Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 05:57 am BST

PDB ID	:	9S0B / pdb_00009s0b
Title	:	3 ms Intermediate-state of CBD of TtCarH at 30 mJ/cm2 laser fluence (TR-SFX, SACLA), refined against extrapolated structure factors
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:

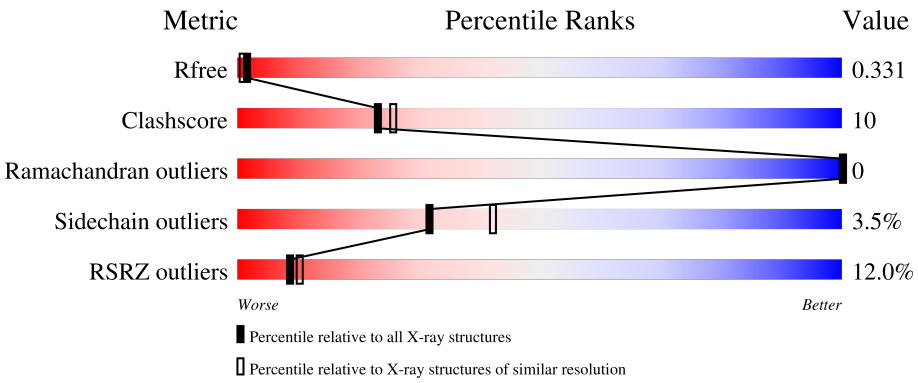
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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	7%, 76%, 15%, 8%
1	B	215	13%, 73%, 15%, •, 8%
1	C	215	14%, 75%, 15%, 9%
1	D	215	11%, 78%, 13%, 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6748 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	1531	979	282	268	2	0	5	0
1	B	197	1516	971	277	266	2	0	4	0
1	C	195	1493	954	276	261	2	0	4	0
1	D	196	1491	955	269	265	2	0	2	0

There are 28 discrepancies between the modelled and reference sequences:

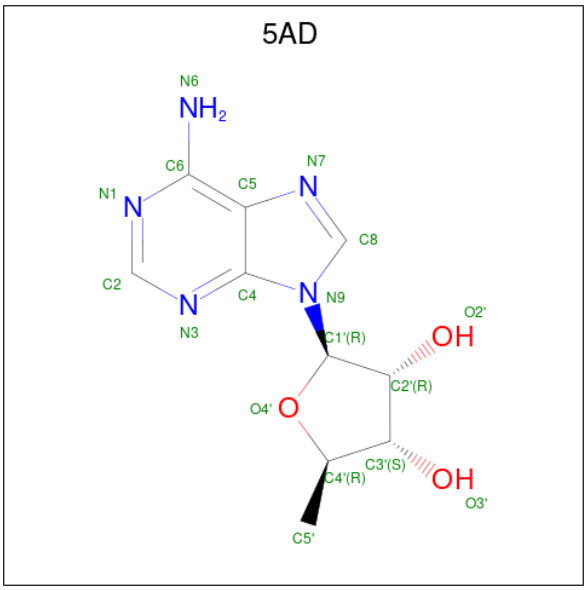
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLY	-	expression tag	UNP Q746J7
A	287	HIS	-	expression tag	UNP Q746J7
A	288	HIS	-	expression tag	UNP Q746J7
A	289	HIS	-	expression tag	UNP Q746J7
A	290	HIS	-	expression tag	UNP Q746J7
A	291	HIS	-	expression tag	UNP Q746J7
A	292	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

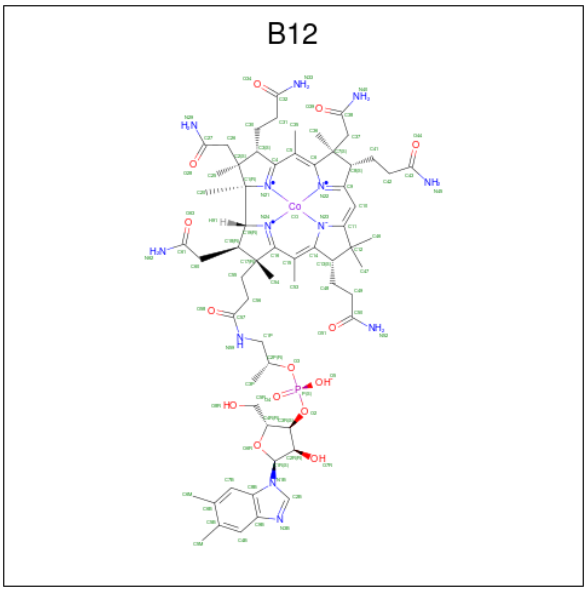
Chain	Residue	Modelled	Actual	Comment	Reference
D	286	GLY	-	expression tag	UNP Q746J7
D	287	HIS	-	expression tag	UNP Q746J7
D	288	HIS	-	expression tag	UNP Q746J7
D	289	HIS	-	expression tag	UNP Q746J7
D	290	HIS	-	expression tag	UNP Q746J7
D	291	HIS	-	expression tag	UNP Q746J7
D	292	HIS	-	expression tag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

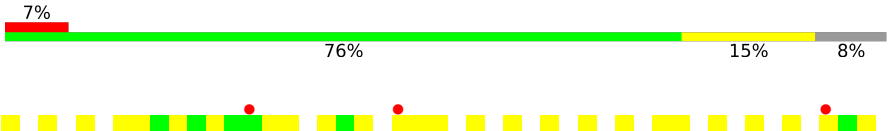
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	88	88	88	0	0
4	B	70	70	70	0	0
4	C	60	60	60	0	0
4	D	63	63	63	0	0

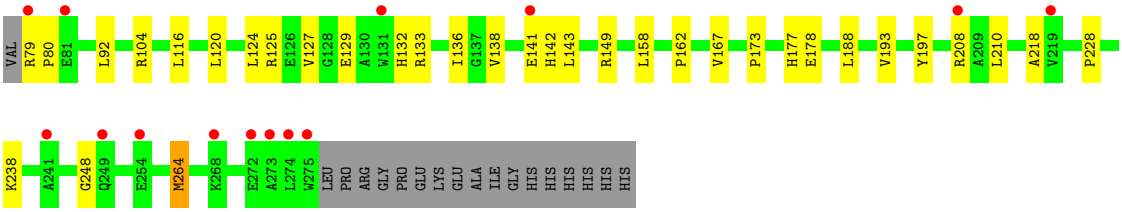
3 Residue-property plots (i)

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

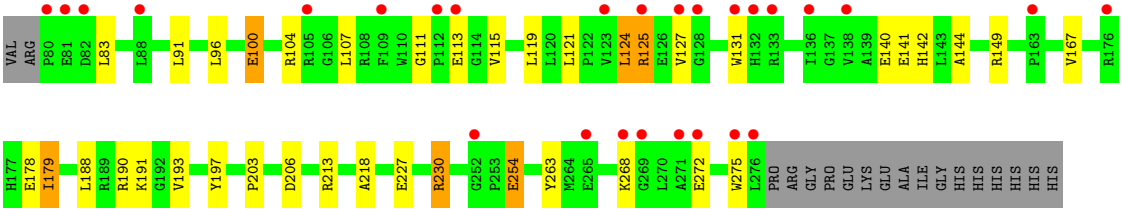
Chain A:





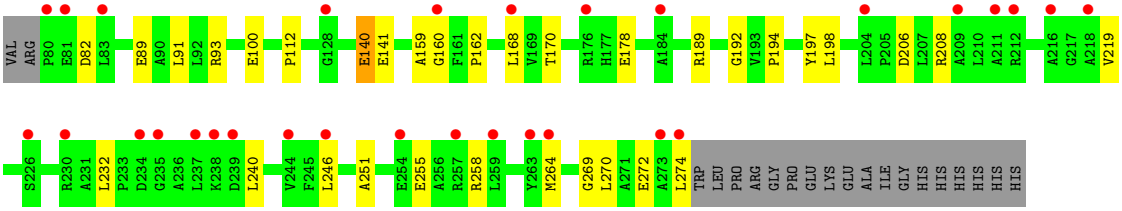
• Molecule 1: Probable transcriptional regulator

Chain B:



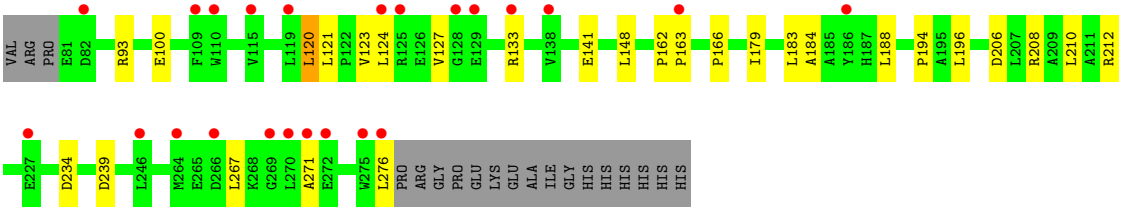
• Molecule 1: Probable transcriptional regulator

Chain C:



• Molecule 1: Probable transcriptional regulator

Chain D:


VAL
ARG
PRO
E81
D82
R93
E100
F109
W110
V115
L119
L120
L121
P122
V123
L124
R125
E126
V127
G128
E129
R133
V138
E141
L148
P162
P163
P166
I179
L183
A184
A185
Y186
H187
L188
P194
A195
L196
D206
L207
R208
A209
L210
A211
R212
E227
D234
D239
L246
M264
E265
D266
L267
K268
G269
L270
A271
E272
W275
L276
PRO
ARG
GLY
PRO
GLU
LYS
GLU
ALA
ILE
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.80Å 71.08Å 207.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.31 – 2.35 29.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.31-2.35) 99.7 (29.31-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.281 , 0.330 0.281 , 0.331	Depositor DCC
R_{free} test set	1998 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.56$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6748	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: B12, 5AD

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	0.26	0/1578	0.41	0/2143
1	B	0.25	0/1554	0.41	0/2111
1	C	0.26	0/1532	0.45	2/2079 (0.1%)
1	D	0.25	0/1525	0.41	0/2073
All	All	0.25	0/6189	0.42	2/8406 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	159	ALA	CA-C-N	-6.58	108.51	121.41
1	C	159	ALA	C-N-CA	-6.58	108.51	121.41

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	1531	0	1575	27	0
1	B	1516	0	1550	31	0
1	C	1493	0	1537	22	0
1	D	1491	0	1520	19	0
2	A	18	0	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	0	13	6	0
2	C	18	0	12	3	0
2	D	18	0	12	4	0
3	A	91	0	88	14	0
3	B	91	0	88	15	0
3	C	91	0	88	11	0
3	D	91	0	88	11	0
4	A	88	0	0	3	0
4	B	70	0	0	6	0
4	C	60	0	0	2	0
4	D	63	0	0	6	0
All	All	6748	0	6584	135	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 10.

