Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 11:15 am BST

PDB ID	:	9S0F / pdb_00009s0f
Title	:	Dark-state of CBD of TtCarH (TR-SFX, SwissFEL)
Authors	:	Rios-Santacruz, R.; Coquelle, N.; Colletier, J.P.; De Zitter, E.; Schiro, G.; Weik, M.
Deposited on	:	2025-07-16
Resolution	:	2.35 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 (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:

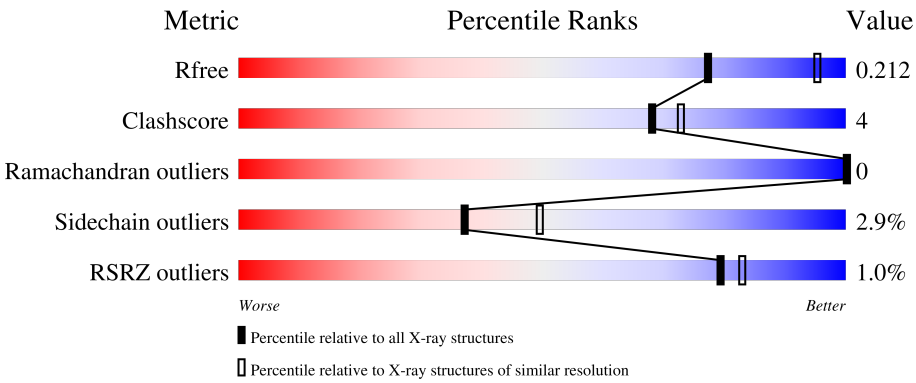
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	215	90% • 8%
1	B	215	% 83% 8% 8%
1	C	215	82% 9% 8%
1	D	215	2% 84% 7% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6899 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 Probable transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	1534	980	282	270	2	0	6	0
1	B	197	1524	977	277	268	2	0	6	0
1	C	197	1528	977	281	268	2	0	5	0
1	D	197	1524	980	273	269	2	0	6	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLY	-	expression tag	UNP Q746J7
A	287	HIS	-	expression tag	UNP Q746J7
A	288	HIS	-	expression tag	UNP Q746J7
A	289	HIS	-	expression tag	UNP Q746J7
A	290	HIS	-	expression tag	UNP Q746J7
A	291	HIS	-	expression tag	UNP Q746J7
A	292	HIS	-	expression tag	UNP Q746J7
B	286	GLY	-	expression tag	UNP Q746J7
B	287	HIS	-	expression tag	UNP Q746J7
B	288	HIS	-	expression tag	UNP Q746J7
B	289	HIS	-	expression tag	UNP Q746J7
B	290	HIS	-	expression tag	UNP Q746J7
B	291	HIS	-	expression tag	UNP Q746J7
B	292	HIS	-	expression tag	UNP Q746J7
C	286	GLY	-	expression tag	UNP Q746J7
C	287	HIS	-	expression tag	UNP Q746J7
C	288	HIS	-	expression tag	UNP Q746J7
C	289	HIS	-	expression tag	UNP Q746J7
C	290	HIS	-	expression tag	UNP Q746J7
C	291	HIS	-	expression tag	UNP Q746J7
C	292	HIS	-	expression tag	UNP Q746J7

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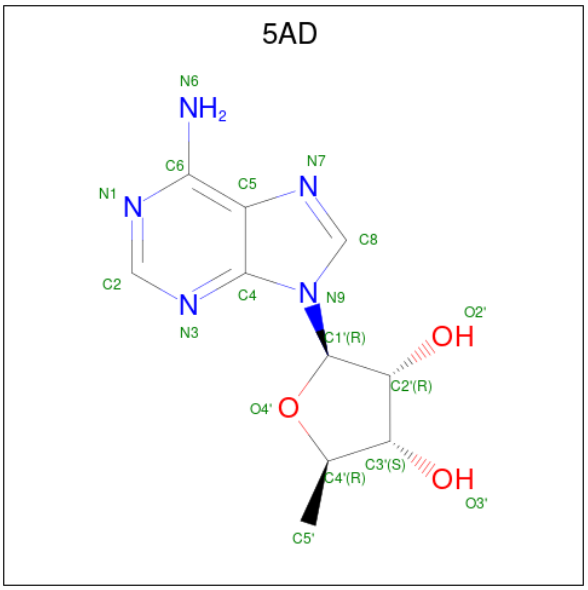
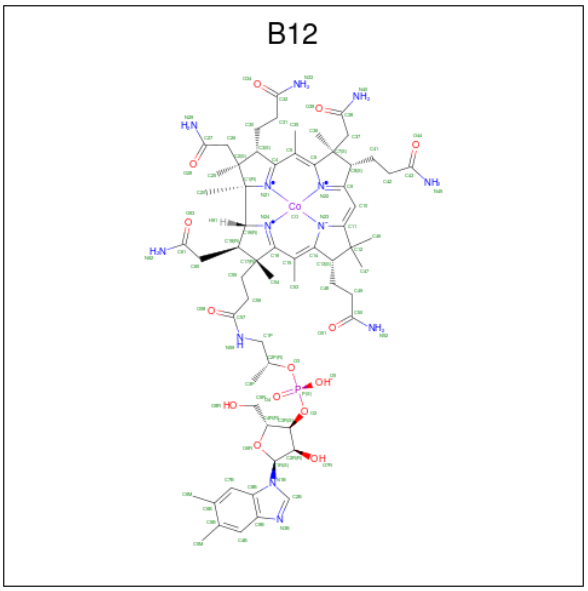
Chain	Residue	Modelled	Actual	Comment	Reference
D	286	GLY	-	expression tag	UNP Q746J7
D	287	HIS	-	expression tag	UNP Q746J7
D	288	HIS	-	expression tag	UNP Q746J7
D	289	HIS	-	expression tag	UNP Q746J7
D	290	HIS	-	expression tag	UNP Q746J7
D	291	HIS	-	expression tag	UNP Q746J7
D	292	HIS	-	expression tag	UNP Q746J7

- Molecule 2 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

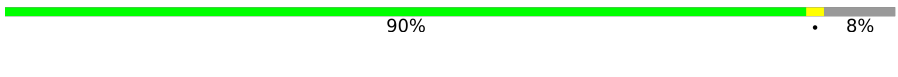
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	98	98	98	0	0
4	B	118	119	119	0	1
4	C	70	70	70	0	0
4	D	66	66	66	0	0

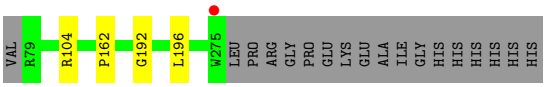
3 Residue-property plots (i)

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: Probable transcriptional regulator

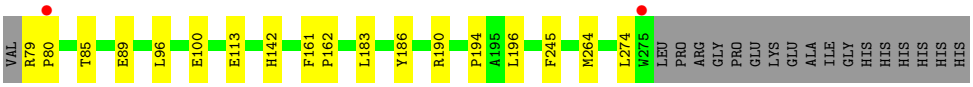
Chain A:





- Molecule 1: Probable transcriptional regulator

Chain B:

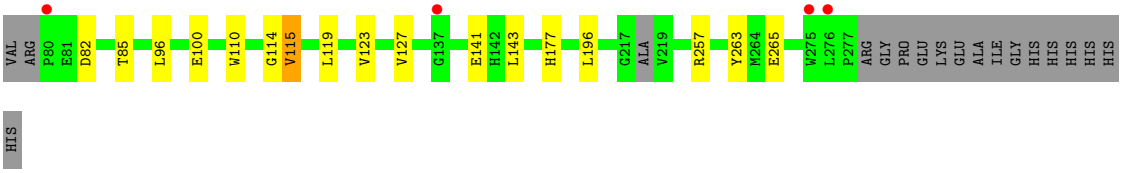


- Molecule 1: Probable transcriptional regulator

Chain C:

- Molecule 1: Probable transcriptional regulator

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.52Å 72.13Å 209.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.35 48.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.50-2.35) 100.0 (48.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.161 , 0.211 0.161 , 0.212	Depositor DCC
R_{free} test set	2109 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6899	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: 5AD, B12

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	0.36	0/1572	0.49	0/2135
1	B	0.36	0/1568	0.51	0/2131
1	C	0.33	0/1566	0.46	0/2127
1	D	0.35	0/1559	0.49	0/2119
All	All	0.35	0/6265	0.49	0/8512

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1534	0	1568	3	0
1	B	1524	0	1566	9	0
1	C	1528	0	1564	9	0
1	D	1524	0	1558	7	0
2	A	18	0	12	1	0
2	B	18	0	12	0	0
2	C	18	0	12	1	0
2	D	18	0	12	2	0
3	A	91	0	88	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	91	0	88	2	0
3	C	91	0	88	7	0
3	D	91	0	88	7	0
4	A	98	0	0	1	0
4	B	119	0	0	0	0
4	C	70	0	0	1	0
4	D	66	0	0	0	0
All	All	6899	0	6656	48	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.

