



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:36 AM UTC

PDB ID : 2XIJ / pdb_00002xij
Title : Crystal structure of human methylmalonyl-CoA mutase in complex with adenosylcobalamin
Authors : Yue, W.W.; Froese, D.S.; Kochan, G.; Chaikuad, A.; Krojer, T.; Muniz, J.; Vollmar, M.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Bountra, C.; Oppermann, U.
Deposited on : 2010-06-30
Resolution : 1.95 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](#) ①) 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

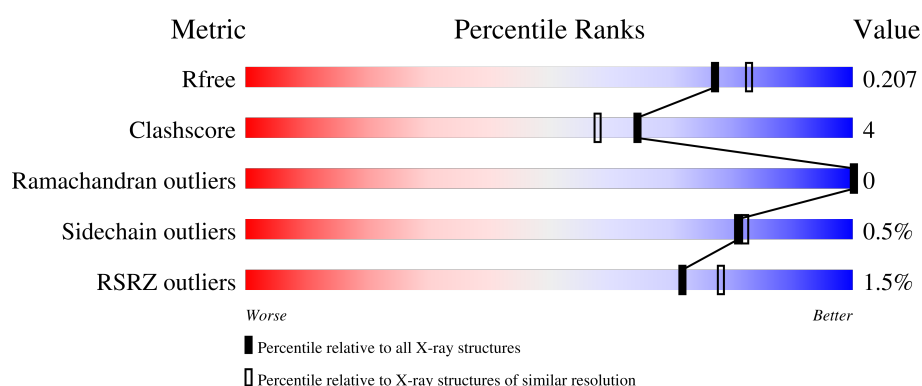
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	762	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BTB	A	1756	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6165 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.

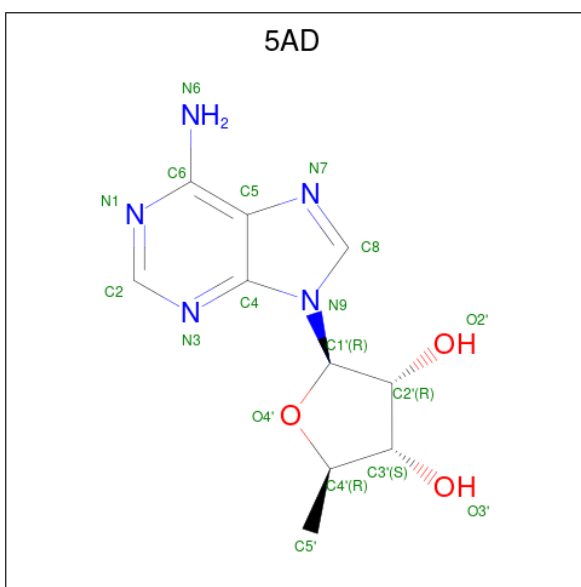
- Molecule 1 is a protein called METHYLMALONYL-COA MUTASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	6	0
			5464	3459	936	1037	32			

There are 24 discrepancies between the modelled and reference sequences:

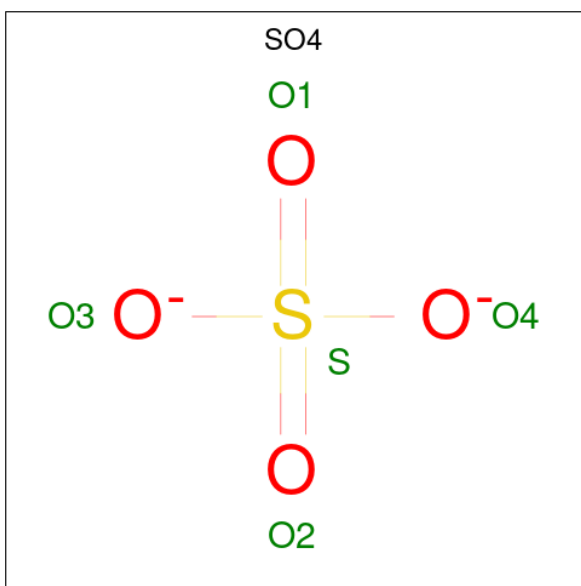
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P22033
A	751	ALA	-	expression tag	UNP P22033
A	752	GLU	-	expression tag	UNP P22033
A	753	ASN	-	expression tag	UNP P22033
A	754	LEU	-	expression tag	UNP P22033
A	755	TYR	-	expression tag	UNP P22033
A	756	PHE	-	expression tag	UNP P22033
A	757	GLN	-	expression tag	UNP P22033
A	758	SER	-	expression tag	UNP P22033
A	759	HIS	-	expression tag	UNP P22033
A	760	HIS	-	expression tag	UNP P22033
A	761	HIS	-	expression tag	UNP P22033
A	762	HIS	-	expression tag	UNP P22033
A	763	HIS	-	expression tag	UNP P22033
A	764	HIS	-	expression tag	UNP P22033
A	765	ASP	-	expression tag	UNP P22033
A	766	TYR	-	expression tag	UNP P22033
A	767	LYS	-	expression tag	UNP P22033
A	768	ASP	-	expression tag	UNP P22033
A	769	ASP	-	expression tag	UNP P22033
A	770	ASP	-	expression tag	UNP P22033
A	771	ASP	-	expression tag	UNP P22033
A	772	LYS	-	expression tag	UNP P22033
A	499	THR	ALA	variant	UNP P22033