All (135) 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:401:5AD:H4'	3:B:402:B12:N24	1.81	0.95
1:B:107:LEU:HA	1:B:115:VAL:HG11	1.63	0.80
1:C:232:LEU:O	1:C:258:ARG:NH2	2.20	0.74
1:D:93:ARG:NH2	4:D:502:HOH:O	2.21	0.71
3:D:402:B12:H401	3:D:402:B12:H8	1.56	0.69
1:D:120:LEU:HD23	1:D:148:LEU:HD22	1.77	0.66
1:C:178:GLU:HG2	3:C:402:B12:H522	1.60	0.66
1:B:124:LEU:HD13	3:B:402:B12:H1P2	1.78	0.66
2:C:401:5AD:H5'3	3:C:402:B12:H261	1.78	0.65
3:C:402:B12:H362	3:C:402:B12:H351	1.78	0.65
1:B:124:LEU:HD11	1:B:179:ILE:HD12	1.78	0.65
1:B:113:GLU:HB2	1:B:190:ARG:NH1	2.10	0.65
2:A:401:5AD:H5'3	3:A:402:B12:H261	1.81	0.62
3:B:402:B12:H8	3:B:402:B12:H401	1.66	0.61
3:A:402:B12:H251	3:A:402:B12:H291	1.66	0.60
1:C:178:GLU:HB2	1:C:197:TYR:OH	2.02	0.59
2:A:401:5AD:O4'	3:A:402:B12:N22	2.36	0.59
3:B:402:B12:H601	3:B:402:B12:H262	1.85	0.58
1:A:188:LEU:HB3	1:A:193:VAL:HB	1.85	0.57
1:B:188:LEU:HB3	1:B:193:VAL:HB	1.86	0.57
1:B:272:GLU:HA	1:B:275:TRP:CE2	2.39	0.57
1:B:263:TYR:OH	4:B:502:HOH:O	2.16	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:402:B12:N33	4:B:501:HOH:O	2.14	0.56
1:B:113:GLU:OE1	1:B:190:ARG:HD3	2.06	0.56
1:C:208:ARG:HB2	1:C:240:LEU:HD23	1.87	0.56
3:A:402:B12:H351	3:A:402:B12:H362	1.88	0.55
1:B:149:ARG:NH1	4:B:506:HOH:O	2.40	0.55
1:A:177:HIS:CE1	3:A:402:B12:H412	2.42	0.55
3:A:402:B12:H401	3:A:402:B12:H8	1.72	0.54
1:B:131:TRP:CZ2	2:B:401:5AD:H5'2	2.42	0.54
1:B:100:GLU:O	1:B:104:ARG:HG2	2.08	0.54
2:B:401:5AD:H5'3	3:B:402:B12:H261	1.91	0.53
1:A:210:LEU:HD13	1:B:140:GLU:HG3	1.89	0.53
2:B:401:5AD:C5'	3:B:402:B12:H261	2.39	0.53
1:A:79[B]:ARG:HB3	1:A:80:PRO:HD3	1.91	0.53
3:D:402:B12:H362	3:D:402:B12:H351	1.91	0.53
1:A:178:GLU:HB2	1:A:197:TYR:OH	2.09	0.53
1:C:168:LEU:HB2	1:C:219:VAL:HG22	1.91	0.52
2:D:401:5AD:H5'3	3:D:402:B12:H261	1.91	0.52
1:B:272:GLU:HG3	1:B:275:TRP:CH2	2.44	0.52
1:D:166:PRO:HA	1:D:194:PRO:HB2	1.91	0.51
2:C:401:5AD:N1	4:C:504:HOH:O	2.34	0.51
1:B:91:LEU:HD13	1:B:144:ALA:HA	1.92	0.51
1:B:167:VAL:HG22	1:B:218:ALA:HB3	1.92	0.51
3:A:402:B12:H353	3:A:402:B12:H311	1.93	0.51
1:D:133:ARG:NH1	4:D:512:HOH:O	2.43	0.51
1:A:149:ARG:HH11	1:B:149:ARG:HH21	1.59	0.50
1:D:123:VAL:O	1:D:127:VAL:HG23	2.11	0.50
1:A:208:ARG:NH2	4:A:509:HOH:O	2.45	0.49
1:C:246:LEU:HD21	1:C:251:ALA:HB1	1.94	0.49
1:A:162:PRO:HB3	1:C:192:GLY:HA3	1.95	0.49
3:D:402:B12:H531	3:D:402:B12:H552	1.95	0.49
2:B:401:5AD:H4'	3:B:402:B12:N21	2.27	0.49
3:B:402:B12:H2B	3:B:402:B12:O2	2.13	0.49
1:A:104:ARG:NH1	4:A:511:HOH:O	2.46	0.49
1:D:212:ARG:NH1	4:D:513:HOH:O	2.46	0.49
1:A:125:ARG:NH1	4:A:508:HOH:O	2.42	0.48
1:A:129:GLU:O	1:A:133:ARG:HG3	2.13	0.48
1:B:254:GLU:H	1:B:254:GLU:CD	2.20	0.48
1:D:234:ASP:OD2	4:D:501:HOH:O	2.20	0.48
3:B:402:B12:O28	3:B:402:B12:H3	2.14	0.47
1:D:121:LEU:HD21	1:D:183:LEU:HD11	1.95	0.47
1:D:124:LEU:HD22	3:D:402:B12:H552	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:NH1	1:B:149:ARG:HH21	2.13	0.47
3:A:402:B12:H363	3:A:402:B12:H411	1.67	0.47
2:B:401:5AD:H5'1	3:B:402:B12:C4	2.45	0.46
1:C:89:GLU:O	1:C:93:ARG:HG2	2.15	0.46
2:D:401:5AD:H5'1	3:D:402:B12:C4	2.46	0.46
1:D:206:ASP:OD1	1:D:206:ASP:N	2.48	0.46
1:A:79[A]:ARG:HB3	1:A:80:PRO:HD3	1.97	0.46
3:A:402:B12:H601	3:A:402:B12:H262	1.98	0.46
1:A:173:PRO:O	1:A:228:PRO:HB3	2.15	0.46
1:C:141:GLU:OE2	3:C:402:B12:H532	2.15	0.46
3:D:402:B12:H253	3:D:402:B12:H301	1.85	0.45
1:A:141:GLU:OE1	2:A:401:5AD:O2'	2.35	0.45
1:C:206:ASP:O	4:C:501:HOH:O	2.21	0.45
1:D:239:ASP:HB3	4:D:538:HOH:O	2.15	0.45
1:B:141:GLU:CD	1:B:141:GLU:C	2.85	0.45
1:B:178:GLU:HB2	1:B:197:TYR:OH	2.16	0.45
1:B:213:ARG:NH1	4:B:504:HOH:O	2.32	0.45
1:B:121:LEU:O	1:B:125:ARG:HG3	2.17	0.44
1:B:191:LYS:HZ3	1:B:268:LYS:HE3	1.83	0.44
1:B:141:GLU:OE2	3:B:402:B12:H532	2.17	0.44
1:B:111:GLY:O	1:B:115:VAL:HG13	2.18	0.44
1:B:113:GLU:HB2	1:B:190:ARG:HH11	1.80	0.44
1:A:158:LEU:HD23	1:C:112:PRO:HG3	2.00	0.44
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.83	0.43
3:D:402:B12:HM53	3:D:402:B12:HM61	1.81	0.43
1:C:140:GLU:HG3	1:D:210:LEU:HD13	2.01	0.43
1:A:177:HIS:CD2	3:A:402:B12:H202	2.54	0.43
1:A:138:VAL:HG12	1:A:142:HIS:CE1	2.54	0.43
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.85	0.43
3:D:402:B12:H261	3:D:402:B12:H91	1.75	0.43
3:C:402:B12:H552	3:C:402:B12:H531	1.99	0.43
1:C:255:GLU:OE1	1:C:258:ARG:NH1	2.52	0.42
1:D:141:GLU:CD	1:D:141:GLU:C	2.87	0.42
1:D:196:LEU:HD23	1:D:196:LEU:HA	1.83	0.42
1:C:82:ASP:OD1	1:C:82:ASP:N	2.52	0.42
1:C:269:GLY:HA2	1:C:272:GLU:HG3	2.01	0.42
1:A:116:LEU:HA	1:A:120:LEU:HB3	2.00	0.42
1:A:127:VAL:HG13	1:A:136:ILE:HD11	2.00	0.42
1:A:141:GLU:CD	1:A:141:GLU:C	2.87	0.42
3:B:402:B12:H362	3:B:402:B12:H351	2.01	0.42
2:C:401:5AD:H5'1	3:C:402:B12:C4	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:B12:H253	3:A:402:B12:H301	1.84	0.42
3:B:402:B12:H541	3:B:402:B12:H602	1.86	0.42
1:C:91:LEU:HD23	1:C:91:LEU:HA	1.93	0.42
3:C:402:B12:H91	3:C:402:B12:H262	1.62	0.42
1:C:264:MET:HA	1:C:264:MET:HE2	2.02	0.42
3:B:402:B12:H201	3:B:402:B12:H18	1.83	0.41
1:C:170:THR:HB	1:C:198:LEU:HB2	2.01	0.41
3:C:402:B12:H353	3:C:402:B12:H311	2.02	0.41
3:D:402:B12:H8	3:D:402:B12:N40	2.30	0.41
1:C:160:GLY:O	1:C:189[B]:ARG:HG2	2.20	0.41
1:D:141:GLU:OE1	2:D:401:5AD:O2'	2.38	0.41
1:C:264:MET:O	3:C:402:B12:HM62	2.20	0.41
1:C:162:PRO:HG2	1:C:194:PRO:HD3	2.03	0.41
1:D:184:ALA:HA	1:D:267:LEU:HD22	2.03	0.41
2:D:401:5AD:H5'3	3:D:402:B12:H91	2.03	0.41
1:B:227:GLU:HG3	4:B:512:HOH:O	2.20	0.41
1:A:248:GLY:HA2	3:A:402:B12:O7R	2.21	0.41
1:A:264:MET:HE3	1:A:264:MET:HB2	1.62	0.41
1:B:203:PRO:HB2	1:B:206:ASP:OD2	2.20	0.41
1:B:230:ARG:HD2	4:B:512:HOH:O	2.21	0.41
1:C:264:MET:HG3	1:C:270[A]:LEU:HD13	2.03	0.40
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.83	0.40
3:A:402:B12:H201	3:A:402:B12:H18	1.90	0.40
3:C:402:B12:H201	3:C:402:B12:H18	1.81	0.40
1:D:162:PRO:HA	1:D:163:PRO:HD3	1.95	0.40
1:A:141:GLU:OE2	3:A:402:B12:H532	2.22	0.40
1:A:167:VAL:HG22	1:A:218:ALA:HB3	2.03	0.40
3:C:402:B12:N40	3:C:402:B12:H8	2.36	0.40
1:D:188:LEU:HD23	1:D:271:ALA:HB2	2.03	0.40
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.89	0.40
1:D:208:ARG:NH2	4:D:507:HOH:O	2.32	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	199/215 (93%)	195 (98%)	4 (2%)	0	100	100
1	B	198/215 (92%)	194 (98%)	4 (2%)	0	100	100
1	C	196/215 (91%)	191 (97%)	5 (3%)	0	100	100
1	D	195/215 (91%)	188 (96%)	7 (4%)	0	100	100
All	All	788/860 (92%)	768 (98%)	20 (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%)	147 (97%)	4 (3%)	40	54
1	B	148/161 (92%)	139 (94%)	9 (6%)	17	20
1	C	146/161 (91%)	143 (98%)	3 (2%)	47	61
1	D	146/161 (91%)	142 (97%)	4 (3%)	39	52
All	All	591/644 (92%)	571 (97%)	20 (3%)	32	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	143	LEU
1	A	238	LYS
1	A	264	MET
1	B	96	LEU
1	B	100	GLU
1	B	124	LEU
1	B	125	ARG
1	B	127	VAL
1	B	142	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	179	ILE
1	B	230	ARG
1	B	254	GLU
1	C	100	GLU
1	C	140	GLU
1	C	274	LEU
1	D	100	GLU
1	D	120	LEU
1	D	179	ILE
1	D	276	LEU