All (48) 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:C:238:LYS:HG3	1:C:260:GLY:HA3	1.74	0.70
3:B:402:B12:H362	3:B:402:B12:H351	1.76	0.68
1:A:104:ARG:NH2	4:A:503:HOH:O	2.29	0.64
3:A:402:B12:H351	3:A:402:B12:H362	1.79	0.63
3:C:402:B12:H362	3:C:402:B12:H351	1.84	0.59
2:D:401:5AD:H5'3	3:D:402:B12:N24	2.15	0.58
3:D:402:B12:H362	3:D:402:B12:H351	1.86	0.57
1:B:113:GLU:OE2	1:B:190:ARG:HD3	2.06	0.55
1:B:161:PHE:CZ	1:B:196:LEU:HD13	2.42	0.55
1:C:93:ARG:HD3	4:C:546:HOH:O	2.08	0.54
1:D:141:GLU:OE2	3:D:402:B12:H532	2.07	0.54
2:D:401:5AD:H5'3	3:D:402:B12:C19	2.38	0.54
2:C:401:5AD:H5'3	3:C:402:B12:C19	2.40	0.51
1:C:208:ARG:HH12	1:C:239:ASP:HB3	1.76	0.51
3:C:402:B12:H8	3:C:402:B12:N40	2.27	0.50
1:C:268:LYS:NZ	1:C:272:GLU:OE2	2.46	0.49
1:B:186:TYR:CZ	1:B:190:ARG:HD2	2.50	0.46
1:C:162:PRO:HG2	1:C:192:GLY:O	2.15	0.46
3:C:402:B12:H8	3:C:402:B12:H401	1.81	0.46
1:D:115:VAL:HG22	1:D:119:LEU:HD23	1.98	0.46
3:B:402:B12:H8	3:B:402:B12:H401	1.81	0.46
1:C:227:GLU:HG3	1:C:230:ARG:NH1	2.31	0.45
1:B:79:ARG:HB2	1:B:80:PRO:HD3	1.98	0.45
3:A:402:B12:H363	3:A:402:B12:H411	1.76	0.44
1:D:110:TRP:HB3	1:D:114:GLY:HA3	1.99	0.44
3:A:402:B12:H552	3:A:402:B12:H531	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:B12:H473	3:A:402:B12:H481	1.86	0.44
3:C:402:B12:H262	3:C:402:B12:H91	1.82	0.44
1:B:245:PHE:CD1	1:B:264:MET:HE3	2.53	0.43
1:D:123:VAL:O	1:D:127:VAL:HG23	2.18	0.43
3:C:402:B12:O28	3:C:402:B12:H3	2.17	0.43
3:C:402:B12:H203	3:C:402:B12:H301	2.01	0.42
3:D:402:B12:H253	3:D:402:B12:H301	1.89	0.42
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.87	0.42
1:A:162:PRO:HG2	1:A:192:GLY:O	2.19	0.42
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.93	0.42
1:C:178:GLU:HB2	1:C:197:TYR:OH	2.19	0.42
1:D:263:TYR:CE2	1:D:265:GLU:HG2	2.55	0.42
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.78	0.41
3:A:402:B12:H401	3:A:402:B12:H8	1.85	0.41
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.91	0.41
3:A:402:B12:O28	3:A:402:B12:H3	2.21	0.41
1:D:177:HIS:CD2	3:D:402:B12:H202	2.56	0.41
1:B:162:PRO:O	1:B:194:PRO:HB3	2.21	0.41
1:C:170:THR:OG1	1:C:171:THR:N	2.54	0.41
2:A:401:5AD:H5'3	3:A:402:B12:C19	2.51	0.40
1:D:177:HIS:HE1	3:D:402:B12:H412	1.86	0.40
1:B:85:THR:O	1:B:89:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/215 (93%)	197 (98%)	3 (2%)	0	100	100
1	B	200/215 (93%)	197 (98%)	3 (2%)	0	100	100
1	C	199/215 (93%)	195 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	197/215 (92%)	192 (98%)	5 (2%)	0	100	100
All	All	796/860 (93%)	781 (98%)	15 (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	151/161 (94%)	151 (100%)	0	100	100
1	B	151/161 (94%)	148 (98%)	3 (2%)	48	63
1	C	150/161 (93%)	144 (96%)	6 (4%)	28	37
1	D	151/161 (94%)	143 (95%)	8 (5%)	20	25
All	All	603/644 (94%)	586 (97%)	17 (3%)	37	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	LEU
1	B	100	GLU
1	B	142	HIS
1	C	81	GLU
1	C	93	ARG
1	C	221	LEU
1	C	240	LEU
1	C	257	ARG
1	C	258	ARG
1	D	82	ASP
1	D	85	THR
1	D	96	LEU
1	D	100	GLU
1	D	115	VAL
1	D	143	LEU
1	D	196	LEU

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Mol	Chain	Res	Type
1	D	257	ARG

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

Mol	Chain	Res	Type
1	A	153	GLN
1	C	153	GLN
1	C	249	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	5AD	C	401	-	20,20,20	1.76	4 (20%)	27,30,30	2.41	12 (44%)
3	B12	C	402	1	93,101,101	1.13	6 (6%)	146,166,166	1.70	37 (25%)
3	B12	D	402	1	93,101,101	1.07	5 (5%)	146,166,166	1.68	33 (22%)
2	5AD	A	401	-	20,20,20	1.63	4 (20%)	27,30,30	2.19	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5AD	B	401	-	20,20,20	1.60	4 (20%)	27,30,30	2.27	10 (37%)
2	5AD	D	401	-	20,20,20	1.68	4 (20%)	27,30,30	2.43	7 (25%)
3	B12	B	402	1	93,101,101	1.17	8 (8%)	146,166,166	1.60	30 (20%)
3	B12	A	402	1	93,101,101	1.16	6 (6%)	146,166,166	1.64	28 (19%)

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	5AD	C	401	-	-	0/4/20/20	0/3/3/3
3	B12	C	402	1	-	19/56/223/223	0/3/11/11
3	B12	D	402	1	-	20/56/223/223	0/3/11/11
2	5AD	A	401	-	-	0/4/20/20	0/3/3/3
2	5AD	B	401	-	-	0/4/20/20	0/3/3/3
2	5AD	D	401	-	-	0/4/20/20	0/3/3/3
3	B12	B	402	1	-	17/56/223/223	0/3/11/11
3	B12	A	402	1	-	18/56/223/223	0/3/11/11

