wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 12:16 PM EDT

PDB ID	:	4LEM
Title	:	Crystal structure of the Delta-pyrroline-5-carboxylate dehydrogenase from Mycobacterium tuberculosis
Authors	:	Lagautriere, T.; Bashiri, G.; Baker, E.N.
Deposited on	:	2013-06-26
Resolution	:	2.27 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:

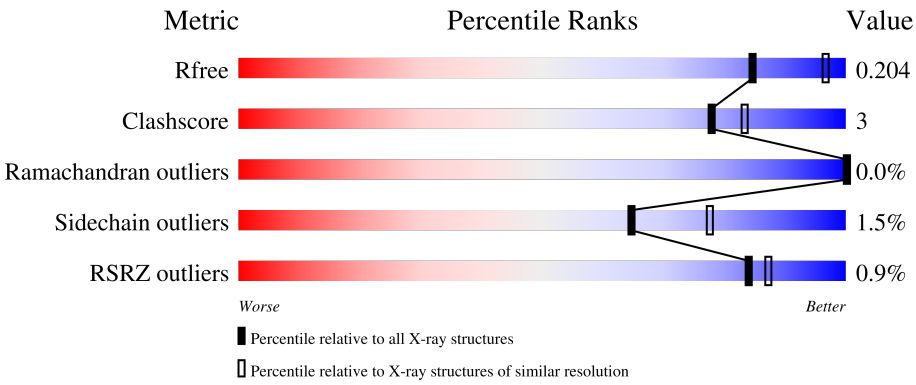
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	89% 7% •
1	B	563	89% 7% • •
1	C	563	% 90% 7% •
1	D	563	89% 7% • •
1	E	563	2% 87% 7% • •

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Mol	Chain	Length	Quality of chain
1	F	563	2% 87% 8%

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	C	601	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27828 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 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	543	4168	2641	737	779	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	540	4144	2628	731	774	11	0	0	0
1	F	538	4127	2617	730	769	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 O50443
A	-18	GLY	-	EXPRESSION TAG	UNP O50443
A	-17	SER	-	EXPRESSION TAG	UNP O50443
A	-16	SER	-	EXPRESSION TAG	UNP O50443
A	-15	HIS	-	EXPRESSION TAG	UNP O50443
A	-14	HIS	-	EXPRESSION TAG	UNP O50443
A	-13	HIS	-	EXPRESSION TAG	UNP O50443
A	-12	HIS	-	EXPRESSION TAG	UNP O50443
A	-11	HIS	-	EXPRESSION TAG	UNP O50443
A	-10	HIS	-	EXPRESSION TAG	UNP O50443
A	-9	SER	-	EXPRESSION TAG	UNP O50443
A	-8	SER	-	EXPRESSION TAG	UNP O50443
A	-7	GLY	-	EXPRESSION TAG	UNP O50443
A	-6	LEU	-	EXPRESSION TAG	UNP O50443
A	-5	VAL	-	EXPRESSION TAG	UNP O50443
A	-4	PRO	-	EXPRESSION TAG	UNP O50443
A	-3	ARG	-	EXPRESSION TAG	UNP O50443

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP O50443
A	-1	SER	-	EXPRESSION TAG	UNP O50443
A	0	HIS	-	EXPRESSION TAG	UNP O50443
A	505	ASP	GLY	ENGINEERED MUTATION	UNP O50443
B	-19	MET	-	EXPRESSION TAG	UNP O50443
B	-18	GLY	-	EXPRESSION TAG	UNP O50443
B	-17	SER	-	EXPRESSION TAG	UNP O50443
B	-16	SER	-	EXPRESSION TAG	UNP O50443
B	-15	HIS	-	EXPRESSION TAG	UNP O50443
B	-14	HIS	-	EXPRESSION TAG	UNP O50443
B	-13	HIS	-	EXPRESSION TAG	UNP O50443
B	-12	HIS	-	EXPRESSION TAG	UNP O50443
B	-11	HIS	-	EXPRESSION TAG	UNP O50443
B	-10	HIS	-	EXPRESSION TAG	UNP O50443
B	-9	SER	-	EXPRESSION TAG	UNP O50443
B	-8	SER	-	EXPRESSION TAG	UNP O50443
B	-7	GLY	-	EXPRESSION TAG	UNP O50443
B	-6	LEU	-	EXPRESSION TAG	UNP O50443
B	-5	VAL	-	EXPRESSION TAG	UNP O50443
B	-4	PRO	-	EXPRESSION TAG	UNP O50443
B	-3	ARG	-	EXPRESSION TAG	UNP O50443
B	-2	GLY	-	EXPRESSION TAG	UNP O50443
B	-1	SER	-	EXPRESSION TAG	UNP O50443
B	0	HIS	-	EXPRESSION TAG	UNP O50443
B	505	ASP	GLY	ENGINEERED MUTATION	UNP O50443
C	-19	MET	-	EXPRESSION TAG	UNP O50443
C	-18	GLY	-	EXPRESSION TAG	UNP O50443
C	-17	SER	-	EXPRESSION TAG	UNP O50443
C	-16	SER	-	EXPRESSION TAG	UNP O50443
C	-15	HIS	-	EXPRESSION TAG	UNP O50443
C	-14	HIS	-	EXPRESSION TAG	UNP O50443
C	-13	HIS	-	EXPRESSION TAG	UNP O50443
C	-12	HIS	-	EXPRESSION TAG	UNP O50443
C	-11	HIS	-	EXPRESSION TAG	UNP O50443
C	-10	HIS	-	EXPRESSION TAG	UNP O50443
C	-9	SER	-	EXPRESSION TAG	UNP O50443
C	-8	SER	-	EXPRESSION TAG	UNP O50443
C	-7	GLY	-	EXPRESSION TAG	UNP O50443
C	-6	LEU	-	EXPRESSION TAG	UNP O50443
C	-5	VAL	-	EXPRESSION TAG	UNP O50443
C	-4	PRO	-	EXPRESSION TAG	UNP O50443
C	-3	ARG	-	EXPRESSION TAG	UNP O50443

