Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 02:19 PM EDT

PDB ID	:	7RUV
Title	:	Structure of Human ATP:Cobalamin Adenosyltransferase E193K bound to adenosylcobalamin
Authors	:	Mascarenhas, R.; Gouda, H.; Koutmos, M.; Banerjee, R.
Deposited on	:	2021-08-18
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

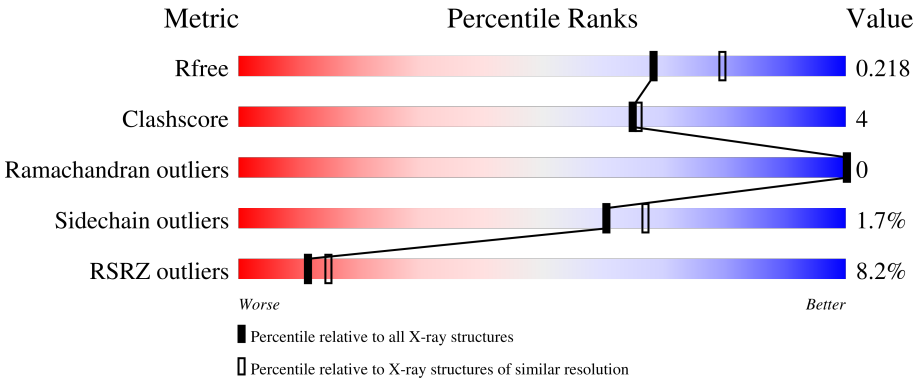
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	196	6% 71% 5% 23%
1	B	196	8% 72% · 25%
1	C	196	6% 74% · 23%
1	D	196	6% 73% · 23%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5180 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 Corrinoid adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1163	742	195	221	5			
1	B	147	Total	C	N	O	S	0	0	0
			1137	728	191	212	6			
1	C	151	Total	C	N	O	S	0	0	0
			1160	739	194	221	6			
1	D	151	Total	C	N	O	S	0	0	0
			1162	741	196	221	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP Q96EY8
A	193	LYS	GLU	engineered mutation	UNP Q96EY8
B	55	MET	-	initiating methionine	UNP Q96EY8
B	193	LYS	GLU	engineered mutation	UNP Q96EY8
C	55	MET	-	initiating methionine	UNP Q96EY8
C	193	LYS	GLU	engineered mutation	UNP Q96EY8
D	55	MET	-	initiating methionine	UNP Q96EY8
D	193	LYS	GLU	engineered mutation	UNP Q96EY8

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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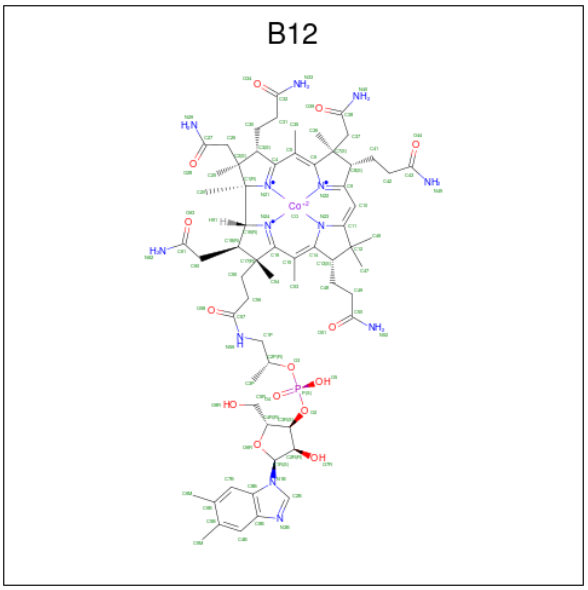
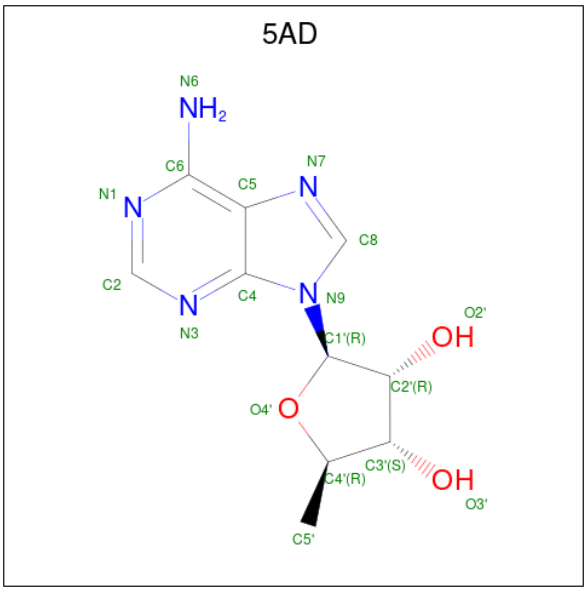
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



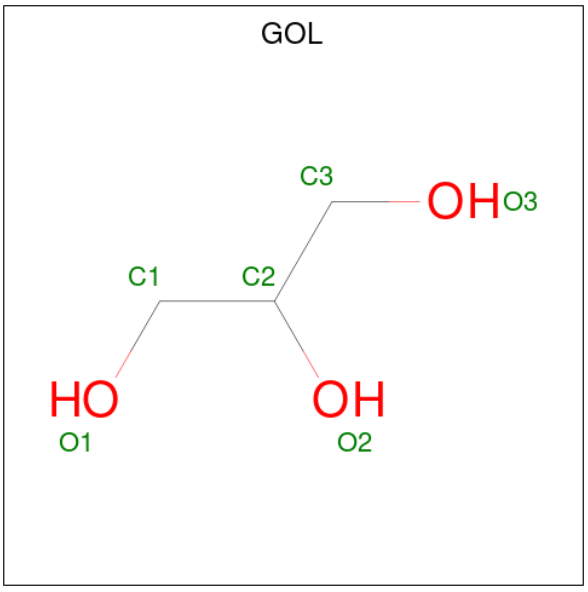
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Co N O P 91 62 1 13 14 1	0	0
4	B	1	Total C Co N O P 91 62 1 13 14 1	0	0
4	C	1	Total C Co N O P 91 62 1 13 14 1	0	0
4	D	1	Total C Co N O P 91 62 1 13 14 1	0	0

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



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

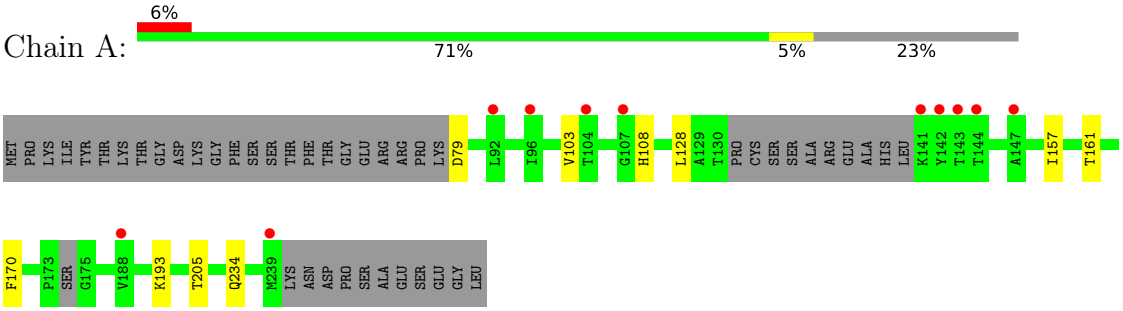
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0
7	B	24	Total O 24 24	0	0
7	C	32	Total O 32 32	0	0
7	D	21	Total O 21 21	0	0

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.

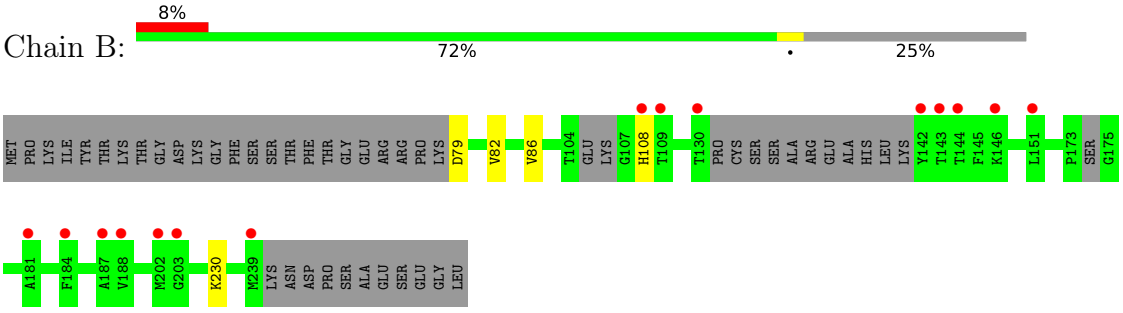
• Molecule 1: Corrinoid adenosyltransferase

Chain A:



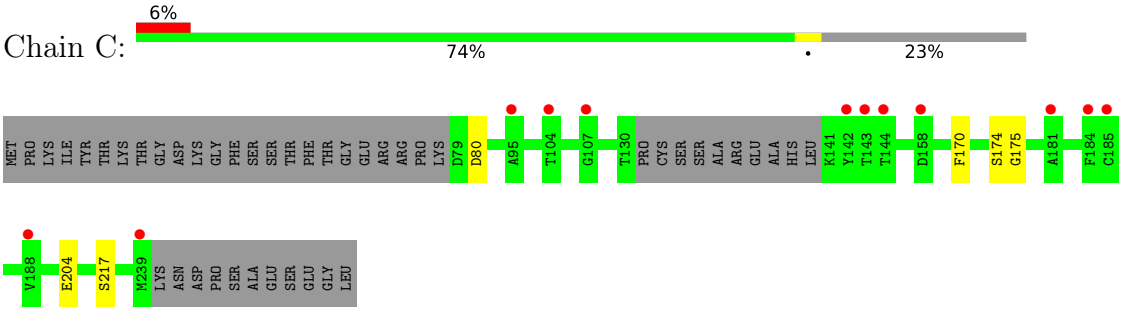
• Molecule 1: Corrinoid adenosyltransferase

Chain B:



