64.27Å	Depositor
a, b, c, α , β , γ	90.00° 101.15° 90.00°	Depositor
Resolution (Å)	50.64 - 2.50	Depositor
Resolution (A)	50.64 - 2.50	EDS
% Data completeness	99.0 (50.64-2.50)	Depositor
(in resolution range)	99.3 (50.64 - 2.50)	EDS
R _{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.66 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D.	0.249 , 0.279	Depositor
R, R_{free}	0.249 , 0.278	DCC
R_{free} test set	816 reflections (5.26%)	wwPDB-VP
Wilson B-factor $(Å^2)$	49.1	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.41 , 49.3	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5035	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.45% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: $\mathrm{B}12$

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 RMSZ	lengths	Bond angles		
			# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/1238	0.44	0/1676	
1	В	0.26	0/1203	0.45	0/1625	
All	All	0.26	0/2441	0.44	0/3301	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	А	1214	1158	1157	10	0
1	В	1179	1150	1149	4	0
2	А	68	72	69	10	0
2	В	91	89	88	1	0
3	А	9	0	0	0	0
3	В	5	0	0	0	0
All	All	2566	2469	2463	25	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 5.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash
2:A:301:B12:H531	2:A:301:B12:H543	1.37	$\frac{\text{overlap (Å)}}{1.04}$
1:A:136:SER:O	1:A:139:THR:HG22	1.83	0.77
2:A:301:B12:H531	2:A:301:B12:C54	2.16	0.72
2:A:301:B12:H533	2:A:301:B12:H492	1.75	0.67
1:A:150:ILE:HG12	1:A:176:LEU:HD13	1.85	0.57
2:B:301:B12:H552	2:B:301:B12:H531	1.87	0.56
2:A:301:B12:H362	2:A:301:B12:H351	1.89	0.54
2:A:301:B12:H8	2:A:301:B12:O39	2.07	0.54
2:A:301:B12:H561	2:A:301:B12:O63	2.07	0.53
1:A:190:SER:OG	1:A:191:GLU:N	2.43	0.52
2:A:301:B12:H353	2:A:301:B12:H302	1.93	0.51
2:A:301:B12:O39	2:A:301:B12:H473	2.11	0.51
1:B:269:LEU:HD12	1:B:270:TRP:CD1	2.48	0.48
1:A:182:THR:HG22	1:A:200:LEU:CD1	2.43	0.48
1:A:287:SER:O	1:A:291:LYS:HG3	2.14	0.47
1:B:155:GLU:HA	1:B:158:ARG:HB2	2.00	0.44
2:A:301:B12:H521	2:A:301:B12:H13	1.83	0.43
1:A:135:ASN:HB2	1:A:139:THR:HG21	2.01	0.43
1:A:148:CYS:HB3	1:A:176:LEU:HD11	2.01	0.42
1:B:250:ARG:NH2	1:B:256:VAL:O	2.52	0.42
1:A:226:ASP:OD1	1:A:228:SER:OG	2.34	0.41
2:A:301:B12:C61	2:A:301:B12:H262	2.50	0.41
1:A:164:LEU:HD21	1:A:240:ASN:O	2.20	0.41
1:A:237:TYR:O	1:A:238:THR:HG23	2.20	0.41
1:B:148:CYS:HB3	1:B:176:LEU:HD11	2.03	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	Perce	ntiles
1	А	152/192~(79%)	145~(95%)	7 (5%)	0	100	100
1	В	145/192~(76%)	140 (97%)	5(3%)	0	100	100
All	All	297/384~(77%)	285~(96%)	12~(4%)	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 side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	128/168~(76%)	126~(98%)	2(2%)	62 84
1	В	127/168~(76%)	124 (98%)	3(2%)	49 74
All	All	255/336~(76%)	250~(98%)	5(2%)	55 79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	237	TYR
1	А	248	ARG
1	В	158	ARG
1	В	159	LYS
1	В	246	ASP

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

Mol	Chain	Res	Type
1	А	151	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)

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	Turne	Chain	Res Link		Boi	nd lengt	hs	Bo	nd angle	es
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	B12	В	301	-	90,101,101	1.03	4 (4%)	137,166,166	1.49	23 (16%)
2	B12	А	301	-	66,75,101	1.47	7 (10%)	104,125,166	2.27	27 (25%)

