wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 01:58 PM EDT

PDB ID	:	4NS3 / pdb_00004ns3
Title	:	Crystal structure of the Delta-pyrroline-5-carboxylate dehydrogenase from Mycobacterium tuberculosis bound with NAD and cobalamin
Authors	:	Lagautriere, T.; Bashiri, G.; Baker, E.N.
Deposited on	:	2013-11-27
Resolution	:	2.38 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 (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 (i)) were used in the production of this report:

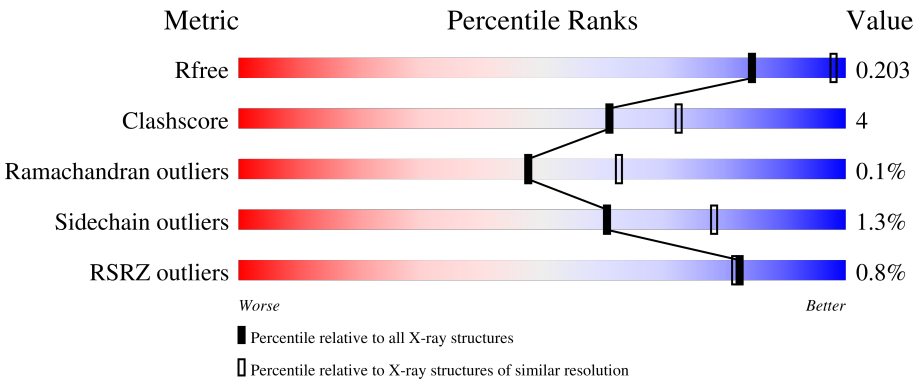
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	563	90% 6% • •
1	B	563	87% 8% • •
1	C	563	88% 8% •
1	D	563	90% 7% •
1	E	563	2% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	563	2% 85% 9% 5%

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
2	B12	A	601	X	-	-	-
2	B12	B	601	X	-	-	-
2	B12	C	601	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27892 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 Delta-1-pyrroline-5-carboxylate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	4161	2636	736	778	11	0	0	0
1	B	542	4163	2638	736	778	11	0	0	0
1	C	544	4176	2645	738	782	11	0	0	0
1	D	544	4171	2642	738	780	11	0	0	0
1	E	532	4072	2581	723	757	11	0	0	0
1	F	535	4100	2597	727	765	11	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP L7N4Z6
A	-18	GLY	-	expression tag	UNP L7N4Z6
A	-17	SER	-	expression tag	UNP L7N4Z6
A	-16	SER	-	expression tag	UNP L7N4Z6
A	-15	HIS	-	expression tag	UNP L7N4Z6
A	-14	HIS	-	expression tag	UNP L7N4Z6
A	-13	HIS	-	expression tag	UNP L7N4Z6
A	-12	HIS	-	expression tag	UNP L7N4Z6
A	-11	HIS	-	expression tag	UNP L7N4Z6
A	-10	HIS	-	expression tag	UNP L7N4Z6
A	-9	SER	-	expression tag	UNP L7N4Z6
A	-8	SER	-	expression tag	UNP L7N4Z6
A	-7	GLY	-	expression tag	UNP L7N4Z6
A	-6	LEU	-	expression tag	UNP L7N4Z6
A	-5	VAL	-	expression tag	UNP L7N4Z6
A	-4	PRO	-	expression tag	UNP L7N4Z6
A	-3	ARG	-	expression tag	UNP L7N4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP L7N4Z6
A	-1	SER	-	expression tag	UNP L7N4Z6
A	0	HIS	-	expression tag	UNP L7N4Z6
A	505	ASP	GLY	engineered mutation	UNP L7N4Z6
B	-19	MET	-	expression tag	UNP L7N4Z6
B	-18	GLY	-	expression tag	UNP L7N4Z6
B	-17	SER	-	expression tag	UNP L7N4Z6
B	-16	SER	-	expression tag	UNP L7N4Z6
B	-15	HIS	-	expression tag	UNP L7N4Z6
B	-14	HIS	-	expression tag	UNP L7N4Z6
B	-13	HIS	-	expression tag	UNP L7N4Z6
B	-12	HIS	-	expression tag	UNP L7N4Z6
B	-11	HIS	-	expression tag	UNP L7N4Z6
B	-10	HIS	-	expression tag	UNP L7N4Z6
B	-9	SER	-	expression tag	UNP L7N4Z6
B	-8	SER	-	expression tag	UNP L7N4Z6
B	-7	GLY	-	expression tag	UNP L7N4Z6
B	-6	LEU	-	expression tag	UNP L7N4Z6
B	-5	VAL	-	expression tag	UNP L7N4Z6
B	-4	PRO	-	expression tag	UNP L7N4Z6
B	-3	ARG	-	expression tag	UNP L7N4Z6
B	-2	GLY	-	expression tag	UNP L7N4Z6
B	-1	SER	-	expression tag	UNP L7N4Z6
B	0	HIS	-	expression tag	UNP L7N4Z6
B	505	ASP	GLY	engineered mutation	UNP L7N4Z6
C	-19	MET	-	expression tag	UNP L7N4Z6
C	-18	GLY	-	expression tag	UNP L7N4Z6
C	-17	SER	-	expression tag	UNP L7N4Z6
C	-16	SER	-	expression tag	UNP L7N4Z6
C	-15	HIS	-	expression tag	UNP L7N4Z6
C	-14	HIS	-	expression tag	UNP L7N4Z6
C	-13	HIS	-	expression tag	UNP L7N4Z6
C	-12	HIS	-	expression tag	UNP L7N4Z6
C	-11	HIS	-	expression tag	UNP L7N4Z6
C	-10	HIS	-	expression tag	UNP L7N4Z6
C	-9	SER	-	expression tag	UNP L7N4Z6
C	-8	SER	-	expression tag	UNP L7N4Z6
C	-7	GLY	-	expression tag	UNP L7N4Z6
C	-6	LEU	-	expression tag	UNP L7N4Z6
C	-5	VAL	-	expression tag	UNP L7N4Z6
C	-4	PRO	-	expression tag	UNP L7N4Z6
C	-3	ARG	-	expression tag	UNP L7N4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP L7N4Z6
C	-1	SER	-	expression tag	UNP L7N4Z6
C	0	HIS	-	expression tag	UNP L7N4Z6
C	505	ASP	GLY	engineered mutation	UNP L7N4Z6
D	-19	MET	-	expression tag	UNP L7N4Z6
D	-18	GLY	-	expression tag	UNP L7N4Z6
D	-17	SER	-	expression tag	UNP L7N4Z6
D	-16	SER	-	expression tag	UNP L7N4Z6
D	-15	HIS	-	expression tag	UNP L7N4Z6
D	-14	HIS	-	expression tag	UNP L7N4Z6
D	-13	HIS	-	expression tag	UNP L7N4Z6
D	-12	HIS	-	expression tag	UNP L7N4Z6
D	-11	HIS	-	expression tag	UNP L7N4Z6
D	-10	HIS	-	expression tag	UNP L7N4Z6
D	-9	SER	-	expression tag	UNP L7N4Z6
D	-8	SER	-	expression tag	UNP L7N4Z6
D	-7	GLY	-	expression tag	UNP L7N4Z6
D	-6	LEU	-	expression tag	UNP L7N4Z6
D	-5	VAL	-	expression tag	UNP L7N4Z6
D	-4	PRO	-	expression tag	UNP L7N4Z6
D	-3	ARG	-	expression tag	UNP L7N4Z6
D	-2	GLY	-	expression tag	UNP L7N4Z6
D	-1	SER	-	expression tag	UNP L7N4Z6
D	0	HIS	-	expression tag	UNP L7N4Z6
D	505	ASP	GLY	engineered mutation	UNP L7N4Z6
E	-19	MET	-	expression tag	UNP L7N4Z6
E	-18	GLY	-	expression tag	UNP L7N4Z6
E	-17	SER	-	expression tag	UNP L7N4Z6
E	-16	SER	-	expression tag	UNP L7N4Z6
E	-15	HIS	-	expression tag	UNP L7N4Z6
E	-14	HIS	-	expression tag	UNP L7N4Z6
E	-13	HIS	-	expression tag	UNP L7N4Z6
E	-12	HIS	-	expression tag	UNP L7N4Z6
E	-11	HIS	-	expression tag	UNP L7N4Z6
E	-10	HIS	-	expression tag	UNP L7N4Z6
E	-9	SER	-	expression tag	UNP L7N4Z6
E	-8	SER	-	expression tag	UNP L7N4Z6
E	-7	GLY	-	expression tag	UNP L7N4Z6
E	-6	LEU	-	expression tag	UNP L7N4Z6
E	-5	VAL	-	expression tag	UNP L7N4Z6
E	-4	PRO	-	expression tag	UNP L7N4Z6
E	-3	ARG	-	expression tag	UNP L7N4Z6

