Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 03:31 am BST

PDB ID	:	8C31 / pdb_00008c31
Title	:	Dark state 1.8 Angstrom crystal structure of cobalamin binding domain belonging to a light-dependent transcription regulator TtCarH obtained under aerobic condition
Authors	:	Poddar, H.; Leys, D.
Deposited on	:	2022-12-23
Resolution	:	1.80 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:

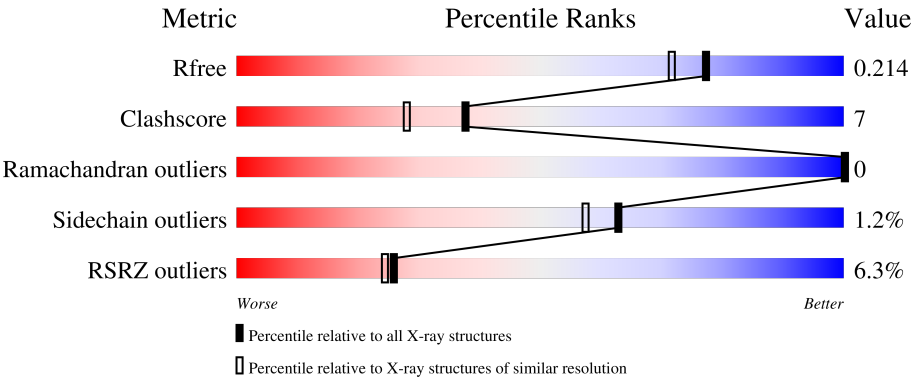
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	12% 78% 12% 10%
1	B	215	6% 83% 7% • 8%
1	C	215	2% 87% • 8%
1	D	215	3% 82% 7% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	B	301	-	-	X	-
3	B12	B	302	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6897 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
1	A	194	Total	C	N	O	S	0	1	0
			1475	946	266	261	2			
1	B	198	Total	C	N	O	S	0	0	0
			1498	960	273	263	2			
1	C	197	Total	C	N	O	S	0	0	0
			1488	951	271	264	2			
1	D	194	Total	C	N	O	S	0	1	0
			1467	938	268	259	2			

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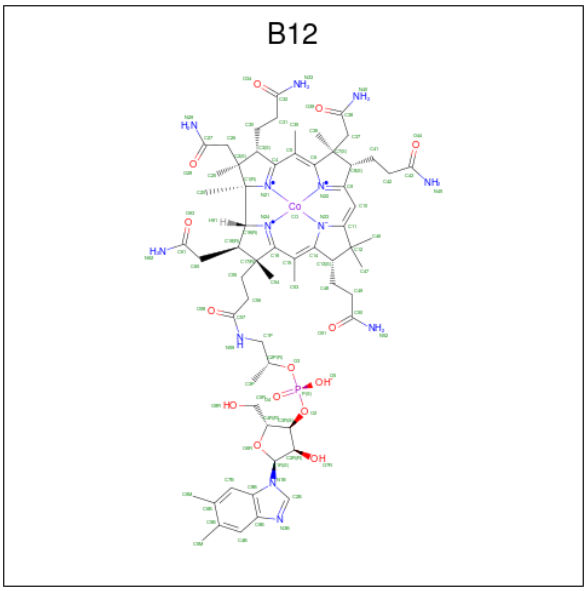
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Chain	Residue	Modelled	Actual	Comment	Reference
D	286	GLY	-	expression tag	UNP Q746J7
D	287	HIS	-	expression tag	UNP Q746J7
D	288	HIS	-	expression tag	UNP Q746J7
D	289	HIS	-	expression tag	UNP Q746J7
D	290	HIS	-	expression tag	UNP Q746J7
D	291	HIS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

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	C	1	Total Br 1 1	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).



