



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 PM UTC

PDB ID : 5UL3 / pdb_00005ul3
Title : Structure of Cobalamin-dependent S-adenosylmethionine radical enzyme OxsB
with aqua-cobalamin bound
Authors : Bridwell-Rabb, J.; Drennan, C.L.
Deposited on : 2017-01-24
Resolution : 1.80 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

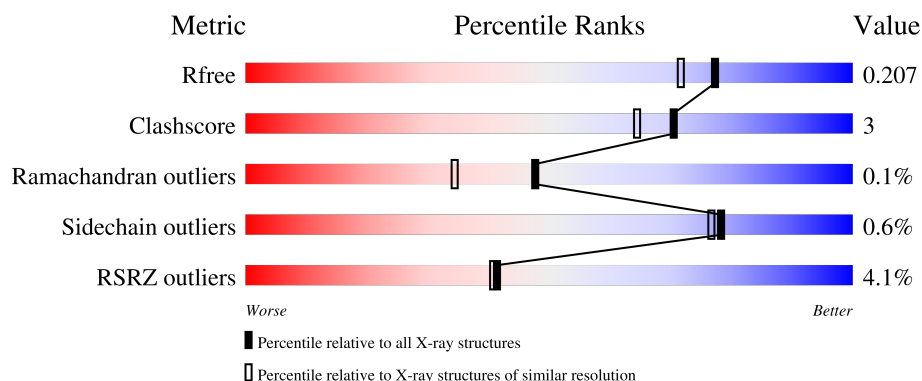
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

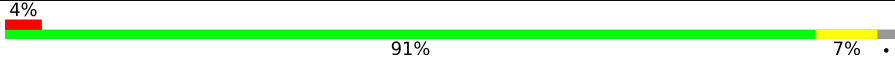
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	744	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7090 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 OxsB protein.

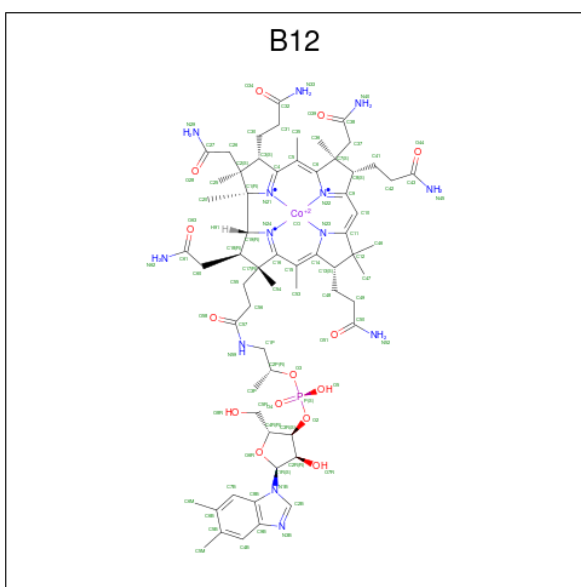
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	6186	3926	1032	1193	35	0	33	0

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



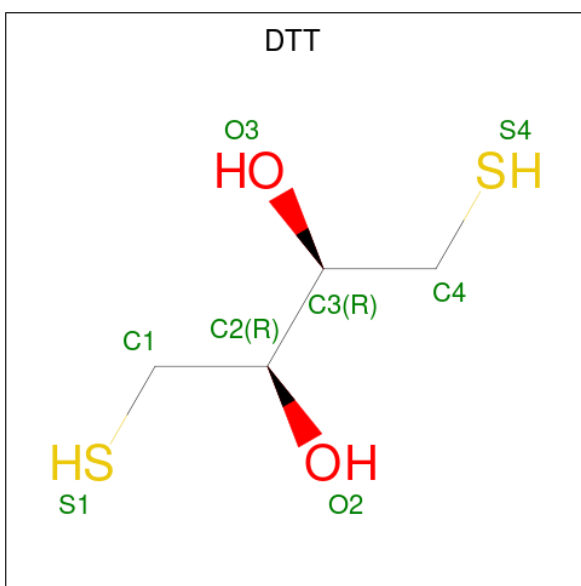
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $\text{C}_{62}\text{H}_{89}\text{CoN}_{13}\text{O}_{14}\text{P}$).