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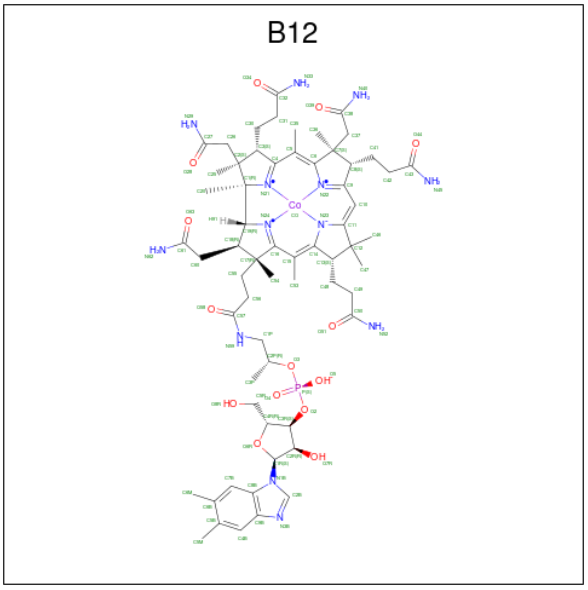
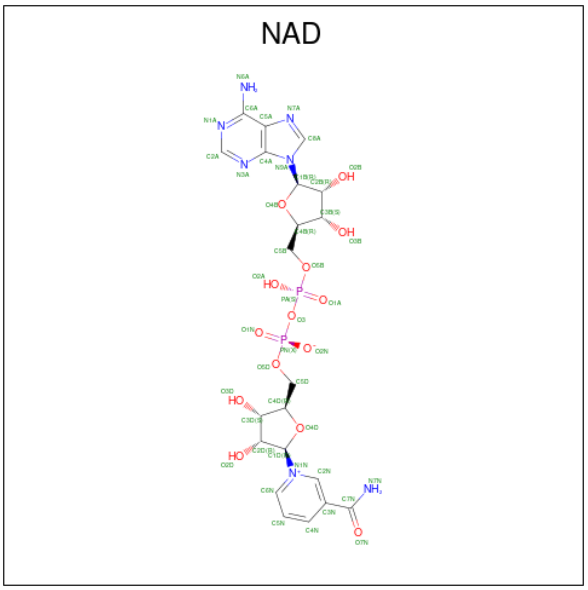
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP L7N4Z6
E	-1	SER	-	expression tag	UNP L7N4Z6
E	0	HIS	-	expression tag	UNP L7N4Z6
E	505	ASP	GLY	conflict	UNP L7N4Z6
F	-19	MET	-	expression tag	UNP L7N4Z6
F	-18	GLY	-	expression tag	UNP L7N4Z6
F	-17	SER	-	expression tag	UNP L7N4Z6
F	-16	SER	-	expression tag	UNP L7N4Z6
F	-15	HIS	-	expression tag	UNP L7N4Z6
F	-14	HIS	-	expression tag	UNP L7N4Z6
F	-13	HIS	-	expression tag	UNP L7N4Z6
F	-12	HIS	-	expression tag	UNP L7N4Z6
F	-11	HIS	-	expression tag	UNP L7N4Z6
F	-10	HIS	-	expression tag	UNP L7N4Z6
F	-9	SER	-	expression tag	UNP L7N4Z6
F	-8	SER	-	expression tag	UNP L7N4Z6
F	-7	GLY	-	expression tag	UNP L7N4Z6
F	-6	LEU	-	expression tag	UNP L7N4Z6
F	-5	VAL	-	expression tag	UNP L7N4Z6
F	-4	PRO	-	expression tag	UNP L7N4Z6
F	-3	ARG	-	expression tag	UNP L7N4Z6
F	-2	GLY	-	expression tag	UNP L7N4Z6
F	-1	SER	-	expression tag	UNP L7N4Z6
F	0	HIS	-	expression tag	UNP L7N4Z6
F	505	ASP	GLY	engineered mutation	UNP L7N4Z6

- Molecule 2 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	E	1	28	11	5	10	2	0	0
3	F	1	26	10	5	9	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	537	537	537	0	0
4	B	482	482	482	0	0
4	C	480	480	480	0	0

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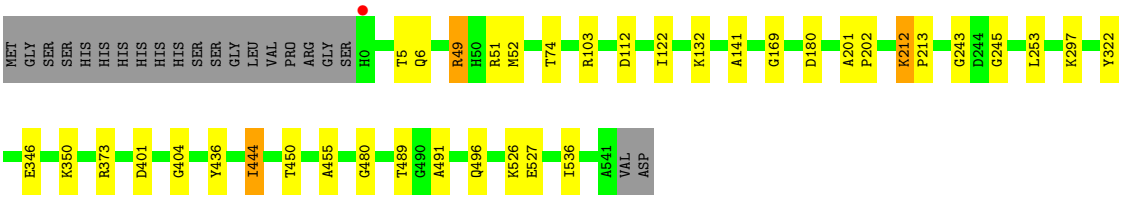
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	484	484	484	0	0
			Total	O		
4	E	316	316	316	0	0
			Total	O		
4	F	332	332	332	0	0

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.

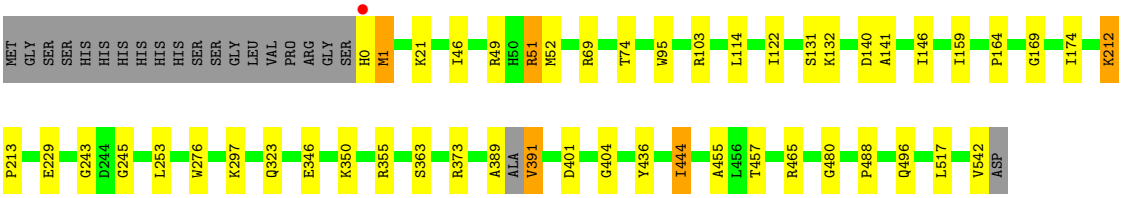
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase

Chain A:



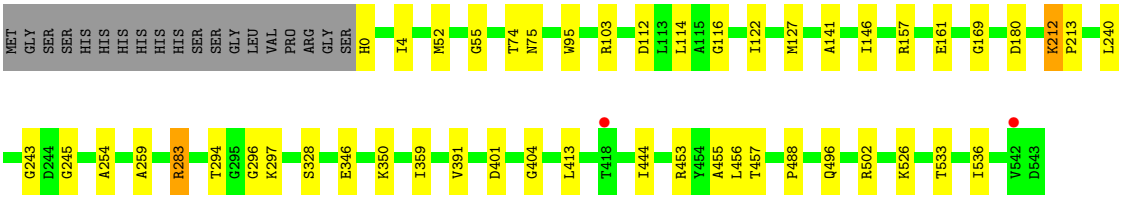
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase

Chain B:



• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase

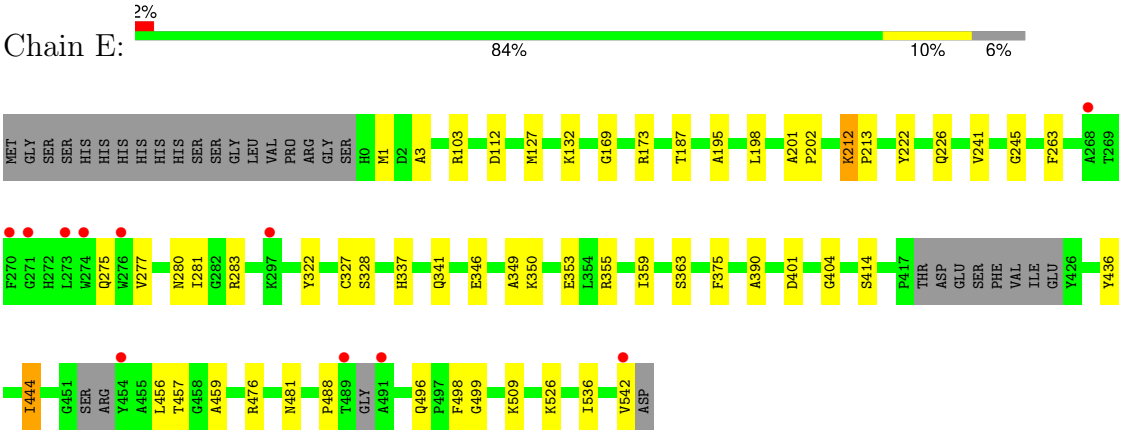
Chain C:



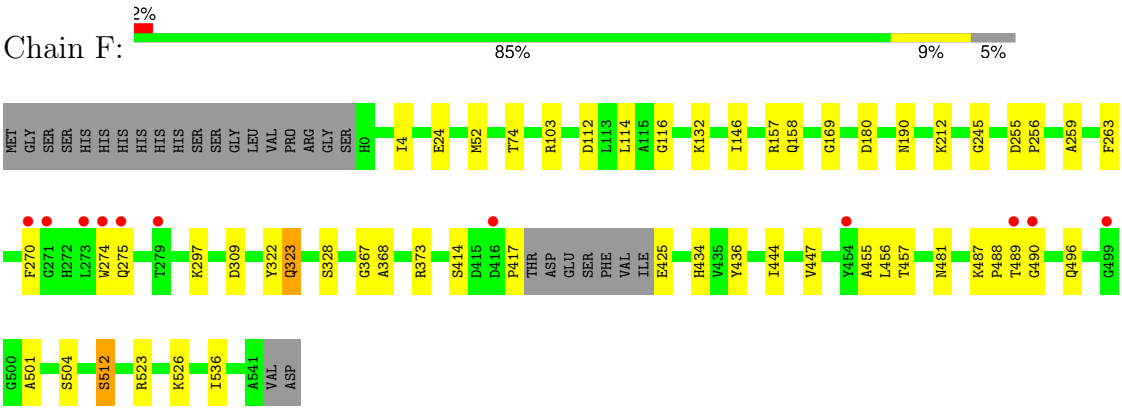
• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase

Chain D:

• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase



• Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.85Å 164.85Å 260.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.05 – 2.38 20.05 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.05-2.38) 99.7 (20.05-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.38Å)	Xtriage
Refinement program	PHENIX 1.9_1692, REFMAC 5.8.0049	Depositor
R, R_{free}	0.157 , 0.205 0.156 , 0.203	Depositor DCC
R_{free} test set	8211 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27892	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.74	0/4253	0.78	0/5800
1	B	0.73	0/4254	0.77	0/5800
1	C	0.73	0/4268	0.79	2/5821 (0.0%)
1	D	0.73	0/4263	0.81	5/5814 (0.1%)
1	E	0.65	0/4159	0.78	1/5668 (0.0%)
1	F	0.67	0/4189	0.80	5/5711 (0.1%)
All	All	0.71	0/25386	0.79	13/34614 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	307	ARG	CA-C-N	6.68	126.19	119.24
1	D	307	ARG	C-N-CA	6.68	126.19	119.24
1	F	116	GLY	CA-C-N	6.58	126.52	119.28
1	F	116	GLY	C-N-CA	6.58	126.52	119.28
1	F	323	GLN	CA-CB-CG	5.50	125.09	114.10

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	4161	0	4066	23	0
1	B	4163	0	4069	37	0
1	C	4176	0	4079	32	0
1	D	4171	0	4070	27	0
1	E	4072	0	3981	35	0
1	F	4100	0	4009	44	0
2	A	91	0	87	5	0
2	B	91	0	87	6	0
2	C	91	0	87	10	0
2	D	91	0	86	10	0
3	E	28	0	12	0	0
3	F	26	0	12	0	0
4	A	537	0	0	5	0
4	B	482	0	0	5	0
4	C	480	0	0	2	0
4	D	484	0	0	8	0
4	E	316	0	0	4	0
4	F	332	0	0	5	0
All	All	27892	0	24645	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 210 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:B:46:ILE:HD12	1:B:51:ARG:HH21	1.44	0.82
1:E:275:GLN:OE1	4:E:971:HOH:O	1.99	0.81
1:F:323:GLN:HE21	1:F:367:GLY:C	1.98	0.72
1:C:52:MET:HE3	1:C:74:THR:HG23	1.74	0.70
1:E:103:ARG:NH2	4:E:957:HOH:O	2.21	0.68

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	539/563 (96%)	524 (97%)	14 (3%)	1 (0%)	43	56
1	B	537/563 (95%)	526 (98%)	10 (2%)	1 (0%)	43	56
1	C	541/563 (96%)	530 (98%)	11 (2%)	0	100	100
1	D	541/563 (96%)	522 (96%)	19 (4%)	0	100	100
1	E	523/563 (93%)	510 (98%)	13 (2%)	0	100	100
1	F	530/563 (94%)	514 (97%)	16 (3%)	0	100	100
All	All	3211/3378 (95%)	3126 (97%)	83 (3%)	2 (0%)	48	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	480	GLY
1	A	480	GLY

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	421/439 (96%)	414 (98%)	7 (2%)	53	72
1	B	422/439 (96%)	414 (98%)	8 (2%)	50	69
1	C	423/439 (96%)	417 (99%)	6 (1%)	59	77
1	D	421/439 (96%)	419 (100%)	2 (0%)	81	90
1	E	410/439 (93%)	405 (99%)	5 (1%)	63	79
1	F	413/439 (94%)	408 (99%)	5 (1%)	63	79
All	All	2510/2634 (95%)	2477 (99%)	33 (1%)	61	78

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	158	GLN

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Mol	Chain	Res	Type
1	F	414	SER
1	F	536	ILE
1	B	391	VAL
1	B	323	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	0	HIS
1	D	341	GLN
1	E	38	HIS
1	D	434	HIS
1	B	38	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	F	327	1	8,9,10	1.01	0	6,9,11	0.91	0
1	CME	B	327	1	8,9,10	0.87	0	6,9,11	0.53	0
1	CME	E	327	1	8,9,10	1.08	1 (12%)	6,9,11	0.88	0
1	CME	D	327	1	8,9,10	1.01	0	6,9,11	0.58	0
1	CME	A	327	1	8,9,10	0.96	0	6,9,11	0.42	0
1	CME	C	327	1	8,9,10	1.05	0	6,9,11	0.94	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
1	CME	F	327	1	-	2/5/8/10	-
1	CME	B	327	1	-	0/5/8/10	-
1	CME	E	327	1	-	2/5/8/10	-
1	CME	D	327	1	-	0/5/8/10	-
1	CME	A	327	1	-	0/5/8/10	-
1	CME	C	327	1	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	327	CME	CB-SG	-2.22	1.74	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	327	CME	CE-SD-SG-CB
1	F	327	CME	CE-SD-SG-CB
1	F	327	CME	CZ-CE-SD-SG
1	E	327	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides 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	D	601	-	94,101,101	1.52	12 (12%)	149,166,166	2.79	43 (28%)
2	B12	C	601	-	94,101,101	1.44	12 (12%)	149,166,166	2.39	35 (23%)
3	NAD	F	601	-	25,28,48	1.04	3 (12%)	37,42,73	1.89	9 (24%)
3	NAD	E	601	-	30,30,48	1.17	3 (10%)	43,46,73	1.84	9 (20%)
2	B12	B	601	-	94,101,101	1.54	12 (12%)	149,166,166	2.52	38 (25%)
2	B12	A	601	-	94,101,101	1.52	12 (12%)	149,166,166	2.58	35 (23%)