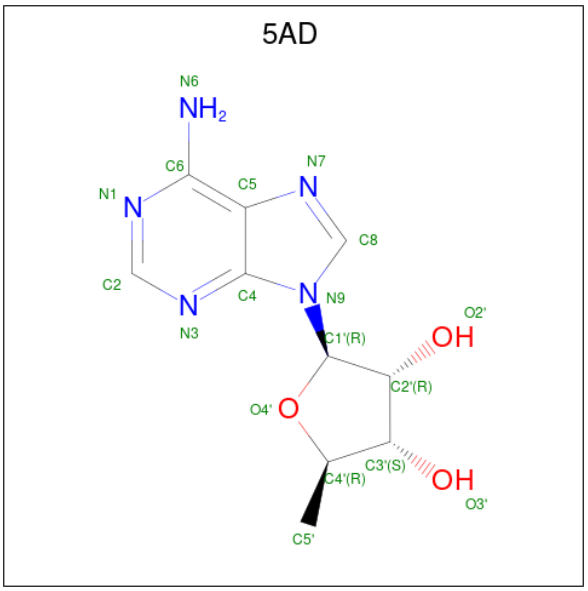
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Co N O P 91 62 1 13 14 1	0	0
3	B	1	Total C Co N O P 91 62 1 13 14 1	0	0

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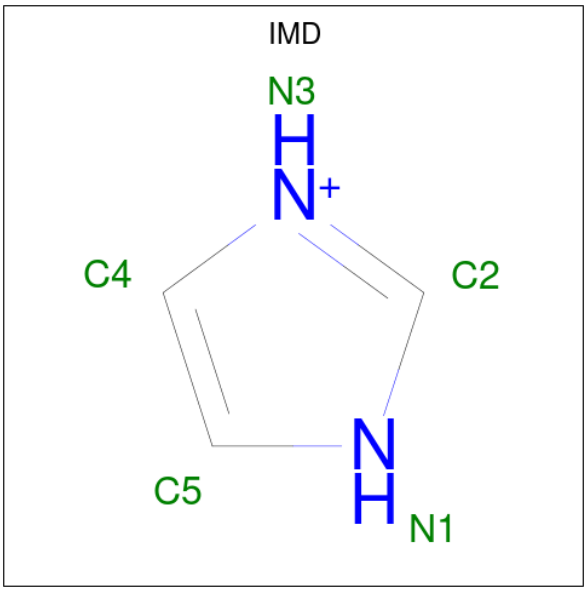
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	D	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



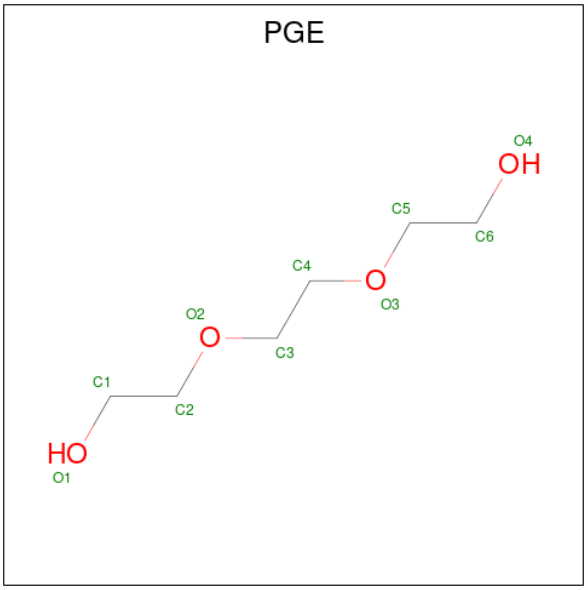
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	10	5	3		
4	B	1	Total	C	N	O	0	0
			18	10	5	3		
4	C	1	Total	C	N	O	0	0
			18	10	5	3		
4	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