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	5AD	C5-C4	5.52	1.49	1.39
2	A	401	5AD	C5-C4	5.16	1.48	1.39
2	D	401	5AD	C5-C4	5.08	1.48	1.39
2	B	401	5AD	C5-C4	5.03	1.48	1.39
3	A	402	B12	C14-N23	4.58	1.40	1.35
3	B	402	B12	C14-N23	4.54	1.40	1.35
3	C	402	B12	C14-N23	3.89	1.40	1.35
3	D	402	B12	C14-N23	3.34	1.39	1.35
3	A	402	B12	C35-C5	3.24	1.57	1.50
3	C	402	B12	C54-C17	3.20	1.60	1.54
3	B	402	B12	C35-C5	3.19	1.57	1.50
2	C	401	5AD	C5-C6	3.15	1.49	1.41
2	D	401	5AD	C5-C6	2.99	1.49	1.41
3	D	402	B12	C54-C17	2.92	1.59	1.54
3	B	402	B12	C54-C17	2.85	1.59	1.54
3	D	402	B12	C35-C5	2.84	1.56	1.50
3	A	402	B12	C54-C17	2.83	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	5AD	C8-N7	2.82	1.36	1.31
2	A	401	5AD	C5-C6	2.80	1.48	1.41
3	C	402	B12	C35-C5	2.70	1.56	1.50
2	B	401	5AD	C8-N7	2.69	1.36	1.31
2	B	401	5AD	C5-C6	2.55	1.48	1.41
2	A	401	5AD	C8-N7	2.53	1.36	1.31
3	D	402	B12	C6B-C5B	2.42	1.46	1.40
3	C	402	B12	C2B-N1B	-2.35	1.33	1.37
3	B	402	B12	C48-C13	2.33	1.59	1.54
3	B	402	B12	C55-C17	-2.28	1.49	1.54
2	B	401	5AD	C5-N7	-2.25	1.34	1.39
2	D	401	5AD	C5-N7	-2.23	1.34	1.39
2	C	401	5AD	C8-N7	2.22	1.35	1.31
3	B	402	B12	C53-C15	2.20	1.55	1.50
3	B	402	B12	C6B-C5B	2.17	1.46	1.40
2	C	401	5AD	C5-N7	-2.14	1.35	1.39
2	A	401	5AD	C5-N7	-2.13	1.35	1.39
3	A	402	B12	C48-C13	2.12	1.59	1.54
3	C	402	B12	C48-C13	2.11	1.59	1.54
3	B	402	B12	C2B-N1B	-2.11	1.33	1.37
3	D	402	B12	C41-C8	2.10	1.59	1.54
3	A	402	B12	C6B-C5B	2.07	1.46	1.40
3	C	402	B12	C53-C15	2.06	1.55	1.50
3	A	402	B12	C30-C3	2.04	1.59	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	B12	C2P-C1P-N59	-7.98	101.17	112.93
2	D	401	5AD	C5-C4-N3	-7.35	117.16	126.75
3	A	402	B12	C2P-C1P-N59	-6.69	103.06	112.93
3	C	402	B12	C2P-C1P-N59	-6.66	103.11	112.93
2	A	401	5AD	C5-C4-N3	-6.09	118.80	126.75
2	C	401	5AD	C5-C4-N3	-5.94	119.00	126.75
2	B	401	5AD	C5-C4-N3	-5.83	119.15	126.75
2	D	401	5AD	N3-C4-N9	5.31	135.84	127.08
2	A	401	5AD	N3-C4-N9	4.68	134.78	127.08
2	B	401	5AD	N3-C4-N9	4.60	134.65	127.08
3	A	402	B12	C55-C17-C16	4.54	125.61	116.65
2	C	401	5AD	N3-C4-N9	4.44	134.40	127.08
2	D	401	5AD	C2-N3-C4	4.32	121.96	111.75
3	C	402	B12	C55-C17-C16	4.18	124.91	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	B12	O6R-C1R-N1B	-4.15	99.88	108.06
3	D	402	B12	C18-C17-C16	4.06	105.60	100.67
3	B	402	B12	C2P-C1P-N59	-3.98	107.07	112.93
2	B	401	5AD	C2-N3-C4	3.93	121.05	111.75
3	A	402	B12	C16-C15-C14	-3.89	115.35	121.25
2	C	401	5AD	C4-C5-N7	-3.88	105.89	110.62
3	D	402	B12	C55-C17-C16	3.88	124.30	116.65
2	C	401	5AD	C5'-C4'-C3'	-3.83	111.67	115.70
3	D	402	B12	C9B-C8B-N1B	3.78	106.94	105.35
3	C	402	B12	C18-C17-C16	3.76	105.23	100.67
3	A	402	B12	C13-C14-C15	-3.73	118.61	124.32
3	B	402	B12	C55-C17-C16	3.69	123.94	116.65
3	B	402	B12	C2-C1-C19	-3.68	112.79	118.60
3	D	402	B12	C1P-N59-C57	-3.67	114.69	122.69
2	D	401	5AD	C4-C5-N7	-3.64	106.18	110.62
3	B	402	B12	C18-C17-C16	3.63	105.08	100.67
3	B	402	B12	C1P-N59-C57	-3.62	114.81	122.69
2	B	401	5AD	N3-C2-N1	-3.58	123.00	128.60
3	D	402	B12	C16-C15-C14	-3.56	115.84	121.25
3	C	402	B12	C1P-N59-C57	-3.55	114.96	122.69
3	B	402	B12	C16-C15-C14	-3.54	115.87	121.25
2	A	401	5AD	C2-N3-C4	3.48	119.97	111.75
2	A	401	5AD	C4-C5-N7	-3.47	106.40	110.62
3	B	402	B12	C56-C55-C17	-3.45	108.86	115.52
3	D	402	B12	C17-C16-N24	-3.43	105.86	111.15
2	C	401	5AD	C2-N3-C4	3.41	119.81	111.75
3	D	402	B12	C13-C14-C15	-3.39	119.14	124.32
3	C	402	B12	C16-C15-C14	-3.38	116.12	121.25
2	C	401	5AD	O4'-C1'-N9	3.35	114.66	108.06
3	C	402	B12	C54-C17-C16	-3.33	95.09	112.40
3	A	402	B12	C15-C16-N24	3.32	127.20	122.42
3	C	402	B12	C15-C16-N24	3.32	127.20	122.42
3	A	402	B12	C54-C17-C16	-3.23	95.62	112.40
2	A	401	5AD	C5-N7-C8	3.23	108.10	103.51
3	D	402	B12	C54-C17-C16	-3.22	95.66	112.40
3	B	402	B12	C9B-C8B-N1B	3.21	106.70	105.35
3	A	402	B12	C56-C55-C17	-3.20	109.36	115.52
3	B	402	B12	C15-C16-N24	3.14	126.95	122.42
3	A	402	B12	C18-C17-C16	3.10	104.44	100.67
3	B	402	B12	C13-C14-C15	-3.08	119.61	124.32
3	D	402	B12	C56-C55-C17	-3.06	109.63	115.52
3	D	402	B12	C54-C17-C18	-3.04	108.50	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	B12	C2-C1-C19	-2.99	113.88	118.60
2	D	401	5AD	C5-N7-C8	2.99	107.76	103.51
3	C	402	B12	C13-C14-C15	-2.99	119.75	124.32
2	C	401	5AD	C5-N7-C8	2.98	107.75	103.51
3	B	402	B12	C55-C56-C57	-2.98	104.72	111.23
2	B	401	5AD	C5'-C4'-C3'	-2.98	112.57	115.70
3	B	402	B12	C54-C17-C16	-2.97	97.00	112.40
3	B	402	B12	C1-C19-C18	-2.90	117.13	121.88
2	B	401	5AD	C4-C5-N7	-2.83	107.17	110.62
3	D	402	B12	C15-C16-N24	2.83	126.49	122.42
3	D	402	B12	C5M-C5B-C6B	-2.82	114.95	120.74
3	C	402	B12	C2-C26-C27	-2.82	107.28	115.22
3	D	402	B12	C7B-C8B-C9B	2.81	125.85	122.52
3	B	402	B12	C17-C16-N24	-2.80	106.83	111.15
3	C	402	B12	C17-C16-N24	-2.80	106.84	111.15
3	A	402	B12	C9B-C8B-N1B	2.79	106.53	105.35
3	C	402	B12	C41-C8-C9	-2.78	106.30	111.19
3	B	402	B12	C54-C17-C18	-2.77	108.89	112.98
3	C	402	B12	C9B-C8B-N1B	2.77	106.52	105.35
3	A	402	B12	C54-C17-C18	-2.75	108.92	112.98
3	A	402	B12	C8B-C9B-N3B	-2.75	106.94	109.97
3	A	402	B12	C5M-C5B-C6B	-2.74	115.12	120.74
3	A	402	B12	C13-C14-N23	2.73	112.82	109.10
3	D	402	B12	C53-C15-C16	2.73	125.08	120.38
3	C	402	B12	O2-C3R-C4R	-2.72	100.23	110.08
3	B	402	B12	C53-C15-C16	2.72	125.05	120.38
3	D	402	B12	C4B-C5B-C6B	2.71	123.55	119.67
3	C	402	B12	C2-C1-C19	-2.70	114.34	118.60
2	C	401	5AD	C2'-C1'-N9	-2.70	106.47	113.30
3	A	402	B12	C9B-N3B-C2B	2.70	107.65	104.44
3	C	402	B12	C5M-C5B-C6B	-2.68	115.23	120.74
3	B	402	B12	C7B-C8B-C9B	2.67	125.68	122.52
3	B	402	B12	C18-C19-N24	2.66	106.35	102.31
3	C	402	B12	C54-C17-C18	-2.64	109.08	112.98
3	A	402	B12	C53-C15-C16	2.63	124.91	120.38
2	D	401	5AD	N3-C2-N1	-2.61	124.52	128.60
3	D	402	B12	C8B-C9B-N3B	-2.60	107.10	109.97
2	A	401	5AD	N3-C2-N1	-2.59	124.55	128.60
3	D	402	B12	C13-C14-N23	2.59	112.63	109.10
3	A	402	B12	C3R-C2R-C1R	2.57	105.58	99.89
3	A	402	B12	C7B-C8B-C9B	2.56	125.55	122.52
3	D	402	B12	C9B-C4B-C5B	-2.51	116.10	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	5AD	N3-C2-N1	-2.51	124.67	128.60
2	B	401	5AD	C5-N7-C8	2.51	107.08	103.51
3	C	402	B12	C13-C14-N23	2.51	112.51	109.10
3	C	402	B12	C3R-C2R-C1R	2.44	105.29	99.89
3	C	402	B12	C7B-C8B-C9B	2.43	125.40	122.52
3	A	402	B12	C4B-C5B-C6B	2.40	123.11	119.67
3	B	402	B12	C8B-C9B-N3B	-2.40	107.32	109.97
3	A	402	B12	C49-C48-C13	-2.40	107.81	114.73
3	C	402	B12	O28-C27-N29	-2.38	116.01	122.50
3	D	402	B12	C2-C1-C19	-2.37	114.86	118.60
2	B	401	5AD	C4-N9-C8	2.36	108.29	105.73
2	C	401	5AD	C3'-C2'-C1'	2.36	105.90	101.43
3	C	402	B12	C4B-C5B-C6B	2.36	123.04	119.67
3	C	402	B12	C56-C55-C17	-2.35	110.98	115.52
3	C	402	B12	C42-C43-N45	2.34	123.80	116.51
3	C	402	B12	C1-C19-C18	-2.34	118.04	121.88
3	C	402	B12	C47-C12-C46	-2.33	105.42	109.35
3	A	402	B12	C17-C16-N24	-2.33	107.56	111.15
3	C	402	B12	C37-C7-C8	-2.32	102.17	108.39
2	B	401	5AD	C6-C5-N7	2.31	136.31	132.02
3	C	402	B12	C18-C19-N24	2.30	105.81	102.31
3	C	402	B12	C35-C5-C4	-2.29	112.13	116.79
3	C	402	B12	C8B-C9B-N3B	-2.27	107.46	109.97
2	C	401	5AD	C6-C5-N7	2.27	136.24	132.02
3	B	402	B12	O2-C3R-C4R	-2.25	101.94	110.08
3	D	402	B12	O28-C27-N29	-2.25	116.36	122.50
3	D	402	B12	O44-C43-N45	-2.24	116.38	122.50
3	D	402	B12	C3R-C2R-C1R	2.23	104.82	99.89
3	C	402	B12	O39-C38-C37	-2.21	115.00	121.99
3	C	402	B12	C12-C11-N23	2.19	114.89	111.83
3	D	402	B12	O2-C3R-C2R	2.19	119.62	111.68
3	B	402	B12	C31-C32-N33	2.19	123.31	116.51
3	A	402	B12	C30-C3-C2	-2.17	114.49	119.09
3	D	402	B12	C1-C19-C18	-2.17	118.31	121.88
3	C	402	B12	C36-C7-C37	2.16	114.37	110.80
3	D	402	B12	C35-C5-C4	-2.16	112.39	116.79
3	D	402	B12	C9B-N3B-C2B	2.16	107.01	104.44
2	D	401	5AD	C6-C5-N7	2.15	136.02	132.02
3	D	402	B12	C49-C48-C13	-2.14	108.54	114.73
3	A	402	B12	O28-C27-N29	-2.14	116.65	122.50
2	A	401	5AD	C3'-C2'-C1'	2.14	105.50	101.43
3	B	402	B12	C42-C43-N45	2.14	123.17	116.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	B12	C5M-C5B-C6B	-2.13	116.37	120.74
2	A	401	5AD	C4-N9-C8	2.13	108.03	105.73
3	B	402	B12	C9B-N3B-C2B	2.12	106.97	104.44
2	C	401	5AD	C4-N9-C8	2.10	108.01	105.73
3	B	402	B12	C54-C17-C55	-2.09	105.80	109.25
3	C	402	B12	O44-C43-N45	-2.09	116.80	122.50
2	A	401	5AD	N9-C8-N7	-2.09	111.06	113.91
3	A	402	B12	C31-C32-N33	2.09	123.01	116.51
3	B	402	B12	C13-C14-N23	2.09	111.94	109.10
3	D	402	B12	C7B-C8B-N1B	-2.08	127.20	131.41
3	C	402	B12	O5-P-O4	2.08	122.54	112.24
2	A	401	5AD	C6-C5-N7	2.07	135.88	132.02
3	C	402	B12	C2R-C1R-N1B	2.07	118.54	113.30
3	A	402	B12	C4B-C9B-N3B	2.06	134.05	130.51
3	D	402	B12	O2-C3R-C4R	-2.05	102.66	110.08
3	A	402	B12	C41-C8-C9	-2.05	107.58	111.19
3	D	402	B12	C2-C3-C4	2.04	103.95	101.63
3	B	402	B12	C30-C3-C4	2.04	114.38	109.63
3	A	402	B12	C18-C60-C61	-2.04	108.89	113.97
3	A	402	B12	O44-C43-N45	-2.03	116.95	122.50
2	B	401	5AD	C3'-C2'-C1'	2.03	105.29	101.43
3	D	402	B12	C41-C8-C9	-2.03	107.61	111.19
3	B	402	B12	O28-C27-N29	-2.03	116.96	122.50
3	B	402	B12	C20-C1-C19	2.02	111.30	109.36
3	C	402	B12	C53-C15-C16	2.01	123.83	120.38
3	B	402	B12	C3R-C2R-C1R	2.00	104.32	99.89
3	D	402	B12	C4R-O6R-C1R	2.00	113.89	109.47