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP O50443
C	-1	SER	-	EXPRESSION TAG	UNP O50443
C	0	HIS	-	EXPRESSION TAG	UNP O50443
C	505	ASP	GLY	ENGINEERED MUTATION	UNP O50443
D	-19	MET	-	EXPRESSION TAG	UNP O50443
D	-18	GLY	-	EXPRESSION TAG	UNP O50443
D	-17	SER	-	EXPRESSION TAG	UNP O50443
D	-16	SER	-	EXPRESSION TAG	UNP O50443
D	-15	HIS	-	EXPRESSION TAG	UNP O50443
D	-14	HIS	-	EXPRESSION TAG	UNP O50443
D	-13	HIS	-	EXPRESSION TAG	UNP O50443
D	-12	HIS	-	EXPRESSION TAG	UNP O50443
D	-11	HIS	-	EXPRESSION TAG	UNP O50443
D	-10	HIS	-	EXPRESSION TAG	UNP O50443
D	-9	SER	-	EXPRESSION TAG	UNP O50443
D	-8	SER	-	EXPRESSION TAG	UNP O50443
D	-7	GLY	-	EXPRESSION TAG	UNP O50443
D	-6	LEU	-	EXPRESSION TAG	UNP O50443
D	-5	VAL	-	EXPRESSION TAG	UNP O50443
D	-4	PRO	-	EXPRESSION TAG	UNP O50443
D	-3	ARG	-	EXPRESSION TAG	UNP O50443
D	-2	GLY	-	EXPRESSION TAG	UNP O50443
D	-1	SER	-	EXPRESSION TAG	UNP O50443
D	0	HIS	-	EXPRESSION TAG	UNP O50443
D	505	ASP	GLY	ENGINEERED MUTATION	UNP O50443
E	-19	MET	-	EXPRESSION TAG	UNP O50443
E	-18	GLY	-	EXPRESSION TAG	UNP O50443
E	-17	SER	-	EXPRESSION TAG	UNP O50443
E	-16	SER	-	EXPRESSION TAG	UNP O50443
E	-15	HIS	-	EXPRESSION TAG	UNP O50443
E	-14	HIS	-	EXPRESSION TAG	UNP O50443
E	-13	HIS	-	EXPRESSION TAG	UNP O50443
E	-12	HIS	-	EXPRESSION TAG	UNP O50443
E	-11	HIS	-	EXPRESSION TAG	UNP O50443
E	-10	HIS	-	EXPRESSION TAG	UNP O50443
E	-9	SER	-	EXPRESSION TAG	UNP O50443
E	-8	SER	-	EXPRESSION TAG	UNP O50443
E	-7	GLY	-	EXPRESSION TAG	UNP O50443
E	-6	LEU	-	EXPRESSION TAG	UNP O50443
E	-5	VAL	-	EXPRESSION TAG	UNP O50443
E	-4	PRO	-	EXPRESSION TAG	UNP O50443
E	-3	ARG	-	EXPRESSION TAG	UNP O50443

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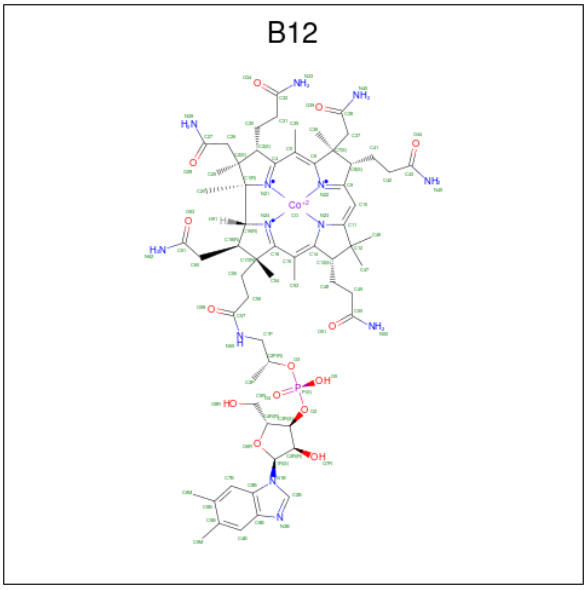
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP O50443
E	-1	SER	-	EXPRESSION TAG	UNP O50443
E	0	HIS	-	EXPRESSION TAG	UNP O50443
E	505	ASP	GLY	ENGINEERED MUTATION	UNP O50443
F	-19	MET	-	EXPRESSION TAG	UNP O50443
F	-18	GLY	-	EXPRESSION TAG	UNP O50443
F	-17	SER	-	EXPRESSION TAG	UNP O50443
F	-16	SER	-	EXPRESSION TAG	UNP O50443
F	-15	HIS	-	EXPRESSION TAG	UNP O50443
F	-14	HIS	-	EXPRESSION TAG	UNP O50443
F	-13	HIS	-	EXPRESSION TAG	UNP O50443
F	-12	HIS	-	EXPRESSION TAG	UNP O50443
F	-11	HIS	-	EXPRESSION TAG	UNP O50443
F	-10	HIS	-	EXPRESSION TAG	UNP O50443
F	-9	SER	-	EXPRESSION TAG	UNP O50443
F	-8	SER	-	EXPRESSION TAG	UNP O50443
F	-7	GLY	-	EXPRESSION TAG	UNP O50443
F	-6	LEU	-	EXPRESSION TAG	UNP O50443
F	-5	VAL	-	EXPRESSION TAG	UNP O50443
F	-4	PRO	-	EXPRESSION TAG	UNP O50443
F	-3	ARG	-	EXPRESSION TAG	UNP O50443
F	-2	GLY	-	EXPRESSION TAG	UNP O50443
F	-1	SER	-	EXPRESSION TAG	UNP O50443
F	0	HIS	-	EXPRESSION TAG	UNP O50443
F	505	ASP	GLY	ENGINEERED MUTATION	UNP O50443

- Molecule 2 is COBALAMIN (three-letter code: 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	F	1	1	1	0	0

- Molecule 4 is water.

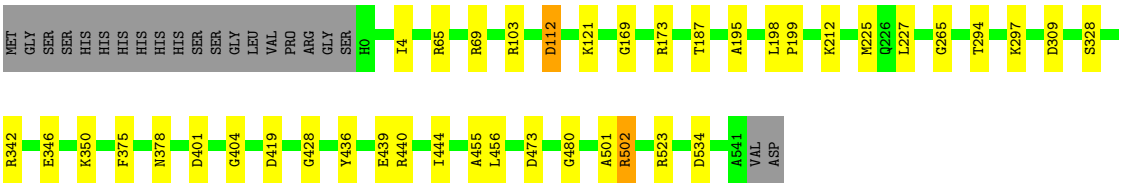
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	491	491	491	0	0
4	B	473	473	473	0	0
4	C	480	480	480	0	0
4	D	439	439	439	0	0
4	E	309	309	309	0	0
4	F	322	322	322	0	0

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.