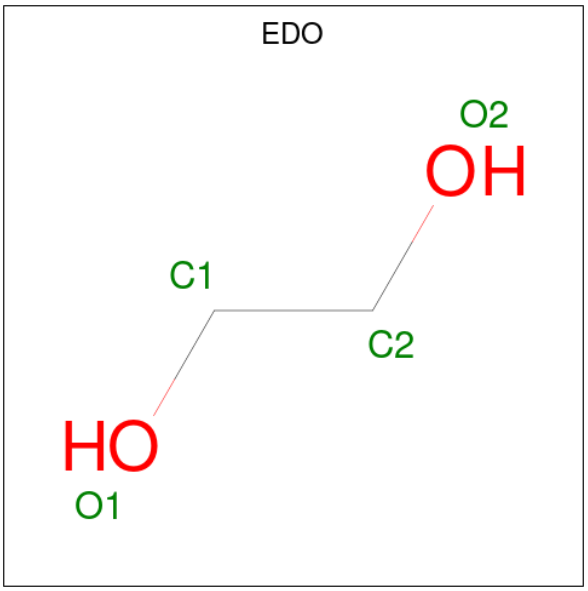
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 6 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

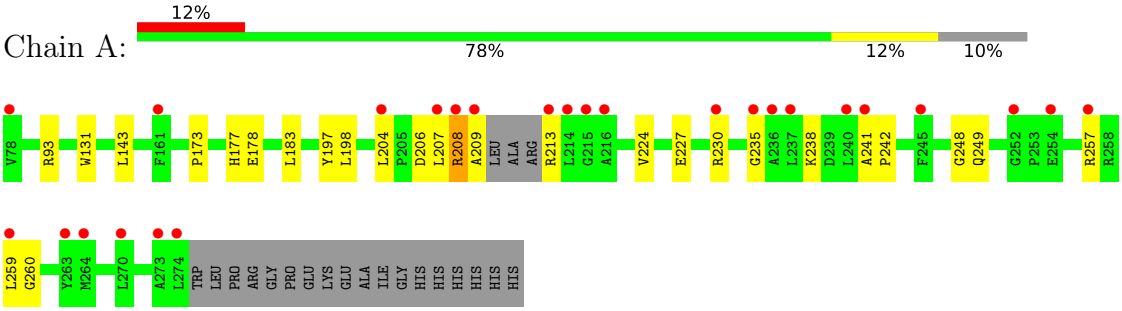
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	94	Total O 94 94	0	0
8	B	112	Total O 112 112	0	0
8	C	150	Total O 150 150	0	0
8	D	134	Total O 134 134	0	0

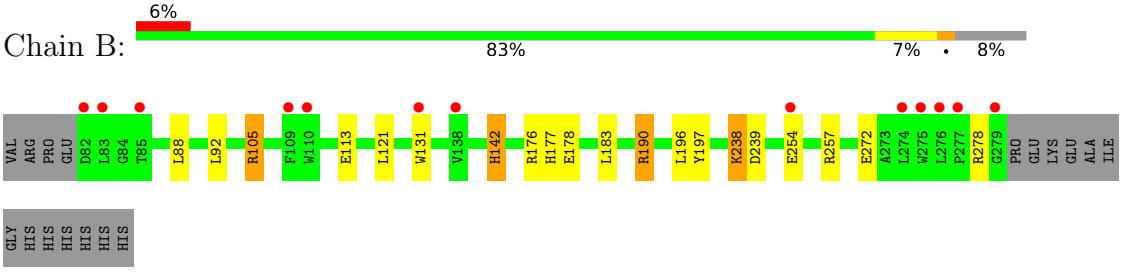
3 Residue-property plots

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.

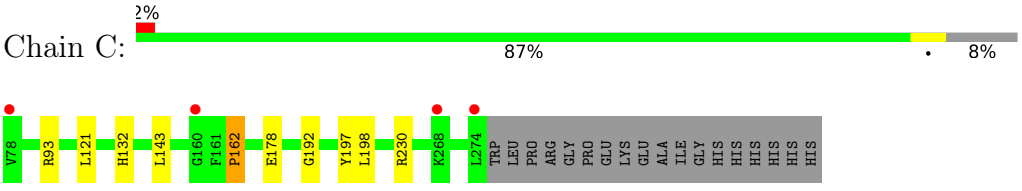
• Molecule 1: Probable transcriptional regulator