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	В	301	-	-	24/52/223/223	0/3/11/11
2	B12	А	301	-	-	18/40/191/223	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	301	B12	C14-N23	7.33	1.44	1.35
2	А	301	B12	C9-N22	3.92	1.40	1.30
2	А	301	B12	C19-N24	-3.62	1.42	1.48
2	В	301	B12	C14-N23	3.17	1.39	1.35
2	А	301	B12	C10-C9	2.83	1.47	1.39
2	А	301	B12	C14-C15	2.78	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	301	B12	C16-C15	-2.77	1.36	1.44
2	В	301	B12	C54-C17	2.75	1.59	1.54
2	А	301	B12	C11-N23	2.52	1.41	1.37
2	В	301	B12	C35-C5	2.49	1.56	1.50
2	В	301	B12	C6B-C5B	2.10	1.46	1.40

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All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
2	А	301	B12	C20-C1-C19	-9.66	100.04	109.36
2	А	301	B12	C1-C19-C18	7.93	134.90	121.88
2	А	301	B12	C18-C19-N24	7.13	113.16	102.31
2	А	301	B12	C2-C1-C19	6.68	129.15	118.60
2	В	301	B12	C7B-C8B-C9B	5.11	125.60	120.54
2	В	301	B12	C55-C17-C16	4.52	125.58	116.65
2	В	301	B12	C16-C15-C14	-4.34	114.66	121.25
2	А	301	B12	C20-C1-N21	-4.31	103.19	110.27
2	В	301	B12	C15-C16-N24	4.13	128.37	122.42
2	А	301	B12	C30-C3-C2	-4.09	110.44	119.09
2	А	301	B12	C55-C17-C16	-4.08	108.59	116.65
2	А	301	B12	C26-C2-C1	3.97	116.20	110.01
2	В	301	B12	C54-C17-C16	-3.78	92.79	112.40
2	А	301	B12	C25-C2-C1	-3.74	108.14	113.78
2	В	301	B12	C2P-C1P-N59	-3.58	107.65	112.93
2	А	301	B12	C19-C1-N21	3.37	105.61	102.16
2	А	301	B12	C15-C14-N23	-3.37	122.15	126.26
2	А	301	B12	C7-C37-C38	3.29	124.16	114.25
2	А	301	B12	C18-C17-C16	3.26	104.63	100.67
2	В	301	B12	C5B-C4B-C9B	-3.11	116.82	121.22
2	А	301	B12	C3-C4-C5	3.03	128.92	123.81
2	А	301	B12	C30-C3-C4	2.88	116.33	109.63
2	А	301	B12	C56-C55-C17	2.86	121.03	115.52
2	В	301	B12	C55-C17-C18	2.85	116.66	111.15
2	А	301	B12	C2-C3-C4	-2.84	98.40	101.63
2	А	301	B12	C8-C7-C6	2.83	105.78	100.92
2	В	301	B12	C17-C16-N24	-2.82	106.80	111.15
2	А	301	B12	C1-C19-N24	2.81	109.39	106.24
2	В	301	B12	C13-C14-C15	-2.79	120.06	124.32
2	В	301	B12	C37-C7-C8	-2.59	101.46	108.39
2	А	301	B12	C8-C9-C10	-2.58	117.75	123.32
2	А	301	B12	C48-C13-C14	2.57	114.91	108.49
2	В	301	B12	C36-C7-C37	2.56	115.02	110.80

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	301	B12	C56-C57-N59	2.51	120.65	116.42
2	В	301	B12	C54-C17-C18	-2.50	109.29	112.98
2	А	301	B12	C5-C4-N21	-2.48	120.16	124.19
2	В	301	B12	C18-C17-C16	2.45	103.65	100.67
2	А	301	B12	C60-C18-C17	2.41	121.57	115.74
2	В	301	B12	C5M-C5B-C6B	-2.40	115.81	120.74
2	А	301	B12	C17-C16-C15	2.39	130.03	126.26
2	А	301	B12	C56-C57-N59	2.25	120.22	116.42
2	В	301	B12	O28-C27-N29	-2.25	116.36	122.50
2	А	301	B12	C16-C15-C14	2.24	124.65	121.25
2	В	301	B12	C13-C14-N23	2.24	112.15	109.10
2	В	301	B12	C54-C17-C55	-2.19	105.64	109.25
2	А	301	B12	O3-C2P-C3P	-2.14	100.09	109.38
2	В	301	B12	C55-C56-C57	-2.13	106.57	111.23
2	В	301	B12	C31-C32-N33	2.12	123.11	116.51
2	В	301	B12	C4B-C5B-C6B	2.09	123.43	119.91
2	В	301	B12	C41-C8-C9	-2.03	107.62	111.19