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	B12	N59-C1P-C2P-C3P
3	A	402	B12	N59-C1P-C2P-O3
3	A	402	B12	C1P-C2P-O3-P
3	A	402	B12	C3P-C2P-O3-P
3	A	402	B12	C3R-O2-P-O5
3	B	402	B12	N59-C1P-C2P-C3P
3	B	402	B12	N59-C1P-C2P-O3
3	B	402	B12	C3R-O2-P-O4
3	B	402	B12	C3R-O2-P-O5
3	C	402	B12	N59-C1P-C2P-C3P

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Mol	Chain	Res	Type	Atoms
3	C	402	B12	N59-C1P-C2P-O3
3	C	402	B12	C1P-C2P-O3-P
3	C	402	B12	C3P-C2P-O3-P
3	C	402	B12	C3R-C4R-C5R-O8R
3	D	402	B12	N59-C1P-C2P-C3P
3	D	402	B12	N59-C1P-C2P-O3
3	D	402	B12	C3R-O2-P-O5
3	D	402	B12	O6R-C1R-N1B-C8B
3	C	402	B12	O6R-C4R-C5R-O8R
3	D	402	B12	O6R-C4R-C5R-O8R
3	D	402	B12	C3R-C4R-C5R-O8R
3	A	402	B12	C42-C41-C8-C9
3	B	402	B12	C4-C3-C30-C31
3	D	402	B12	C4-C3-C30-C31
3	C	402	B12	C3R-O2-P-O3
3	A	402	B12	C2R-C1R-N1B-C8B
3	A	402	B12	O6R-C1R-N1B-C8B
3	B	402	B12	C2R-C1R-N1B-C8B
3	B	402	B12	O6R-C1R-N1B-C8B
3	C	402	B12	C2R-C1R-N1B-C8B
3	C	402	B12	O6R-C1R-N1B-C8B
3	D	402	B12	C2R-C1R-N1B-C8B
3	B	402	B12	C3R-O2-P-O3
3	B	402	B12	O6R-C4R-C5R-O8R
3	B	402	B12	C2-C3-C30-C31
3	A	402	B12	C3R-O2-P-O3
3	D	402	B12	C3R-O2-P-O3
3	D	402	B12	C2-C3-C30-C31
3	D	402	B12	C42-C41-C8-C9
3	D	402	B12	C2P-O3-P-O2
3	A	402	B12	C3R-O2-P-O4
3	C	402	B12	C3R-O2-P-O4
3	D	402	B12	C55-C56-C57-O58
3	D	402	B12	C3R-O2-P-O4
3	C	402	B12	C18-C17-C55-C56
3	B	402	B12	C1P-C2P-O3-P
3	B	402	B12	C3P-C2P-O3-P
3	D	402	B12	C1P-C2P-O3-P
3	D	402	B12	C3P-C2P-O3-P
3	A	402	B12	C4-C3-C30-C31
3	D	402	B12	C55-C56-C57-N59
3	C	402	B12	C17-C18-C60-C61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	402	B12	C17-C18-C60-C61
3	C	402	B12	C55-C56-C57-O58
3	C	402	B12	C2P-O3-P-O2
3	A	402	B12	C2-C3-C30-C31
3	B	402	B12	C42-C41-C8-C9
3	A	402	B12	C55-C56-C57-O58
3	D	402	B12	C18-C60-C61-O63
3	A	402	B12	C2P-O3-P-O2
3	C	402	B12	C42-C41-C8-C9
3	C	402	B12	C55-C56-C57-N59
3	C	402	B12	C3R-O2-P-O5
3	B	402	B12	C17-C18-C60-C61
3	C	402	B12	C54-C17-C55-C56
3	C	402	B12	C19-C18-C60-C61
3	D	402	B12	C19-C18-C60-C61
3	A	402	B12	C55-C56-C57-N59
3	B	402	B12	C55-C56-C57-O58
3	A	402	B12	C7-C37-C38-O39
3	A	402	B12	C17-C18-C60-C61
3	A	402	B12	C19-C18-C60-C61
3	B	402	B12	C19-C18-C60-C61
3	B	402	B12	C55-C56-C57-N59

There are no ring outliers.

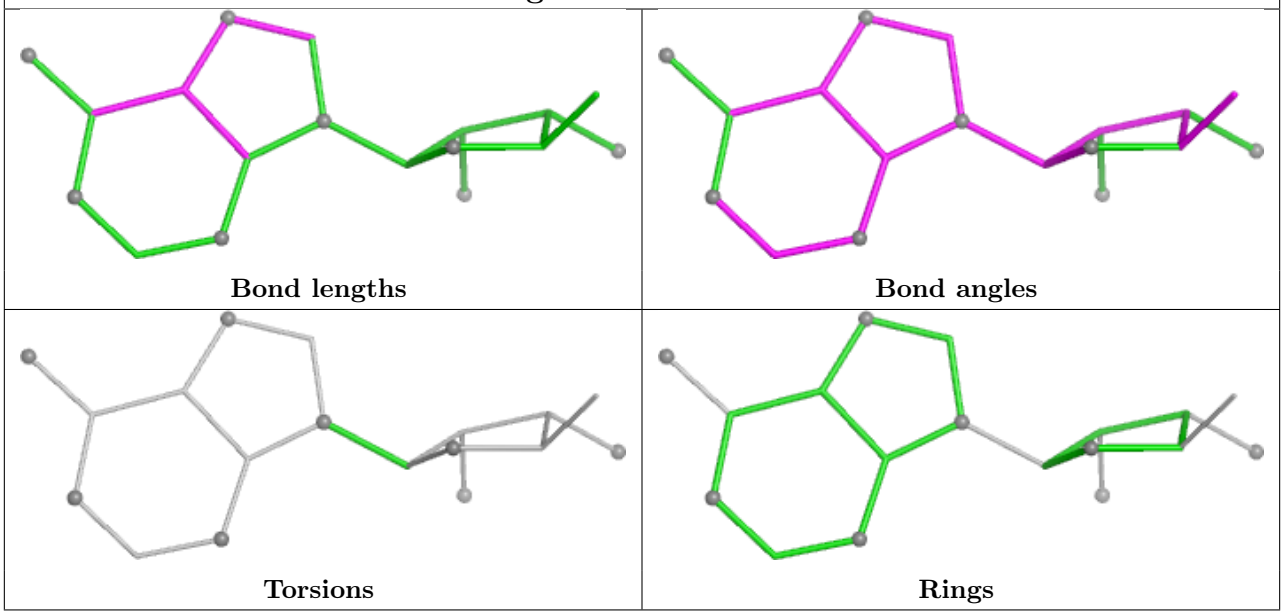
7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	5AD	1	0
3	C	402	B12	7	0
3	D	402	B12	7	0
2	A	401	5AD	1	0
2	D	401	5AD	2	0
3	B	402	B12	2	0
3	A	402	B12	7	0