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

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S		
			8	4	2	2	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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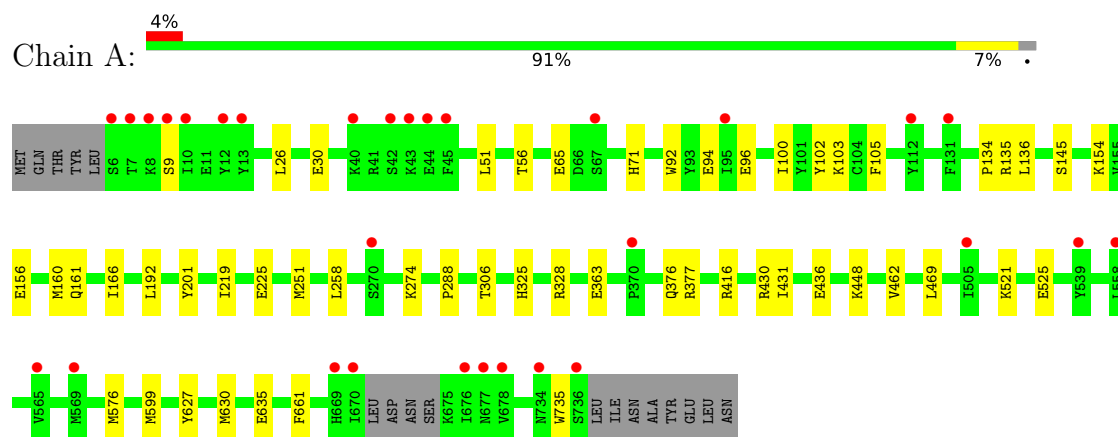
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	689	Total 689	O 689	0	0

- Molecule 1: OxsB protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.36Å 99.59Å 121.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 1.80 49.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-1.80) 100.0 (49.80-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.178 , 0.212 (Not available) , 0.207	Depositor DCC
R_{free} test set	7482 reflections (7.41%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7090	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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: DTT, B12, EDO, SF4, MES

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	0.30	0/6316	0.48	0/8511

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	GLU	Peptide

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	6186	0	6141	38	0
2	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	91	0	88	6	0
4	A	8	0	9	1	0
5	A	12	0	12	0	0
6	A	96	0	144	10	0
7	A	689	0	0	3	0
All	All	7090	0	6394	43	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 3.