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

Mol	Chain	Res	Type
1	A	153	GLN
1	A	249	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	$\#\|Z\| > 2$
3	B12	C	402	1,2	93,101,101	1.05	6 (6%)	146,166,166	1.73	33 (22%)
2	5AD	A	401	3	20,20,20	1.70	3 (15%)	27,30,30	2.49	14 (51%)
3	B12	D	402	1	93,101,101	1.08	6 (6%)	146,166,166	1.65	32 (21%)
3	B12	A	402	1,2	93,101,101	1.05	6 (6%)	146,166,166	1.74	36 (24%)
2	5AD	C	401	3	20,20,20	1.54	3 (15%)	27,30,30	2.43	9 (33%)
2	5AD	B	401	3	20,20,20	1.68	3 (15%)	27,30,30	2.49	12 (44%)
2	5AD	D	401	-	20,20,20	1.66	3 (15%)	27,30,30	2.56	10 (37%)
3	B12	B	402	1,2	93,101,101	1.08	4 (4%)	146,166,166	1.64	27 (18%)

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
3	B12	C	402	1,2	-	18/56/223/223	0/3/11/11
2	5AD	A	401	3	-	0/4/20/20	0/3/3/3
3	B12	D	402	1	-	19/56/223/223	0/3/11/11
3	B12	A	402	1,2	-	23/56/223/223	0/3/11/11
2	5AD	C	401	3	-	0/4/20/20	0/3/3/3
2	5AD	B	401	3	-	0/4/20/20	0/3/3/3
2	5AD	D	401	-	-	0/4/20/20	0/3/3/3
3	B12	B	402	1,2	-	15/56/223/223	0/3/11/11

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	5AD	C5-C4	5.23	1.48	1.39
2	A	401	5AD	C5-C4	5.13	1.48	1.39
2	D	401	5AD	C5-C4	5.06	1.48	1.39
2	C	401	5AD	C5-C4	4.91	1.48	1.39
3	B	402	B12	C14-N23	4.35	1.40	1.35
3	D	402	B12	C14-N23	4.04	1.40	1.35
3	A	402	B12	C14-N23	3.93	1.40	1.35
3	C	402	B12	C14-N23	3.67	1.39	1.35
2	D	401	5AD	C5-C6	3.17	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	5AD	C5-C6	3.13	1.49	1.41
2	B	401	5AD	C5-C6	2.92	1.49	1.41
3	A	402	B12	C35-C5	2.78	1.56	1.50
2	B	401	5AD	C8-N7	2.78	1.36	1.31
3	D	402	B12	C35-C5	2.77	1.56	1.50
2	C	401	5AD	C5-C6	2.72	1.48	1.41
3	D	402	B12	C54-C17	2.72	1.59	1.54
2	D	401	5AD	C8-N7	2.70	1.36	1.31
3	B	402	B12	C35-C5	2.69	1.56	1.50
2	A	401	5AD	C8-N7	2.67	1.36	1.31
3	B	402	B12	C54-C17	2.61	1.59	1.54
3	A	402	B12	C54-C17	2.55	1.59	1.54
3	C	402	B12	C54-C17	2.53	1.58	1.54
3	C	402	B12	C35-C5	2.37	1.55	1.50
2	C	401	5AD	C8-N7	2.32	1.36	1.31
3	A	402	B12	C55-C17	-2.31	1.49	1.54
3	B	402	B12	C6B-C5B	2.30	1.46	1.40
3	A	402	B12	C2B-N1B	-2.26	1.33	1.37
3	C	402	B12	C2B-N1B	-2.25	1.33	1.37
3	C	402	B12	C48-C13	2.18	1.59	1.54
3	C	402	B12	C55-C17	-2.14	1.49	1.54
3	D	402	B12	C48-C13	2.13	1.59	1.54
3	D	402	B12	C2B-N1B	-2.11	1.33	1.37
3	A	402	B12	C30-C3	2.07	1.59	1.54
3	D	402	B12	C55-C17	-2.04	1.50	1.54