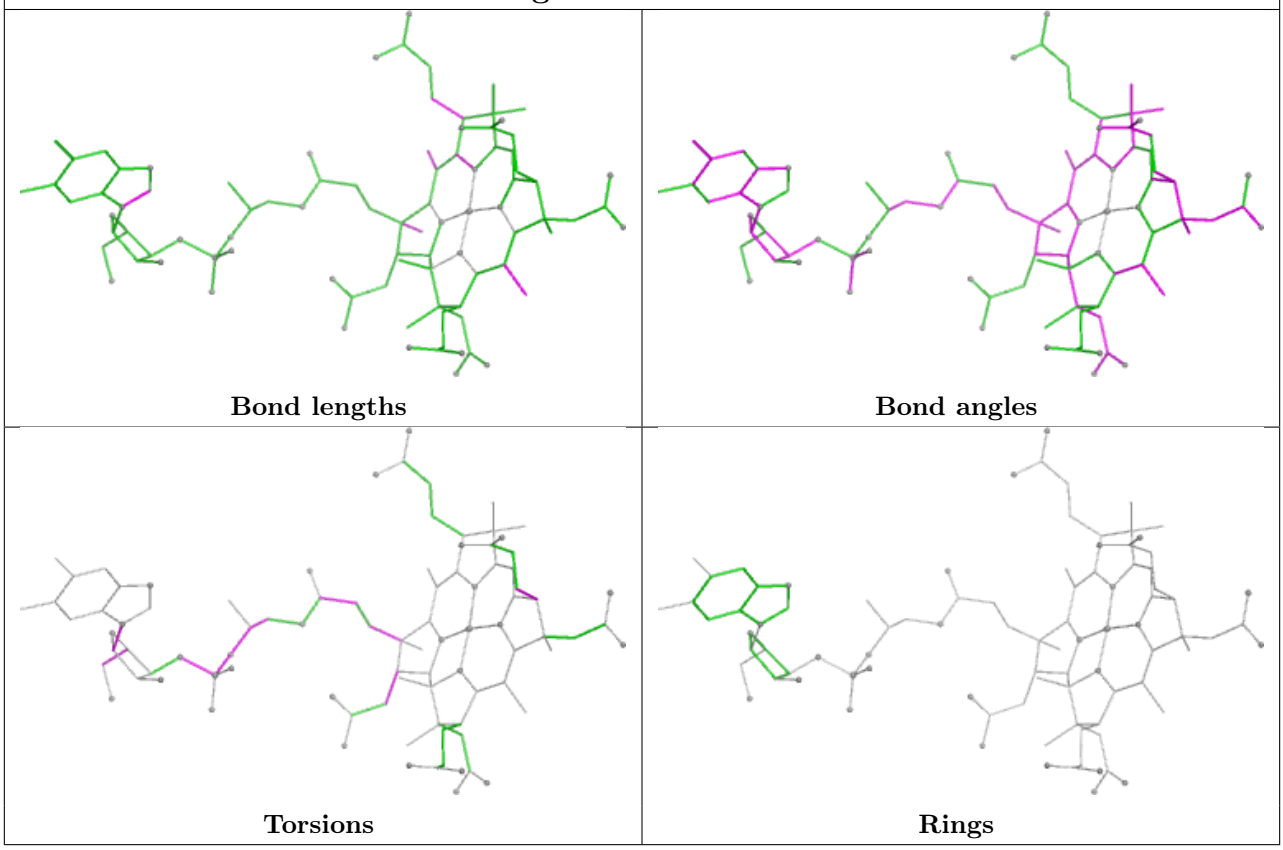
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