- Molecule 2 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: C₁₀H₁₃N₅O₃).



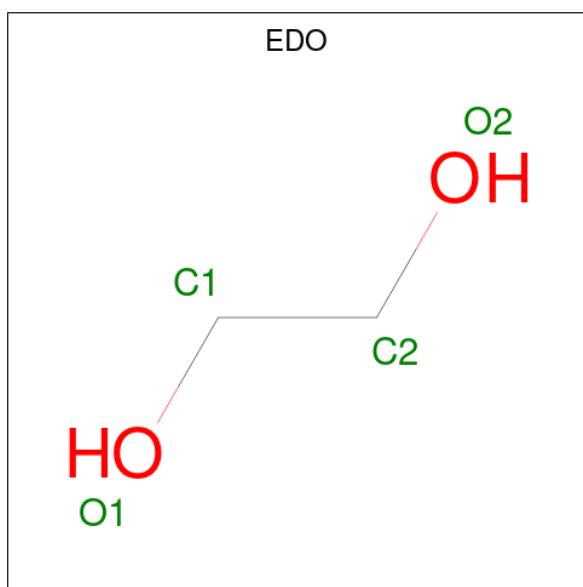
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



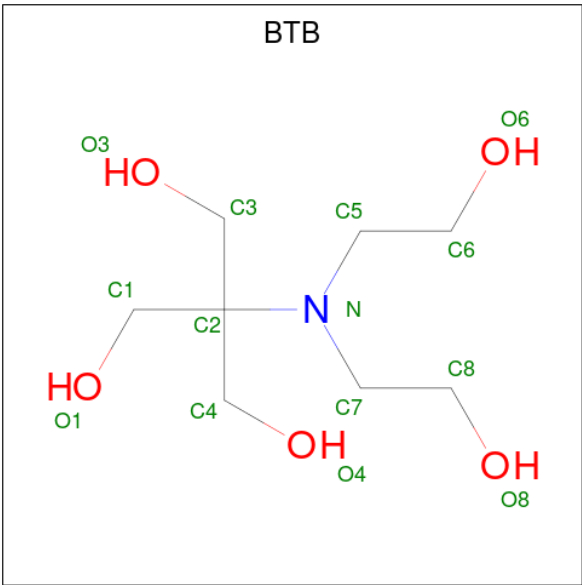
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



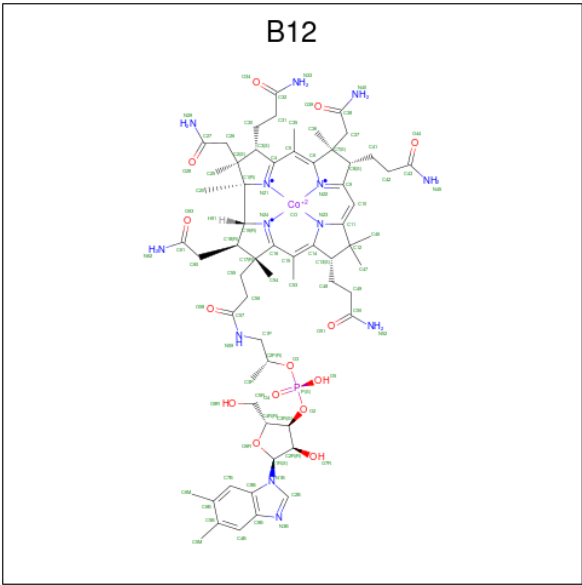
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 8 4 4	0	1
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 8 4 4	0	1
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