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There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	B12	C1-C2-C26-C27
2	А	301	B12	C25-C2-C26-C27
2	А	301	B12	C3-C2-C26-C27
2	А	301	B12	C4-C3-C30-C31
2	А	301	B12	C38-C37-C7-C6
2	А	301	B12	C38-C37-C7-C36
2	А	301	B12	C38-C37-C7-C8
2	А	301	B12	C16-C17-C55-C56
2	А	301	B12	C54-C17-C55-C56
2	А	301	B12	C18-C17-C55-C56
2	В	301	B12	C4-C3-C30-C31
2	В	301	B12	C38-C37-C7-C6
2	В	301	B12	N59-C1P-C2P-O3
2	В	301	B12	C1P-C2P-O3-P
2	В	301	B12	C3P-C2P-O3-P
2	В	301	B12	C2P-O3-P-O2
2	В	301	B12	C3R-C4R-C5R-O8R
2	В	301	B12	C56-C57-N59-C1P
2	В	301	B12	O6R-C4R-C5R-O8R
2	А	301	B12	C2-C3-C30-C31

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\mathbf{Mol}	Chain	Res	Type Atoms		
2	В	301	B12	C2-C3-C30-C31	
2	В	301	B12	O58-C57-N59-C1P	
2	В	301	B12	C2R-C3R-O2-P	
2	В	301	B12	C16-C17-C55-C56	
2	В	301	B12	N59-C1P-C2P-C3P	
2	В	301	B12	C38-C37-C7-C36	
2	В	301	B12	C18-C60-C61-O63	
2	А	301	B12	C3-C30-C31-C32	
2	А	301	B12	C17-C55-C56-C57	
2	В	301	B12	C4R-C3R-O2-P	
2	А	301	B12	C14-C13-C48-C49	
2	В	301	B12	C18-C60-C61-N62	
2	В	301	B12	C41-C42-C43-O44	
2	В	301	B12	C41-C42-C43-N45	
2	В	301	B12	C3R-O2-P-O3	
2	В	301	B12	C42-C41-C8-C9	
2	В	301	B12	C14-C13-C48-C49	
2	В	301	B12	C3R-O2-P-O5	
2	А	301	B12	C17-C18-C60-C61	
2	А	301	B12	C8-C41-C42-C43	
2	А	301	B12	C19-C18-C60-C61	
2	А	301	B12	N59-C1P-C2P-O3	

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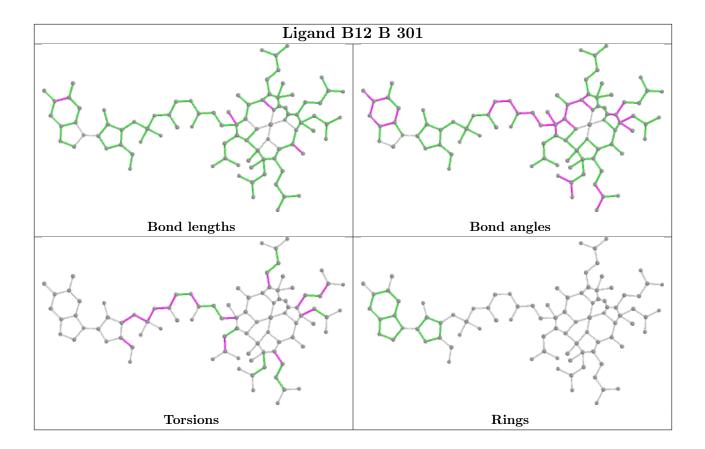
There are no ring outliers.

2 monomers are involved in 11 short contacts:

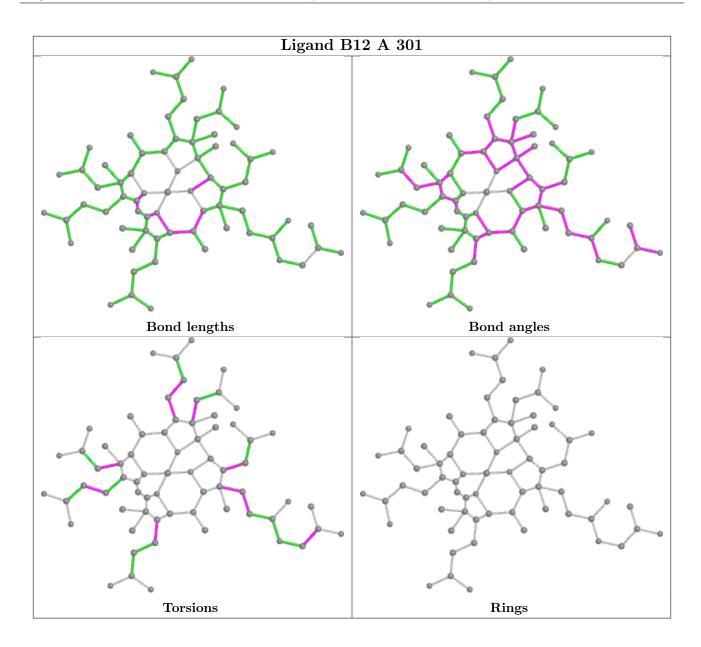
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	301	B12	1	0
2	А	301	B12	10	0

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 sufficient 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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	158/192~(82%)	0.87	9 (5%) 23 25	35, 56, 82, 101	0
1	В	150/192~(78%)	0.71	4 (2%) 54 58	35, 56, 77, 84	0
All	All	308/384~(80%)	0.79	13 (4%) 36 39	35, 56, 81, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	240	ASN	4.9
1	А	236	PRO	4.2
1	В	238	THR	3.1
1	В	165	PHE	2.7
1	А	270	TRP	2.6
1	В	256	VAL	2.5
1	А	241	THR	2.4
1	А	173	LEU	2.2
1	А	252	LEU	2.2
1	В	198	GLU	2.2
1	А	237	TYR	2.2
1	А	265	ILE	2.2
1	А	161	PHE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

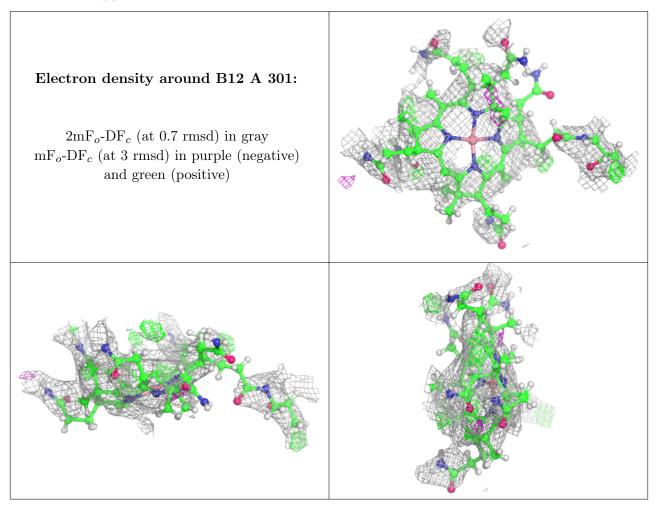


6.4 Ligands (i)

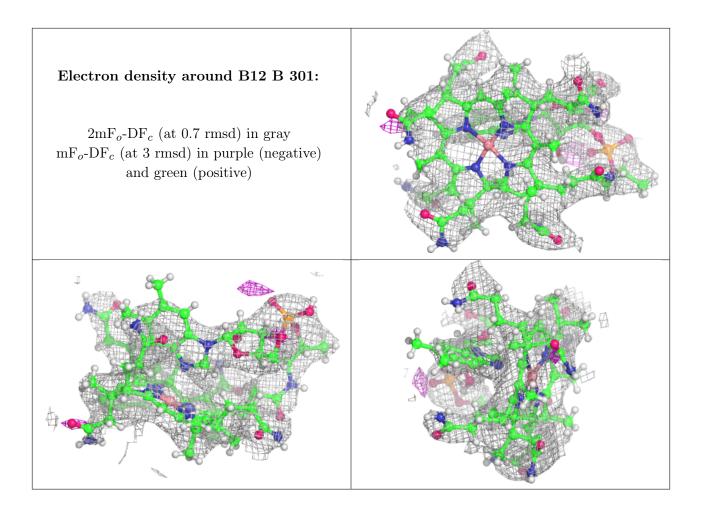
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	B12	А	301	68/91	0.73	0.33	$66,\!111,\!134,\!136$	0
2	B12	В	301	91/91	0.93	0.23	47,72,91,97	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.







6.5 Other polymers (i)

There are no such residues in this entry.