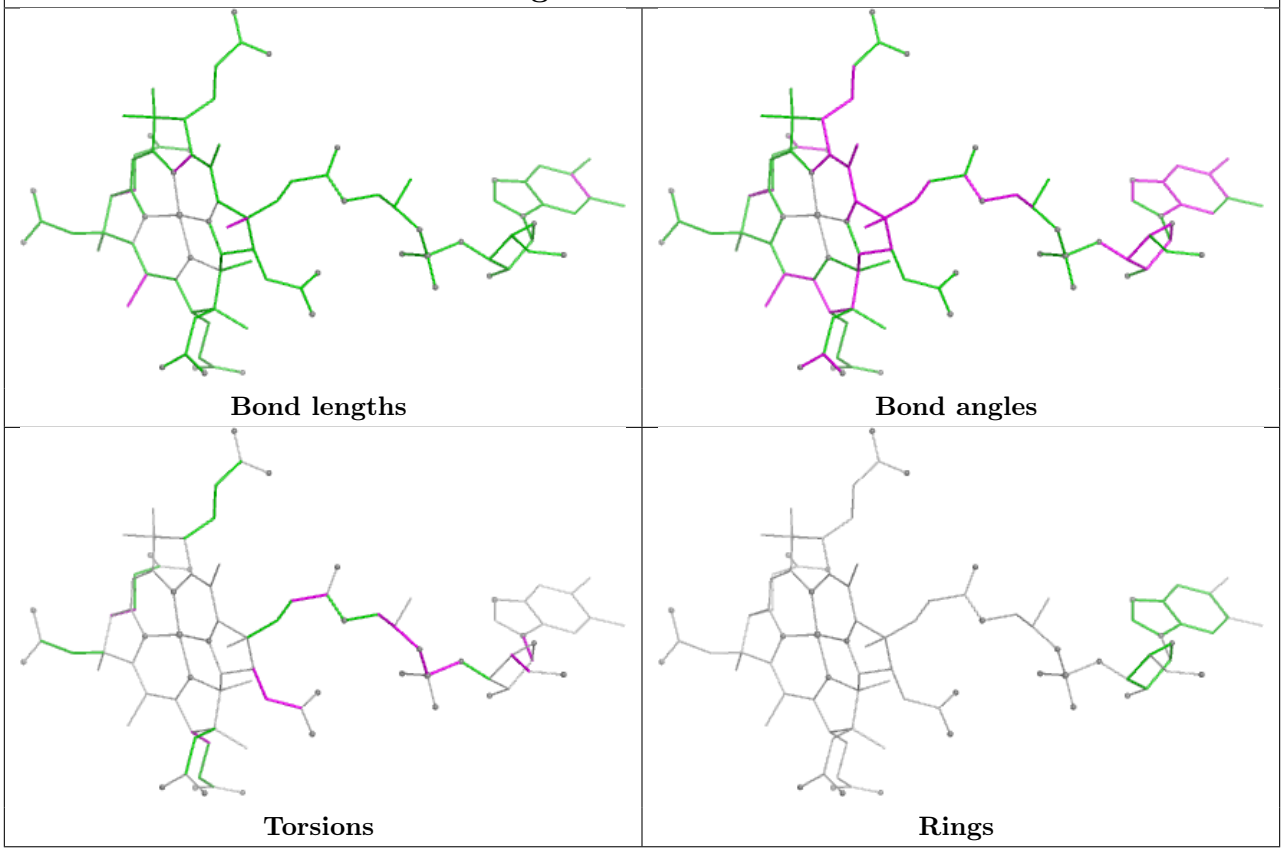
Ligand 5AD C 401



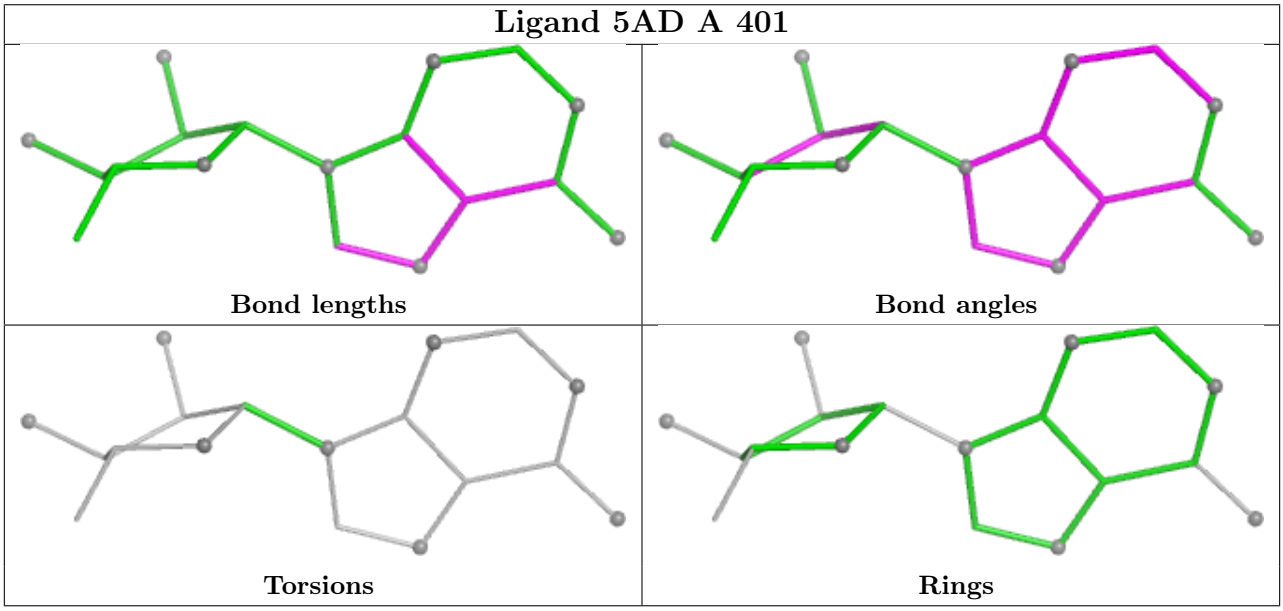
Ligand B12 C 402



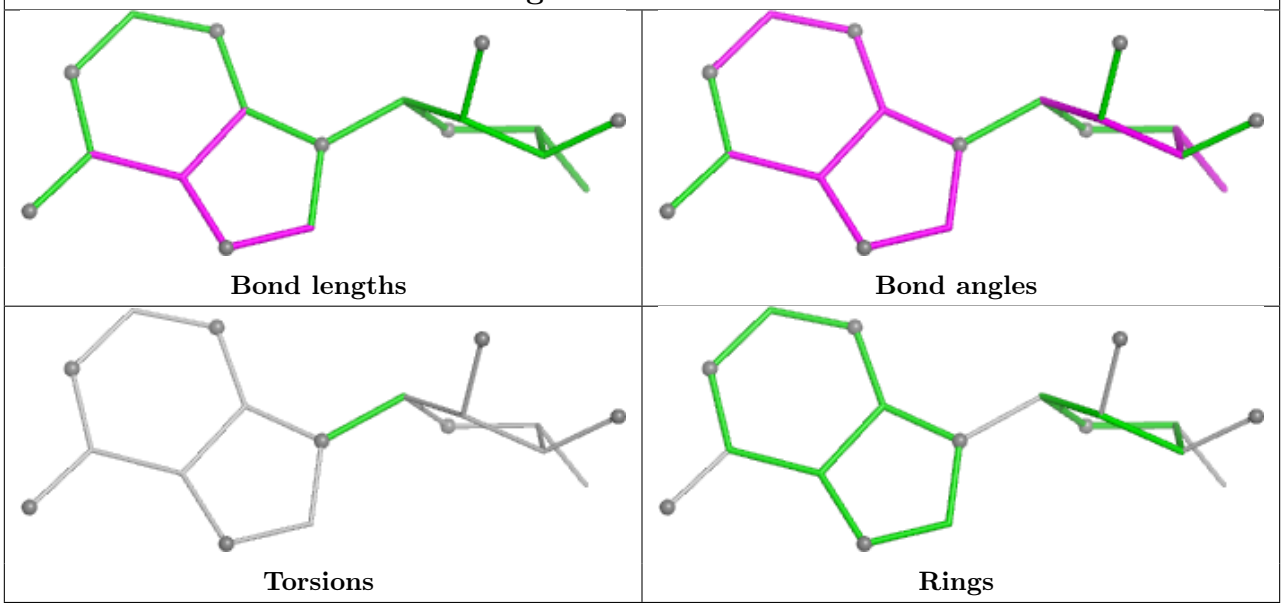
Ligand B12 D 402



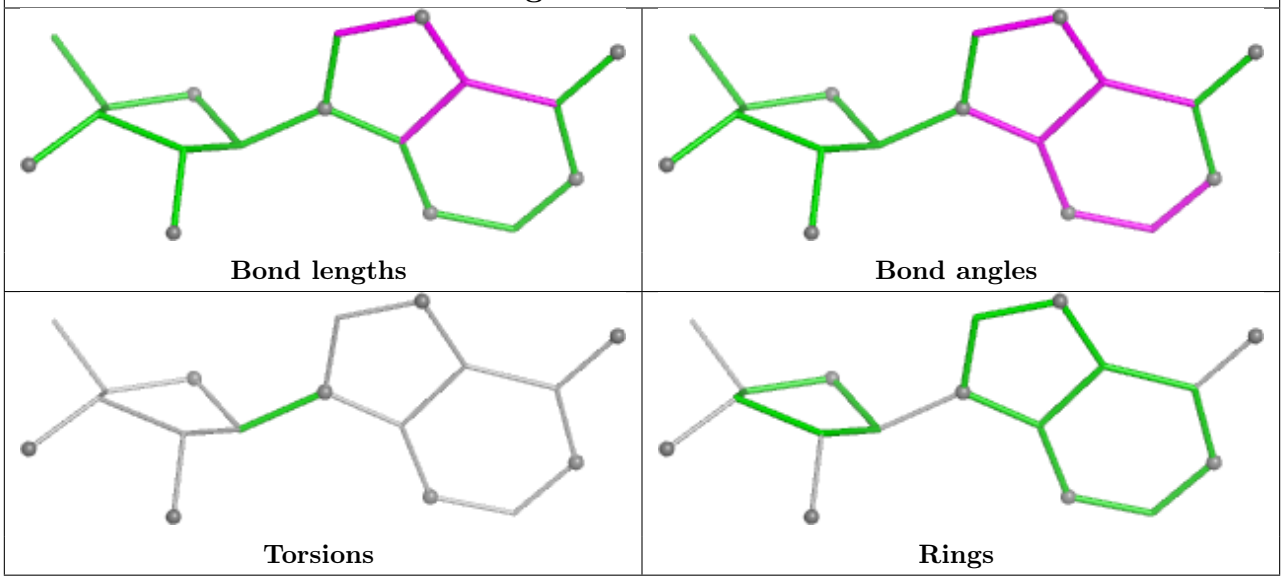
Ligand 5AD A 401



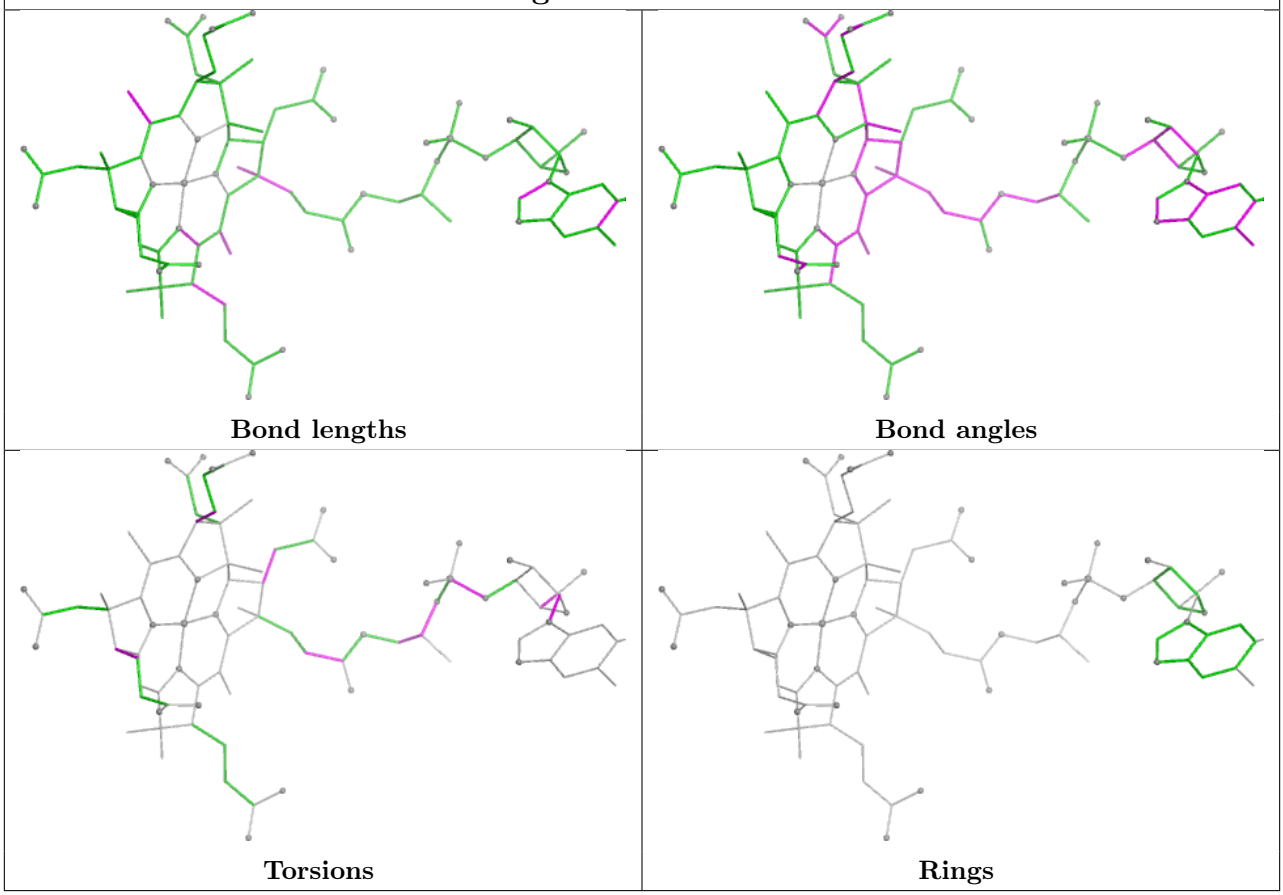
Ligand 5AD B 401



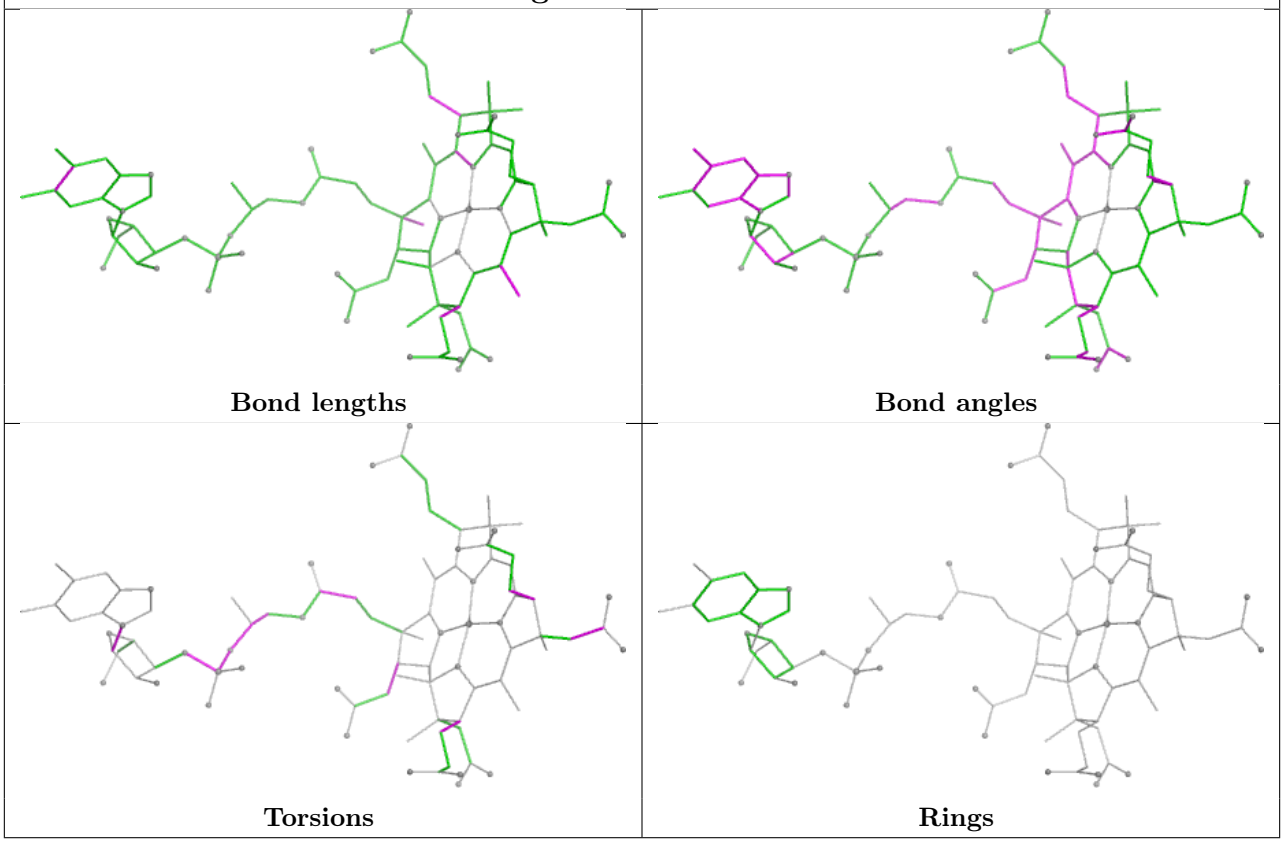
Ligand 5AD D 401



Ligand B12 B 402



Ligand B12 A 402



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	197/215 (91%)	-0.28	1 (0%)	87	90	19, 50, 85, 111	5 (2%)
1	B	197/215 (91%)	-0.29	2 (1%)	79	83	22, 50, 79, 130	5 (2%)
1	C	197/215 (91%)	0.00	1 (0%)	87	90	20, 56, 95, 122	4 (2%)
1	D	197/215 (91%)	0.02	4 (2%)	65	70	21, 58, 92, 124	4 (2%)
All	All	788/860 (91%)	-0.14	8 (1%)	79	83	19, 53, 91, 130	18 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	PRO	3.8
1	B	275	TRP	3.5
1	D	275	TRP	3.1
1	D	80	PRO	2.7
1	A	275	TRP	2.4
1	C	275	TRP	2.3
1	D	276	LEU	2.2
1	D	137	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