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	D	601	-	-	16/56/223/223	0/3/11/11
2	B12	C	601	-	1/1/36/38	15/56/223/223	0/3/11/11
3	NAD	F	601	-	-	4/13/31/62	0/3/3/5
3	NAD	E	601	-	-	5/19/35/62	0/3/3/5
2	B12	B	601	-	1/1/36/38	5/56/223/223	0/3/11/11
2	B12	A	601	-	1/1/36/38	6/56/223/223	0/3/11/11

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	B12	C19-N24	-7.00	1.40	1.49
2	B	601	B12	C19-N24	-6.94	1.40	1.49
2	A	601	B12	C19-N24	-6.16	1.41	1.49
2	C	601	B12	C19-N24	-6.09	1.41	1.49
2	A	601	B12	C14-N23	5.55	1.42	1.35

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	B12	C20-C1-C19	-13.27	96.58	109.35
2	A	601	B12	C20-C1-C19	-12.54	97.28	109.35
2	B	601	B12	C20-C1-C19	-11.97	97.83	109.35
2	C	601	B12	C20-C1-C19	-9.87	99.85	109.35
2	C	601	B12	C1-C19-N24	9.83	117.19	106.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	B12	C19
2	B	601	B12	C19
2	C	601	B12	C19

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	B12	C2-C26-C27-N29
2	C	601	B12	C3-C2-C26-C27
2	C	601	B12	C42-C41-C8-C9
2	C	601	B12	C13-C48-C49-C50
2	D	601	B12	C2-C26-C27-N29

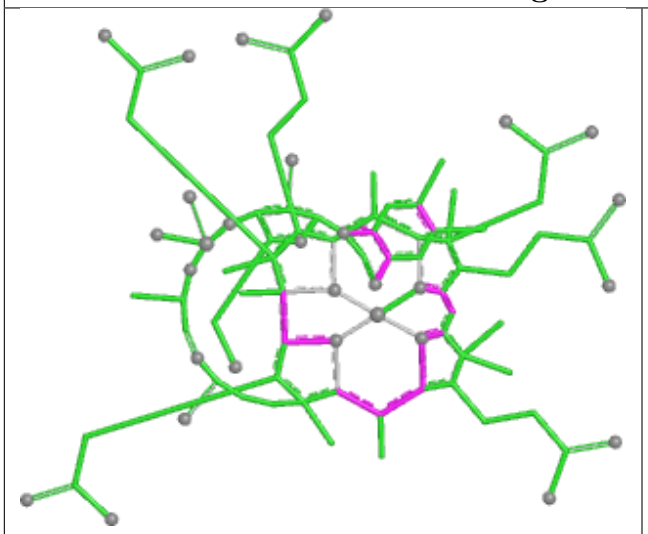
There are no ring outliers.

4 monomers are involved in 31 short contacts:

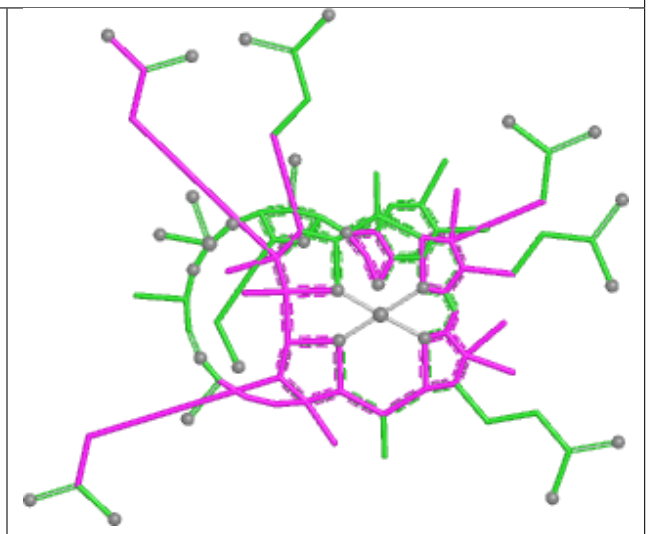
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	B12	10	0
2	C	601	B12	10	0
2	B	601	B12	6	0
2	A	601	B12	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