All (43) 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)
3:A:802:B12:H362	3:A:802:B12:H351	1.76	0.67
1:A:627:TYR:HA	1:A:630:MET:HE3	1.76	0.67
3:A:802:B12:H552	3:A:802:B12:H531	1.79	0.64
1:A:135:ARG:HD3	3:A:802:B12:H491	1.82	0.61
1:A:258:LEU:HB3	6:A:811:EDO:H21	1.83	0.60
1:A:328:ARG:H	6:A:818:EDO:H11	1.69	0.57
1:A:71:HIS:ND1	1:A:102:TYR:OH	2.32	0.56
1:A:462:VAL:HG11	1:A:469:LEU:HD21	1.86	0.56
1:A:377:ARG:HA	6:A:815:EDO:H22	1.89	0.54
1:A:96:GLU:HB3	6:A:825:EDO:H22	1.91	0.53
1:A:328:ARG:NH2	6:A:818:EDO:O1	2.42	0.52
1:A:635:GLU:HG2	1:A:661:PHE:HE1	1.75	0.52
1:A:160:MET:HE1	1:A:192:LEU:HD11	1.93	0.50
1:A:94:GLU:HB3	6:A:825:EDO:H11	1.92	0.50
1:A:92:TRP:HH2	1:A:100:ILE:HD11	1.77	0.50
1:A:521:LYS:NZ	1:A:525:GLU:HG2	2.28	0.49
1:A:92:TRP:CH2	1:A:100:ILE:HD11	2.49	0.48
1:A:635:GLU:HG2	1:A:661:PHE:CE1	2.49	0.48
1:A:51:LEU:HD13	1:A:154:LYS:HE2	1.97	0.47
1:A:136:LEU:HB3	1:A:306[B]:THR:HG22	1.95	0.47
1:A:225[A]:GLU:H	1:A:225[A]:GLU:CD	2.23	0.47
1:A:430:ARG:NE	7:A:903:HOH:O	2.26	0.46
1:A:26:LEU:HD22	1:A:30:GLU:HG2	1.98	0.46
1:A:599:MET:HE2	1:A:735:TRP:HB3	1.96	0.46
1:A:134:PRO:HB3	1:A:161:GLN:HB3	1.99	0.45
1:A:462:VAL:CG1	1:A:469:LEU:HD21	2.46	0.45
1:A:436:GLU:HG2	1:A:448[B]:LYS:HE3	1.99	0.45
3:A:802:B12:H531	3:A:802:B12:C55	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ARG:HD3	1:A:416:ARG:HA	1.77	0.44
3:A:802:B12:H253	3:A:802:B12:H301	1.75	0.44
1:A:103:LYS:HG2	1:A:105:PHE:CZ	2.53	0.44
1:A:166:ILE:HD11	1:A:192:LEU:HD12	1.99	0.43
1:A:376:GLN:HB3	6:A:815:EDO:H11	2.01	0.43
1:A:325:HIS:HD2	7:A:1142:HOH:O	2.02	0.42
1:A:145:SER:HB2	1:A:288:PRO:HG2	2.00	0.42
1:A:251:MET:HE3	6:A:817:EDO:H12	2.02	0.41
1:A:201:TYR:CD1	6:A:820:EDO:H21	2.55	0.41
6:A:822:EDO:O2	7:A:901:HOH:O	2.21	0.41
1:A:219:ILE:HD13	1:A:219:ILE:HA	1.86	0.41
1:A:274:LYS:HD3	1:A:274:LYS:HA	1.86	0.41
1:A:363:GLU:HA	4:A:803:DTT:H41	2.01	0.41
1:A:135:ARG:HD3	3:A:802:B12:C50	2.51	0.40
1:A:448[B]:LYS:HA	1:A:448[B]:LYS:HD3	1.91	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	756/744 (102%)	733 (97%)	22 (3%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	THR

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	704/687 (102%)	700 (99%)	4 (1%)	78	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	156	GLU
1	A	431	ILE
1	A	576	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	HIS
1	A	692	ASN
1	A	722	HIS