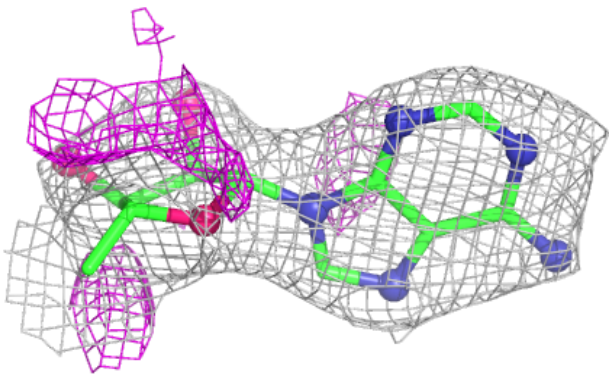
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

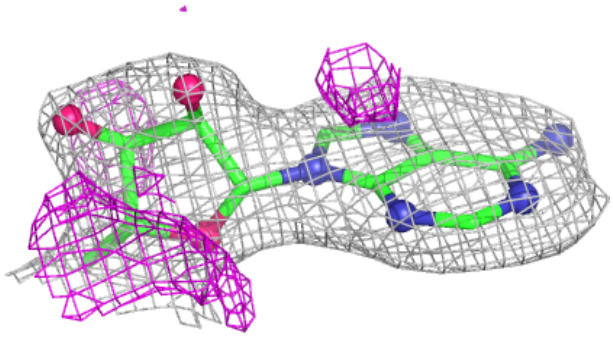
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5AD	D	401	18/18	0.94	0.07	52,57,63,64	0
2	5AD	C	401	18/18	0.95	0.07	40,46,49,49	0
2	5AD	A	401	18/18	0.96	0.06	33,46,51,52	0
2	5AD	B	401	18/18	0.96	0.06	38,51,56,56	0
3	B12	B	402	91/91	0.96	0.07	37,50,64,75	0
3	B12	D	402	91/91	0.96	0.08	44,57,75,83	0
3	B12	C	402	91/91	0.97	0.07	36,49,71,76	0
3	B12	A	402	91/91	0.97	0.07	36,47,65,80	0

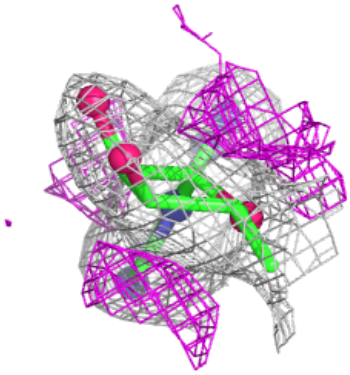
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD D 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

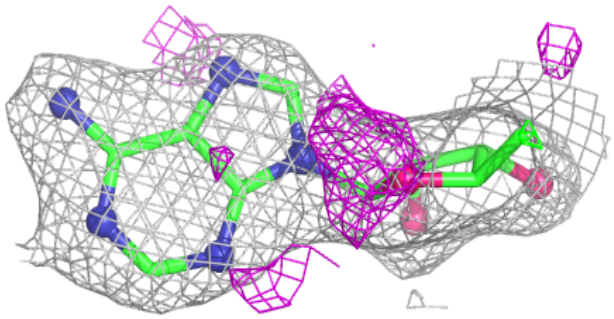


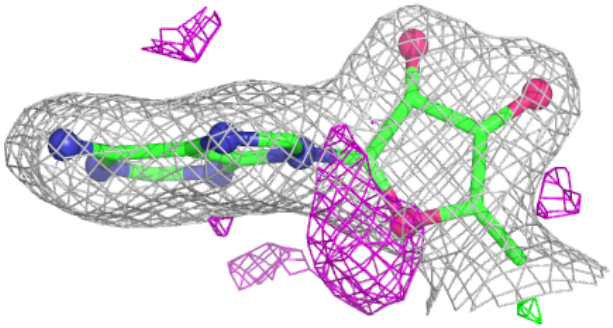


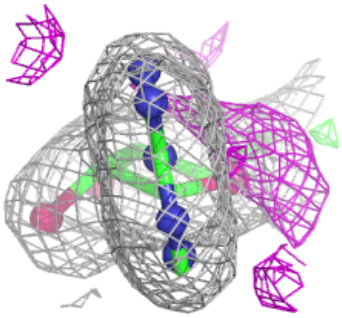


Electron density around 5AD C 401:

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

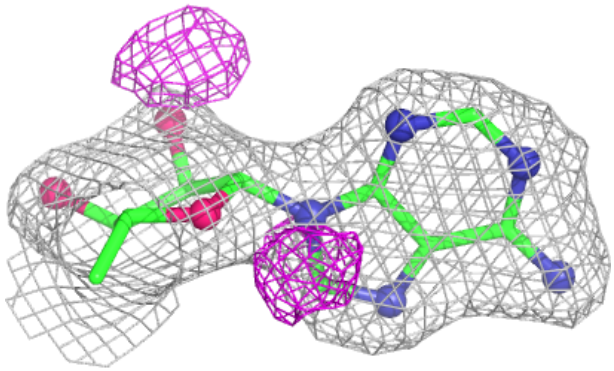


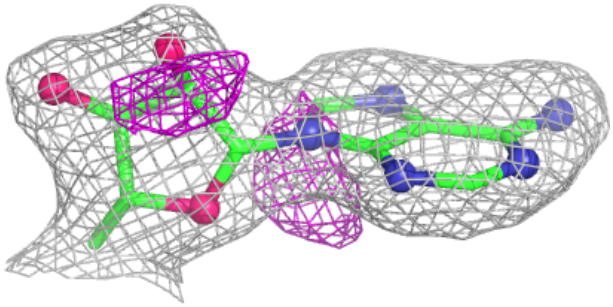


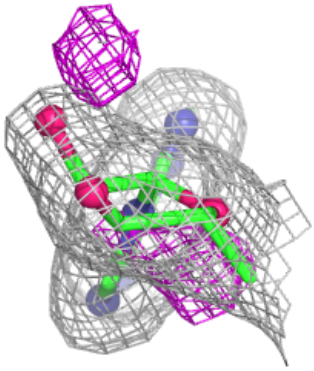


Electron density around 5AD A 401:

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

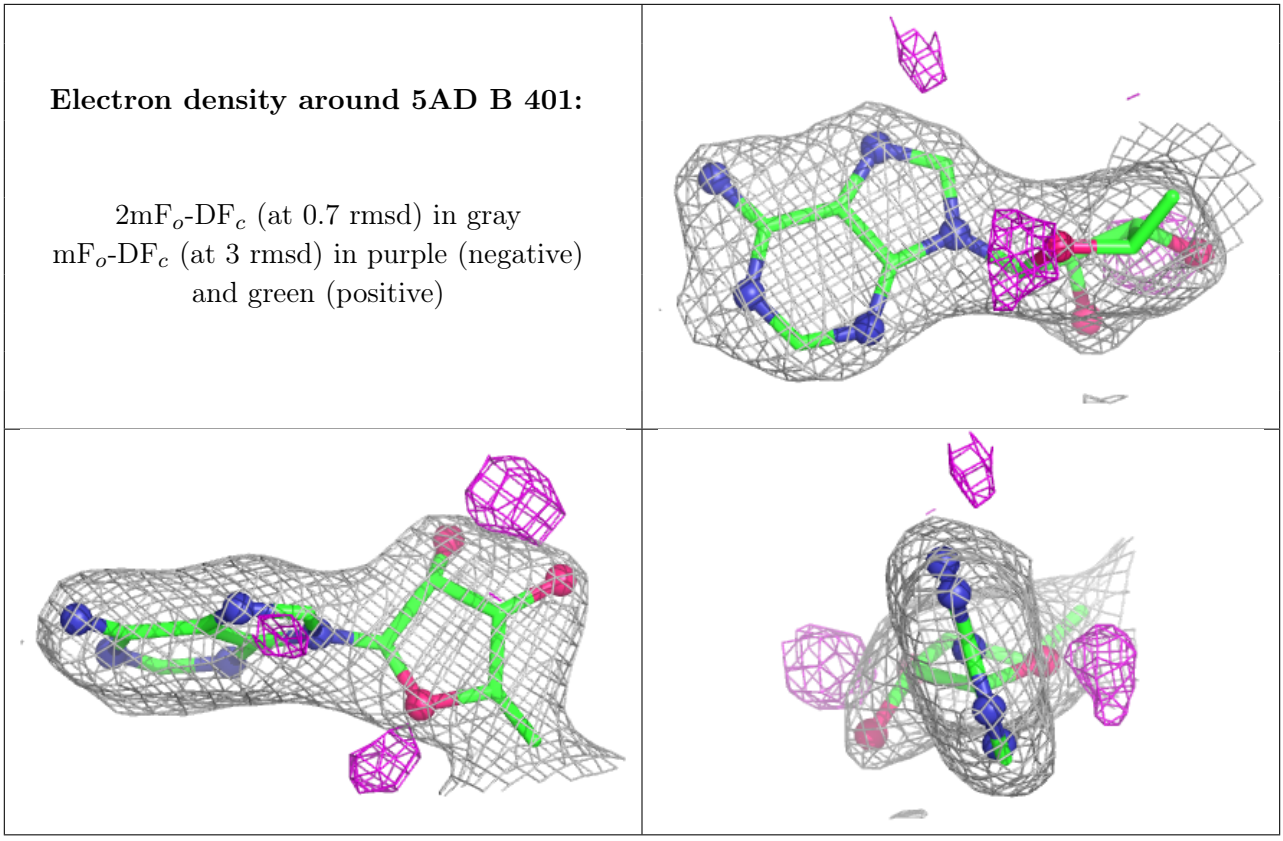






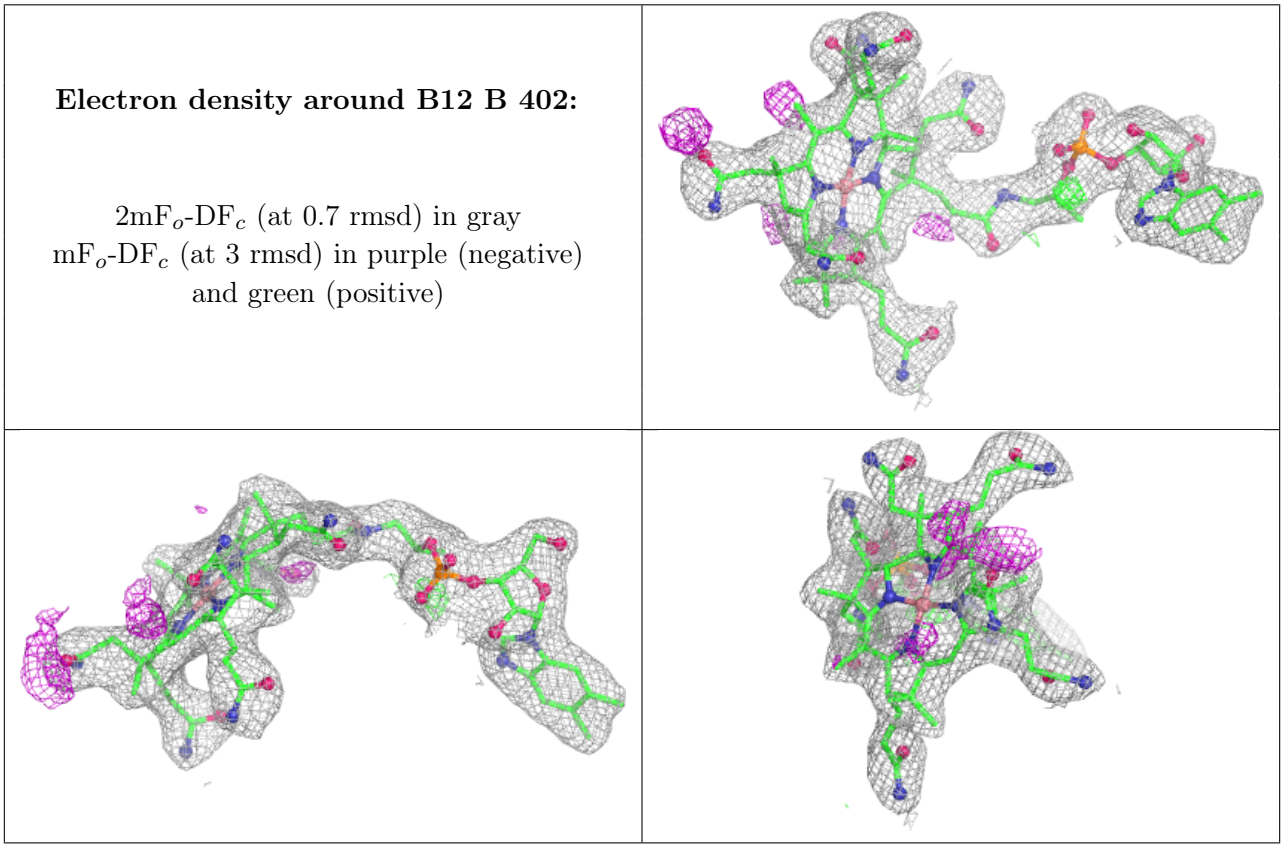
Electron density around 5AD B 401:

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



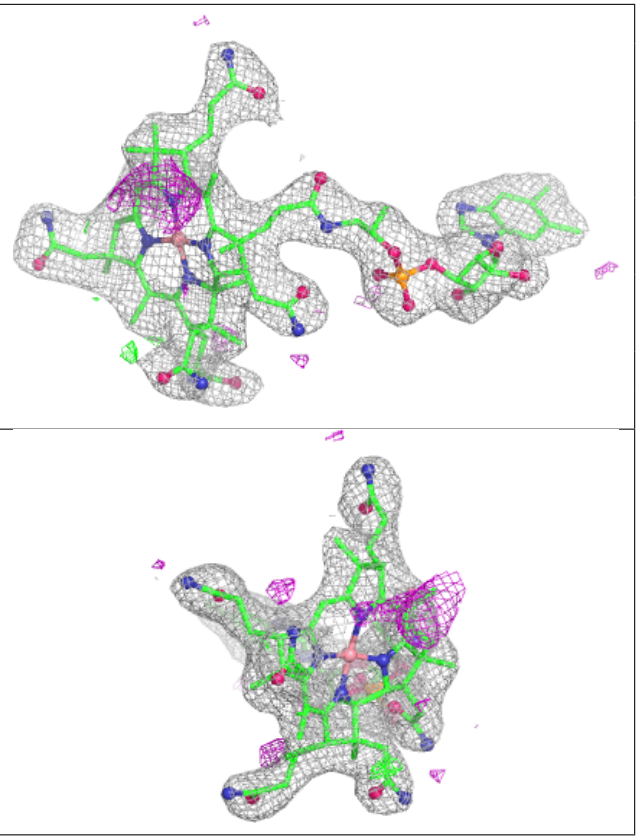
Electron density around B12 B 402:

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



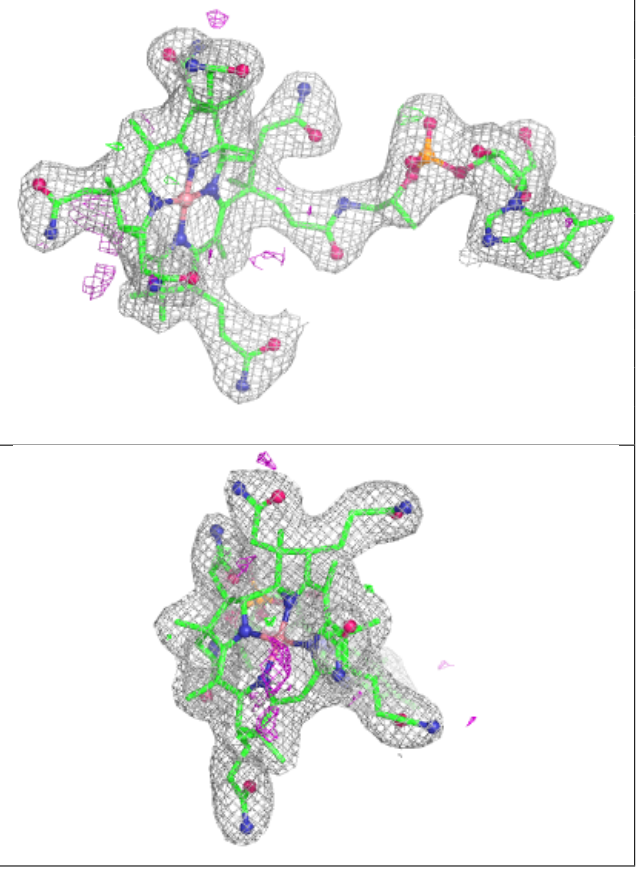
Electron density around B12 D 402:

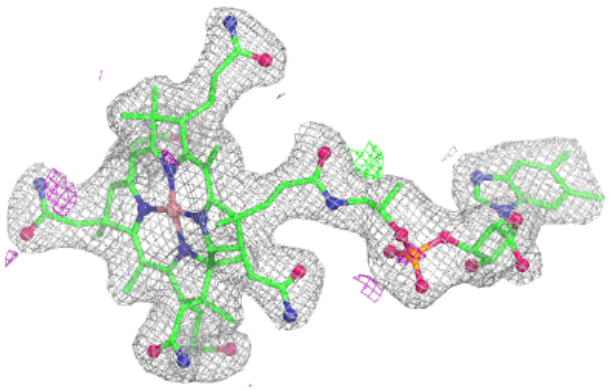
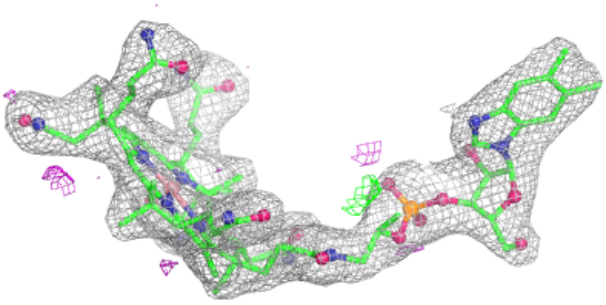
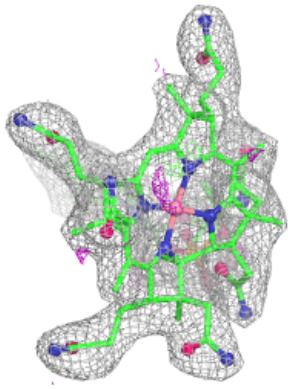
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B12 C 402:

$2mF_o$-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 402: $2mF_o$-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.