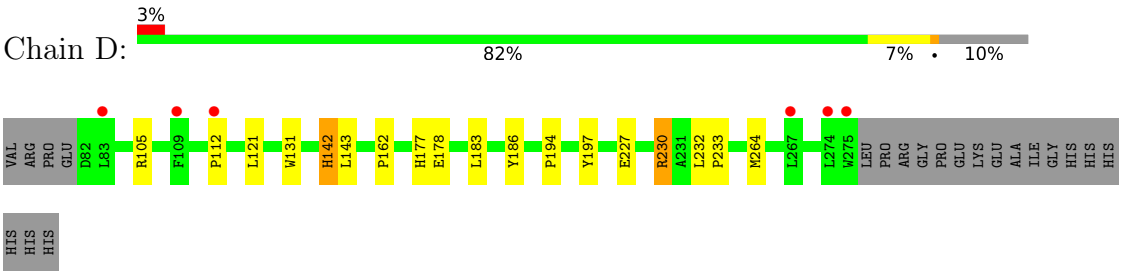
• Molecule 1: Probable transcriptional regulator



• Molecule 1: Probable transcriptional regulator



• Molecule 1: Probable transcriptional regulator



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.11Å 69.70Å 204.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.18 – 1.80 61.18 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (61.18-1.80) 98.3 (61.18-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.170 , 0.209 0.180 , 0.214	Depositor DCC
R_{free} test set	4386 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.5	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	6897	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: 5AD, B12, PGE, BR, IMD, EDO

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	0.67	1/1512 (0.1%)	0.95	1/2055 (0.0%)
1	B	0.64	0/1533	0.94	1/2084 (0.0%)
1	C	0.65	0/1521	0.91	1/2067 (0.0%)
1	D	0.68	0/1502	0.95	0/2040
All	All	0.66	1/6068 (0.0%)	0.94	3/8246 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	2
1	D	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	ARG	NE-CZ	5.25	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	LYS	N-CA-C	6.23	118.07	111.28
1	C	162	PRO	CB-CA-C	-5.82	103.82	110.92
1	A	248	GLY	CA-C-O	-5.26	118.66	122.45

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	176	ARG	Sidechain
1	B	190	ARG	Sidechain
1	B	278	ARG	Sidechain
1	C	230	ARG	Sidechain
1	C	93	ARG	Sidechain
1	D	105	ARG	Sidechain
1	D	230	ARG	Sidechain

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	1475	0	1505	25	0
1	B	1498	0	1534	15	0
1	C	1488	0	1525	10	0
1	D	1467	0	1505	13	0
2	A	1	0	0	0	0
2	B	1	0	0	2	0
2	C	1	0	0	0	0
3	A	91	0	87	14	0
3	B	91	0	87	12	0
3	C	91	0	87	10	0
3	D	91	0	86	6	0
4	A	18	0	12	2	0
4	B	18	0	12	1	0
4	C	18	0	12	0	0
4	D	18	0	12	1	0
5	A	5	0	5	2	0
5	C	5	0	5	0	0
6	C	10	0	14	0	0
7	C	4	0	6	0	0
7	D	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	94	0	0	2	0
8	B	112	0	0	1	0
8	C	150	0	0	1	0
8	D	134	0	0	1	0
All	All	6897	0	6518	91	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 7.