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

28 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$
6	EDO	A	818	-	3,3,3	0.25	0	2,2,2	0.28	0
6	EDO	A	811	-	3,3,3	0.52	0	2,2,2	0.23	0
5	MES	A	804	-	12,12,12	2.28	1 (8%)	15,16,16	1.60	4 (26%)
6	EDO	A	805	-	3,3,3	0.57	0	2,2,2	0.33	0
6	EDO	A	826	-	3,3,3	0.52	0	2,2,2	0.21	0
6	EDO	A	813	-	3,3,3	0.43	0	2,2,2	0.46	0
4	DTT	A	803	2	7,7,7	0.75	0	4,8,8	1.21	1 (25%)
6	EDO	A	806	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EDO	A	827	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	A	807	-	3,3,3	0.44	0	2,2,2	0.60	0
6	EDO	A	812	-	3,3,3	0.50	0	2,2,2	0.26	0
6	EDO	A	828	-	3,3,3	0.57	0	2,2,2	0.25	0
6	EDO	A	824	-	3,3,3	0.40	0	2,2,2	0.36	0
6	EDO	A	822	-	3,3,3	0.42	0	2,2,2	0.56	0
3	B12	A	802	7	94,101,101	0.76	3 (3%)	149,166,166	0.99	8 (5%)
6	EDO	A	820	-	3,3,3	0.52	0	2,2,2	0.20	0
6	EDO	A	810	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	A	821	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	A	823	-	3,3,3	0.55	0	2,2,2	0.14	0
6	EDO	A	809	-	3,3,3	0.46	0	2,2,2	0.43	0
6	EDO	A	825	-	3,3,3	0.45	0	2,2,2	0.26	0
2	SF4	A	801	4,1	0,12,12	-	-	-	-	-
6	EDO	A	816	-	3,3,3	0.41	0	2,2,2	0.37	0
6	EDO	A	814	-	3,3,3	0.44	0	2,2,2	0.55	0
6	EDO	A	815	-	3,3,3	0.50	0	2,2,2	0.40	0
6	EDO	A	819	-	3,3,3	0.37	0	2,2,2	0.48	0
6	EDO	A	808	-	3,3,3	0.44	0	2,2,2	0.42	0
6	EDO	A	817	-	3,3,3	0.46	0	2,2,2	0.43	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
6	EDO	A	818	-	-	1/1/1/1	-
6	EDO	A	811	-	-	1/1/1/1	-
5	MES	A	804	-	-	1/6/14/14	0/1/1/1
6	EDO	A	805	-	-	1/1/1/1	-
6	EDO	A	826	-	-	0/1/1/1	-
6	EDO	A	813	-	-	1/1/1/1	-
4	DTT	A	803	2	-	6/8/8/8	-
6	EDO	A	806	-	-	1/1/1/1	-
6	EDO	A	827	-	-	0/1/1/1	-
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	A	812	-	-	1/1/1/1	-
6	EDO	A	828	-	-	0/1/1/1	-
6	EDO	A	824	-	-	0/1/1/1	-
6	EDO	A	822	-	-	0/1/1/1	-