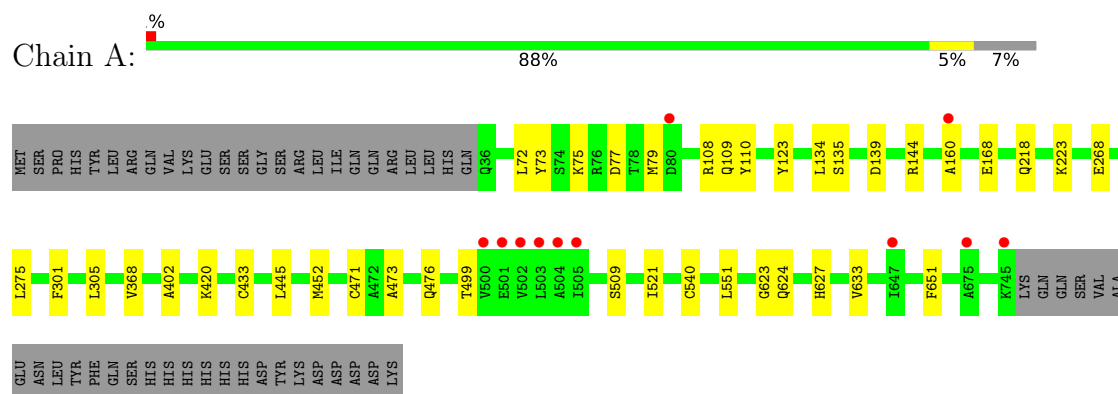
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	528	Total 528	O 528	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: METHYLMALONYL-COA MUTASE, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.36Å 137.72Å 198.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.20 – 1.95 99.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (99.20-1.95) 87.4 (99.20-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0066	Depositor
R, R_{free}	0.158 , 0.199 (Not available) , 0.207	Depositor DCC
R_{free} test set	2956 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6165	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: SO4, B12, BTB, 5AD, EDO

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	0.92	1/5589 (0.0%)	0.73	0/7573