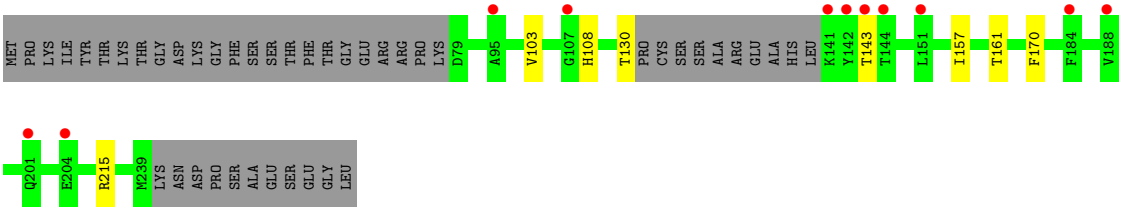
• Molecule 1: Corrinoid adenosyltransferase

Chain C:



• Molecule 1: Corrinoid adenosyltransferase

Chain D:


MET
PRO
LYS
ILE
TYR
THR
LYS
THR
GLY
ASP
LYS
GLY
PHE
SER
SER
THR
PHE
THR
GLY
GLU
ARG
ARG
PRO
LYS
D79
A95
V103
G107
H108
T130
PRO
CYS
SER
SER
ALA
ARG
GLU
ALA
HIS
LEU
K141
Y142
T143
T144
L151
I157
T161
F170
F184
V188
Q201
E204
R215
M239
LYS
ASN
ASP
PRO
SER
ALA
GLU
SER
GLU
GLY
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	121.18Å 121.18Å 169.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.00 – 2.10 33.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (33.00-2.10) 96.0 (33.00-2.10)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.185 , 0.217 0.185 , 0.218	Depositor DCC
R_{free} test set	2625 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5180	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, MG, 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	0.43	0/1182	0.49	0/1598
1	B	0.41	0/1155	0.51	0/1559
1	C	0.40	0/1180	0.50	0/1599
1	D	0.37	0/1182	0.46	0/1601
All	All	0.41	0/4699	0.49	0/6357

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

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	1163	0	1154	4	0
1	B	1137	0	1135	3	0
1	C	1160	0	1141	2	0
1	D	1162	0	1149	5	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	91	0	88	9	0
4	B	91	0	88	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	91	0	88	7	0
4	D	91	0	88	10	0
5	A	18	0	10	1	0
5	B	18	0	10	2	0
5	C	18	0	10	1	0
5	D	18	0	10	2	0
6	C	6	0	8	0	0
7	A	36	0	0	0	0
7	B	24	0	0	0	0
7	C	32	0	0	0	0
7	D	21	0	0	0	0
All	All	5180	0	4979	41	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 (41) 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)
4:A:303:B12:O8R	4:A:303:B12:N62	2.23	0.71
4:B:301:B12:H362	4:B:301:B12:H351	1.80	0.63
4:A:303:B12:H59	4:A:303:B12:H5R2	1.63	0.63
4:C:503:B12:H362	4:C:503:B12:H351	1.80	0.61
4:A:303:B12:H362	4:A:303:B12:H351	1.85	0.59
4:D:301:B12:C61	4:D:301:B12:H252	2.36	0.56
1:D:130:THR:HG21	1:D:143:THR:H	1.71	0.56
4:A:303:B12:H601	4:A:303:B12:H252	1.90	0.54
4:D:301:B12:C16	5:D:302:5AD:H4'	2.40	0.52
4:B:301:B12:C16	5:B:302:5AD:H4'	2.39	0.52
1:A:157:ILE:O	1:A:161:THR:HG23	2.10	0.51
4:A:303:B12:C16	5:A:304:5AD:H4'	2.42	0.50
4:C:503:B12:H5R2	4:C:503:B12:H562	1.92	0.50
1:D:103:VAL:HG13	1:D:108:HIS:HB2	1.94	0.49
1:A:128:LEU:HD23	1:A:205:THR:HG21	1.93	0.49
4:C:503:B12:C16	5:C:504:5AD:H4'	2.43	0.49
4:D:301:B12:H621	4:D:301:B12:H18	1.54	0.49
4:C:503:B12:H543	4:C:503:B12:H531	1.96	0.48
4:D:301:B12:H362	4:D:301:B12:H351	1.96	0.48
4:B:301:B12:H331	4:B:301:B12:HM52	1.79	0.47
4:D:301:B12:H562	4:D:301:B12:O8R	2.16	0.46
1:A:170:PHE:CZ	4:A:303:B12:H202	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:303:B12:H5R2	4:A:303:B12:N59	2.29	0.46
1:D:130:THR:HG22	1:D:143:THR:OG1	2.15	0.46
1:C:170:PHE:CZ	4:C:503:B12:H202	2.52	0.45
1:D:170:PHE:CZ	4:D:301:B12:H202	2.52	0.44
4:B:301:B12:H552	4:B:301:B12:H531	1.99	0.44
1:B:79:ASP:HB3	1:B:82:VAL:HG23	2.00	0.44
1:B:230:LYS:HA	1:B:230:LYS:HD2	1.66	0.44
4:D:301:B12:H253	4:D:301:B12:H301	1.79	0.43
4:D:301:B12:H262	4:D:301:B12:H91	1.80	0.43
4:B:301:B12:N24	5:B:302:5AD:H4'	2.34	0.42
4:A:303:B12:H621	4:A:303:B12:C5R	2.32	0.42
1:C:174:SER:OG	1:C:175:GLY:N	2.52	0.42
4:C:503:B12:H5R1	4:C:503:B12:H621	1.84	0.42
1:D:157:ILE:O	1:D:161:THR:OG1	2.34	0.41
1:B:86:VAL:HG11	4:D:301:B12:H13	2.02	0.41
4:D:301:B12:N24	5:D:302:5AD:H4'	2.34	0.41
1:A:103:VAL:HG13	1:A:108:HIS:HB2	2.03	0.41
4:A:303:B12:H543	4:A:303:B12:H531	2.02	0.40
4:C:503:B12:H3	4:C:503:B12:N29	2.37	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	144/196 (74%)	144 (100%)	0	0	100	100
1	B	139/196 (71%)	136 (98%)	3 (2%)	0	100	100
1	C	147/196 (75%)	143 (97%)	4 (3%)	0	100	100
1	D	147/196 (75%)	143 (97%)	4 (3%)	0	100	100
All	All	577/784 (74%)	566 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	122/164 (74%)	119 (98%)	3 (2%)	47	52
1	B	119/164 (73%)	118 (99%)	1 (1%)	81	86
1	C	121/164 (74%)	118 (98%)	3 (2%)	47	52
1	D	121/164 (74%)	120 (99%)	1 (1%)	81	86
All	All	483/656 (74%)	475 (98%)	8 (2%)	60	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	193	LYS
1	A	234	GLN
1	B	108	HIS
1	C	80	ASP
1	C	204	GLU
1	C	217	SER
1	D	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	B12	C	503	-	90,101,101	1.07	6 (6%)	137,166,166	1.63	27 (19%)
5	5AD	C	504	-	17,20,20	2.01	5 (29%)	15,30,30	1.82	4 (26%)
5	5AD	B	302	-	17,20,20	1.75	4 (23%)	15,30,30	1.77	4 (26%)
4	B12	D	301	-	90,101,101	1.06	4 (4%)	137,166,166	1.63	24 (17%)
4	B12	A	303	-	90,101,101	1.08	4 (4%)	137,166,166	1.58	26 (18%)
5	5AD	D	302	-	17,20,20	2.13	6 (35%)	15,30,30	1.76	4 (26%)
4	B12	B	301	-	90,101,101	1.05	3 (3%)	137,166,166	1.59	27 (19%)
5	5AD	A	304	-	17,20,20	1.98	5 (29%)	15,30,30	1.82	5 (33%)
6	GOL	C	501	-	5,5,5	0.66	0	5,5,5	1.09	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
4	B12	C	503	-	-	7/52/223/223	0/3/11/11
5	5AD	C	504	-	-	0/0/20/20	0/3/3/3
5	5AD	B	302	-	-	0/0/20/20	0/3/3/3
4	B12	D	301	-	-	9/52/223/223	0/3/11/11
4	B12	A	303	-	-	8/52/223/223	0/3/11/11
5	5AD	D	302	-	-	0/0/20/20	0/3/3/3
4	B12	B	301	-	-	5/52/223/223	0/3/11/11
5	5AD	A	304	-	-	0/0/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	501	-	-	2/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	302	5AD	O4'-C1'	4.76	1.47	1.41
5	C	504	5AD	O4'-C1'	4.23	1.47	1.41
4	D	301	B12	C14-N23	4.10	1.40	1.35
5	A	304	5AD	C2'-C1'	3.93	1.59	1.53
5	C	504	5AD	C2'-C1'	3.86	1.59	1.53
4	A	303	B12	C14-N23	3.63	1.39	1.35
5	C	504	5AD	O2'-C2'	-3.55	1.34	1.43
5	D	302	5AD	O2'-C2'	-3.51	1.34	1.43
5	B	302	5AD	C2'-C1'	3.46	1.59	1.53
5	A	304	5AD	O4'-C1'	3.44	1.45	1.41
5	B	302	5AD	O2'-C2'	-3.43	1.34	1.43
4	B	301	B12	C14-N23	3.30	1.39	1.35
5	A	304	5AD	O2'-C2'	-3.26	1.35	1.43
4	B	301	B12	C54-C17	3.17	1.60	1.54
5	B	302	5AD	O3'-C3'	-3.16	1.35	1.43
5	D	302	5AD	O3'-C3'	-3.13	1.35	1.43
5	A	304	5AD	O3'-C3'	-3.11	1.35	1.43
4	C	503	B12	C14-N23	3.05	1.39	1.35
5	D	302	5AD	C3'-C4'	2.98	1.56	1.52
4	B	301	B12	C35-C5	2.94	1.57	1.50
4	A	303	B12	C35-C5	2.92	1.57	1.50
4	C	503	B12	C54-C17	2.91	1.59	1.54
5	C	504	5AD	O3'-C3'	-2.78	1.36	1.43
5	C	504	5AD	C2-N3	2.74	1.36	1.32
4	D	301	B12	C54-C17	2.73	1.59	1.54
5	A	304	5AD	C2-N3	2.56	1.36	1.32
5	D	302	5AD	C2'-C1'	2.54	1.57	1.53
4	C	503	B12	C35-C5	2.52	1.56	1.50
4	A	303	B12	C54-C17	2.46	1.58	1.54
4	D	301	B12	C35-C5	2.28	1.55	1.50
5	D	302	5AD	C2-N3	2.27	1.35	1.32
5	B	302	5AD	C4-N3	2.24	1.38	1.35
4	D	301	B12	C55-C17	-2.19	1.49	1.54
4	C	503	B12	C3R-C4R	2.14	1.58	1.52
4	C	503	B12	C30-C3	2.12	1.59	1.54
4	C	503	B12	C6B-C5B	2.04	1.46	1.40
4	A	303	B12	C6B-C5B	2.00	1.45	1.40