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	5AD	C5-C4-N3	-6.50	118.27	126.75
2	B	401	5AD	C5-C4-N3	-5.88	119.08	126.75
2	A	401	5AD	C5-C4-N3	-5.84	119.13	126.75
2	C	401	5AD	C5-C4-N3	-5.73	119.28	126.75
3	B	402	B12	C1-C19-C18	-5.71	112.50	121.88
2	C	401	5AD	C5'-C4'-C3'	-5.63	109.79	115.70
2	D	401	5AD	C5'-C4'-C3'	-5.57	109.85	115.70
3	A	402	B12	C1-C19-C18	-5.25	113.26	121.88
3	D	402	B12	C1P-N59-C57	-5.20	111.38	122.69
3	D	402	B12	C18-C17-C16	5.14	106.91	100.67
3	B	402	B12	C18-C17-C16	4.94	106.68	100.67
3	B	402	B12	C54-C17-C18	-4.92	105.71	112.98
3	A	402	B12	C18-C17-C16	4.88	106.60	100.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	5AD	N3-C4-N9	4.84	135.06	127.08
2	D	401	5AD	N3-C4-N9	4.83	135.04	127.08
2	C	401	5AD	N3-C4-N9	4.76	134.93	127.08
2	A	401	5AD	N3-C4-N9	4.70	134.83	127.08
2	B	401	5AD	C5'-C4'-C3'	-4.61	110.86	115.70
3	C	402	B12	C54-C17-C18	-4.48	106.37	112.98
3	B	402	B12	C55-C17-C16	4.30	125.15	116.65
3	A	402	B12	C54-C17-C18	-4.30	106.63	112.98
3	C	402	B12	C1P-N59-C57	-4.25	113.44	122.69
3	C	402	B12	C1-C19-C18	-4.17	115.04	121.88
3	C	402	B12	C18-C17-C16	4.09	105.64	100.67
3	C	402	B12	C16-C15-C14	-4.07	115.07	121.25
2	D	401	5AD	C4-C5-N7	-3.96	105.80	110.62
3	B	402	B12	C55-C56-C57	-3.95	102.61	111.23
2	D	401	5AD	C2-N3-C4	3.90	120.97	111.75
3	A	402	B12	C55-C56-C57	-3.90	102.72	111.23
3	D	402	B12	C15-C16-N24	3.87	128.00	122.42
3	D	402	B12	C55-C17-C16	3.84	124.23	116.65
3	A	402	B12	C16-C15-C14	-3.84	115.43	121.25
3	D	402	B12	C9B-C8B-N1B	3.82	106.96	105.35
2	C	401	5AD	C2-N3-C4	3.72	120.55	111.75
2	A	401	5AD	C5'-C4'-C3'	-3.68	111.84	115.70
2	A	401	5AD	C2-N3-C4	3.66	120.39	111.75
3	D	402	B12	C2P-C1P-N59	-3.65	107.56	112.93
3	B	402	B12	C1P-N59-C57	-3.64	114.76	122.69
3	D	402	B12	C54-C17-C18	-3.61	107.65	112.98
2	B	401	5AD	C2-N3-C4	3.59	120.23	111.75
3	C	402	B12	C15-C16-N24	3.58	127.58	122.42
3	C	402	B12	C55-C17-C16	3.57	123.69	116.65
3	D	402	B12	C16-C15-C14	-3.56	115.85	121.25
3	D	402	B12	C54-C17-C16	-3.49	94.30	112.40
3	C	402	B12	C54-C17-C16	-3.49	94.31	112.40
3	A	402	B12	C55-C17-C16	3.48	123.53	116.65
3	B	402	B12	C18-C19-N24	3.48	107.61	102.31
3	A	402	B12	C25-C2-C1	-3.47	108.55	113.78
3	D	402	B12	C56-C55-C17	-3.46	108.84	115.52
3	B	402	B12	C54-C17-C16	-3.40	94.73	112.40
3	C	402	B12	C2P-C1P-N59	-3.40	107.92	112.93
3	A	402	B12	C15-C16-N24	3.36	127.27	122.42
2	B	401	5AD	C4-C5-N7	-3.34	106.55	110.62
3	A	402	B12	C54-C17-C16	-3.33	95.11	112.40
2	A	401	5AD	C4-C5-N7	-3.32	106.57	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	B12	C15-C16-N24	3.32	127.20	122.42
3	C	402	B12	C56-C55-C17	-3.30	109.16	115.52
2	D	401	5AD	C5-N7-C8	3.27	108.16	103.51
2	B	401	5AD	C4-N9-C8	3.26	109.27	105.73
2	A	401	5AD	O3'-C3'-C2'	-3.25	101.30	111.82
3	D	402	B12	C13-C14-C15	-3.23	119.38	124.32
3	B	402	B12	C16-C15-C14	-3.23	116.36	121.25
3	C	402	B12	C13-C14-C15	-3.18	119.46	124.32
3	C	402	B12	C9B-C8B-N1B	3.13	106.67	105.35
3	C	402	B12	C55-C56-C57	-3.12	104.41	111.23
2	C	401	5AD	N3-C2-N1	-3.10	123.75	128.60
3	C	402	B12	C49-C48-C13	-3.07	105.86	114.73
3	A	402	B12	C5M-C5B-C6B	-3.06	114.46	120.74
2	B	401	5AD	N3-C2-N1	-3.03	123.86	128.60
3	A	402	B12	C2-C3-C4	3.02	105.06	101.63
3	C	402	B12	C5M-C5B-C6B	-3.01	114.56	120.74
3	D	402	B12	C1-C19-C18	-3.01	116.94	121.88
2	A	401	5AD	N3-C2-N1	-3.00	123.91	128.60
3	A	402	B12	C4B-C5B-C6B	2.99	123.96	119.67
3	C	402	B12	C26-C2-C1	-2.96	105.39	110.01
2	C	401	5AD	C4-C5-N7	-2.96	107.01	110.62
3	D	402	B12	C17-C16-N24	-2.96	106.59	111.15
3	C	402	B12	C20-C1-N21	2.95	115.11	110.27
3	C	402	B12	C18-C19-N24	2.94	106.79	102.31
2	B	401	5AD	C5-N7-C8	2.94	107.68	103.51
3	A	402	B12	C17-C16-N24	-2.93	106.63	111.15
3	B	402	B12	C9B-C8B-N1B	2.92	106.58	105.35
2	A	401	5AD	C4-N9-C8	2.90	108.88	105.73
3	D	402	B12	C53-C15-C16	2.89	125.35	120.38
2	A	401	5AD	C5-N7-C8	2.89	107.61	103.51
3	A	402	B12	C1P-N59-C57	-2.88	116.42	122.69
3	C	402	B12	C20-C1-C19	-2.88	106.58	109.36
2	C	401	5AD	C4-N9-C8	2.88	108.84	105.73
2	D	401	5AD	N3-C2-N1	-2.86	124.13	128.60
3	C	402	B12	C41-C8-C9	-2.85	106.16	111.19
3	A	402	B12	O28-C27-N29	-2.83	114.76	122.50
3	D	402	B12	C7B-C8B-C9B	2.81	125.85	122.52
3	D	402	B12	C4B-C5B-C6B	2.79	123.66	119.67
3	A	402	B12	C7B-C8B-C9B	2.77	125.81	122.52
3	D	402	B12	C18-C19-N24	2.77	106.53	102.31
3	A	402	B12	C18-C19-N24	2.77	106.52	102.31
3	A	402	B12	C13-C14-C15	-2.77	120.09	124.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	B12	C8B-C9B-N3B	-2.76	106.92	109.97
3	B	402	B12	C17-C16-N24	-2.76	106.90	111.15
3	C	402	B12	C7B-C8B-C9B	2.74	125.77	122.52
3	D	402	B12	C13-C14-N23	2.72	112.80	109.10
3	A	402	B12	C53-C15-C16	2.67	124.97	120.38
2	A	401	5AD	O3'-C3'-C4'	2.64	116.94	110.47
3	A	402	B12	C36-C7-C37	2.62	115.12	110.80
3	B	402	B12	C49-C48-C13	-2.59	107.25	114.73
3	C	402	B12	C4B-C5B-C6B	2.55	123.32	119.67
3	B	402	B12	C7B-C8B-C9B	2.53	125.52	122.52
2	C	401	5AD	C5-N7-C8	2.52	107.09	103.51
3	D	402	B12	C55-C56-C57	-2.51	105.76	111.23
2	A	401	5AD	O2'-C2'-C3'	-2.50	103.73	111.82
3	B	402	B12	C35-C5-C4	-2.48	111.74	116.79
2	B	401	5AD	C3'-C2'-C1'	2.45	106.08	101.43
3	B	402	B12	C1-C2-C3	-2.43	98.49	101.60
3	A	402	B12	C18-C60-C61	-2.43	107.92	113.97
3	C	402	B12	C17-C16-N24	-2.42	107.41	111.15
2	B	401	5AD	N9-C8-N7	-2.39	110.64	113.91
3	A	402	B12	C8B-C9B-N3B	-2.39	107.33	109.97
2	D	401	5AD	C6-C5-N7	2.36	136.42	132.02
3	A	402	B12	C9B-C8B-N1B	2.32	106.33	105.35
3	C	402	B12	C36-C7-C37	2.32	114.62	110.80
3	D	402	B12	C5M-C5B-C6B	-2.31	116.01	120.74
3	B	402	B12	C2-C3-C4	2.30	104.25	101.63
3	C	402	B12	C53-C15-C16	2.30	124.33	120.38
3	C	402	B12	C35-C5-C4	-2.29	112.12	116.79
3	A	402	B12	C49-C48-C13	-2.29	108.12	114.73
3	A	402	B12	C2-C1-N21	2.29	104.96	101.77
2	A	401	5AD	C6-C5-N7	2.29	136.28	132.02
2	D	401	5AD	C4-N9-C8	2.28	108.20	105.73
3	D	402	B12	C9B-C4B-C5B	-2.27	116.54	120.71
3	A	402	B12	C3R-C2R-C1R	2.26	104.89	99.89
3	B	402	B12	C2P-C1P-N59	-2.25	109.61	112.93
3	B	402	B12	C47-C12-C46	-2.24	105.56	109.35
3	D	402	B12	O39-C38-C37	-2.24	114.91	121.99
3	C	402	B12	C3R-C2R-C1R	2.24	104.84	99.89
3	B	402	B12	O28-C27-N29	-2.23	116.42	122.50
3	A	402	B12	C9B-N3B-C2B	2.22	107.08	104.44
3	B	402	B12	C13-C14-C15	-2.22	120.94	124.32
3	A	402	B12	O39-C38-C37	-2.21	114.99	121.99
3	D	402	B12	C2-C3-C4	2.20	104.14	101.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	5AD	N9-C8-N7	-2.20	110.90	113.91
3	B	402	B12	C4B-C5B-C6B	2.20	122.82	119.67
3	A	402	B12	C56-C55-C17	-2.20	111.28	115.52
3	C	402	B12	C13-C14-N23	2.19	112.09	109.10
3	C	402	B12	C9B-N3B-C2B	2.19	107.05	104.44
3	D	402	B12	C13-C12-C11	2.19	103.44	100.97
2	B	401	5AD	O2'-C2'-C3'	-2.19	104.74	111.82
2	C	401	5AD	C6-C5-N7	2.19	136.10	132.02
3	A	402	B12	C42-C43-N45	2.18	123.29	116.51
3	D	402	B12	C8B-C9B-N3B	-2.17	107.57	109.97
3	A	402	B12	C31-C32-N33	2.17	123.26	116.51
2	B	401	5AD	C6-C5-N7	2.17	136.05	132.02
3	C	402	B12	O3-C2P-C1P	-2.16	102.60	106.92
3	A	402	B12	C1-C2-C3	-2.15	98.85	101.60
3	D	402	B12	C31-C32-N33	2.14	123.17	116.51
3	D	402	B12	C36-C7-C37	2.14	114.32	110.80
3	D	402	B12	C3R-C2R-C1R	2.12	104.60	99.89
3	D	402	B12	C48-C13-C14	2.12	113.78	108.49
3	A	402	B12	C9B-C4B-C5B	-2.12	116.82	120.71
2	A	401	5AD	C3'-C2'-C1'	2.12	105.45	101.43
3	C	402	B12	C9B-C4B-C5B	-2.11	116.84	120.71
3	B	402	B12	C20-C1-N21	2.09	113.70	110.27
3	D	402	B12	C7B-C8B-N1B	-2.09	127.19	131.41
3	B	402	B12	C31-C32-N33	2.09	123.02	116.51
3	B	402	B12	C5M-C5B-C6B	-2.08	116.47	120.74
3	A	402	B12	C56-C57-N59	-2.07	112.93	116.42
3	D	402	B12	C3P-C2P-C1P	-2.07	107.38	111.39
3	A	402	B12	C2-C26-C27	-2.05	109.47	115.22
3	D	402	B12	O3-C2P-C1P	-2.04	102.84	106.92
3	B	402	B12	C48-C13-C12	-2.02	110.95	116.63
3	A	402	B12	O5-P-O4	2.02	122.24	112.24
3	C	402	B12	C4B-C9B-N3B	2.02	133.97	130.51
2	D	401	5AD	N9-C8-N7	-2.02	111.16	113.91
3	B	402	B12	C8B-C9B-N3B	-2.01	107.75	109.97

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	B12	C2-C26-C27-O28
3	A	402	B12	C2-C3-C30-C31
3	A	402	B12	C4-C3-C30-C31

Continued on next page...

Continued from previous page...

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	O6R-C1R-N1B-C8B
3	C	402	B12	N59-C1P-C2P-C3P
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-O2-P-O5
3	C	402	B12	O6R-C1R-N1B-C8B
3	C	402	B12	C3R-C4R-C5R-O8R
3	D	402	B12	C1-C2-C26-C27
3	D	402	B12	C25-C2-C26-C27
3	D	402	B12	C3-C2-C26-C27
3	D	402	B12	C1P-C2P-O3-P
3	D	402	B12	C3P-C2P-O3-P
3	D	402	B12	C3R-O2-P-O5
3	C	402	B12	O6R-C4R-C5R-O8R
3	D	402	B12	C3R-C4R-C5R-O8R
3	D	402	B12	O6R-C4R-C5R-O8R
3	C	402	B12	C2-C3-C30-C31
3	C	402	B12	C4-C3-C30-C31
3	D	402	B12	C4-C3-C30-C31
3	A	402	B12	C2-C26-C27-N29
3	D	402	B12	C7-C37-C38-N40
3	B	402	B12	O6R-C4R-C5R-O8R
3	A	402	B12	C3R-O2-P-O3
3	C	402	B12	C3R-O2-P-O3
3	D	402	B12	C3R-O2-P-O3
3	A	402	B12	C7-C37-C38-N40
3	B	402	B12	C7-C37-C38-N40
3	D	402	B12	C7-C37-C38-O39
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	C	402	B12	C2R-C1R-N1B-C8B
3	B	402	B12	C4-C3-C30-C31
3	A	402	B12	C7-C37-C38-O39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	402	B12	C7-C37-C38-O39
3	D	402	B12	C2-C3-C30-C31
3	B	402	B12	C2P-O3-P-O2
3	A	402	B12	C42-C41-C8-C9
3	B	402	B12	C3R-C4R-C5R-O8R
3	C	402	B12	C42-C41-C8-C9
3	A	402	B12	C3R-O2-P-O4
3	C	402	B12	C3R-O2-P-O4
3	D	402	B12	C3R-O2-P-O4
3	A	402	B12	C18-C17-C55-C56
3	A	402	B12	C55-C56-C57-O58
3	A	402	B12	C55-C56-C57-N59
3	D	402	B12	C2R-C1R-N1B-C8B
3	D	402	B12	O6R-C1R-N1B-C8B
3	B	402	B12	C2-C3-C30-C31
3	A	402	B12	C38-C37-C7-C36
3	A	402	B12	C25-C2-C26-C27
3	B	402	B12	C17-C18-C60-C61
3	D	402	B12	C17-C18-C60-C61
3	A	402	B12	C12-C13-C48-C49
3	B	402	B12	C55-C56-C57-O58
3	A	402	B12	C54-C17-C55-C56
3	C	402	B12	C55-C56-C57-O58
3	B	402	B12	C19-C18-C60-C61
3	C	402	B12	C17-C18-C60-C61
3	D	402	B12	C19-C18-C60-C61
3	D	402	B12	C2R-C1R-N1B-C2B
3	B	402	B12	C55-C56-C57-N59
3	C	402	B12	C55-C56-C57-N59
3	C	402	B12	C19-C18-C60-C61

There are no ring outliers.