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	ALA	CA-CB	5.59	1.62	1.53

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	A	5464	0	5383	29	0
2	A	18	0	12	1	0
3	A	10	0	0	0	0
4	A	40	0	60	2	0
5	A	14	0	19	11	0
6	A	91	0	88	13	0
7	A	528	0	0	4	1
All	All	6165	0	5562	44	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (44) 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)
6:A:800:B12:H362	6:A:800:B12:H351	1.54	0.87
6:A:800:B12:H552	6:A:800:B12:H531	1.60	0.81
6:A:800:B12:H473	6:A:800:B12:C49	2.09	0.74
1:A:368:VAL:HG23	7:A:2262:HOH:O	1.89	0.71
6:A:800:B12:H473	6:A:800:B12:H492	1.70	0.70
1:A:268:GLU:HB3	6:A:800:B12:H532	1.74	0.69
1:A:123:TYR:CD2	1:A:134:LEU:HD22	2.28	0.68
1:A:110:TYR:H	5:A:1756:BTB:H51	1.59	0.68
1:A:135:SER:OG	5:A:1756:BTB:H82	1.96	0.63
1:A:109:GLN:H	5:A:1756:BTB:C3	2.11	0.62
1:A:75:LYS:HG2	1:A:79:MET:HE3	1.80	0.62
6:A:800:B12:H492	6:A:800:B12:C47	2.34	0.58
6:A:800:B12:H531	6:A:800:B12:C55	2.32	0.57
1:A:72:LEU:HG	1:A:73:TYR:N	2.21	0.56
1:A:109:GLN:H	5:A:1756:BTB:H32	1.70	0.55
1:A:77:ASP:HB3	1:A:433[A]:CYS:SG	2.48	0.54
1:A:160:ALA:HB1	6:A:800:B12:N40	2.22	0.54
6:A:800:B12:H362	6:A:800:B12:C35	2.32	0.54
1:A:110:TYR:HA	5:A:1756:BTB:H81	1.89	0.53
2:A:1746:5AD:H3'	7:A:2198:HOH:O	2.09	0.53
6:A:800:B12:H203	6:A:800:B12:H301	1.91	0.52
1:A:108:ARG:HA	5:A:1756:BTB:H31	1.92	0.51
1:A:139:ASP:HA	1:A:160:ALA:HB3	1.93	0.51
5:A:1756:BTB:C8	5:A:1756:BTB:H61	2.42	0.50
1:A:452:MET:C	1:A:452:MET:SD	2.94	0.50
5:A:1756:BTB:O6	5:A:1756:BTB:H71	2.12	0.49
1:A:301:PHE:CZ	1:A:305:LEU:HD21	2.48	0.49
1:A:445:LEU:HD11	4:A:1750[A]:EDO:H11	1.94	0.49
1:A:275:LEU:HD12	1:A:471[A]:CYS:SG	2.54	0.48
1:A:452:MET:HG2	7:A:2323:HOH:O	2.12	0.48
1:A:420:LYS:HE2	7:A:2300:HOH:O	2.16	0.44
1:A:476:GLN:CB	1:A:633:VAL:HG21	2.47	0.44
1:A:144:ARG:HD3	1:A:624:GLN:OE1	2.19	0.42
6:A:800:B12:O28	6:A:800:B12:H3	2.18	0.42
1:A:473:ALA:HA	1:A:633:VAL:HG23	2.00	0.42
1:A:168:GLU:HG3	1:A:521:ILE:HD12	2.01	0.41
6:A:800:B12:C49	6:A:800:B12:C47	2.89	0.41
1:A:218:GLN:HE21	4:A:1754[B]:EDO:H12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:OG	5:A:1756:BTB:C8	2.66	0.41
1:A:623:GLY:O	1:A:651:PHE:HA	2.21	0.41
5:A:1756:BTB:H31	5:A:1756:BTB:H52	1.79	0.41
5:A:1756:BTB:C8	5:A:1756:BTB:C6	2.99	0.41
1:A:627:HIS:CE1	6:A:800:B12:N22	2.88	0.40
1:A:540:CYS:HB2	1:A:551:LEU:CD1	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2005:HOH:O	7:A:2052:HOH:O[4_555]	1.87	0.33

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	714/762 (94%)	702 (98%)	12 (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	568/636 (89%)	565 (100%)	3 (0%)	81 82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LYS
1	A	499	THR
1	A	509	SER