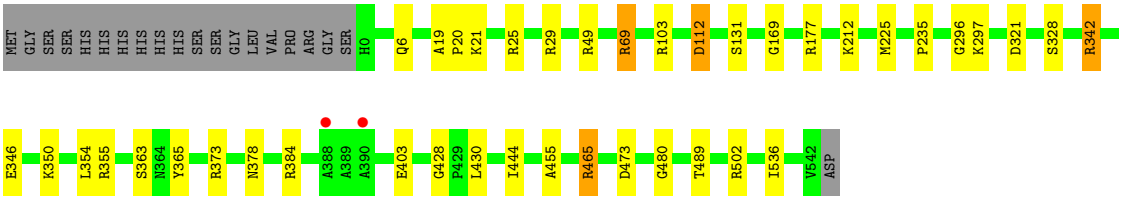
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain A:



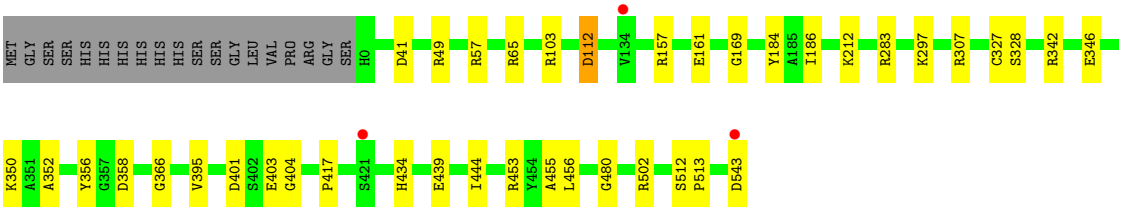
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain B:



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

Chain C:

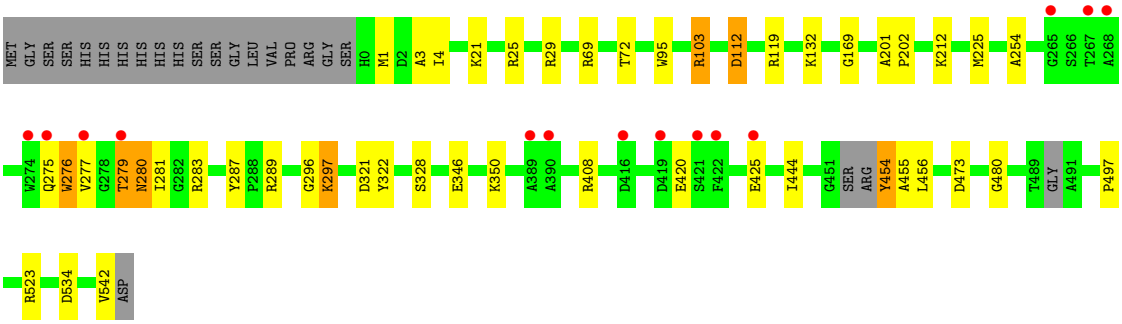


• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain D:

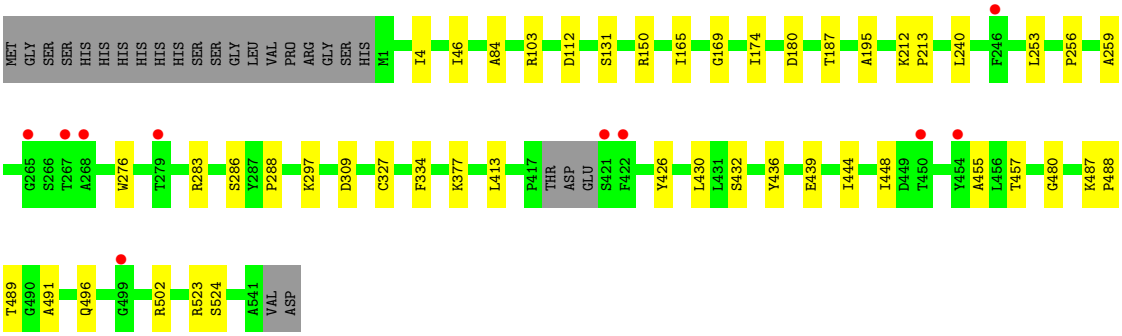
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.30Å 164.30Å 259.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.01 – 2.27 20.01 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.01-2.27) 99.6 (20.01-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.148 , 0.204 0.155 , 0.204	Depositor DCC
R_{free} test set	9351 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.6	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	0.96	EDS
Total number of atoms	27828	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: MG, B12, CME

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	0.86	1/4253 (0.0%)	0.90	13/5800 (0.2%)
1	B	0.85	0/4260	0.93	18/5810 (0.3%)
1	C	0.86	2/4268 (0.0%)	0.92	12/5821 (0.2%)
1	D	0.82	0/4263	0.89	10/5814 (0.2%)
1	E	0.81	1/4234 (0.0%)	0.92	13/5772 (0.2%)
1	F	0.82	1/4217 (0.0%)	0.89	4/5749 (0.1%)
All	All	0.84	5/25495 (0.0%)	0.91	70/34766 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	439	GLU	CD-OE1	5.73	1.31	1.25
1	A	439	GLU	CG-CD	5.42	1.60	1.51
1	C	439	GLU	CD-OE1	5.25	1.31	1.25
1	E	276	TRP	CB-CG	-5.21	1.40	1.50
1	C	439	GLU	CG-CD	5.03	1.59	1.51

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	103	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	465	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	C	103	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	C	502	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	C	103	ARG	NE-CZ-NH2	7.66	124.13	120.30

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	18	0
1	B	4168	0	4075	18	0
1	C	4176	0	4079	18	0
1	D	4171	0	4070	21	0
1	E	4144	0	4046	29	0
1	F	4127	0	4041	25	0
2	A	91	0	87	8	0
2	B	91	0	87	9	0
2	C	91	0	87	7	0
2	D	91	0	86	8	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	491	0	0	1	0
4	B	473	0	0	5	0
4	C	480	0	0	3	0
4	D	439	0	0	2	0
4	E	309	0	0	3	0
4	F	322	0	0	2	0
All	All	27828	0	24724	145	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.

The worst 5 of 145 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)
2:B:601:B12:H362	2:B:601:B12:H351	1.42	1.00
2:D:601:B12:H362	2:D:601:B12:H351	1.48	0.95
1:B:473:ASP:HB2	4:E:613:HOH:O	1.66	0.93
2:A:601:B12:H362	2:A:601:B12:H351	1.70	0.74
2:C:601:B12:H552	2:C:601:B12:H531	1.70	0.73

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%)	525 (97%)	13 (2%)	1 (0%)	47	57
1	B	540/563 (96%)	527 (98%)	13 (2%)	0	100	100
1	C	541/563 (96%)	526 (97%)	15 (3%)	0	100	100
1	D	541/563 (96%)	527 (97%)	14 (3%)	0	100	100
1	E	533/563 (95%)	513 (96%)	20 (4%)	0	100	100
1	F	533/563 (95%)	513 (96%)	20 (4%)	0	100	100
All	All	3227/3378 (96%)	3131 (97%)	95 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	419 (100%)	2 (0%)	88	94
1	B	422/439 (96%)	413 (98%)	9 (2%)	53	68
1	C	423/439 (96%)	418 (99%)	5 (1%)	71	82
1	D	421/439 (96%)	415 (99%)	6 (1%)	67	79
1	E	419/439 (95%)	409 (98%)	10 (2%)	49	63
1	F	417/439 (95%)	412 (99%)	5 (1%)	71	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2523/2634 (96%)	2486 (98%)	37 (2%)	65 77