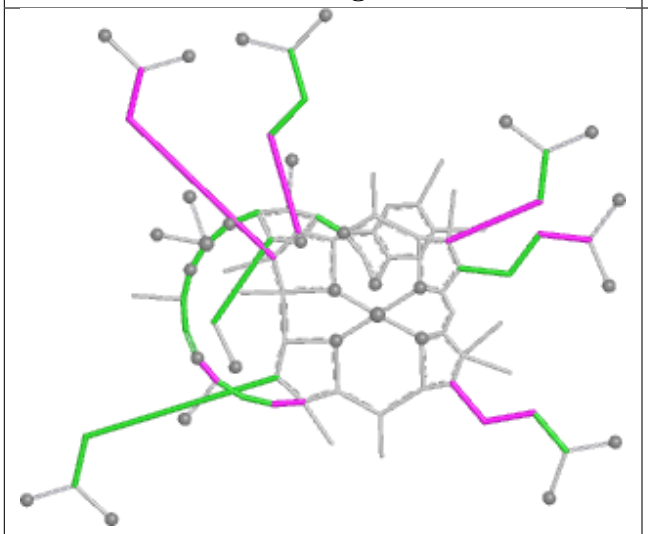
Ligand B12 D 601



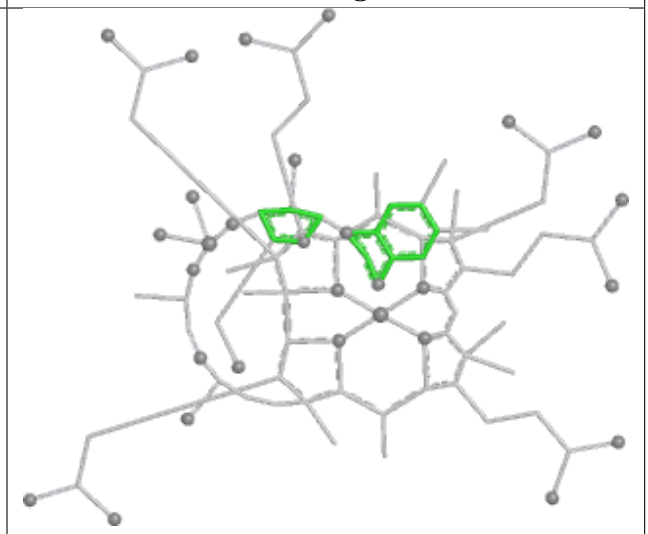
Bond lengths



Bond angles

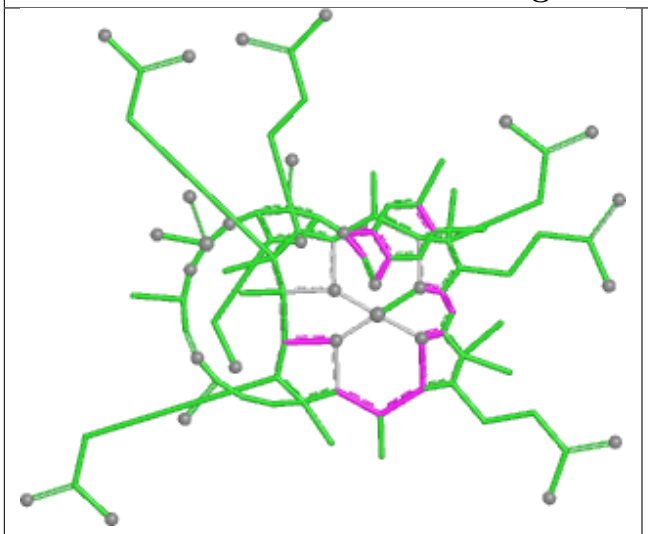


Torsions

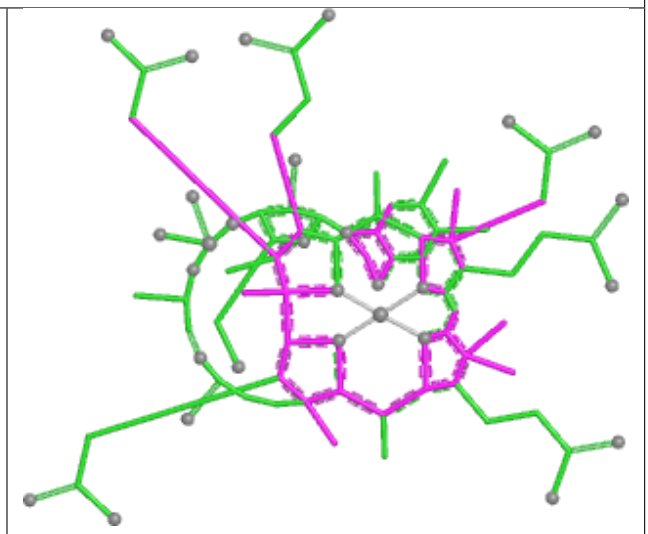


Rings

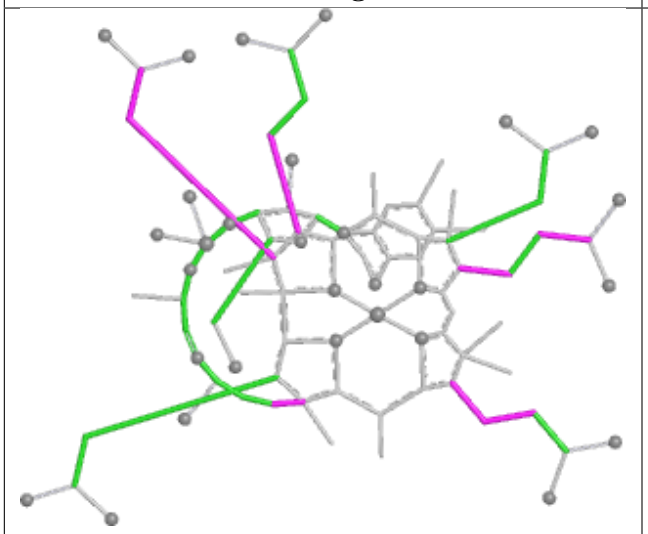
Ligand B12 C 601



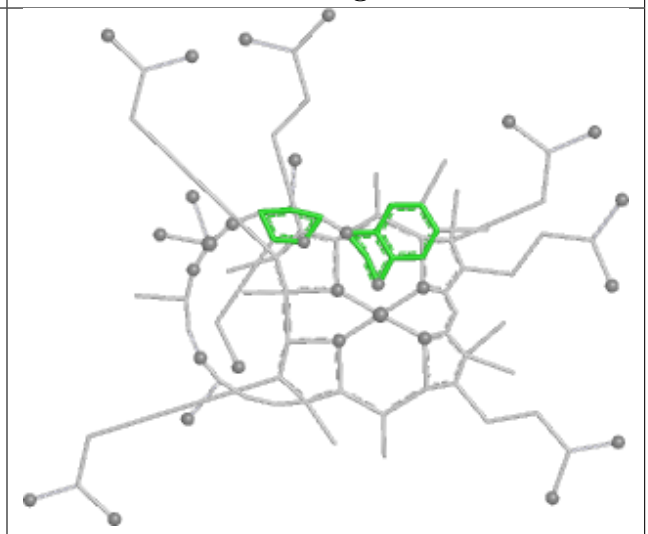
Bond lengths



Bond angles

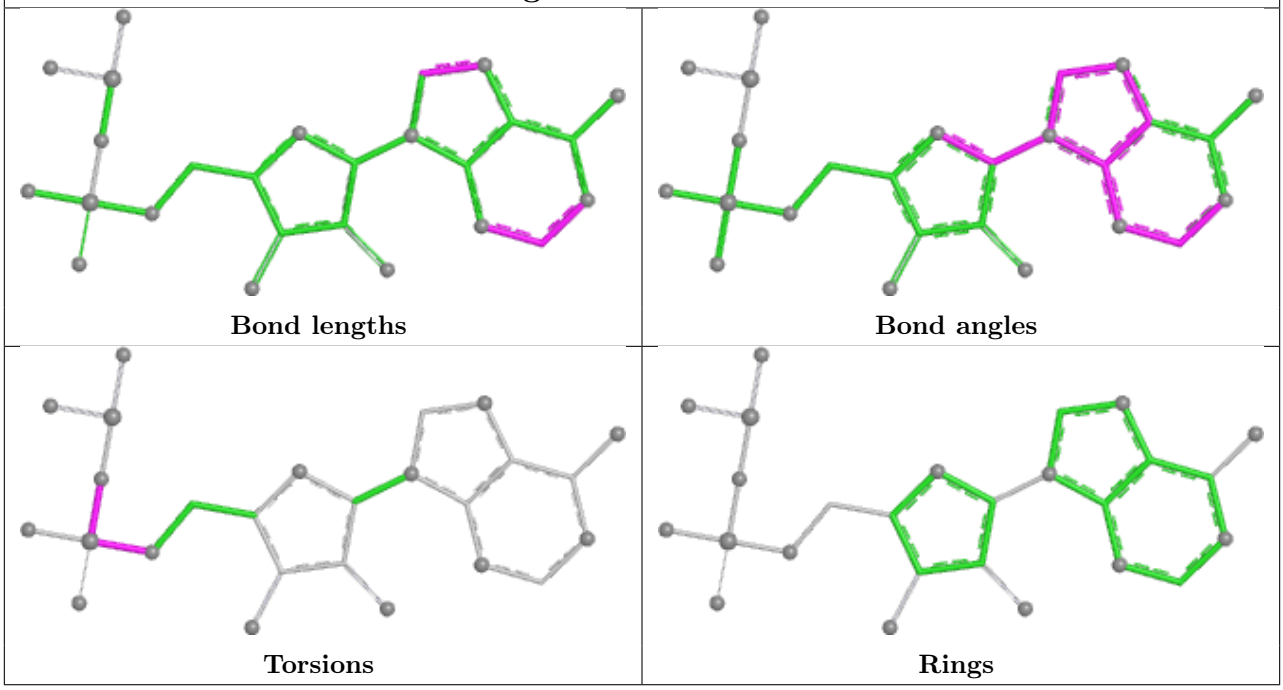


Torsions

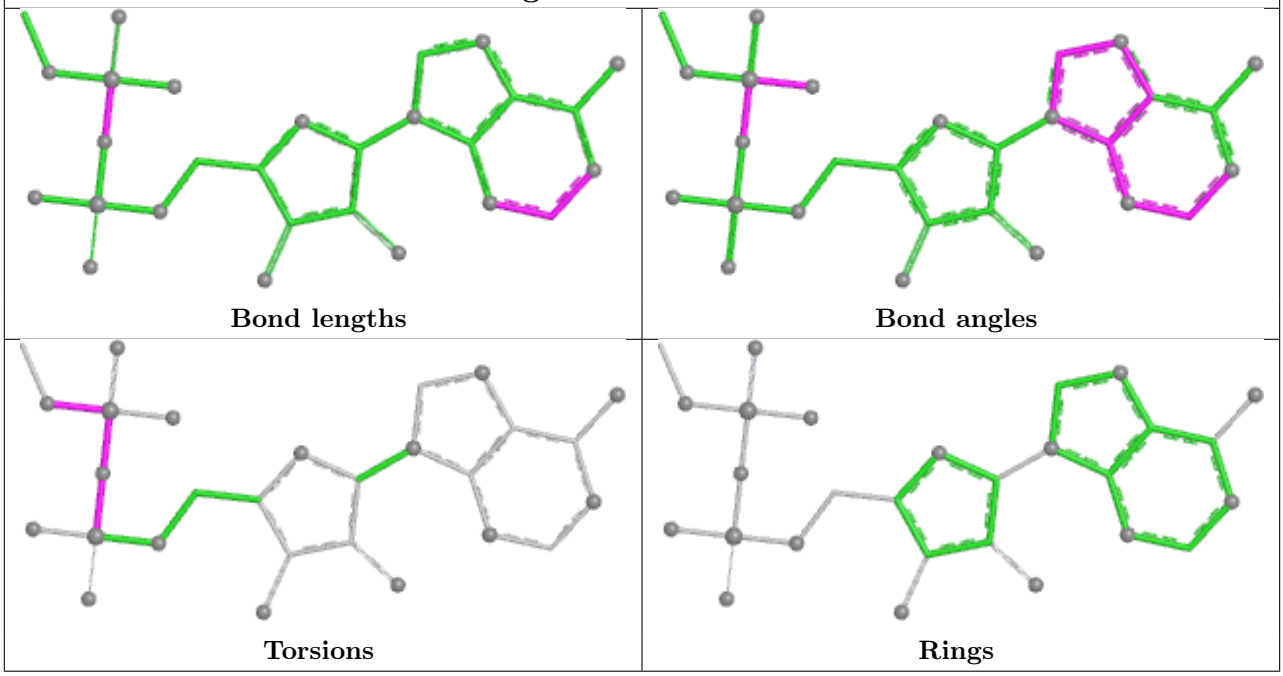


Rings

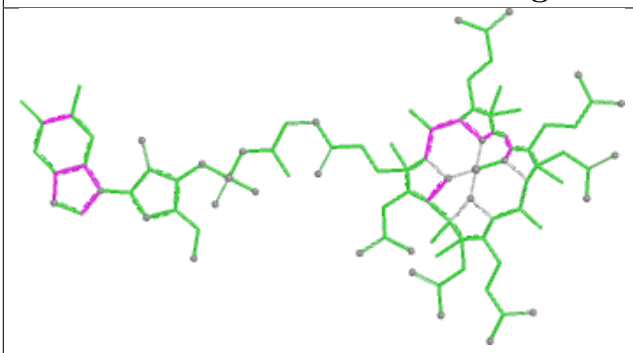
Ligand NAD F 601



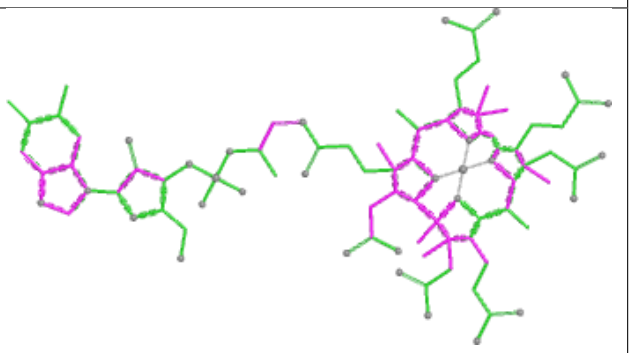
Ligand NAD E 601



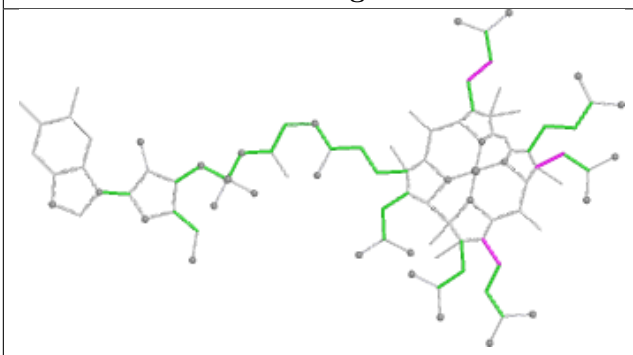
Ligand B12 B 601



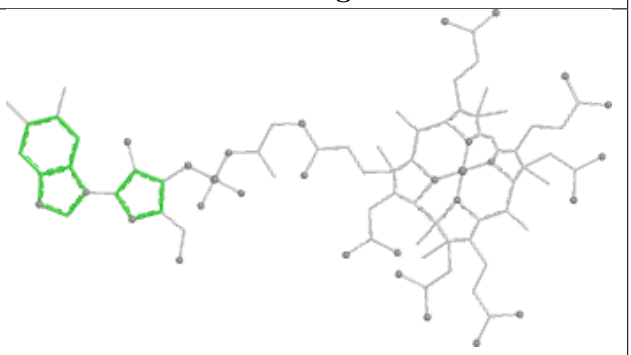
Bond lengths



Bond angles

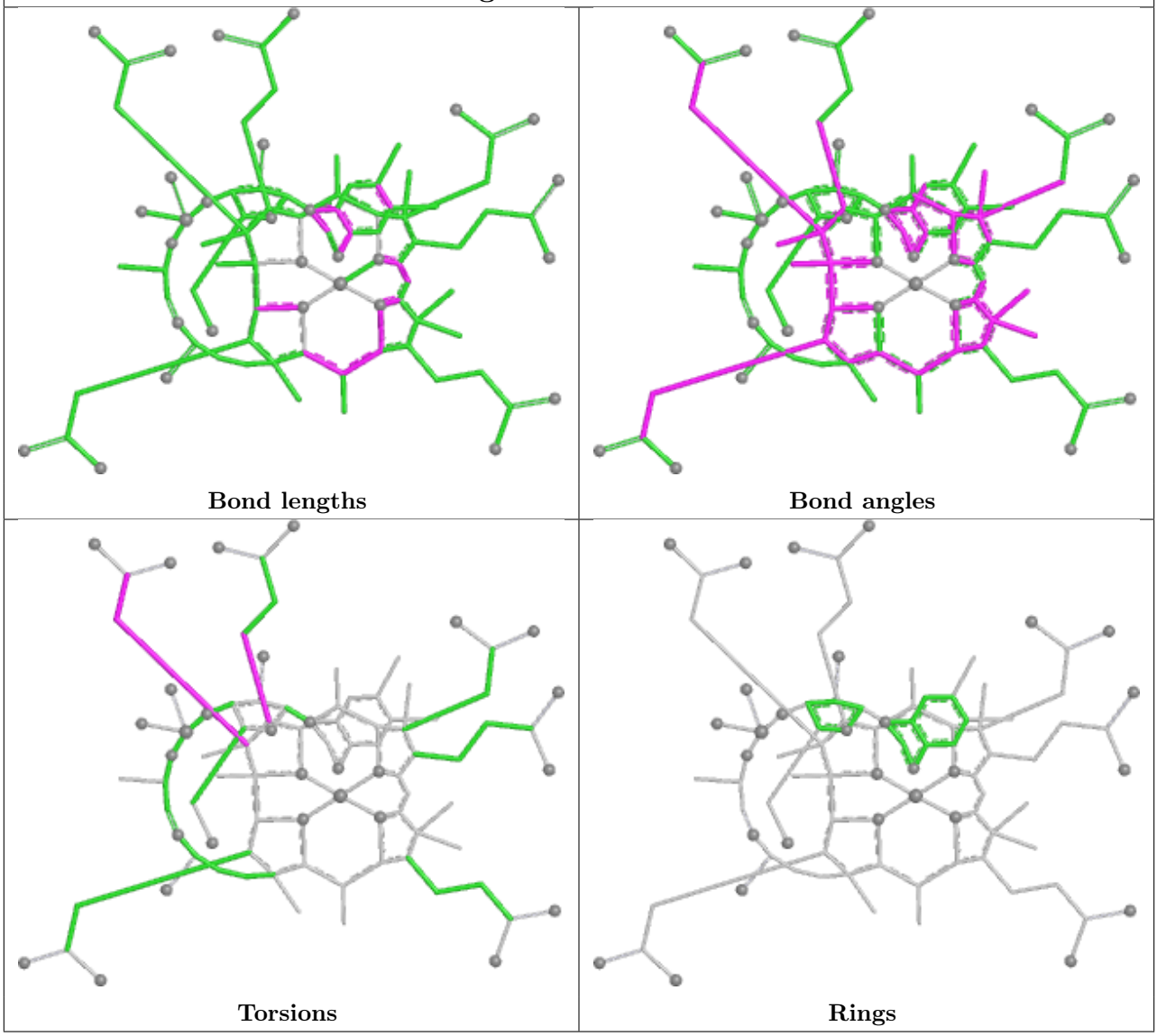


Torsions



Rings

Ligand B12 A 601



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	541/563 (96%)	-0.81	1 (0%)	91	90	11, 18, 33, 61	0
1	B	541/563 (96%)	-0.79	1 (0%)	91	90	10, 19, 37, 56	0
1	C	543/563 (96%)	-0.76	2 (0%)	88	88	12, 18, 36, 61	0
1	D	543/563 (96%)	-0.79	0	100	100	11, 20, 34, 56	0
1	E	531/563 (94%)	-0.39	11 (2%)	63	62	16, 27, 57, 82	0
1	F	534/563 (94%)	-0.45	11 (2%)	63	62	16, 26, 55, 76	0
All	All	3233/3378 (95%)	-0.67	26 (0%)	82	82	10, 21, 44, 82	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	274	TRP	4.8
1	F	270	PHE	4.4
1	E	273	LEU	3.7
1	F	279	THR	3.2
1	E	270	PHE	3.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CME	E	327	10/11	0.91	0.11	43,52,58,60	0
1	CME	F	327	10/11	0.91	0.12	41,47,53,57	0
1	CME	B	327	10/11	0.98	0.05	16,18,24,24	0
1	CME	C	327	10/11	0.98	0.06	21,24,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CME	A	327	10/11	0.99	0.04	14,18,20,22	0
1	CME	D	327	10/11	0.99	0.05	17,20,22,24	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