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	B12	C7B-C8B-C9B	5.95	126.43	120.54
4	A	303	B12	C7B-C8B-C9B	5.77	126.25	120.54
4	D	301	B12	C7B-C8B-C9B	5.58	126.06	120.54
4	A	303	B12	C18-C17-C16	5.08	106.84	100.67
4	D	301	B12	C18-C17-C16	5.07	106.83	100.67
4	C	503	B12	C54-C17-C18	-4.80	105.89	112.98
4	B	301	B12	C7B-C8B-C9B	4.75	125.24	120.54
4	B	301	B12	C18-C17-C16	4.73	106.42	100.67
4	C	503	B12	C18-C17-C16	4.71	106.39	100.67
4	D	301	B12	C54-C17-C18	-4.70	106.04	112.98
4	D	301	B12	C2P-C1P-N59	-4.50	106.30	112.93
4	B	301	B12	C56-C55-C17	-4.41	107.02	115.52
4	C	503	B12	C2P-C1P-N59	-4.29	106.61	112.93
4	B	301	B12	C54-C17-C18	-4.28	106.67	112.98
4	D	301	B12	C1P-N59-C57	-4.22	113.50	122.69
4	A	303	B12	C56-C55-C17	-4.09	107.63	115.52
4	B	301	B12	C2P-C1P-N59	-3.98	107.06	112.93
4	D	301	B12	C56-C55-C17	-3.98	107.85	115.52
4	D	301	B12	C13-C14-C15	-3.79	118.52	124.32
5	C	504	5AD	N3-C2-N1	3.70	134.46	128.68
4	D	301	B12	C16-C15-C14	-3.68	115.66	121.25
4	B	301	B12	C17-C16-N24	-3.68	105.47	111.15
4	A	303	B12	C54-C17-C16	-3.68	93.29	112.40
5	A	304	5AD	N3-C2-N1	3.65	134.38	128.68
4	C	503	B12	C16-C15-C14	-3.65	115.72	121.25
5	D	302	5AD	N3-C2-N1	3.64	134.37	128.68
4	A	303	B12	C17-C16-N24	-3.64	105.55	111.15
4	D	301	B12	C17-C16-N24	-3.63	105.56	111.15
5	B	302	5AD	N3-C2-N1	3.61	134.33	128.68
4	B	301	B12	C15-C16-N24	3.61	127.62	122.42
4	C	503	B12	C54-C17-C16	-3.35	95.01	112.40
4	C	503	B12	C13-C14-C15	-3.32	119.25	124.32
4	A	303	B12	C54-C17-C18	-3.29	108.13	112.98
4	D	301	B12	C54-C17-C16	-3.16	95.97	112.40
5	B	302	5AD	C4-C5-N7	3.15	112.68	109.40
4	D	301	B12	C55-C17-C16	3.15	122.86	116.65
4	C	503	B12	C5M-C5B-C6B	-3.14	114.29	120.74
4	B	301	B12	C54-C17-C16	-3.14	96.09	112.40
4	C	503	B12	C15-C16-N24	3.09	126.88	122.42
4	B	301	B12	C5B-C4B-C9B	-3.09	116.85	121.22
5	D	302	5AD	C4-C5-N7	3.06	112.59	109.40
4	C	503	B12	C1P-N59-C57	-3.04	116.06	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	B12	C5M-C5B-C6B	-3.03	114.53	120.74
4	A	303	B12	C1P-N59-C57	-3.01	116.14	122.69
4	C	503	B12	C5B-C4B-C9B	-3.00	116.97	121.22
4	A	303	B12	C2P-C1P-N59	-2.98	108.54	112.93
4	B	301	B12	C16-C15-C14	-2.98	116.73	121.25
4	A	303	B12	C5B-C4B-C9B	-2.97	117.01	121.22
4	B	301	B12	C13-C14-C15	-2.96	119.80	124.32
4	C	503	B12	C56-C55-C17	-2.95	109.82	115.52
5	A	304	5AD	C5'-C4'-C3'	-2.93	112.62	115.70
4	A	303	B12	C15-C16-N24	2.93	126.64	122.42
4	A	303	B12	C16-C15-C14	-2.92	116.82	121.25
4	D	301	B12	C15-C16-N24	2.92	126.62	122.42
5	B	302	5AD	C5'-C4'-C3'	-2.88	112.68	115.70
4	C	503	B12	C17-C16-N24	-2.86	106.74	111.15
5	C	504	5AD	C4-C5-N7	2.86	112.38	109.40
5	C	504	5AD	C5'-C4'-C3'	-2.86	112.70	115.70
4	C	503	B12	C55-C17-C16	2.85	122.28	116.65
4	D	301	B12	C5B-C4B-C9B	-2.83	117.21	121.22
4	A	303	B12	C1-C19-C18	-2.72	117.42	121.88
4	A	303	B12	C55-C17-C16	2.71	122.01	116.65
4	C	503	B12	O6R-C1R-C2R	-2.71	102.97	106.93
5	A	304	5AD	C2-N1-C6	-2.70	114.14	118.75
5	B	302	5AD	C2-N1-C6	-2.67	114.19	118.75
4	B	301	B12	O58-C57-N59	2.67	128.05	123.01
5	D	302	5AD	C2-N1-C6	-2.63	114.26	118.75
4	B	301	B12	C53-C15-C16	2.62	124.89	120.38
4	B	301	B12	C13-C14-N23	2.62	112.67	109.10
5	C	504	5AD	C2-N1-C6	-2.57	114.36	118.75
4	D	301	B12	C5M-C5B-C6B	-2.57	115.47	120.74
4	B	301	B12	C55-C17-C18	2.57	116.11	111.15
4	A	303	B12	C13-C14-C15	-2.56	120.41	124.32
4	A	303	B12	C5M-C5B-C6B	-2.54	115.53	120.74
4	A	303	B12	C31-C32-N33	2.52	124.36	116.51
5	A	304	5AD	C4-C5-N7	2.51	112.02	109.40
4	C	503	B12	C4B-C9B-C8B	-2.49	118.55	121.10
5	D	302	5AD	C5'-C4'-C3'	-2.48	113.09	115.70
4	A	303	B12	C53-C15-C16	2.45	124.60	120.38
4	C	503	B12	C18-C19-N24	2.42	106.00	102.31
4	C	503	B12	C2-C1-C19	-2.41	114.80	118.60
4	A	303	B12	C26-C2-C1	-2.39	106.28	110.01
4	A	303	B12	C18-C19-N24	2.38	105.93	102.31
4	A	303	B12	C4B-C5B-C6B	2.37	123.91	119.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	B12	C4B-C5B-C6B	2.37	123.90	119.91
4	B	301	B12	C56-C57-N59	-2.33	112.50	116.42
4	A	303	B12	C55-C17-C18	2.31	115.62	111.15
4	A	303	B12	O2-C3R-C2R	2.29	119.99	111.68
4	C	503	B12	C1-C19-C18	-2.29	118.13	121.88
4	C	503	B12	C4B-C5B-C6B	2.27	123.73	119.91
4	B	301	B12	C31-C32-N33	2.25	123.51	116.51
4	A	303	B12	C4B-C9B-C8B	-2.25	118.80	121.10
4	D	301	B12	C4B-C5B-C6B	2.24	123.69	119.91
5	A	304	5AD	C5-C6-N6	2.24	123.75	120.35
4	B	301	B12	C55-C17-C16	2.20	120.99	116.65
4	D	301	B12	C53-C15-C16	2.19	124.15	120.38
4	B	301	B12	C20-C1-C19	2.17	111.44	109.36
4	C	503	B12	O6R-C4R-C5R	-2.17	104.53	109.21
4	C	503	B12	O3-C2P-C1P	-2.16	102.60	106.92
4	B	301	B12	C25-C2-C26	2.16	114.07	109.71
4	C	503	B12	O28-C27-N29	-2.15	116.62	122.50
4	D	301	B12	O2-C3R-C2R	2.15	119.47	111.68
4	D	301	B12	C4B-C9B-C8B	-2.15	118.90	121.10
4	C	503	B12	C55-C17-C18	2.14	115.30	111.15
4	A	303	B12	O6R-C1R-C2R	-2.13	103.81	106.93
4	D	301	B12	O51-C50-C49	-2.13	114.81	121.07
4	D	301	B12	C30-C3-C4	2.13	114.58	109.63
4	C	503	B12	O44-C43-N45	-2.11	116.73	122.50
4	D	301	B12	C2-C26-C27	-2.10	109.31	115.22
4	D	301	B12	C31-C30-C3	-2.10	108.67	114.73
4	A	303	B12	O28-C27-N29	-2.08	116.82	122.50
4	B	301	B12	O28-C27-N29	-2.08	116.83	122.50
4	C	503	B12	O2-C3R-C2R	2.07	119.18	111.68
4	B	301	B12	C2-C1-C19	-2.05	115.36	118.60
4	C	503	B12	C53-C15-C16	2.05	123.91	120.38
4	B	301	B12	C36-C7-C37	2.04	114.17	110.80
4	B	301	B12	O44-C43-N45	-2.04	116.94	122.50
4	B	301	B12	C1-C19-C18	-2.03	118.55	121.88
4	D	301	B12	C25-C2-C26	2.02	113.78	109.71
4	A	303	B12	O44-C43-N45	-2.01	117.00	122.50
4	D	301	B12	O39-C38-C37	-2.01	115.62	121.99