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	425	GLU
1	F	432	SER
1	E	444	ILE
1	F	131	SER
1	C	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	226	GLN
1	E	226	GLN
1	E	280	ASN
1	F	226	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)

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	D	327	1	8,9,10	0.62	0	6,9,11	0.69	0
1	CME	A	327	1	8,9,10	0.96	0	6,9,11	0.88	0
1	CME	C	327	1	8,9,10	1.19	2 (25%)	6,9,11	0.80	0
1	CME	E	327	1	8,9,10	0.72	0	6,9,11	0.62	0

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	0.78	0	6,9,11	1.34	1 (16%)
1	CME	B	327	1	8,9,10	0.80	0	6,9,11	0.75	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	D	327	1	-	0/5/8/10	-
1	CME	A	327	1	-	0/5/8/10	-
1	CME	C	327	1	-	1/5/8/10	-
1	CME	E	327	1	-	1/5/8/10	-
1	CME	F	327	1	-	0/5/8/10	-
1	CME	B	327	1	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	CME	O-C	2.20	1.28	1.20
1	C	327	CME	CB-SG	-2.02	1.75	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	327	CME	CB-SG-SD	3.07	111.80	103.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	-	91,101,101	1.46	13 (14%)	140,166,166	2.53	40 (28%)
2	B12	B	601	-	91,101,101	1.27	7 (7%)	140,166,166	2.15	27 (19%)
2	B12	A	601	-	91,101,101	1.29	8 (8%)	140,166,166	2.13	34 (24%)
2	B12	C	601	-	91,101,101	1.30	8 (8%)	140,166,166	2.11	31 (22%)

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	-	-	14/52/223/223	0/3/11/11
2	B12	C	601	-	1/1/36/38	7/52/223/223	0/3/11/11
2	B12	B	601	-	-	4/52/223/223	0/3/11/11
2	B12	A	601	-	-	5/52/223/223	0/3/11/11

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	B12	C19-N24	-5.88	1.41	1.49
2	B	601	B12	C19-N24	-5.68	1.42	1.49
2	C	601	B12	C9-N22	4.47	1.41	1.30
2	C	601	B12	C6B-C5B	4.40	1.51	1.40
2	D	601	B12	C19-N24	-4.29	1.43	1.49

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	B12	C1-C19-N24	11.94	119.54	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	B12	C1-C19-N24	11.57	119.12	106.25
2	B	601	B12	C20-C1-C19	-10.15	99.58	109.35
2	A	601	B12	C20-C1-C19	-9.95	99.77	109.35
2	D	601	B12	C54-C17-C55	9.64	125.29	109.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	601	B12	C19

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	B12	C2-C26-C27-N29
2	C	601	B12	C1-C2-C26-C27
2	C	601	B12	C25-C2-C26-C27
2	C	601	B12	C3-C2-C26-C27
2	C	601	B12	C38-C37-C7-C6

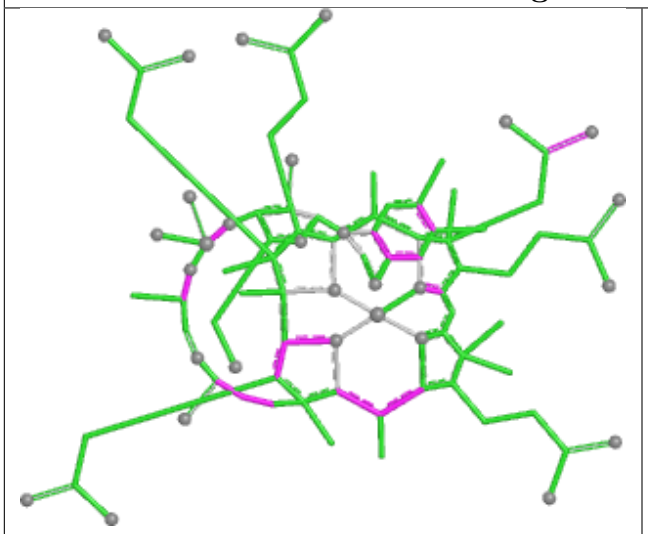
There are no ring outliers.

4 monomers are involved in 32 short contacts:

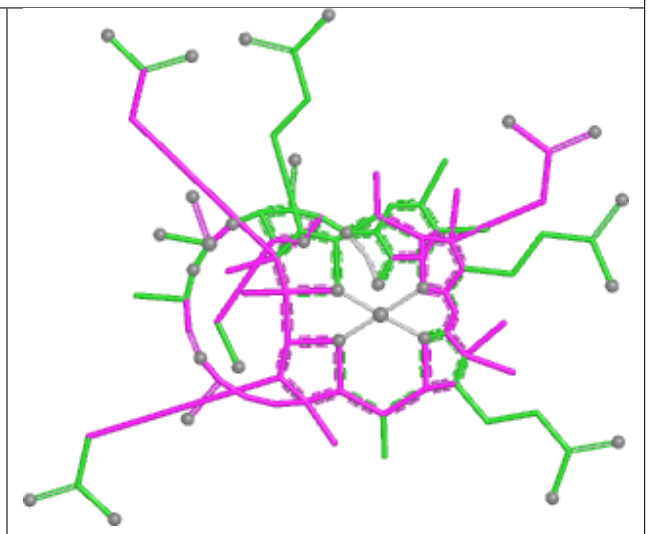
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	B12	8	0
2	B	601	B12	9	0
2	A	601	B12	8	0
2	C	601	B12	7	0

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.