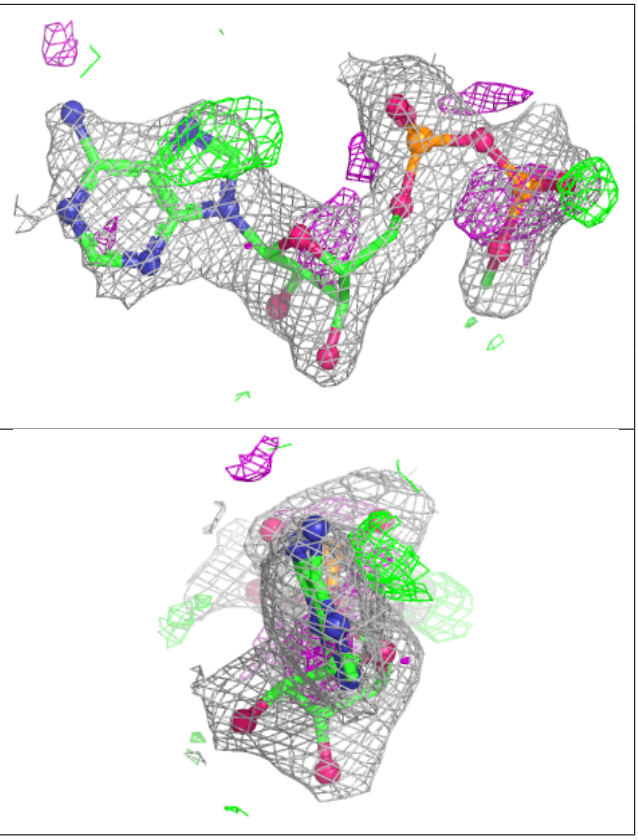
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAD	E	601	28/44	0.80	0.12	38,47,68,79	0
3	NAD	F	601	26/44	0.82	0.10	40,48,59,72	0
2	B12	C	601	91/91	0.89	0.12	29,48,61,67	0
2	B12	D	601	91/91	0.96	0.07	14,21,31,38	0
2	B12	A	601	91/91	0.97	0.06	11,17,21,23	0
2	B12	B	601	91/91	0.97	0.06	14,20,26,37	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 NAD E 601:

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



Electron density around NAD F 601:

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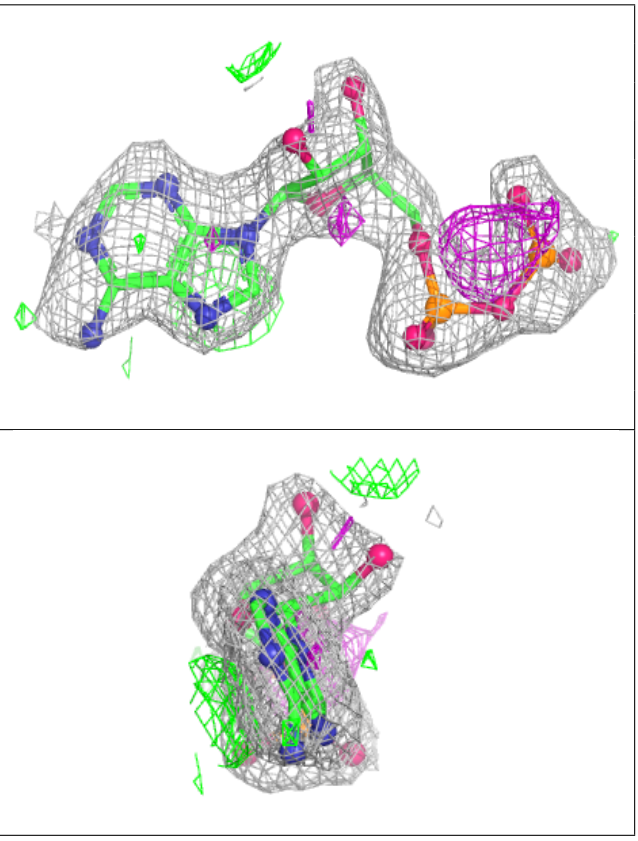
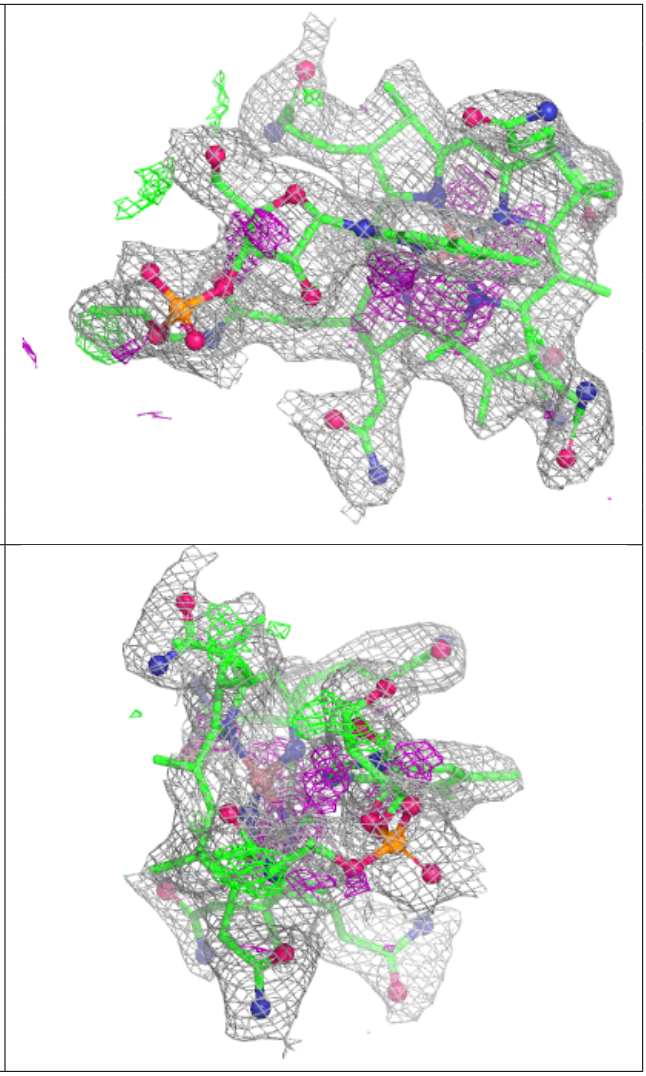
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B12 C 601:

$2mF_o$-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 D 601:

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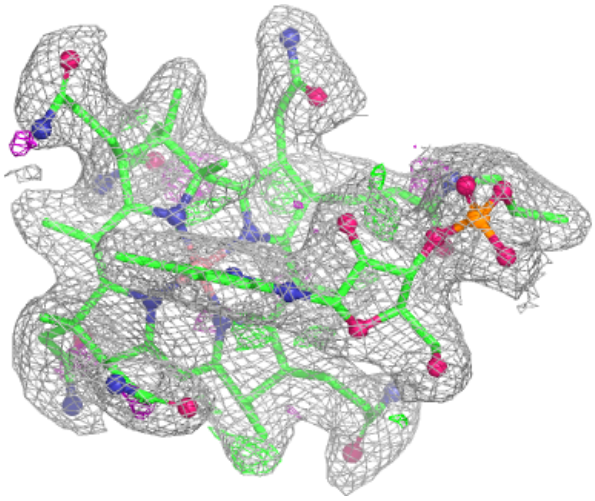
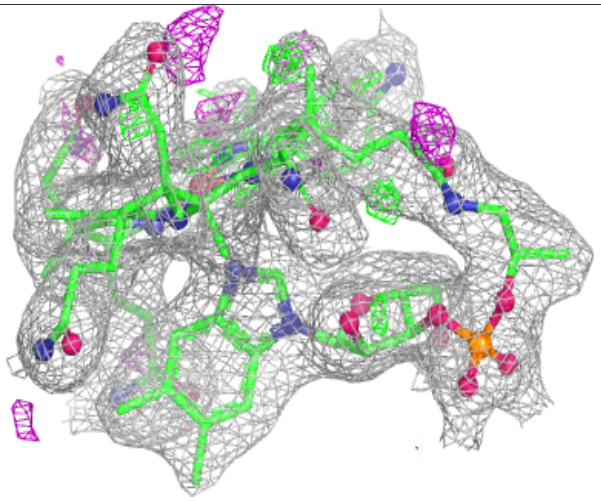
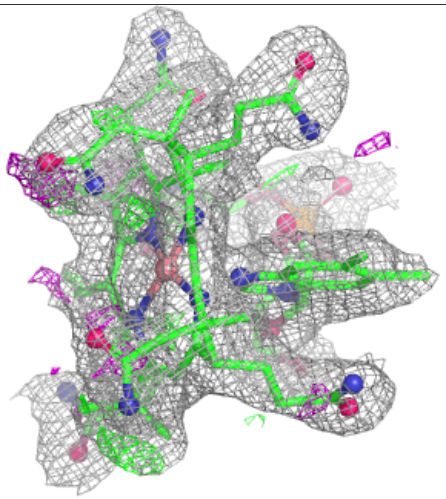
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

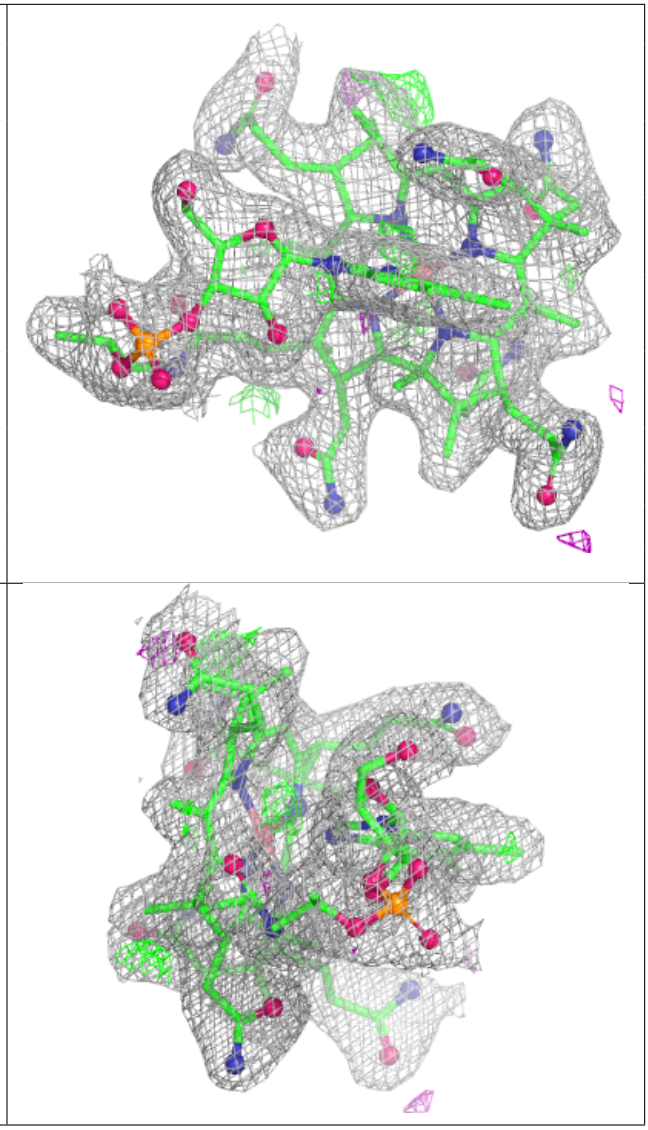






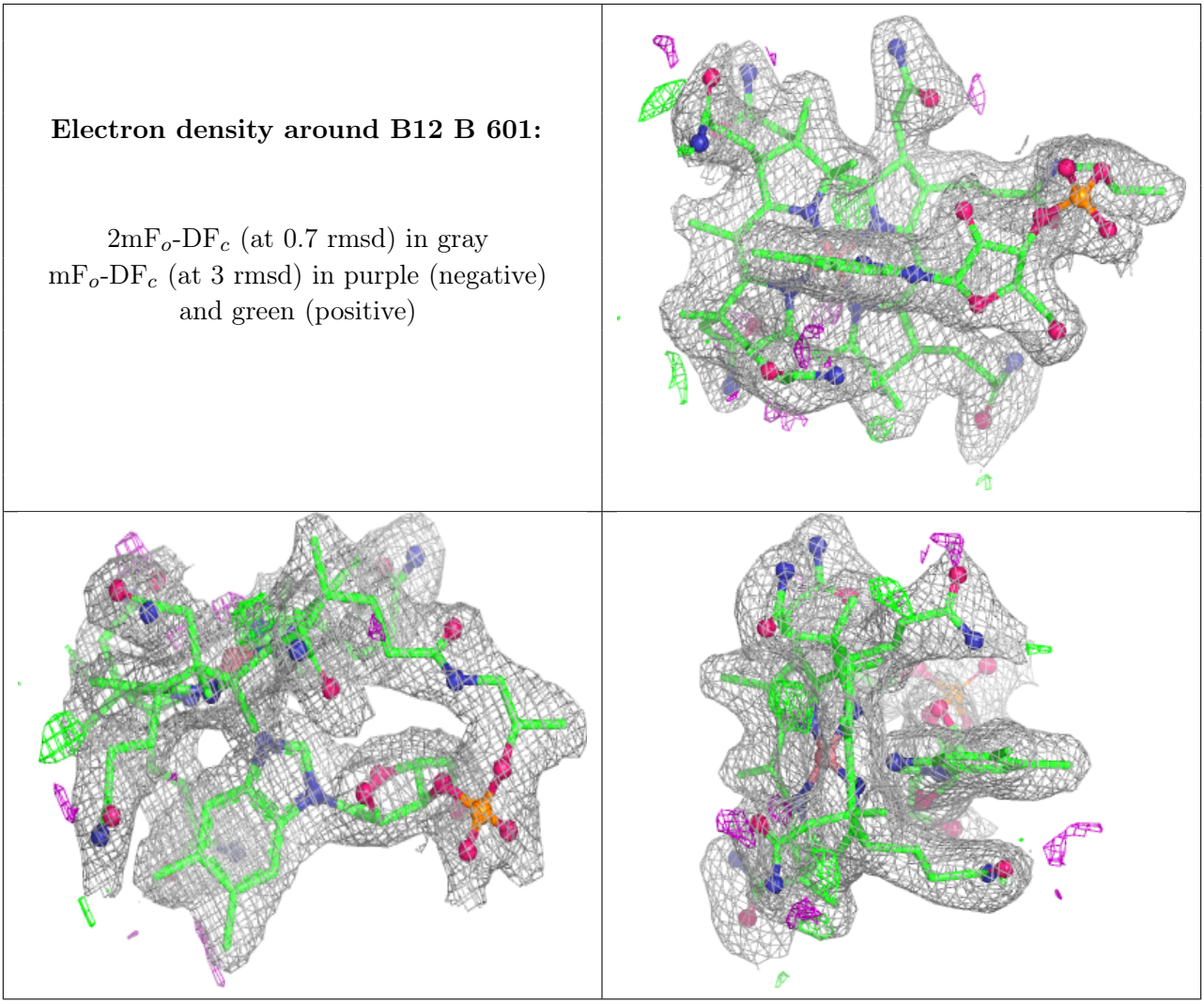
Electron density around B12 A 601:

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



Electron density around B12 B 601:

$2mF_o$-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.