8 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	B12	11	0
2	A	401	5AD	3	0
3	D	402	B12	11	0
3	A	402	B12	14	0
2	C	401	5AD	3	0
2	B	401	5AD	6	0
2	D	401	5AD	4	0

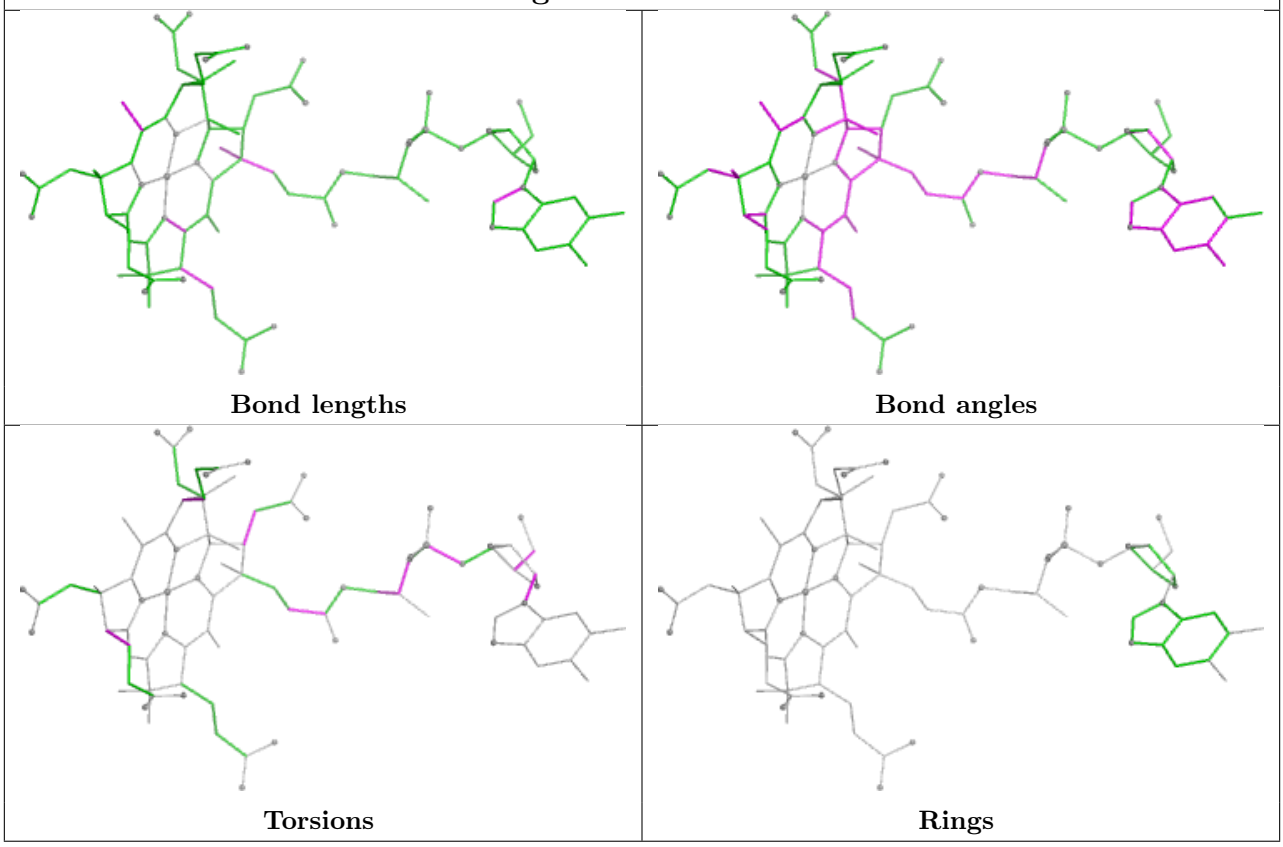
Continued on next page...

Continued from previous page...

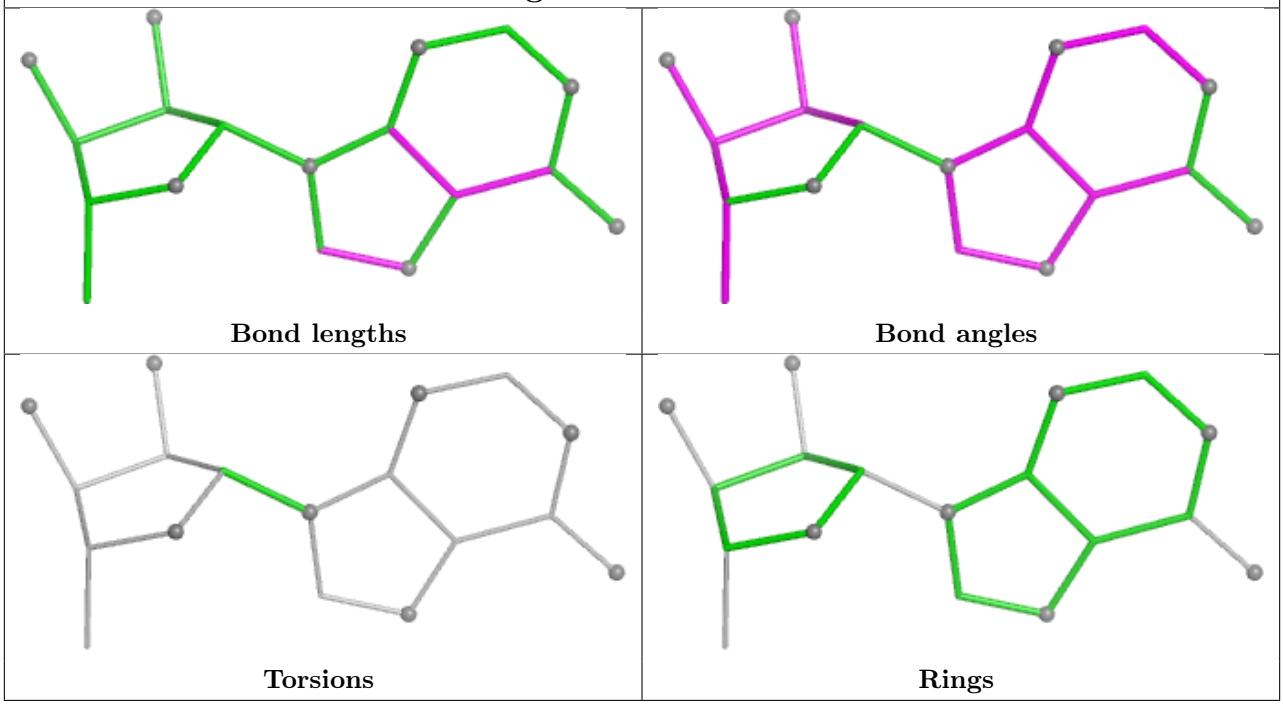
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	B12	15	0

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.