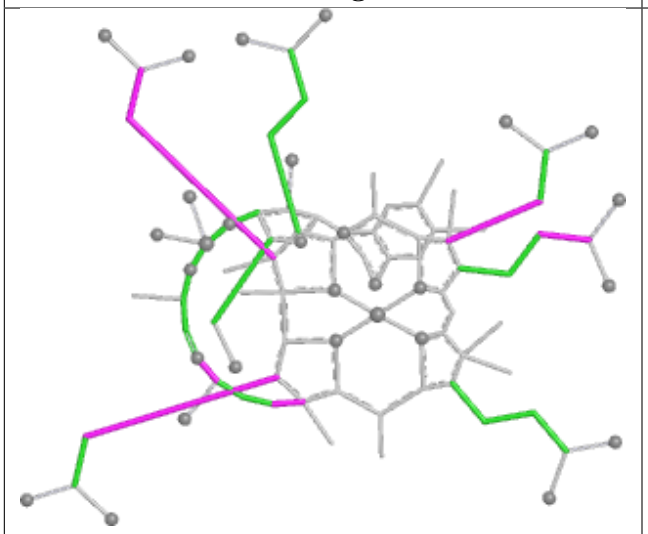
Ligand B12 D 601



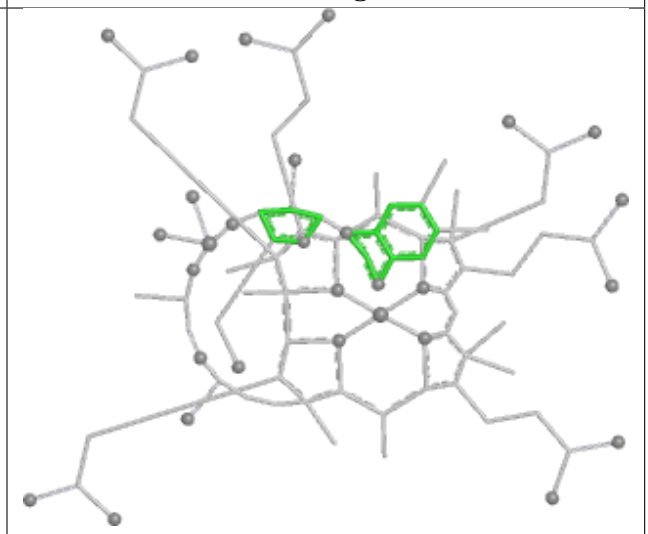
Bond lengths



Bond angles

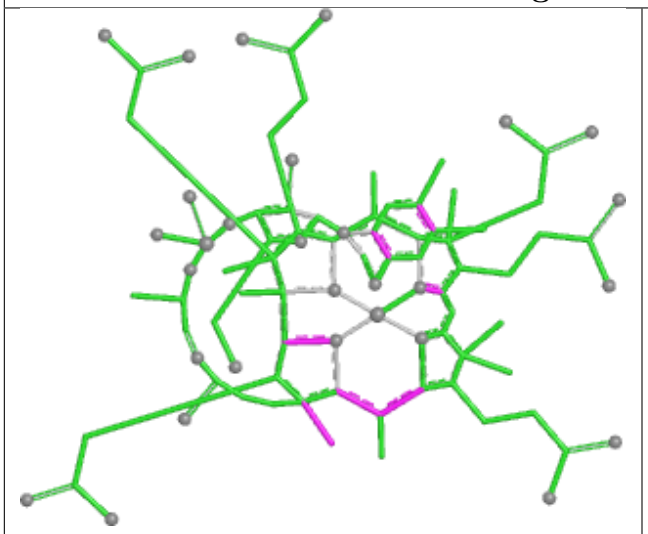


Torsions

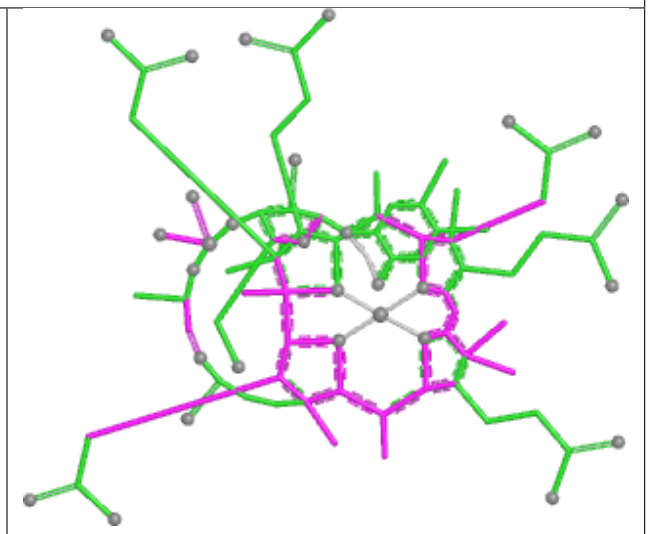


Rings

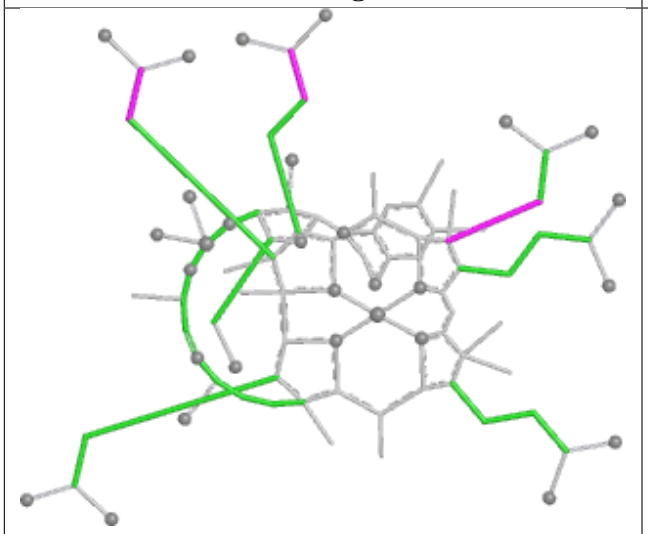
Ligand B12 B 601



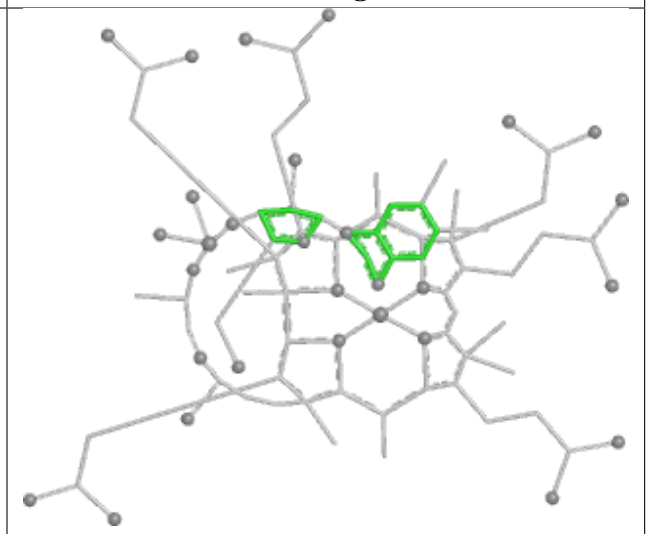
Bond lengths



Bond angles

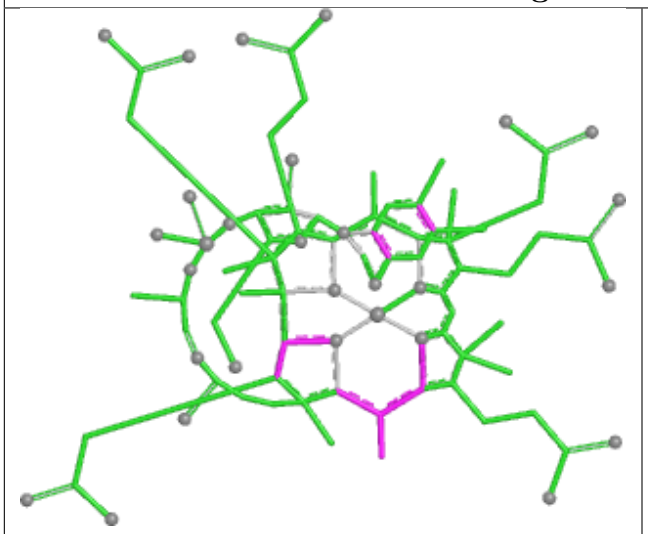


Torsions

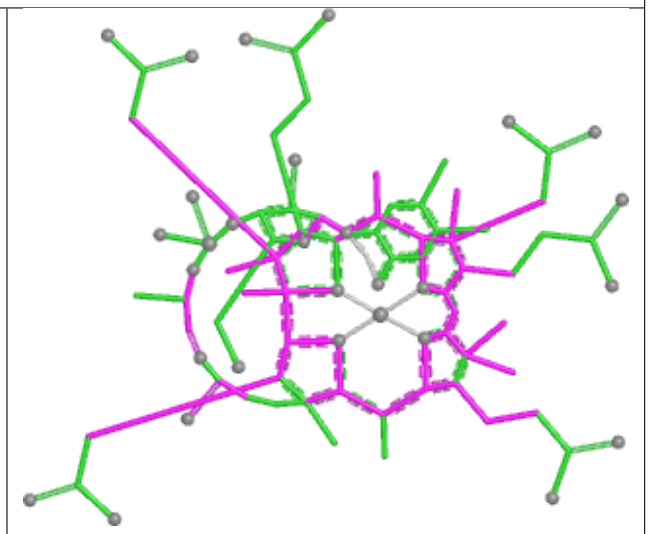


Rings

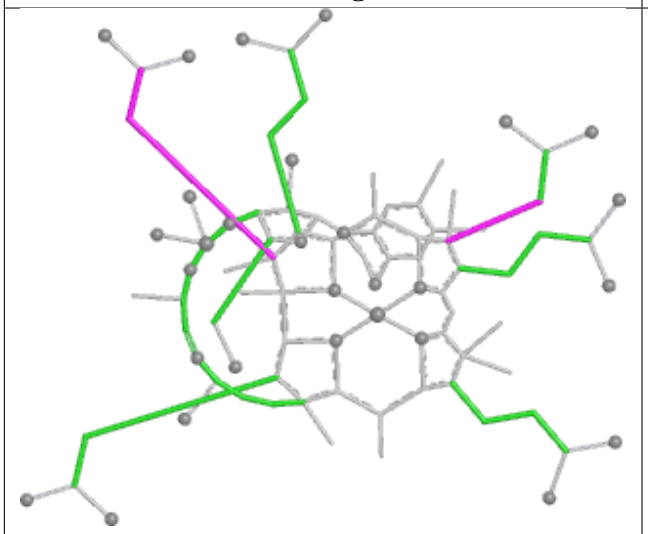
Ligand B12 A 601



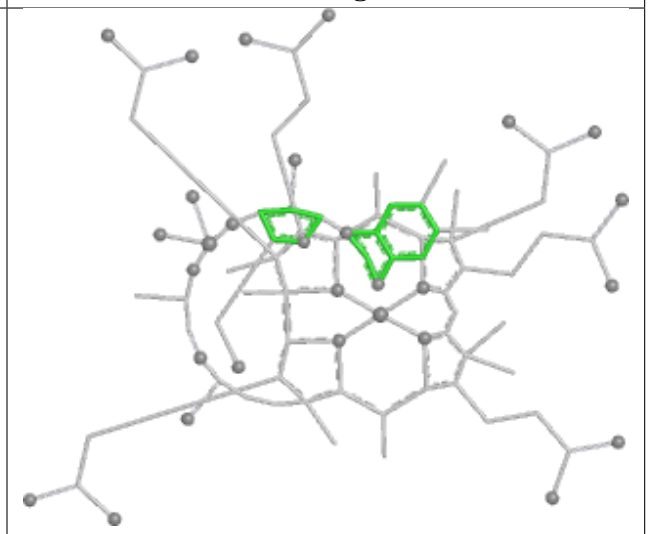
Bond lengths



Bond angles

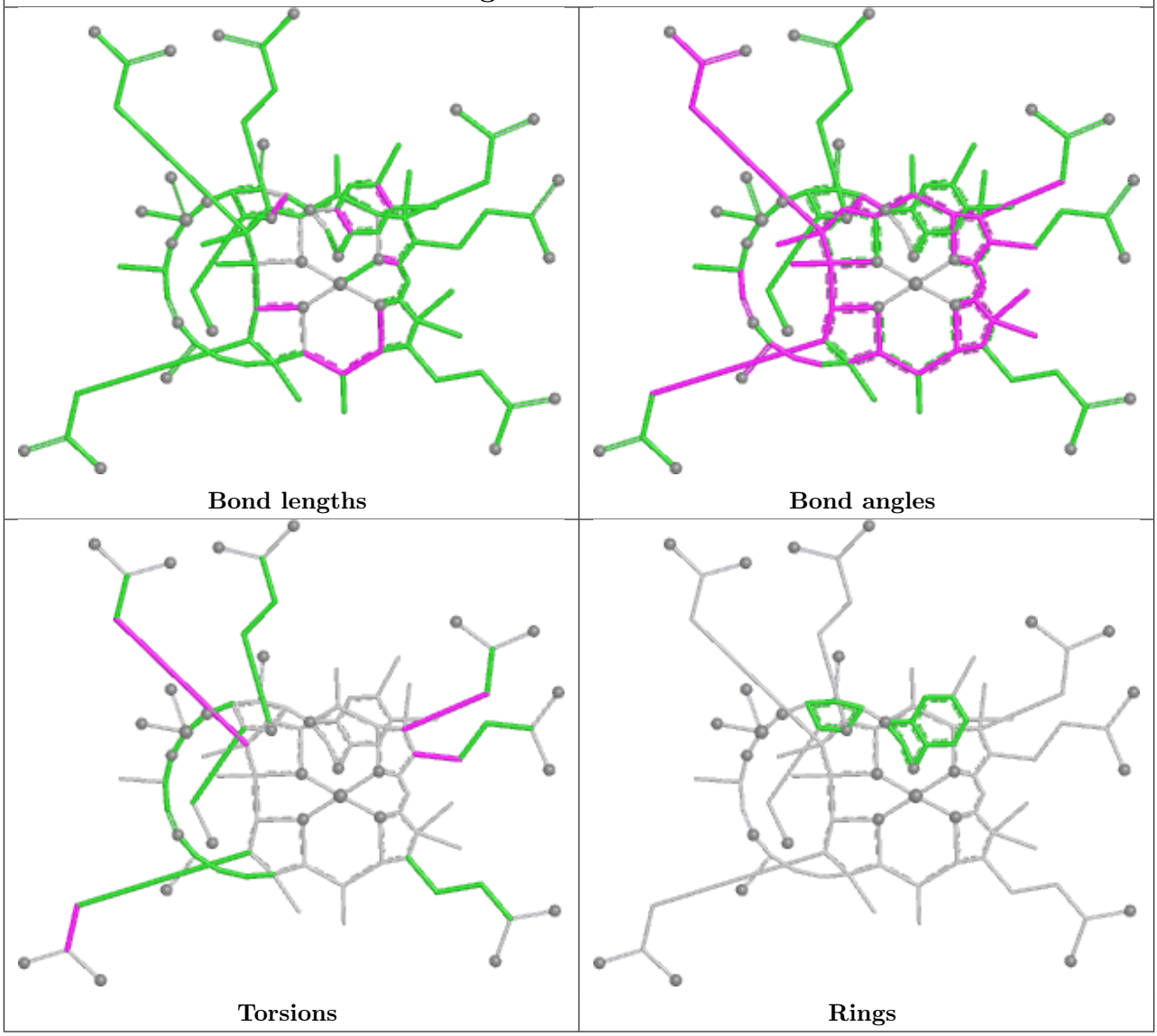


Torsions



Rings

Ligand B12 C 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%)	-0.75	0	100	100	17, 26, 46, 72	0