3	B12	A	802	7	-	8/56/223/223	0/3/11/11
6	EDO	A	820	-	-	0/1/1/1	-
6	EDO	A	810	-	-	0/1/1/1	-
6	EDO	A	821	-	-	1/1/1/1	-
6	EDO	A	823	-	-	0/1/1/1	-
6	EDO	A	809	-	-	1/1/1/1	-
6	EDO	A	825	-	-	0/1/1/1	-
6	EDO	A	816	-	-	1/1/1/1	-
2	SF4	A	801	4,1	-	-	0/6/5/5
6	EDO	A	814	-	-	0/1/1/1	-
6	EDO	A	815	-	-	0/1/1/1	-
6	EDO	A	819	-	-	0/1/1/1	-
6	EDO	A	808	-	-	1/1/1/1	-
6	EDO	A	817	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	MES	C8-S	-7.57	1.67	1.77
3	A	802	B12	C14-N23	4.92	1.41	1.35
3	A	802	B12	C11-N23	-2.15	1.32	1.36
3	A	802	B12	C16-C15	2.11	1.50	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	MES	C5-N4-C3	3.94	117.32	108.84
3	A	802	B12	C9-N22-C6	3.93	110.01	105.28
3	A	802	B12	C19-N24-C16	3.24	110.83	107.29
3	A	802	B12	C10-C9-N22	2.77	128.90	125.74
3	A	802	B12	C55-C56-C57	-2.63	105.38	111.25
3	A	802	B12	C55-C17-C18	-2.55	106.25	111.12
5	A	804	MES	O1S-S-C8	2.36	110.30	106.73
3	A	802	B12	C12-C13-C14	-2.23	98.59	102.26
5	A	804	MES	C7-N4-C5	2.14	116.94	111.24
3	A	802	B12	C30-C3-C2	-2.10	114.37	119.00
4	A	803	DTT	O2-C2-C3	-2.09	105.18	109.57
3	A	802	B12	C41-C8-C9	-2.07	107.58	111.19
5	A	804	MES	O2S-S-C8	2.01	109.77	106.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	DTT	S1-C1-C2-O2
4	A	803	DTT	S1-C1-C2-C3
4	A	803	DTT	C1-C2-C3-C4
4	A	803	DTT	C2-C3-C4-S4
4	A	803	DTT	O3-C3-C4-S4
5	A	804	MES	C8-C7-N4-C5
3	A	802	B12	C4-C3-C30-C31
3	A	802	B12	C2-C3-C30-C31
6	A	809	EDO	O1-C1-C2-O2
6	A	812	EDO	O1-C1-C2-O2
3	A	802	B12	C2R-C1R-N1B-C8B
4	A	803	DTT	C1-C2-C3-O3
3	A	802	B12	C2R-C1R-N1B-C2B
6	A	805	EDO	O1-C1-C2-O2
6	A	821	EDO	O1-C1-C2-O2
3	A	802	B12	C42-C41-C8-C9
3	A	802	B12	O6R-C1R-N1B-C8B
6	A	806	EDO	O1-C1-C2-O2
6	A	816	EDO	O1-C1-C2-O2
3	A	802	B12	C3-C30-C31-C32
6	A	818	EDO	O1-C1-C2-O2
3	A	802	B12	O6R-C1R-N1B-C2B
6	A	813	EDO	O1-C1-C2-O2
6	A	808	EDO	O1-C1-C2-O2
6	A	811	EDO	O1-C1-C2-O2