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	B12	C1P-C2P-O3-P
4	A	303	B12	C3P-C2P-O3-P
4	A	303	B12	O6R-C4R-C5R-O8R
4	B	301	B12	C14-C13-C48-C49
4	B	301	B12	C1P-C2P-O3-P
4	B	301	B12	C3P-C2P-O3-P
4	C	503	B12	C1P-C2P-O3-P
4	C	503	B12	C3P-C2P-O3-P
4	D	301	B12	C14-C13-C48-C49
4	D	301	B12	C18-C60-C61-O63
4	D	301	B12	C18-C60-C61-N62
4	D	301	B12	C1P-C2P-O3-P
4	D	301	B12	C3P-C2P-O3-P
6	C	501	GOL	C1-C2-C3-O3
4	C	503	B12	O6R-C4R-C5R-O8R
4	A	303	B12	C3R-C4R-C5R-O8R
4	A	303	B12	C14-C13-C48-C49
4	C	503	B12	C3R-C4R-C5R-O8R
4	D	301	B12	C16-C17-C55-C56
6	C	501	GOL	O2-C2-C3-O3
4	C	503	B12	C14-C13-C48-C49
4	D	301	B12	C3-C30-C31-C32
4	D	301	B12	C4-C3-C30-C31
4	C	503	B12	C18-C60-C61-O63
4	C	503	B12	C18-C60-C61-N62
4	A	303	B12	C18-C60-C61-O63
4	A	303	B12	C42-C41-C8-C9
4	B	301	B12	O6R-C4R-C5R-O8R
4	D	301	B12	C2-C3-C30-C31
4	A	303	B12	C18-C60-C61-N62
4	B	301	B12	C3-C30-C31-C32

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	B12	7	0
5	C	504	5AD	1	0
5	B	302	5AD	2	0
4	D	301	B12	10	0
4	A	303	B12	9	0
5	D	302	5AD	2	0
4	B	301	B12	5	0

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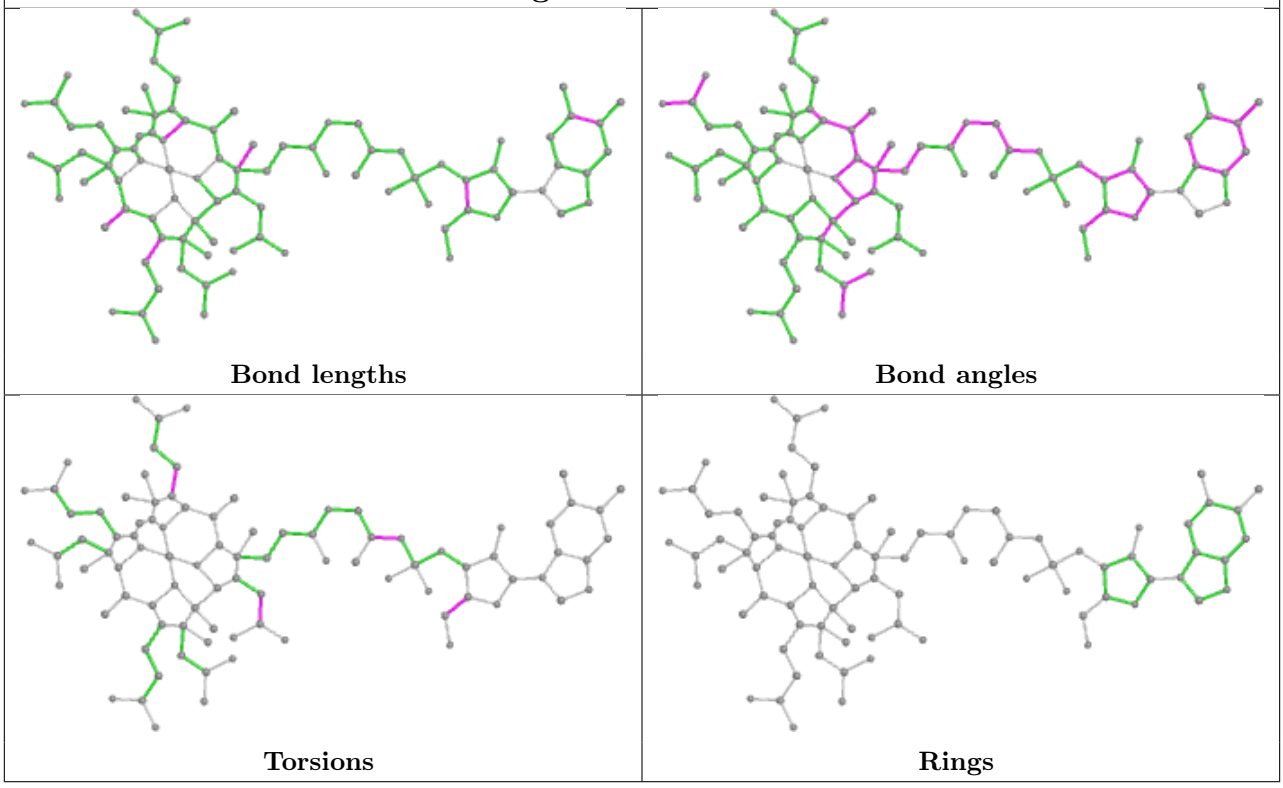
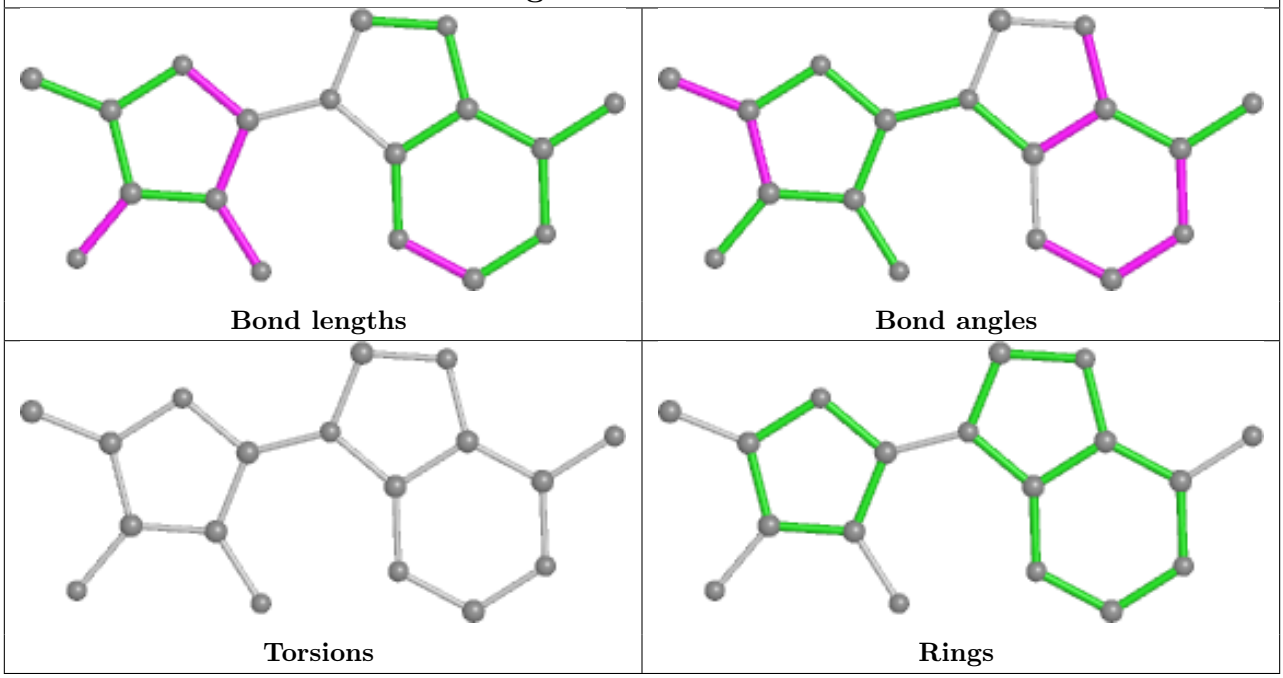
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	5AD	1	0