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	257	ASN
1	A	476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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 >
3	SO4	A	1747	-	4,4,4	0.28	0	6,6,6	0.39	0
4	EDO	A	1757	-	3,3,3	0.64	0	2,2,2	0.24	0
2	5AD	A	1746	-	20,20,20	1.67	5 (25%)	28,30,30	2.20	10 (35%)
4	EDO	A	1754[B]	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	A	1750[B]	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	A	1755	-	3,3,3	0.50	0	2,2,2	0.34	0
3	SO4	A	1748	-	4,4,4	0.43	0	6,6,6	0.14	0
4	EDO	A	1749	-	3,3,3	0.28	0	2,2,2	0.56	0
4	EDO	A	1753	-	3,3,3	0.44	0	2,2,2	0.33	0
4	EDO	A	1752	-	3,3,3	0.32	0	2,2,2	0.35	0
5	BTB	A	1756	-	13,13,13	3.16	5 (38%)	7,16,16	1.02	0
6	B12	A	800	1	94,101,101	1.53	14 (14%)	149,166,166	2.65	40 (26%)
4	EDO	A	1754[A]	-	3,3,3	0.44	0	2,2,2	0.31	0
4	EDO	A	1750[A]	-	3,3,3	0.51	0	2,2,2	0.21	0
4	EDO	A	1751	-	3,3,3	0.35	0	2,2,2	0.47	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1757	-	-	1/1/1/1	-
2	5AD	A	1746	-	-	0/4/20/20	0/3/3/3
4	EDO	A	1754[B]	-	-	0/1/1/1	-
4	EDO	A	1750[B]	-	-	0/1/1/1	-
4	EDO	A	1755	-	-	0/1/1/1	-
4	EDO	A	1749	-	-	1/1/1/1	-
4	EDO	A	1753	-	-	0/1/1/1	-
5	BTB	A	1756	-	-	7/21/21/21	-
4	EDO	A	1752	-	-	1/1/1/1	-
6	B12	A	800	1	-	8/56/223/223	0/3/11/11
4	EDO	A	1754[A]	-	-	1/1/1/1	-
4	EDO	A	1750[A]	-	-	1/1/1/1	-
4	EDO	A	1751	-	-	0/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	800	B12	C14-N23	6.97	1.44	1.35
5	A	1756	BTB	C2-N	6.33	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1756	BTB	C4-C2	5.50	1.59	1.53
5	A	1756	BTB	C5-N	4.91	1.54	1.48
5	A	1756	BTB	C1-C2	4.56	1.58	1.53
6	A	800	B12	C8B-C9B	4.07	1.46	1.40
6	A	800	B12	C12-C13	4.06	1.67	1.55
2	A	1746	5AD	C5-C4	3.90	1.46	1.39
6	A	800	B12	C9-N22	3.49	1.39	1.30
6	A	800	B12	C14-C15	3.05	1.51	1.38
5	A	1756	BTB	C7-N	2.89	1.52	1.48
6	A	800	B12	C6B-C5B	2.82	1.47	1.40
6	A	800	B12	C16-C15	-2.76	1.36	1.44
6	A	800	B12	C1-C2	-2.70	1.52	1.58
6	A	800	B12	C19-N24	-2.70	1.45	1.49
6	A	800	B12	C8B-N1B	-2.69	1.34	1.39
2	A	1746	5AD	C8-N7	2.64	1.36	1.31
6	A	800	B12	C11-N23	2.63	1.41	1.36
2	A	1746	5AD	C5-C6	2.54	1.48	1.41
6	A	800	B12	C9B-N3B	-2.32	1.35	1.39
6	A	800	B12	C48-C13	2.29	1.59	1.54
2	A	1746	5AD	C5-N7	-2.26	1.35	1.39
6	A	800	B12	C2B-N3B	2.17	1.35	1.31