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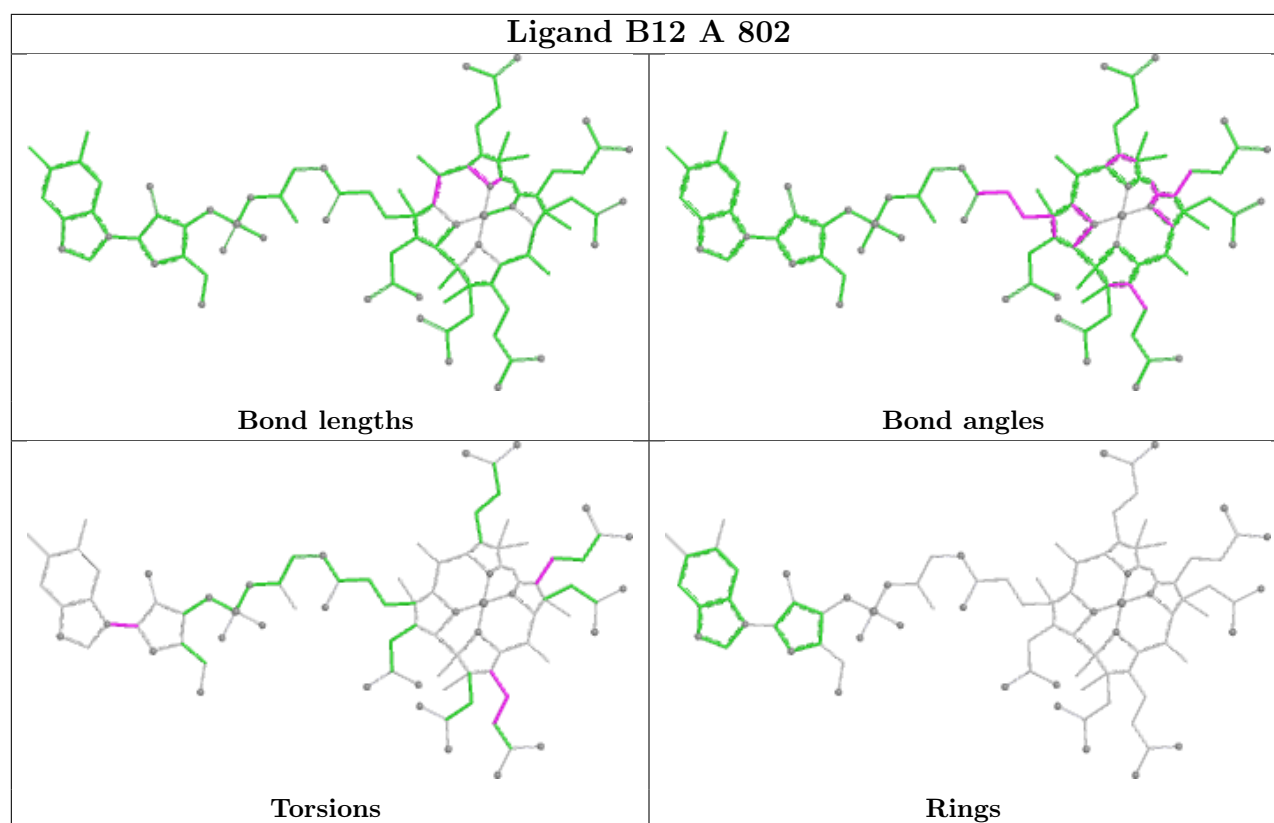
Mol	Chain	Res	Type	Atoms
6	A	817	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	818	EDO	2	0
6	A	811	EDO	1	0
4	A	803	DTT	1	0
6	A	822	EDO	1	0
3	A	802	B12	6	0
6	A	820	EDO	1	0
6	A	825	EDO	2	0
6	A	815	EDO	2	0
6	A	817	EDO	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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/744 (97%)	0.18	30 (4%) 41 41	11, 32, 64, 98	33 (4%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	SER	4.4
1	A	112[A]	TYR	4.0
1	A	670	ILE	4.0
1	A	736	SER	3.8
1	A	45	PHE	3.5
1	A	42	SER	3.4
1	A	539[A]	TYR	3.3
1	A	67[A]	SER	3.2
1	A	7	THR	3.2
1	A	678	VAL	3.0
1	A	676	ILE	3.0
1	A	9	SER	2.9
1	A	95	ILE	2.9
1	A	505	ILE	2.8
1	A	131	PHE	2.7
1	A	44	GLU	2.7
1	A	10	ILE	2.6
1	A	558	LEU	2.6
1	A	8	LYS	2.5
1	A	569	MET	2.4
1	A	734	ASN	2.4
1	A	370	PRO	2.4
1	A	669	HIS	2.3
1	A	12	TYR	2.2
1	A	565	VAL	2.2
1	A	13	TYR	2.1
1	A	270	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	LYS	2.1
1	A	40	LYS	2.0
1	A	677	ASN	2.0