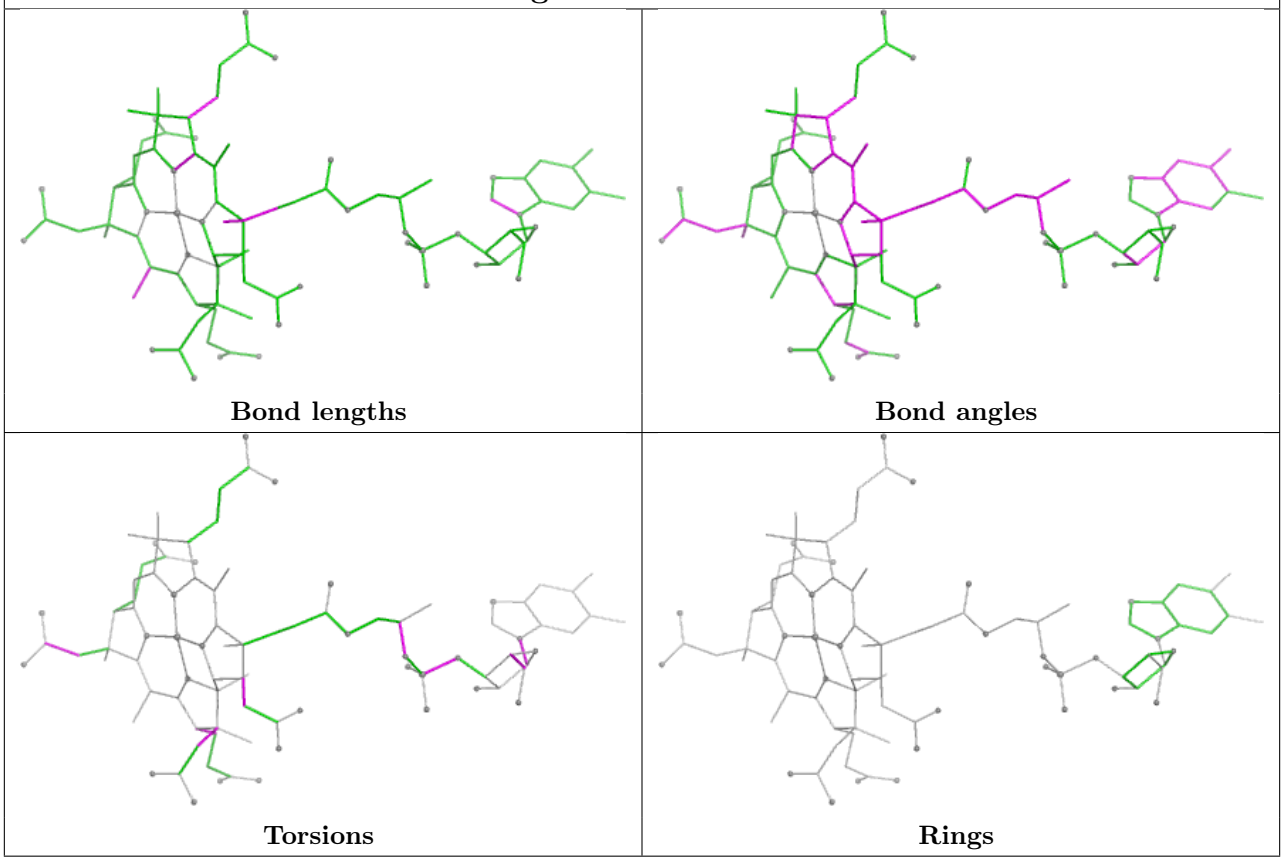
Ligand B12 C 402



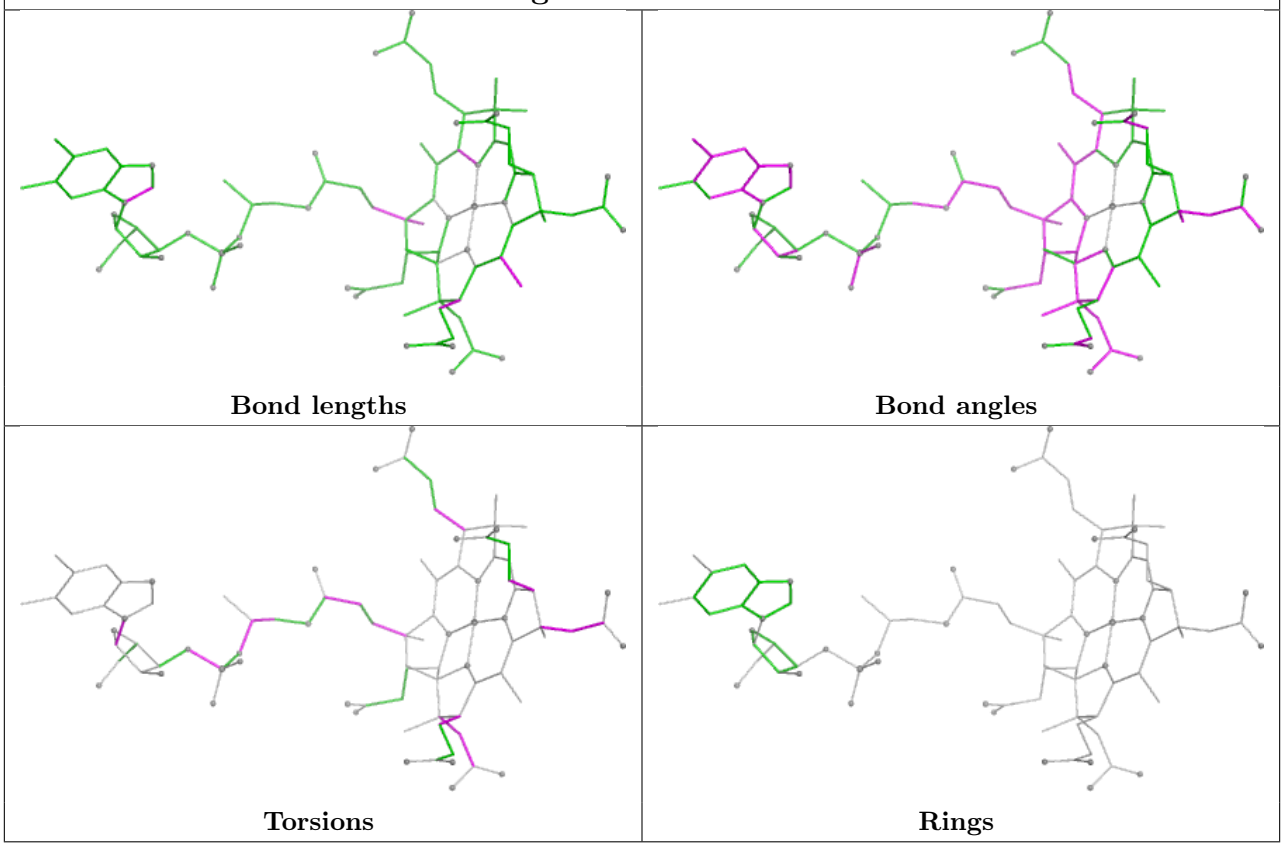
Ligand 5AD A 401



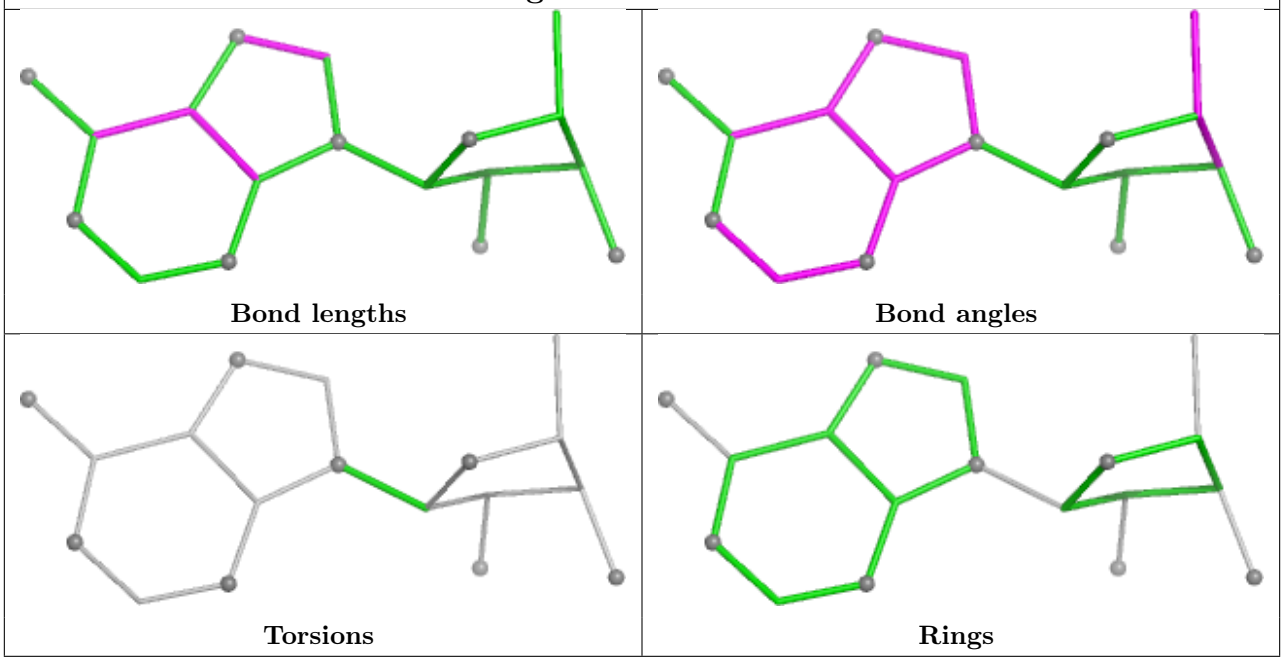
Ligand B12 D 402



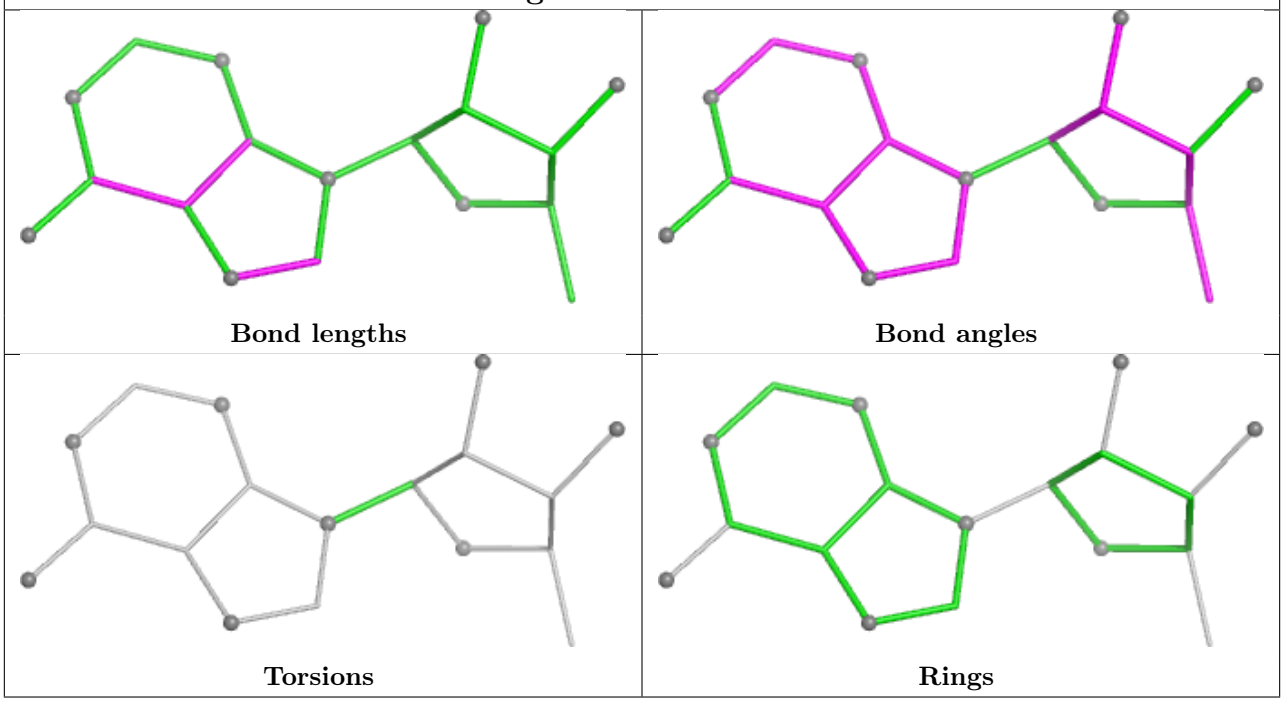
Ligand B12 A 402



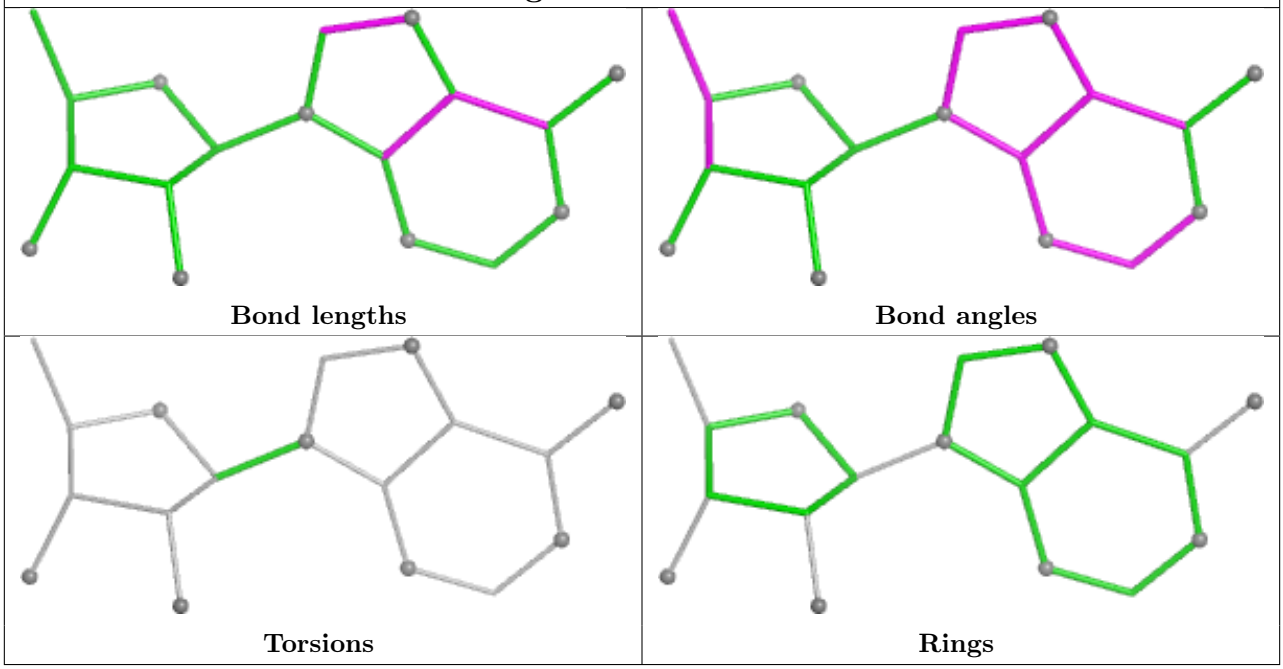
Ligand 5AD C 401



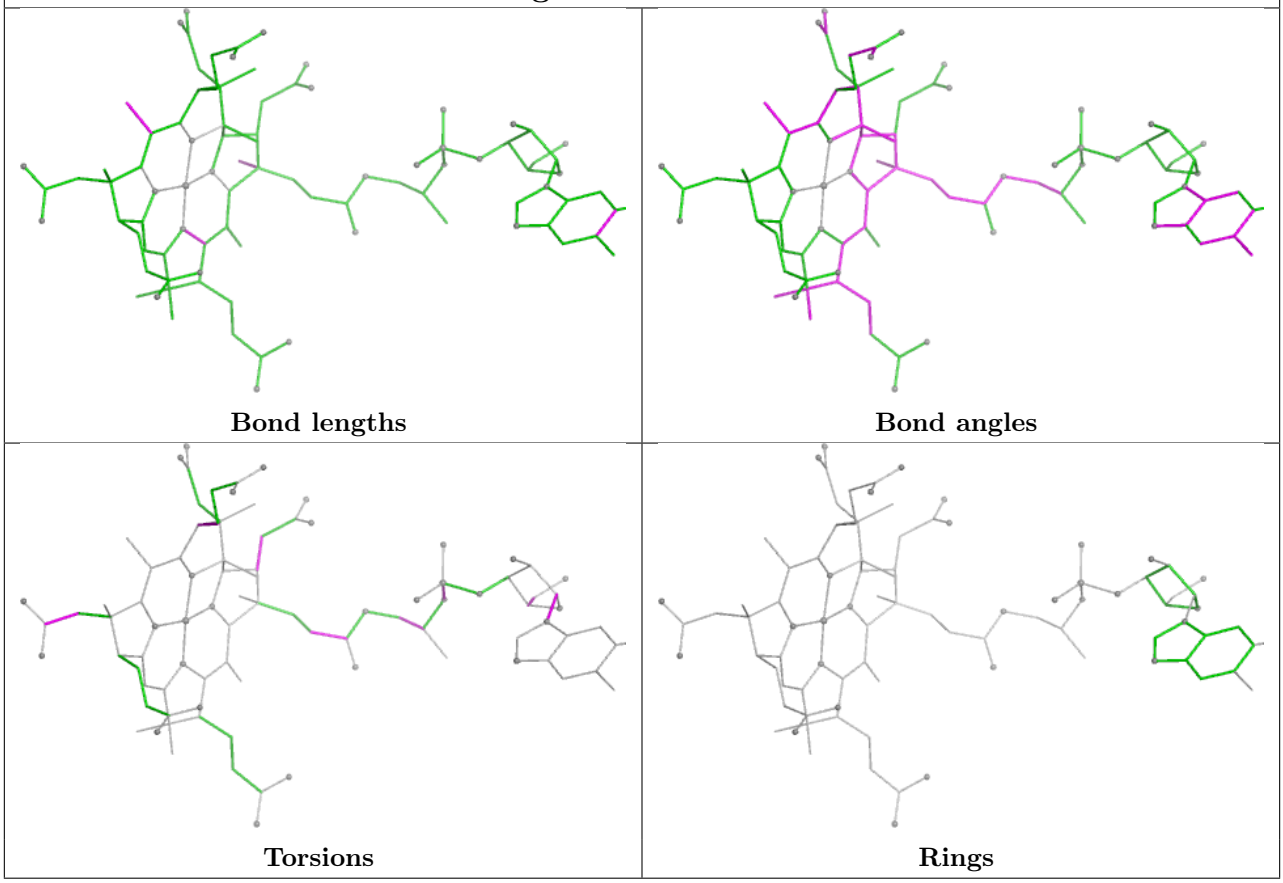
Ligand 5AD B 401



Ligand 5AD D 401



Ligand B12 B 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%)	1.03	14 (7%)	22	25	25, 49, 65, 95	5 (2%)
1	B	197/215 (91%)	1.19	27 (13%)	6	7	22, 52, 72, 87	3 (1%)
1	C	195/215 (90%)	1.20	30 (15%)	5	6	24, 51, 70, 76	3 (1%)
1	D	196/215 (91%)	1.12	23 (11%)	9	11	26, 52, 72, 85	1 (0%)
All	All	785/860 (91%)	1.13	94 (11%)	9	10	22, 51, 71, 95	12 (1%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	GLN	5.5
1	B	275	TRP	5.2
1	A	275	TRP	4.7
1	D	276	LEU	4.7
1	B	269	GLY	4.4
1	B	80	PRO	4.2
1	C	81	GLU	4.2
1	D	275	TRP	4.1
1	B	81	GLU	4.1
1	C	212[A]	ARG	4.0
1	A	272	GLU	3.6
1	B	252	GLY	3.6
1	B	113	GLU	3.6
1	D	128	GLY	3.5
1	A	79[A]	ARG	3.5
1	A	273	ALA	3.2
1	C	239	ASP	3.2
1	A	131	TRP	3.2
1	C	80	PRO	3.2
1	B	276	LEU	3.1
1	C	246	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	226	SER	3.0
1	C	274	LEU	2.9
1	B	268	LYS	2.9
1	A	274	LEU	2.8
1	C	237	LEU	2.8
1	A	268	LYS	2.8
1	D	270[A]	LEU	2.7
1	C	216	ALA	2.7
1	B	127	VAL	2.6
1	C	259	LEU	2.6
1	D	82	ASP	2.6
1	B	125	ARG	2.6
1	B	109	PHE	2.6
1	D	272	GLU	2.5
1	C	218	ALA	2.5
1	D	163	PRO	2.5
1	B	136	ILE	2.5
1	B	138	VAL	2.5
1	B	112	PRO	2.5
1	B	88	LEU	2.4
1	C	235	GLY	2.4
1	C	234	ASP	2.4
1	D	266	ASP	2.4
1	B	163	PRO	2.4
1	C	204	LEU	2.4
1	B	265	GLU	2.4