1	B	542/563 (96%)	-0.74	2 (0%)	92	94	18, 27, 46, 75	0
1	C	543/563 (96%)	-0.70	3 (0%)	89	91	18, 26, 47, 72	0
1	D	543/563 (96%)	-0.72	0	100	100	19, 28, 47, 69	0
1	E	539/563 (95%)	-0.40	14 (2%)	56	62	20, 36, 69, 99	0
1	F	537/563 (95%)	-0.51	10 (1%)	66	72	22, 33, 60, 86	0
All	All	3245/3378 (96%)	-0.64	29 (0%)	84	87	17, 29, 53, 99	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	389	ALA	6.8
1	E	421	SER	4.9
1	E	267	THR	4.4
1	E	279	THR	4.3
1	E	268	ALA	4.3

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	0.94	0.14	48,56,67,68	0
1	CME	F	327	10/11	0.94	0.13	44,46,56,59	0
1	CME	C	327	10/11	0.97	0.08	28,31,44,47	0
1	CME	D	327	10/11	0.98	0.08	27,30,35,37	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	24,27,33,34	0
1	CME	B	327	10/11	0.99	0.05	23,26,33,36	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

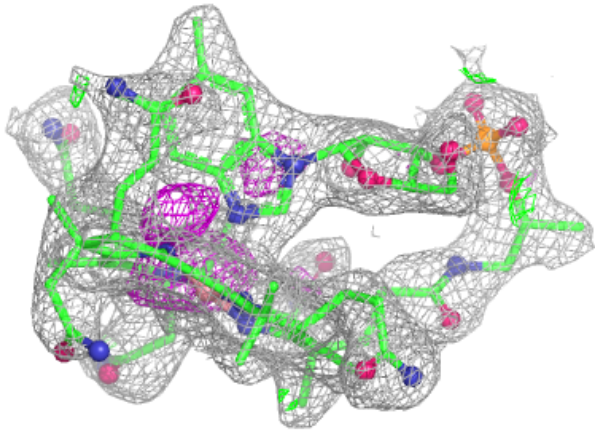
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

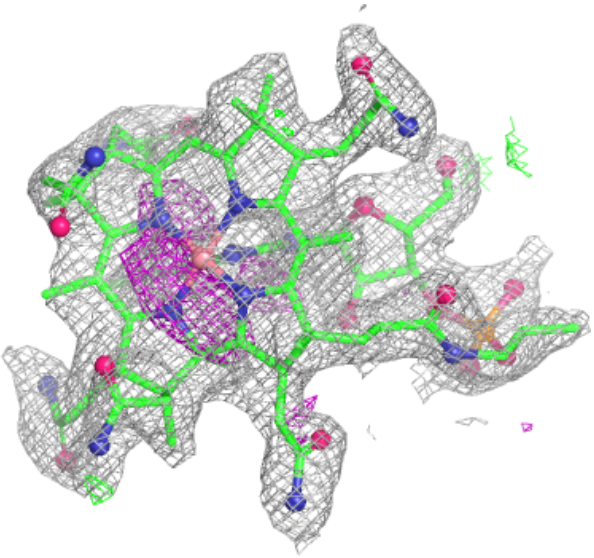
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	602	1/1	0.91	0.07	43,43,43,43	0
3	MG	F	601	1/1	0.91	0.20	52,52,52,52	0
2	B12	C	601	91/91	0.92	0.25	36,51,69,78	0
3	MG	D	602	1/1	0.95	0.10	49,49,49,49	0
2	B12	B	601	91/91	0.96	0.13	20,26,35,44	0
2	B12	D	601	91/91	0.97	0.10	24,30,41,50	0
2	B12	A	601	91/91	0.97	0.08	18,22,28,40	0

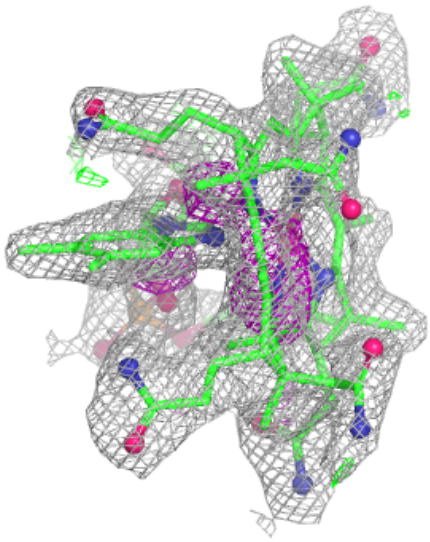
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 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 B 601:

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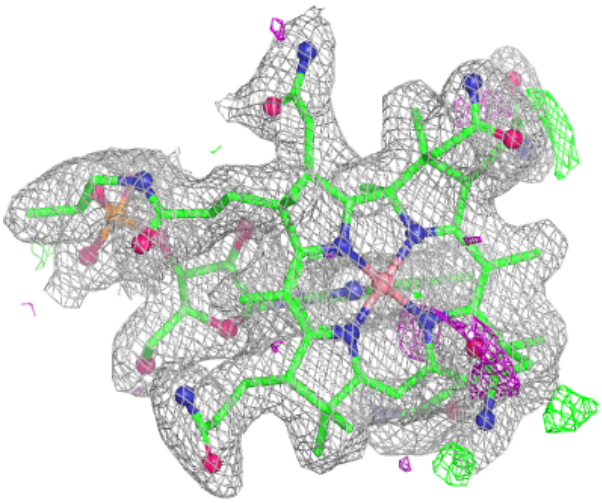
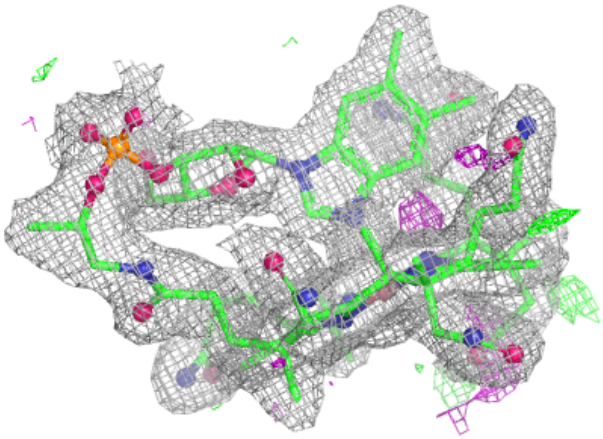
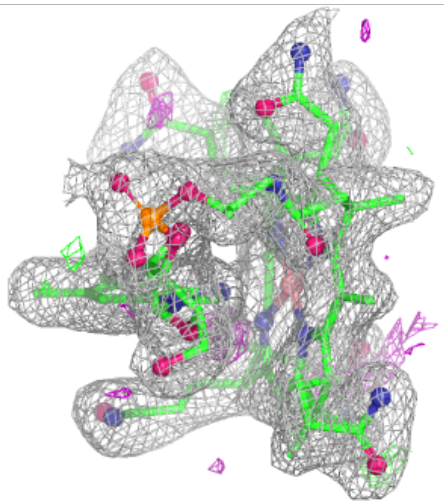
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

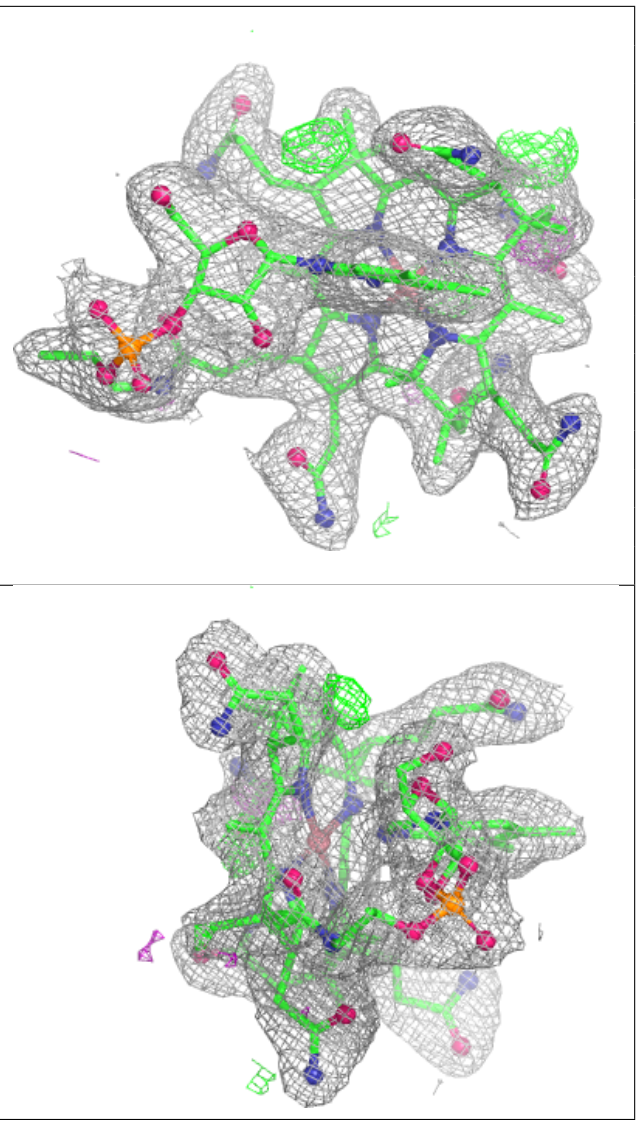






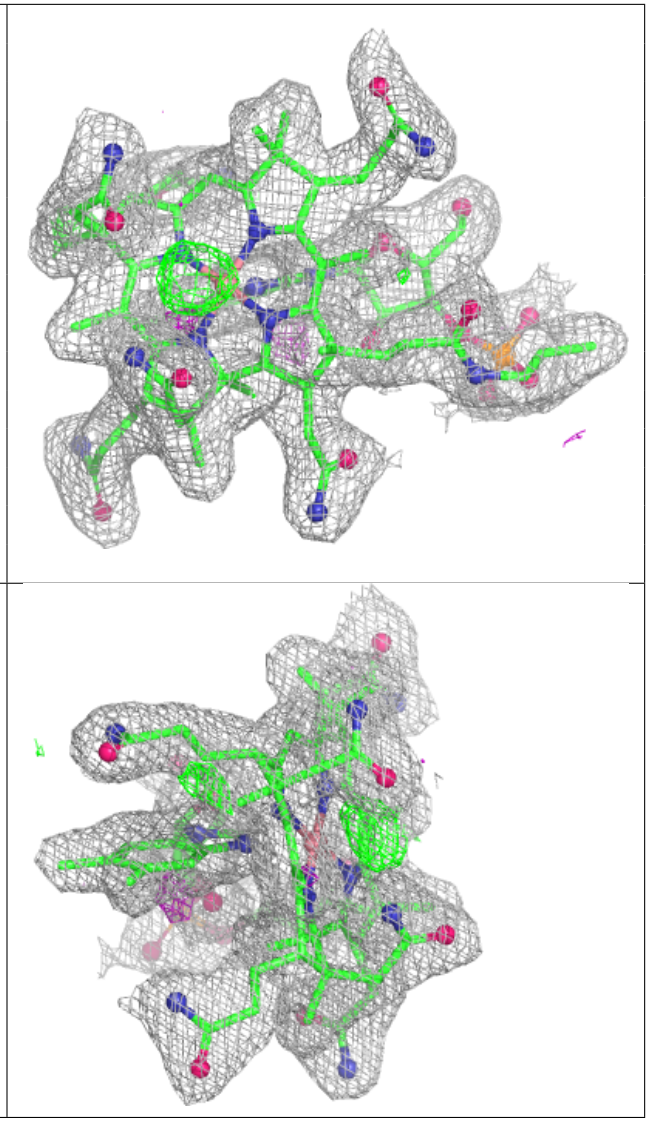
Electron density around B12 D 601:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.