2	A	1746	5AD	C4-N9	-2.14	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	800	B12	C13-C12-C11	-13.66	85.70	100.97
6	A	800	B12	C12-C11-C10	-10.10	110.38	123.40
6	A	800	B12	C20-C1-C19	-8.22	101.44	109.35
6	A	800	B12	C47-C12-C46	8.15	122.90	109.41
6	A	800	B12	C19-C1-N21	7.99	110.36	102.14
6	A	800	B12	C20-C1-N21	-7.69	97.55	110.26
6	A	800	B12	C46-C12-C13	-7.56	82.08	112.74
6	A	800	B12	C47-C12-C13	-6.34	87.03	112.74
6	A	800	B12	C2-C1-N21	5.65	109.63	101.78
2	A	1746	5AD	C5-C4-N3	-5.34	119.36	126.72
6	A	800	B12	C12-C11-N23	5.27	119.08	111.83
6	A	800	B12	C2-C1-C19	4.57	125.73	118.61
6	A	800	B12	C1-C19-C18	4.54	129.27	121.90
2	A	1746	5AD	N3-C2-N1	-4.17	122.27	128.58
2	A	1746	5AD	N3-C4-N9	4.14	134.21	127.17
6	A	800	B12	C9-C10-C11	-4.02	120.22	125.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1746	5AD	C2-N3-C4	3.90	121.36	111.83
6	A	800	B12	C8B-C9B-N3B	-3.77	105.92	110.00
6	A	800	B12	C18-C17-C16	3.54	104.96	100.69
6	A	800	B12	C12-C13-C14	3.51	108.02	102.26
6	A	800	B12	C9B-C8B-N1B	3.26	106.75	105.30
6	A	800	B12	C19-N24-C16	3.23	110.83	107.29
6	A	800	B12	C20-C1-C2	-3.19	108.02	113.28
6	A	800	B12	C18-C19-N24	3.16	107.09	102.33
6	A	800	B12	C9B-N3B-C2B	3.15	108.27	104.40
6	A	800	B12	C37-C7-C6	3.09	116.68	107.11
2	A	1746	5AD	C4-N9-C8	3.08	108.97	105.74
2	A	1746	5AD	C4-C5-N7	-3.06	107.08	110.58
6	A	800	B12	C17-C16-N24	-2.95	106.67	111.17
6	A	800	B12	C1-C19-N24	2.91	109.49	106.25
6	A	800	B12	C3-C4-N21	-2.89	108.39	111.98
6	A	800	B12	C48-C13-C12	2.87	124.72	116.52
2	A	1746	5AD	N9-C8-N7	-2.71	110.09	113.94
2	A	1746	5AD	C5'-C4'-C3'	-2.69	112.88	115.70
6	A	800	B12	C17-C16-C15	2.57	130.32	126.26
6	A	800	B12	C2P-C1P-N59	-2.54	109.18	112.92
6	A	800	B12	C8B-N1B-C2B	2.53	108.56	106.26
2	A	1746	5AD	C5-N7-C8	2.53	107.42	103.45
6	A	800	B12	C54-C17-C18	-2.51	109.38	112.99
6	A	800	B12	C7-C37-C38	-2.49	106.90	114.28
6	A	800	B12	C15-C16-N24	-2.49	118.88	122.42
6	A	800	B12	N1B-C2B-N3B	-2.43	110.49	113.94
6	A	800	B12	C7-C8-C9	2.32	103.83	100.89
6	A	800	B12	C47-C12-C11	2.27	118.18	110.08
6	A	800	B12	C10-C9-N22	2.24	128.29	125.74
6	A	800	B12	C4B-C9B-N3B	2.22	134.25	130.51
6	A	800	B12	C26-C2-C3	2.22	111.29	107.42
2	A	1746	5AD	C6-C5-N7	2.10	136.13	132.09
6	A	800	B12	C25-C2-C1	-2.07	110.65	113.75
6	A	800	B12	O6R-C1R-C2R	-2.04	102.24	106.62