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 oligosaccharides 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.

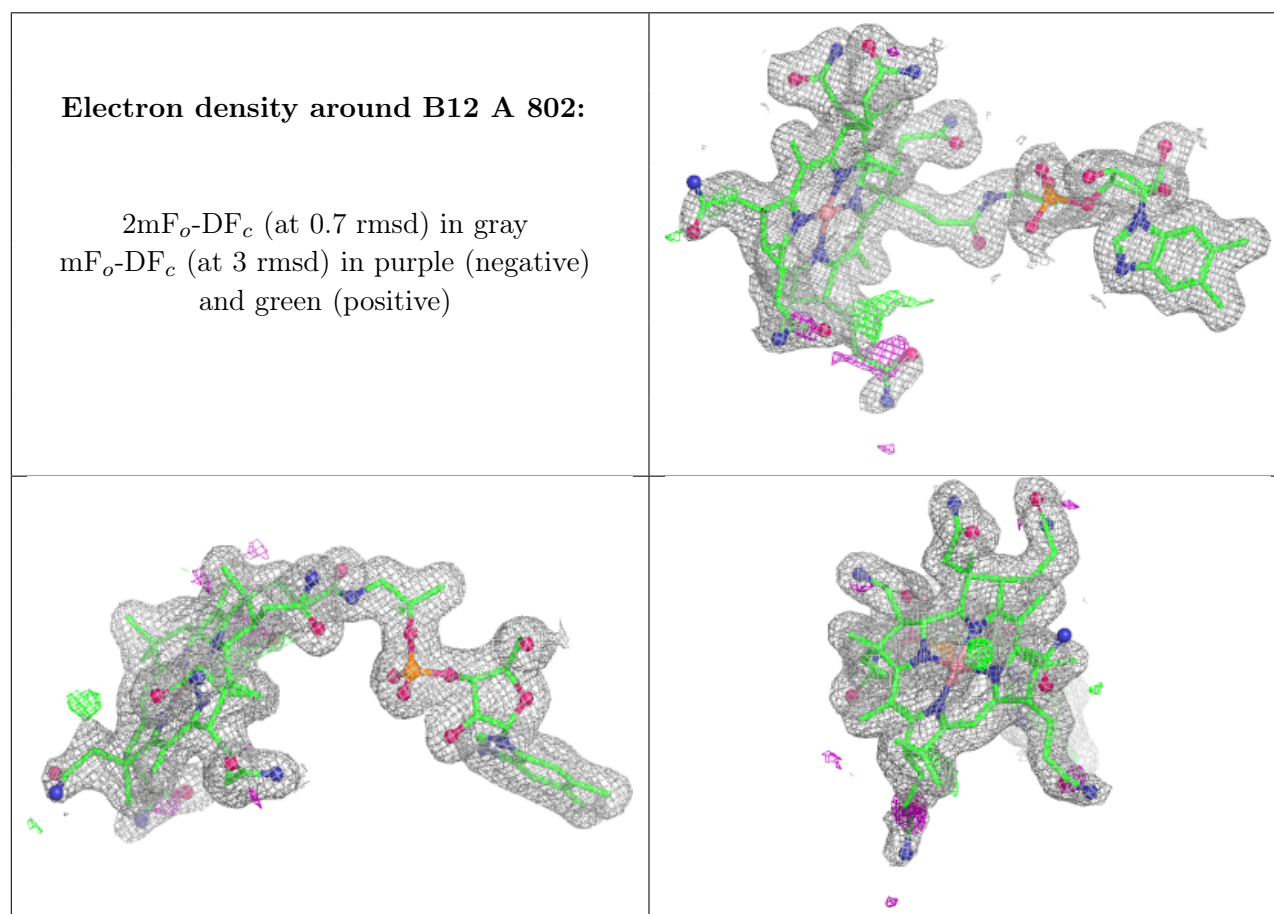
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	813	4/4	0.75	0.22	58,61,62,70	0
6	EDO	A	812	4/4	0.78	0.18	47,54,60,65	0
6	EDO	A	811	4/4	0.78	0.20	41,59,64,70	0
6	EDO	A	810	4/4	0.79	0.18	45,47,64,69	0
6	EDO	A	809	4/4	0.80	0.17	49,50,58,76	0
6	EDO	A	825	4/4	0.80	0.16	50,54,59,62	0
6	EDO	A	826	4/4	0.80	0.16	46,48,49,57	0
6	EDO	A	827	4/4	0.81	0.17	51,58,58,62	0
6	EDO	A	823	4/4	0.83	0.19	38,41,53,56	0
6	EDO	A	814	4/4	0.83	0.15	38,40,53,63	0
6	EDO	A	815	4/4	0.84	0.13	43,48,53,62	0
6	EDO	A	822	4/4	0.84	0.14	46,48,49,61	0
6	EDO	A	821	4/4	0.86	0.16	42,47,51,61	0
6	EDO	A	816	4/4	0.86	0.13	54,59,66,71	0
6	EDO	A	817	4/4	0.86	0.19	48,58,63,66	0
6	EDO	A	806	4/4	0.87	0.14	39,50,54,58	0
5	MES	A	804	12/12	0.89	0.14	43,46,56,58	0
6	EDO	A	818	4/4	0.89	0.15	26,28,42,56	0
6	EDO	A	820	4/4	0.89	0.12	46,49,50,62	0
6	EDO	A	805	4/4	0.92	0.15	37,38,38,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	808	4/4	0.93	0.14	33,36,42,52	0
6	EDO	A	819	4/4	0.94	0.11	33,33,41,41	0
6	EDO	A	807	4/4	0.95	0.13	30,34,36,38	0
4	DTT	A	803	8/8	0.95	0.12	30,42,52,54	0
6	EDO	A	828	4/4	0.95	0.10	34,38,41,42	0
6	EDO	A	824	4/4	0.96	0.11	36,36,39,40	0
3	B12	A	802	91/91	0.98	0.07	19,25,57,63	0
2	SF4	A	801	8/8	0.99	0.03	24,25,28,29	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.