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

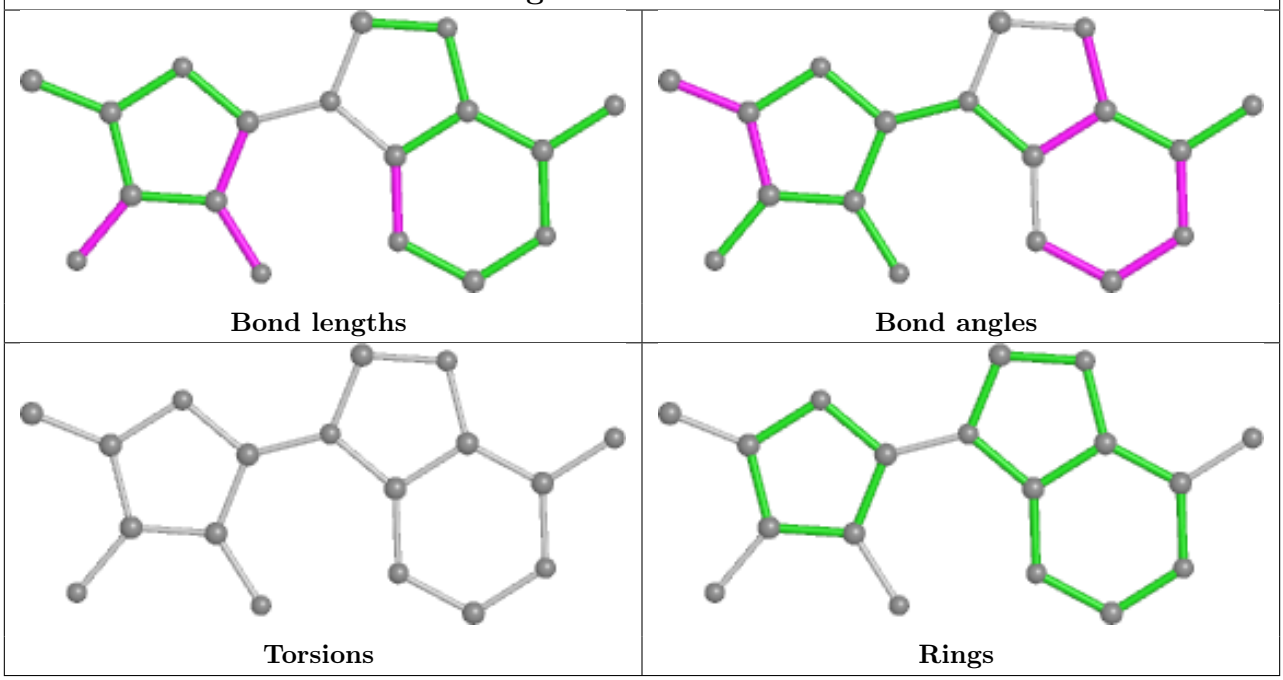
Ligand B12 C 503



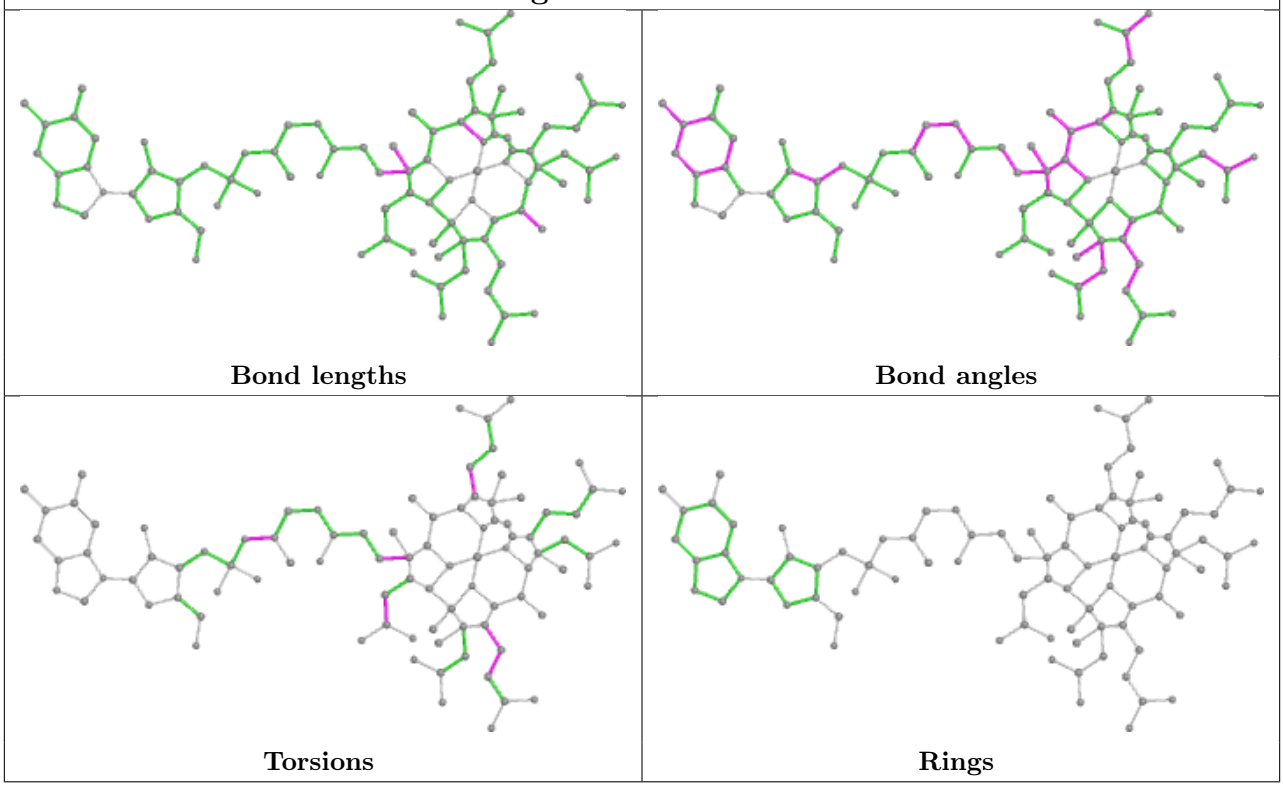
Ligand 5AD C 504



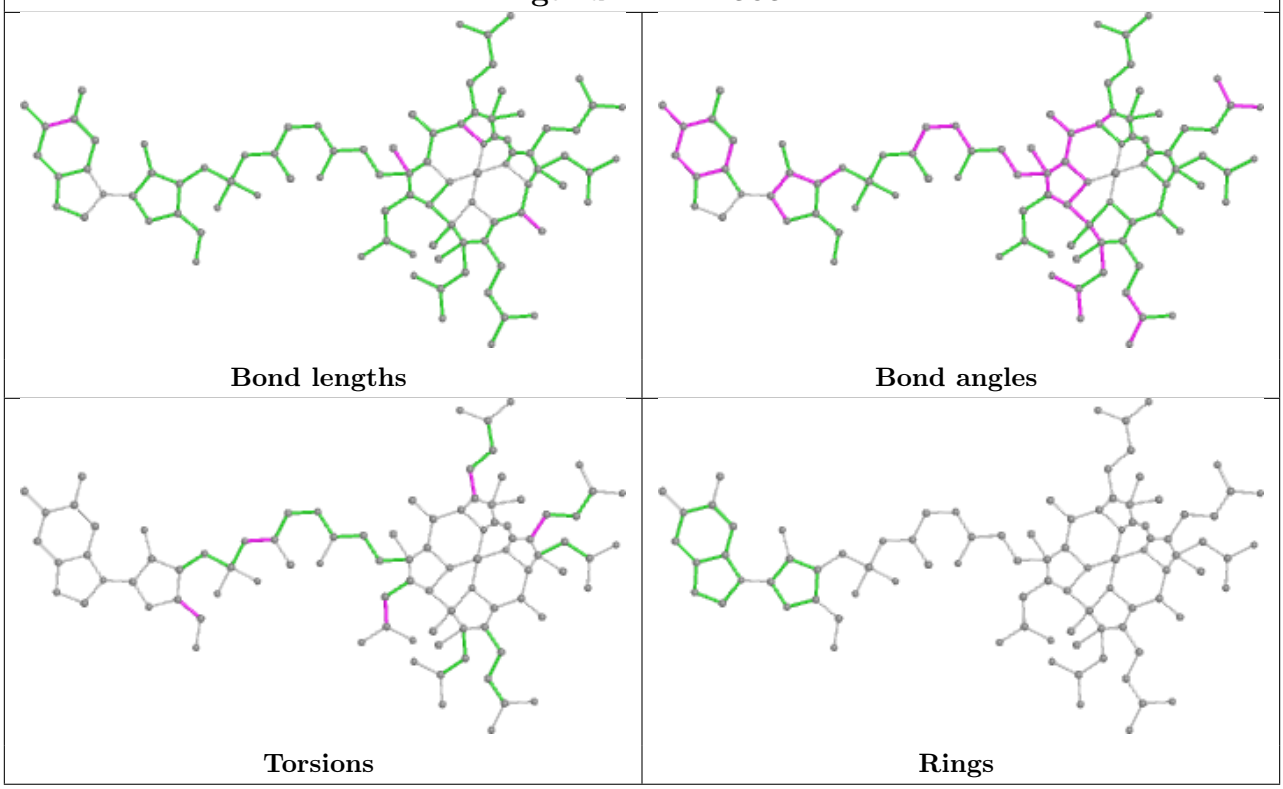
Ligand 5AD B 302



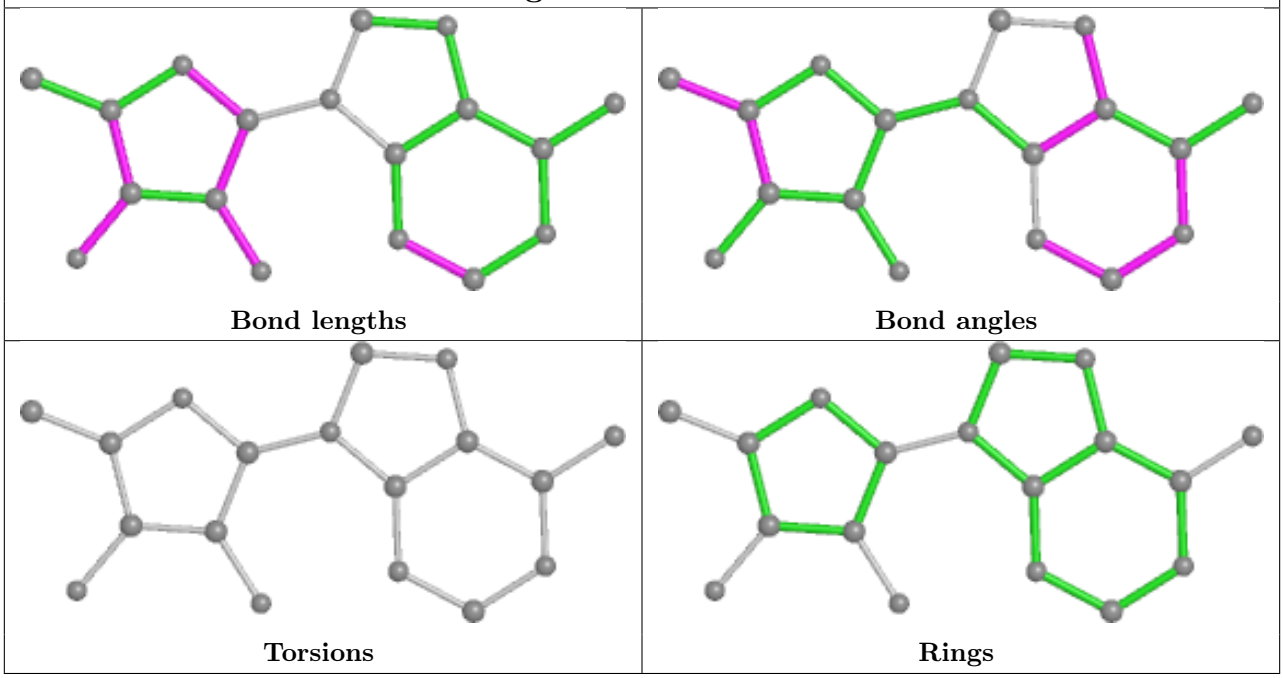
Ligand B12 D 301



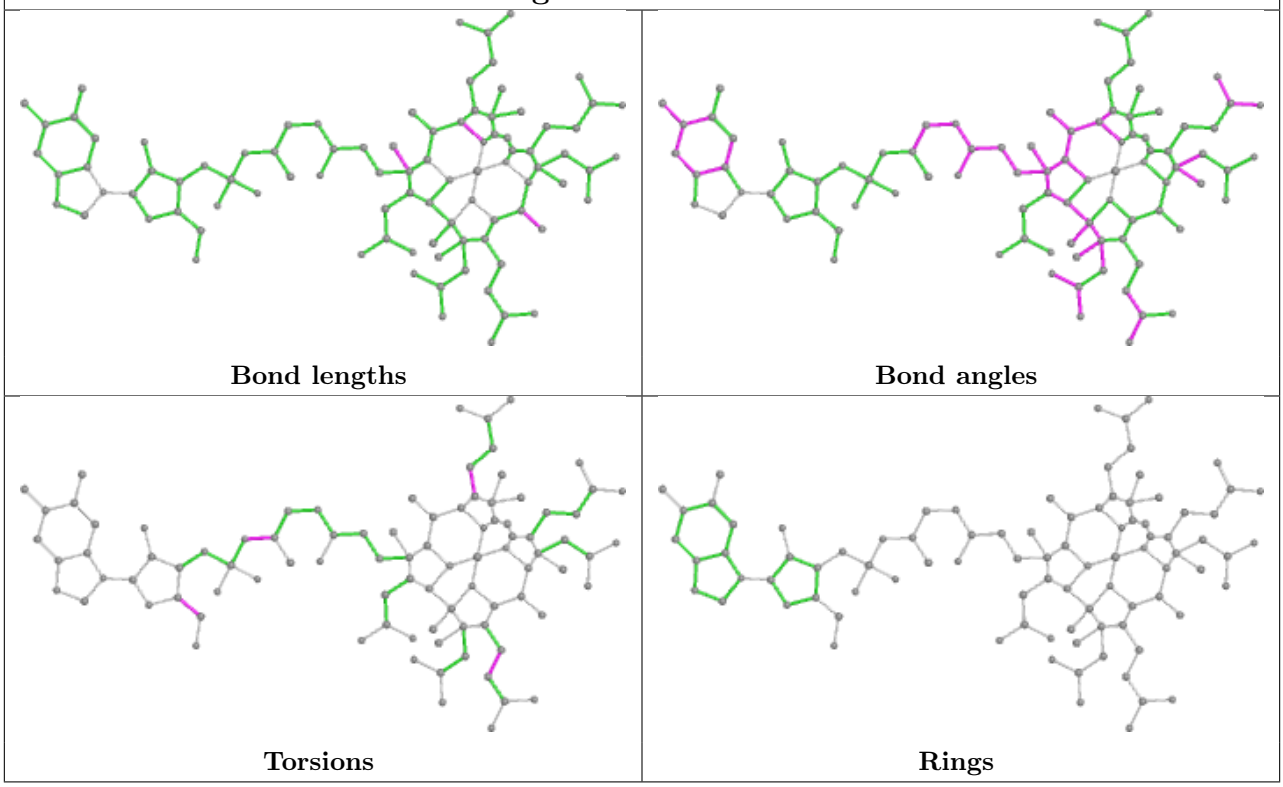
Ligand B12 A 303



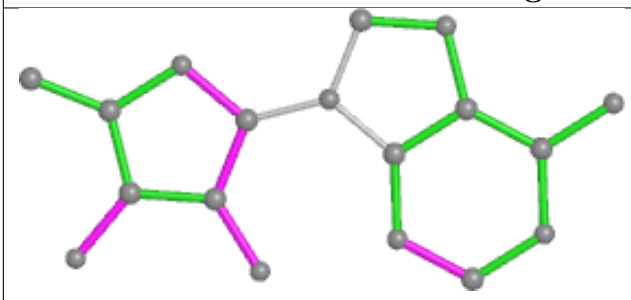
Ligand 5AD D 302



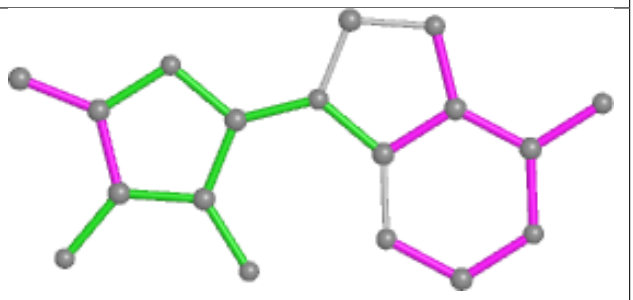
Ligand B12 B 301



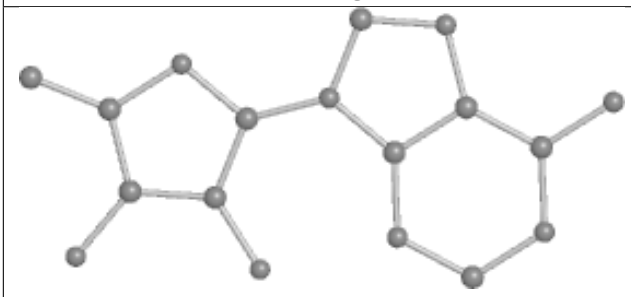
Ligand 5AD A 304



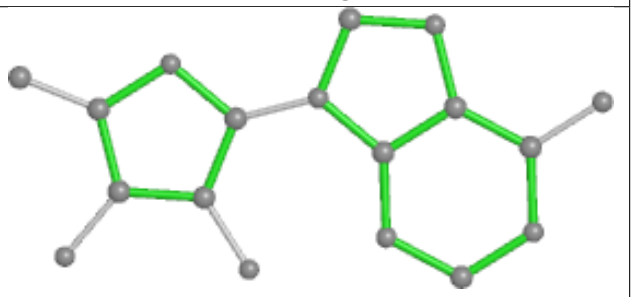
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	150/196 (76%)	0.29	11 (7%) 15 19	32, 43, 69, 91	0
1	B	147/196 (75%)	0.42	15 (10%) 6 8	34, 46, 74, 86	0
1	C	151/196 (77%)	0.29	12 (7%) 12 16	33, 48, 68, 79	0
1	D	151/196 (77%)	0.28	11 (7%) 15 19	34, 48, 73, 87	0
All	All	599/784 (76%)	0.32	49 (8%) 11 15	32, 47, 72, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	TYR	8.0
1	D	142	TYR	5.6
1	A	142	TYR	5.5
1	D	144	THR	4.5
1	C	107	GLY	4.3
1	A	141	LYS	4.3
1	D	107	GLY	4.1
1	B	188	VAL	4.1
1	A	143	THR	4.0
1	B	143	THR	3.9
1	B	144	THR	3.8
1	B	109	THR	3.7
1	A	239	MET	3.7
1	A	144	THR	3.7
1	D	143	THR	3.6
1	A	188	VAL	3.6
1	D	151	LEU	3.5
1	C	143	THR	3.4
1	B	202	MET	3.3
1	B	108	HIS	3.3
1	D	141	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	146	LYS	3.2