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1756	BTB	O1-C1-C2-C3
5	A	1756	BTB	O1-C1-C2-C4
5	A	1756	BTB	C1-C2-C3-O3

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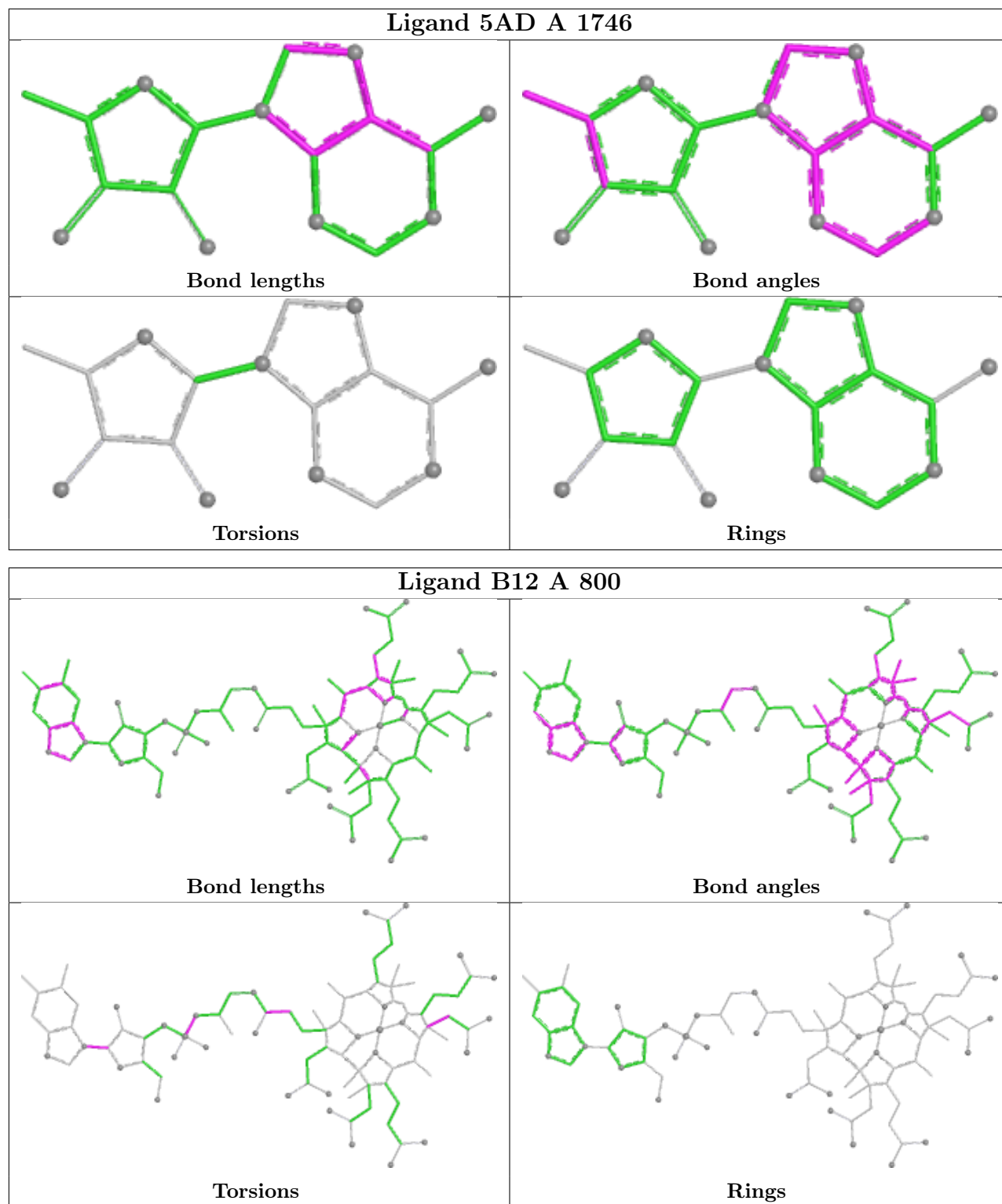
Mol	Chain	Res	Type	Atoms
5	A	1756	BTB	C4-C2-C3-O3
5	A	1756	BTB	N-C2-C4-O4
5	A	1756	BTB	C6-C5-N-C7
5	A	1756	BTB	N-C7-C8-O8
6	A	800	B12	C2R-C1R-N1B-C2B
6	A	800	B12	C2R-C1R-N1B-C8B
4	A	1750[A]	EDO	O1-C1-C2-O2
4	A	1752	EDO	O1-C1-C2-O2
6	A	800	B12	O6R-C1R-N1B-C8B
4	A	1749	EDO	O1-C1-C2-O2
4	A	1757	EDO	O1-C1-C2-O2
4	A	1754[A]	EDO	O1-C1-C2-O2
6	A	800	B12	C38-C37-C7-C36
6	A	800	B12	C55-C56-C57-O58
6	A	800	B12	C55-C56-C57-N59
6	A	800	B12	C2P-O3-P-O5
6	A	800	B12	O6R-C1R-N1B-C2B