1	D	109	PHE	2.3
1	B	272	GLU	2.3
1	B	82	ASP	2.3
1	A	81	GLU	2.3
1	D	124	LEU	2.3
1	C	160	GLY	2.3
1	D	269	GLY	2.3
1	C	211	ALA	2.3
1	D	271	ALA	2.3
1	B	123	VAL	2.3
1	D	138	VAL	2.3
1	B	128	GLY	2.2
1	B	176	ARG	2.2
1	D	186	TYR	2.2
1	B	131	TRP	2.2
1	C	184	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	133	ARG	2.2
1	D	125	ARG	2.2
1	C	128	GLY	2.2
1	B	132	HIS	2.2
1	A	241	ALA	2.2
1	C	168	LEU	2.2
1	C	257	ARG	2.2
1	D	115	VAL	2.2
1	D	129	GLU	2.2
1	D	227	GLU	2.2
1	C	273	ALA	2.2
1	D	119	LEU	2.1
1	D	246	LEU	2.1
1	B	271	ALA	2.1
1	C	209	ALA	2.1
1	D	110	TRP	2.1
1	C	238	LYS	2.1
1	C	83	LEU	2.1
1	A	219	VAL	2.1
1	C	264	MET	2.1
1	A	254[A]	GLU	2.1
1	C	254	GLU	2.1
1	C	263	TYR	2.1
1	A	208	ARG	2.1
1	D	264	MET	2.0
1	A	141	GLU	2.0
1	B	105	ARG	2.0
1	C	176[A]	ARG	2.0
1	C	244	VAL	2.0
1	C	230	ARG	2.0
1	D	133	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

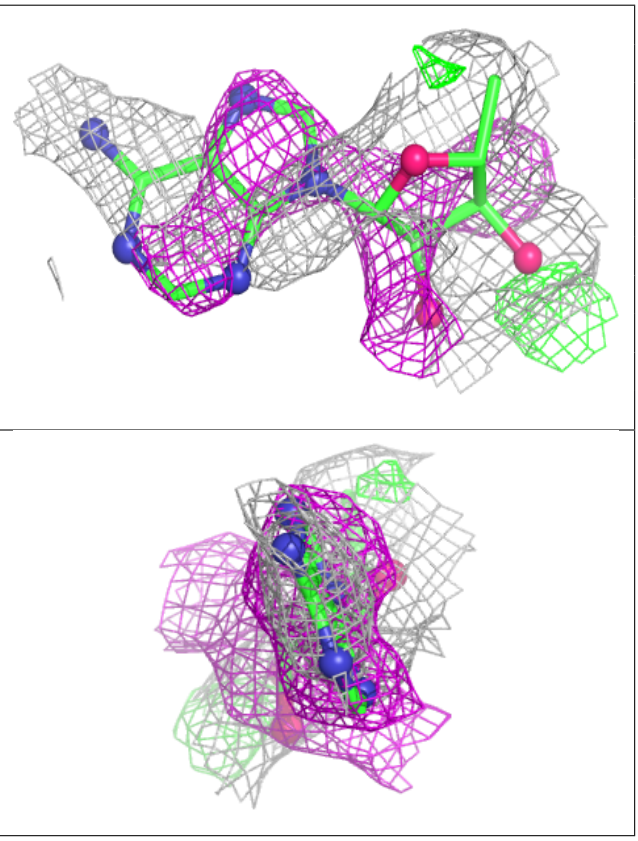
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5AD	B	401	18/18	0.38	0.24	57,62,64,65	0
2	5AD	A	401	18/18	0.44	0.22	50,53,57,61	0
2	5AD	D	401	18/18	0.58	0.20	57,58,60,60	0
2	5AD	C	401	18/18	0.80	0.13	42,43,45,45	0
3	B12	B	402	91/91	0.85	0.14	50,61,65,68	0
3	B12	D	402	91/91	0.86	0.14	48,56,60,64	0
3	B12	A	402	91/91	0.88	0.13	44,53,58,60	0
3	B12	C	402	91/91	0.89	0.12	44,47,57,63	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.

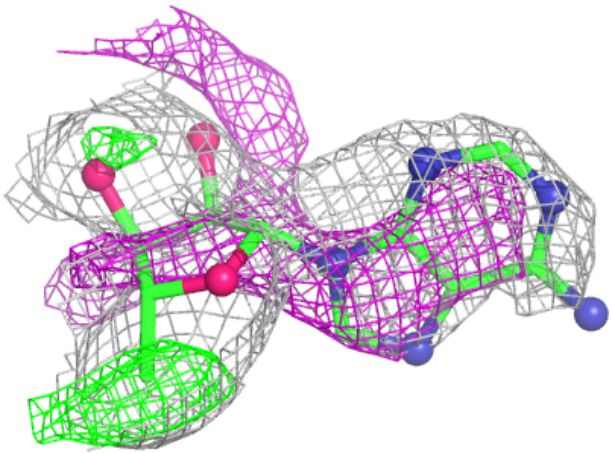
Electron density around 5AD B 401:

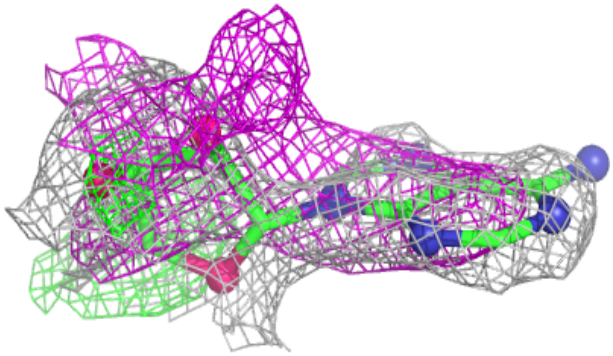
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

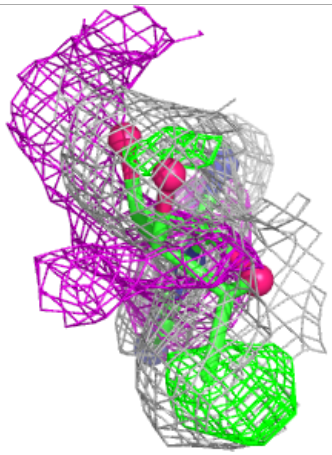


Electron density around 5AD A 401:

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

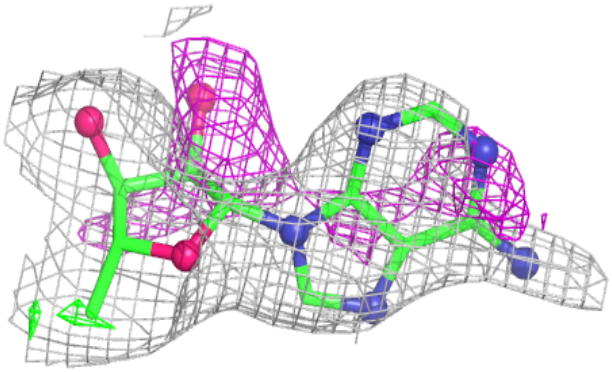


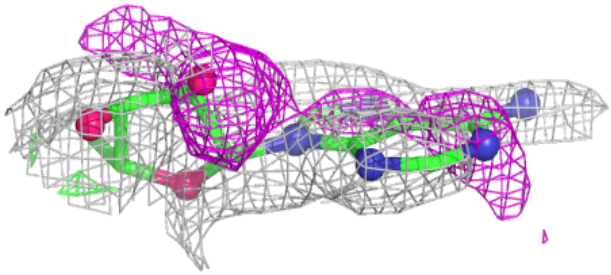


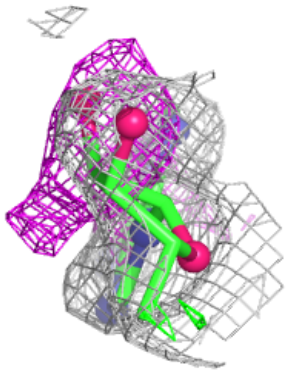


Electron density around 5AD D 401:

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

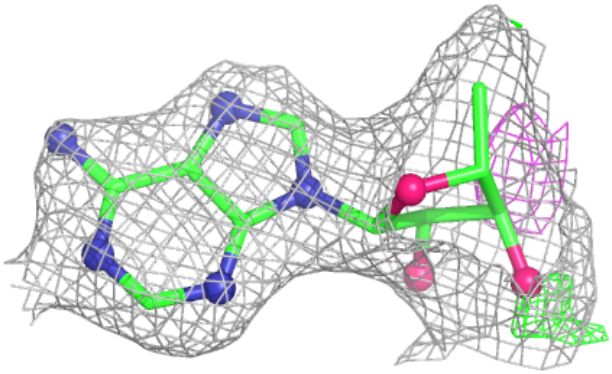


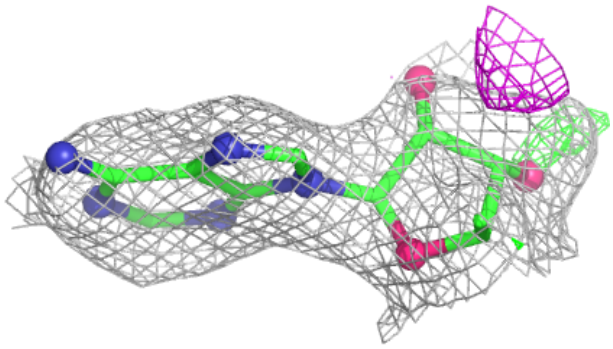


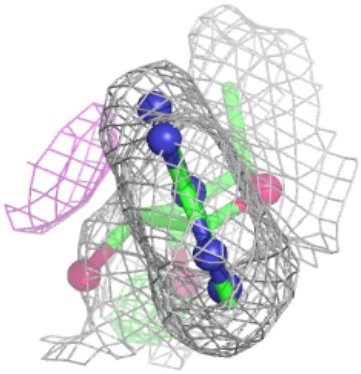


Electron density around 5AD C 401:

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

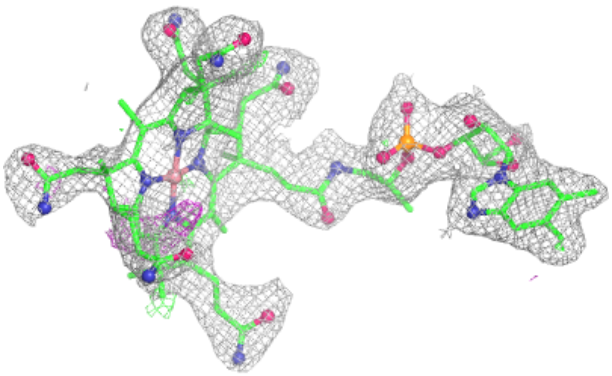


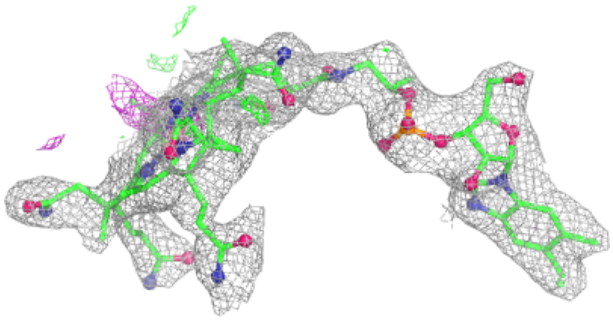


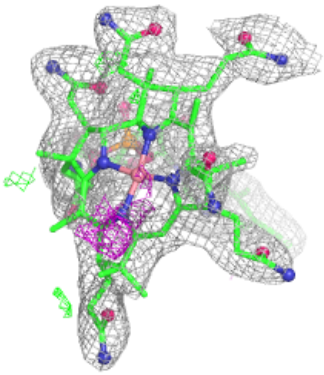


Electron density around B12 B 402:

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

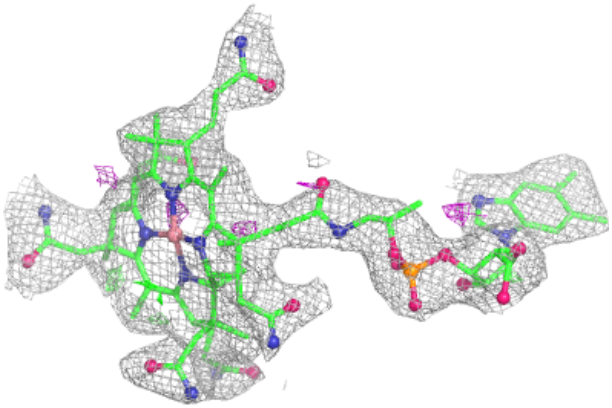


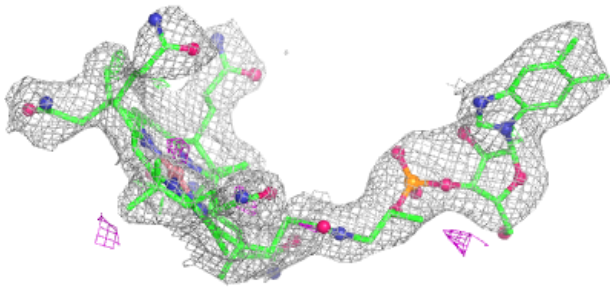


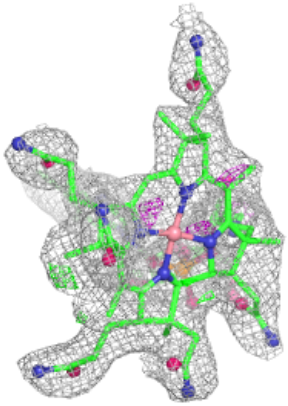


Electron density around B12 D 402:

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

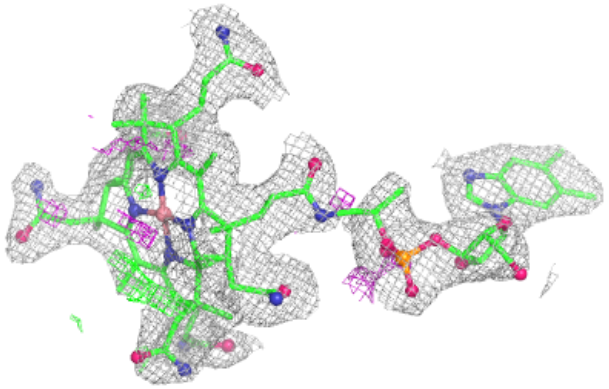


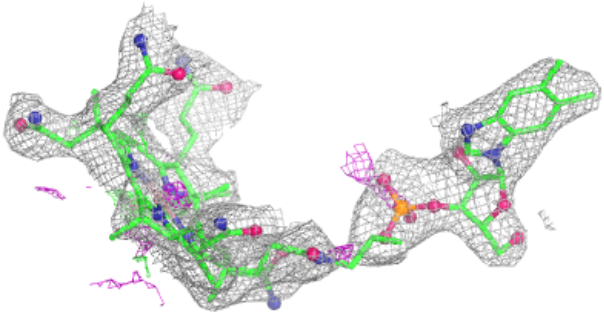


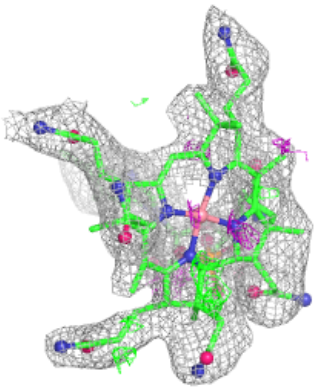


Electron density around B12 A 402:

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

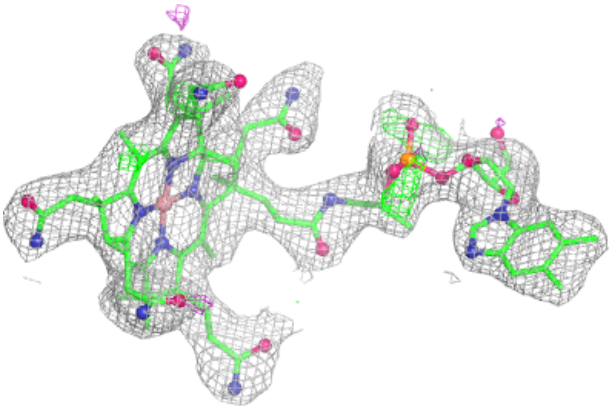


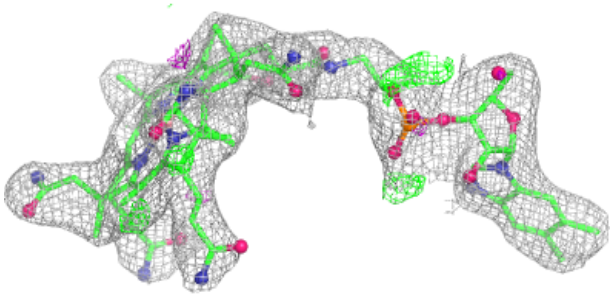


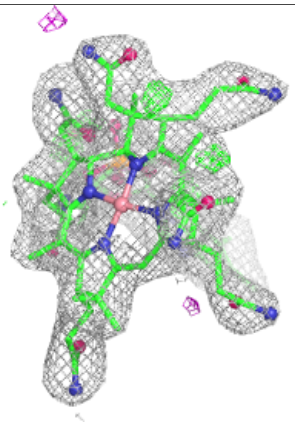


Electron density around B12 C 402:

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







6.5 Other polymers (i)

There are no such residues in this entry.