1	C	144	THR	3.2
1	B	239	MET	3.2
1	C	184	PHE	3.1
1	A	107	GLY	3.0
1	D	95	ALA	3.0
1	B	130	THR	2.9
1	C	239	MET	2.8
1	B	187	ALA	2.8
1	C	181	ALA	2.7
1	B	203	GLY	2.7
1	C	188	VAL	2.6
1	A	104	THR	2.6
1	C	142	TYR	2.6
1	C	104	THR	2.5
1	B	184	PHE	2.5
1	D	201	GLN	2.4
1	D	188	VAL	2.4
1	C	185	CYS	2.4
1	D	204	GLU	2.4
1	C	95	ALA	2.4
1	B	151	LEU	2.2
1	D	184	PHE	2.2
1	C	158	ASP	2.1
1	A	96	ILE	2.1
1	A	147	ALA	2.1
1	A	92	LEU	2.0
1	B	181	ALA	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 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,

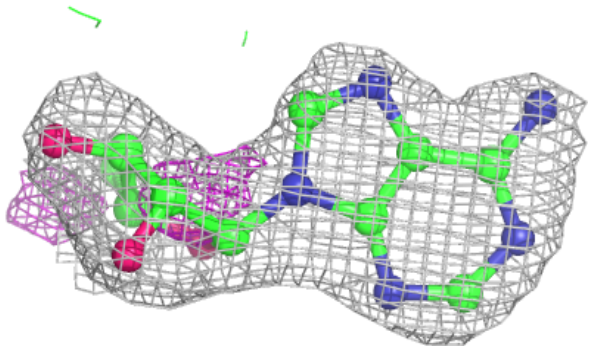
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

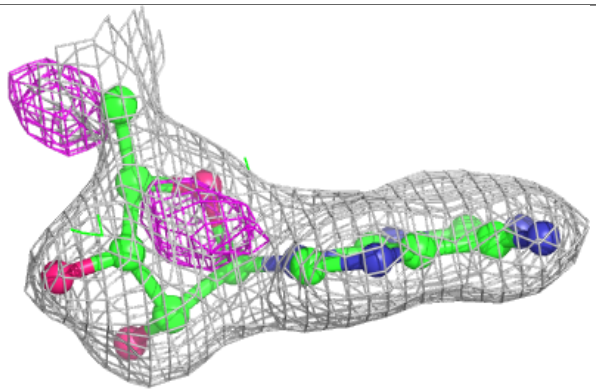
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	501	6/6	0.87	0.19	43,57,61,69	0
3	MG	C	502	1/1	0.91	0.32	36,36,36,36	0
5	5AD	D	302	18/18	0.92	0.17	47,57,62,63	0
5	5AD	A	304	18/18	0.96	0.10	34,41,45,49	0
3	MG	A	302	1/1	0.96	0.29	45,45,45,45	1
4	B12	D	301	91/91	0.96	0.12	41,56,64,77	0
4	B12	B	301	91/91	0.97	0.09	33,40,50,58	0
5	5AD	B	302	18/18	0.97	0.09	32,40,44,45	0
5	5AD	C	504	18/18	0.97	0.10	34,40,43,43	0
4	B12	C	503	91/91	0.97	0.09	32,38,48,54	0
4	B12	A	303	91/91	0.97	0.10	34,41,47,53	0
2	K	A	301	1/1	0.99	0.14	46,46,46,46	1

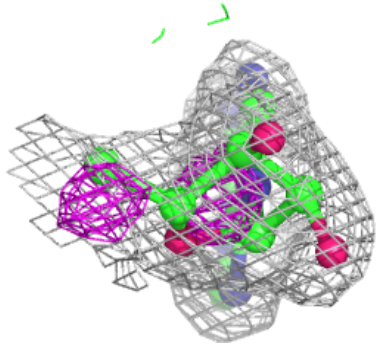
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD D 302:

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

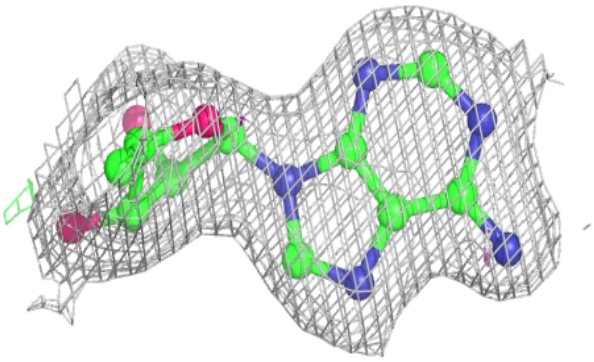


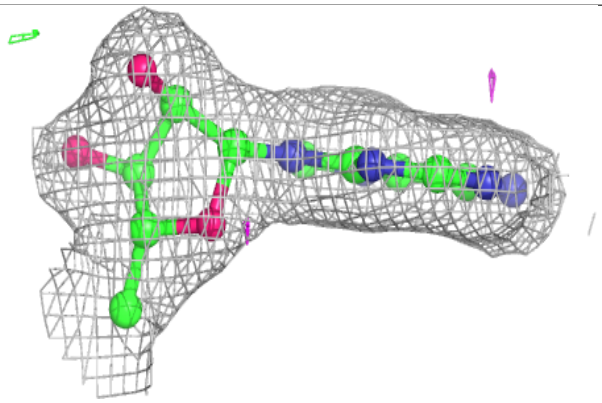


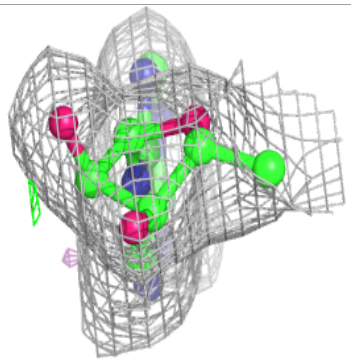


Electron density around 5AD A 304:

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

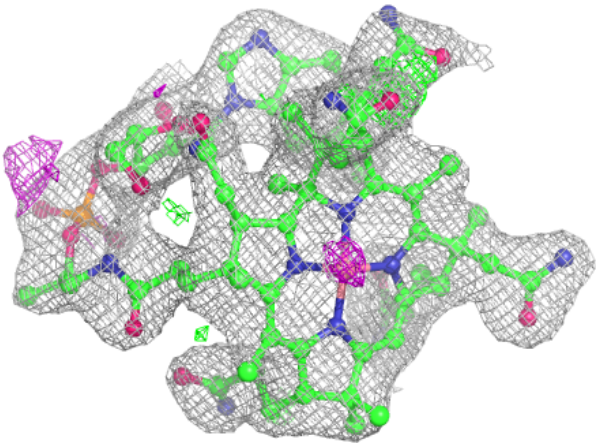


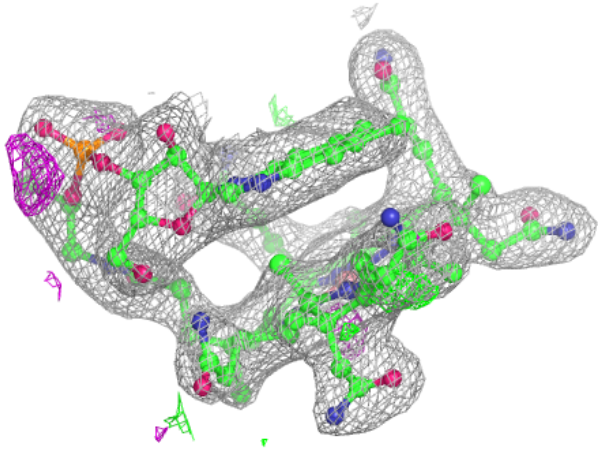


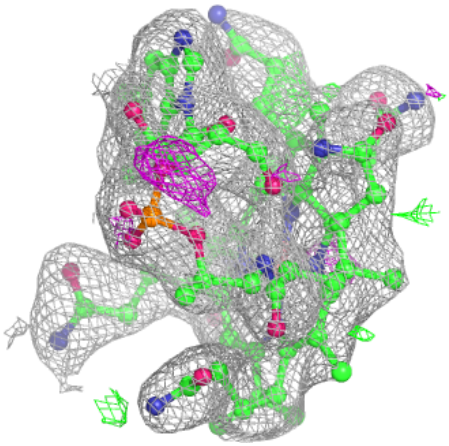


Electron density around B12 D 301:

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

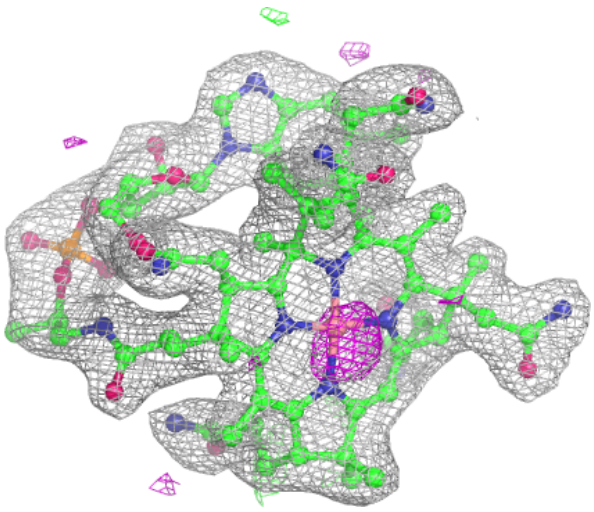


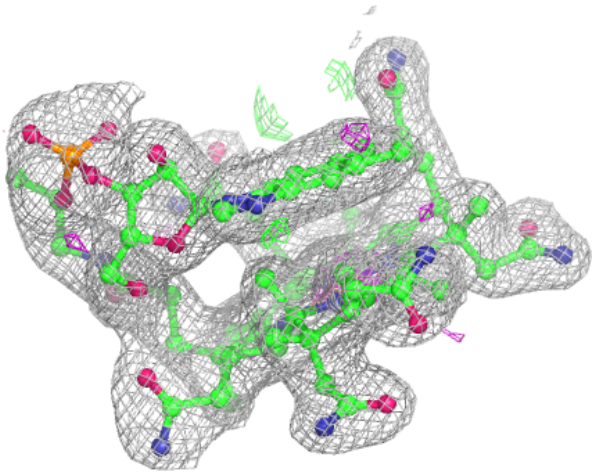


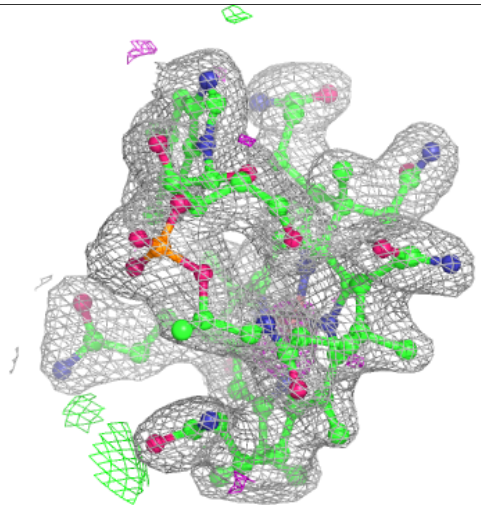


Electron density around B12 B 301:

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

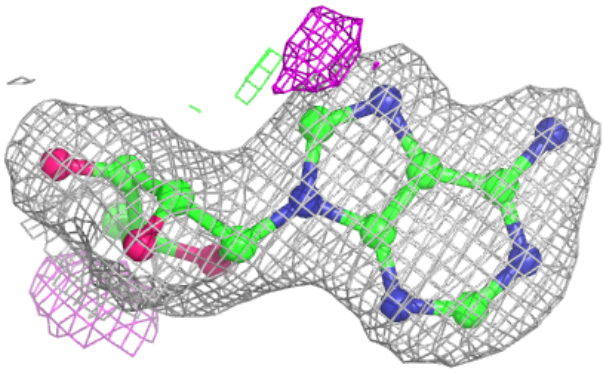


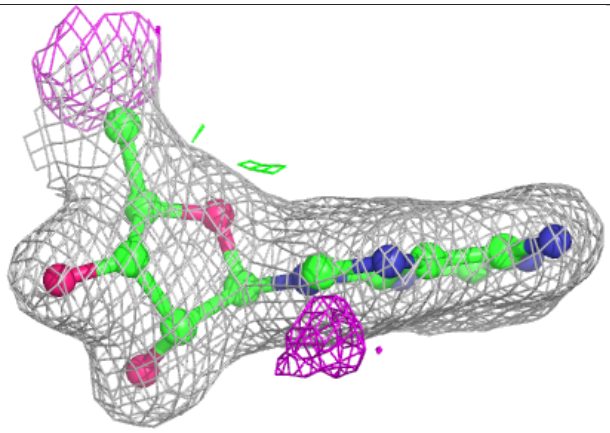


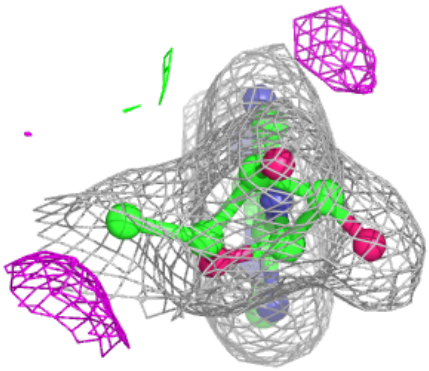


Electron density around 5AD B 302:

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

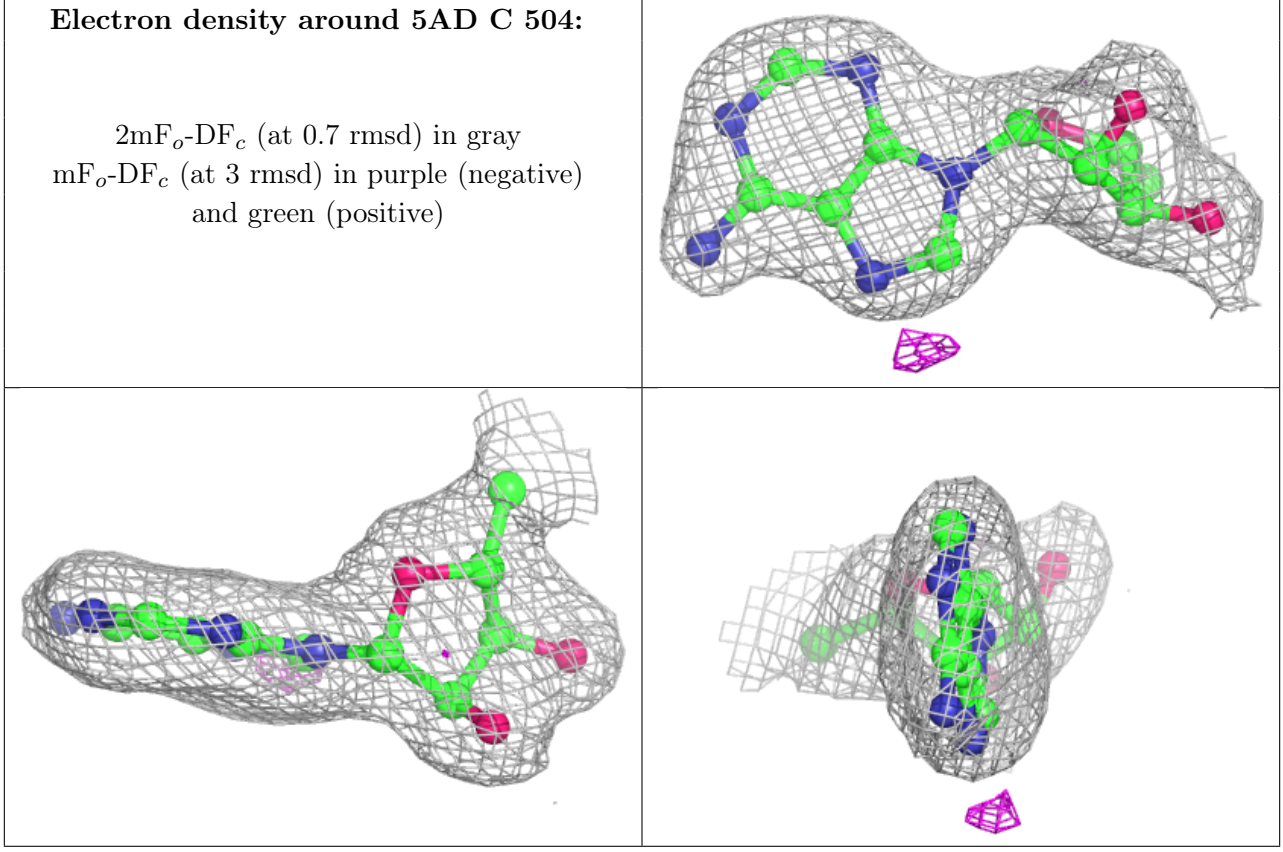






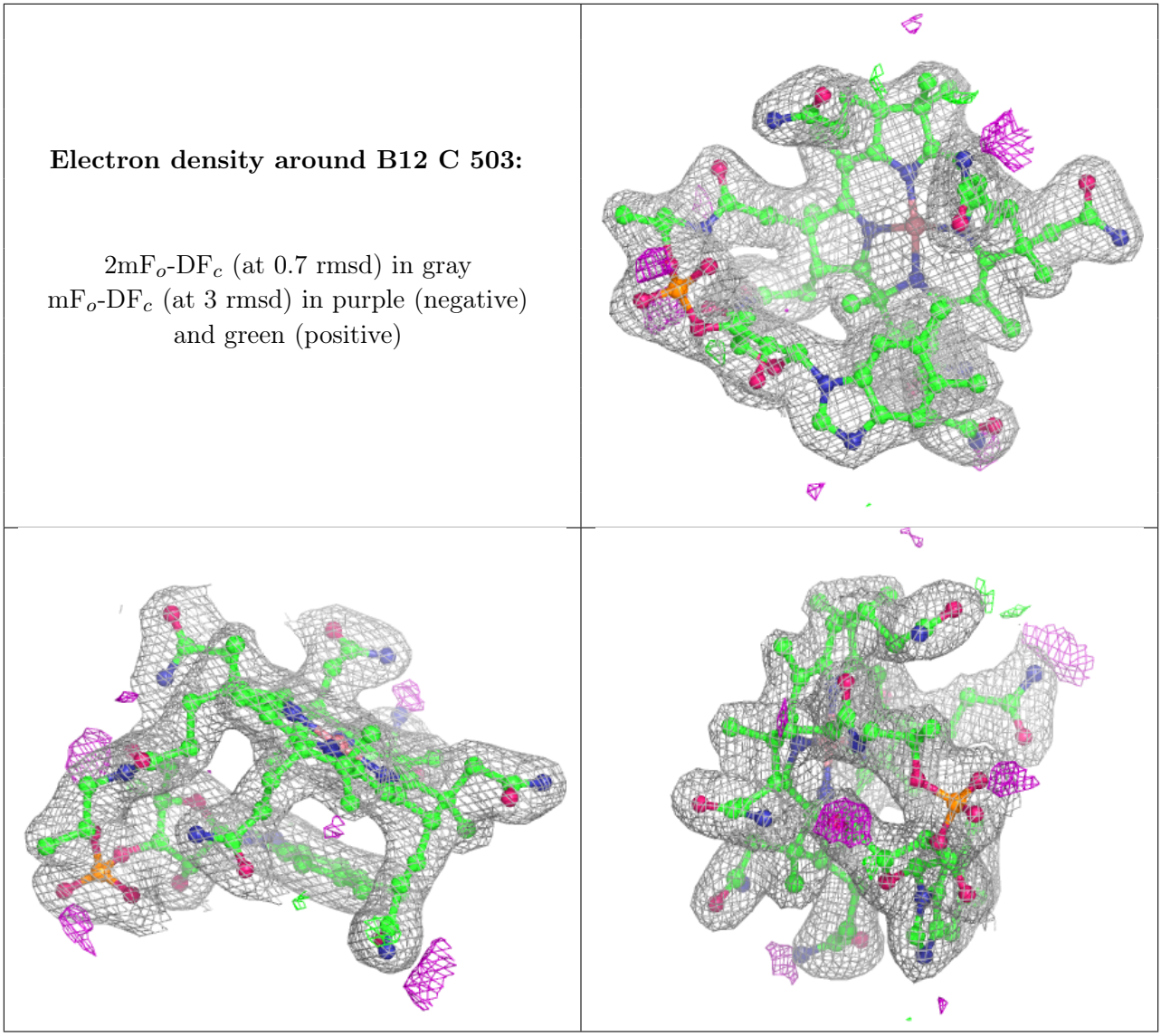
Electron density around 5AD C 504:

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



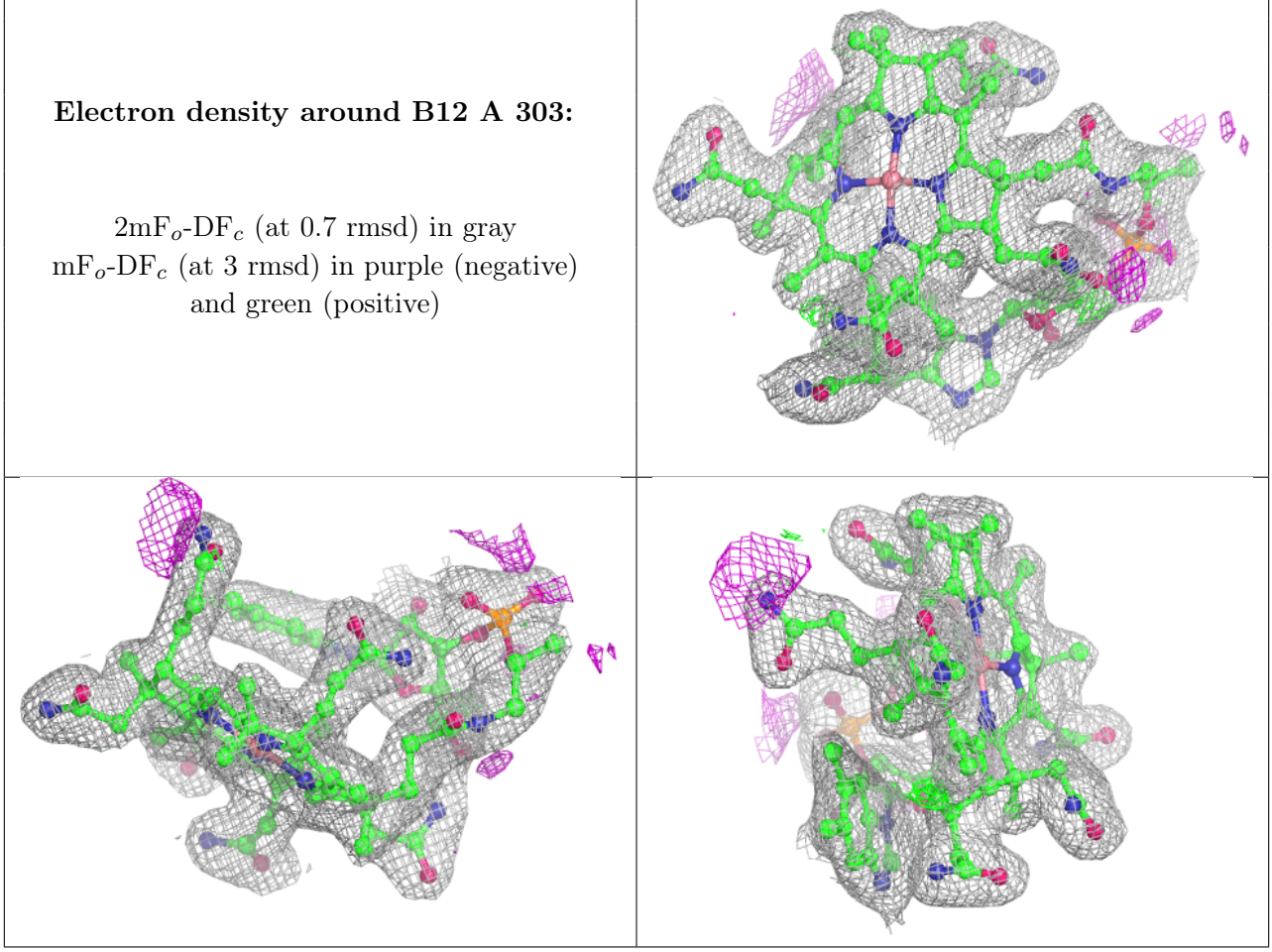
Electron density around B12 C 503:

$2mF_o$-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 303:

$2mF_o$-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.