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1746	5AD	1	0
4	A	1754[B]	EDO	1	0
5	A	1756	BTB	11	0
6	A	800	B12	13	0
4	A	1750[A]	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 ⓘ

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 [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	710/762 (93%)	-0.22	11 (1%) 72 78	14, 26, 49, 92	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	VAL	3.7
1	A	160	ALA	3.1
1	A	502	VAL	2.9
1	A	504	ALA	2.8
1	A	80	ASP	2.7
1	A	675	ALA	2.6
1	A	503	LEU	2.6
1	A	647	ILE	2.2
1	A	745	LYS	2.2
1	A	501	GLU	2.0
1	A	505	ILE	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,

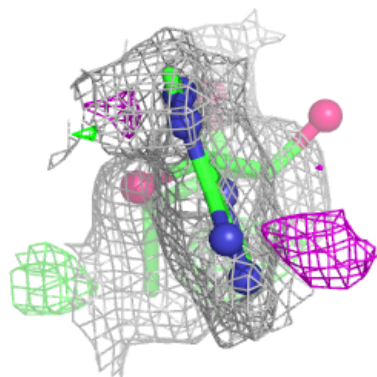
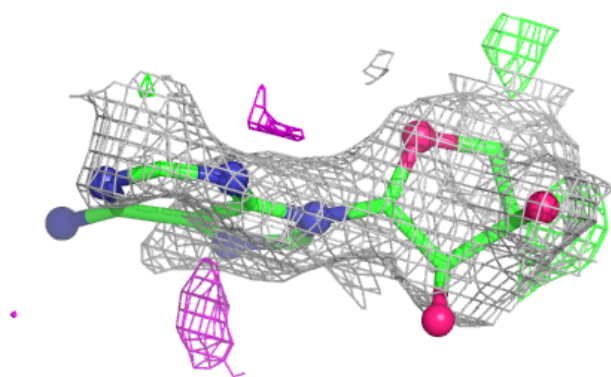
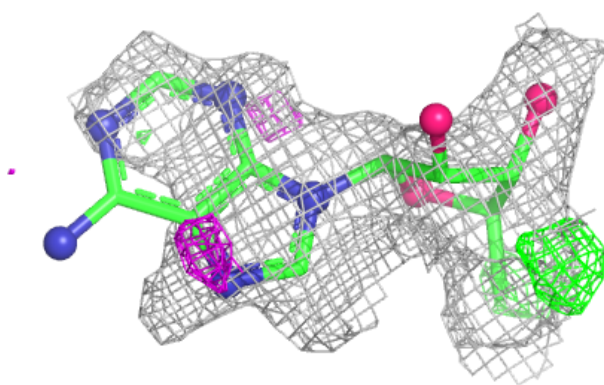
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	1757	4/4	0.78	0.16	43,45,51,54	0
4	EDO	A	1750[B]	4/4	0.81	0.22	26,28,30,36	4
4	EDO	A	1752	4/4	0.81	0.16	42,47,53,56	0
4	EDO	A	1750[A]	4/4	0.81	0.22	27,29,29,34	4
5	BTB	A	1756	14/14	0.84	0.16	35,58,81,84	0
4	EDO	A	1749	4/4	0.85	0.11	30,32,40,43	0
4	EDO	A	1755	4/4	0.86	0.13	45,45,50,54	0
2	5AD	A	1746	18/18	0.91	0.13	16,47,66,67	0
4	EDO	A	1754[B]	4/4	0.92	0.12	38,39,41,52	4
4	EDO	A	1754[A]	4/4	0.92	0.12	20,37,37,51	4
4	EDO	A	1751	4/4	0.93	0.11	35,37,47,53	0
3	SO4	A	1748	5/5	0.95	0.07	45,47,56,57	0
4	EDO	A	1753	4/4	0.96	0.07	27,28,36,38	0
6	B12	A	800	91/91	0.97	0.07	13,19,33,51	0
3	SO4	A	1747	5/5	0.98	0.06	21,26,33,39	5

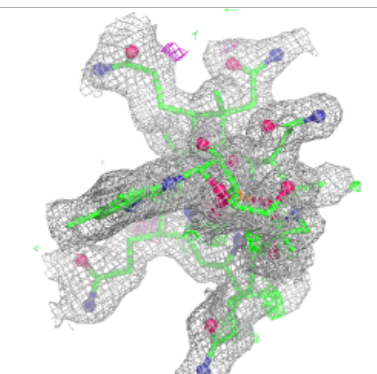
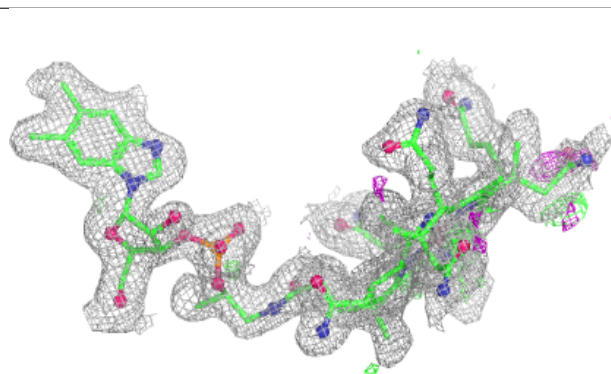
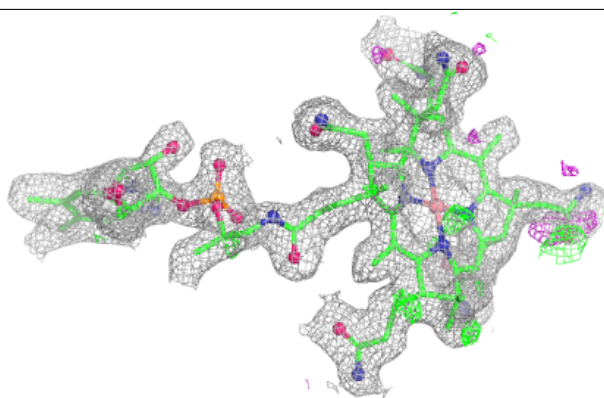
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD A 1746:

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

**Electron density around B12 A 800:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.