All (91) 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)
3:A:302:B12:H351	3:A:302:B12:H362	1.31	1.07
3:D:702:B12:H362	3:D:702:B12:H351	1.49	0.95
3:C:302:B12:H362	3:C:302:B12:H351	1.60	0.82
3:A:302:B12:H552	3:A:302:B12:H531	1.61	0.81
3:A:302:B12:H351	3:A:302:B12:C36	2.10	0.80
1:D:121:LEU:HD21	1:D:183:LEU:HD11	1.68	0.74
1:A:235:GLY:CA	1:A:238:LYS:HE3	2.20	0.71
1:B:113:GLU:HG3	1:B:190:ARG:HH11	1.55	0.70
3:D:702:B12:H552	3:D:702:B12:H531	1.74	0.69
5:A:304:IMD:H2	8:A:408:HOH:O	1.97	0.65
1:A:235:GLY:HA3	1:A:238:LYS:HE3	1.80	0.64
1:D:227:GLU:HG3	1:D:230:ARG:HH12	1.62	0.64
5:A:304:IMD:C2	8:A:408:HOH:O	2.47	0.63
1:B:121:LEU:HD21	1:B:183:LEU:HD11	1.81	0.62
3:D:702:B12:H482	3:D:702:B12:H533	1.81	0.62
1:A:227:GLU:HG3	1:A:230:ARG:HH11	1.67	0.60
3:D:702:B12:H351	3:D:702:B12:C36	2.28	0.60
1:A:235:GLY:HA2	1:A:238:LYS:HE3	1.83	0.59
1:A:173:PRO:CG	1:A:204:LEU:CD1	2.81	0.58
3:A:302:B12:H3	3:A:302:B12:H291	1.68	0.58
1:B:254:GLU:OE1	1:B:257:ARG:NH1	2.36	0.58
1:A:173:PRO:HG2	1:A:204:LEU:HD13	1.86	0.58
1:B:177:HIS:CE1	3:B:302:B12:N22	2.72	0.57
3:A:302:B12:H531	3:A:302:B12:C55	2.31	0.57
3:C:302:B12:H552	3:C:302:B12:H531	1.86	0.56
1:C:121:LEU:CD1	3:C:302:B12:H5R1	2.37	0.54
1:A:173:PRO:CD	1:A:204:LEU:CD1	2.86	0.53
1:B:178:GLU:H	3:B:302:B12:H522	1.54	0.53
1:B:272:GLU:HG3	8:B:402:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD23	1:A:143:LEU:C	2.34	0.53
1:A:178:GLU:H	3:A:302:B12:H522	1.57	0.52
1:A:131:TRP:CD2	4:A:303:5AD:H3'	2.45	0.52
1:C:178:GLU:H	3:C:302:B12:H522	1.59	0.51
1:A:238:LYS:HG2	1:A:260:GLY:HA3	1.94	0.50
3:B:302:B12:H552	3:B:302:B12:H531	1.93	0.50
1:C:143:LEU:C	1:C:143:LEU:HD23	2.36	0.50
3:A:302:B12:C36	3:A:302:B12:C35	2.87	0.49
3:C:302:B12:H482	3:C:302:B12:H533	1.95	0.49
1:D:227:GLU:HG3	1:D:230:ARG:NH1	2.25	0.49
3:B:302:B12:H601	3:B:302:B12:H262	1.95	0.49
3:A:302:B12:H362	3:A:302:B12:C35	2.21	0.48
3:A:302:B12:H3	3:A:302:B12:N29	2.29	0.48
3:C:302:B12:H351	3:C:302:B12:C36	2.39	0.47
1:A:183:LEU:HD12	3:A:302:B12:H3P1	1.96	0.47
1:C:121:LEU:HD11	3:C:302:B12:H5R1	1.96	0.47
1:B:131:TRP:CD2	4:B:303:5AD:H3'	2.50	0.46
3:B:302:B12:H621	3:B:302:B12:H18	1.35	0.46
3:B:302:B12:H541	3:B:302:B12:H602	1.63	0.46
3:B:302:B12:H301	3:B:302:B12:H253	1.63	0.46
3:A:302:B12:H301	3:A:302:B12:H203	1.97	0.46
1:D:112:PRO:HB3	1:D:186:TYR:OH	2.16	0.46
1:B:190:ARG:NH2	2:B:301:BR:BR	3.05	0.45
1:A:207:LEU:C	1:A:209:ALA:H	2.24	0.45
1:D:178:GLU:HB2	1:D:197:TYR:OH	2.17	0.45
3:B:302:B12:H621	3:B:302:B12:H562	1.82	0.45
1:D:162:PRO:O	1:D:194:PRO:HB3	2.17	0.45
1:A:208:ARG:HA	1:A:208:ARG:HD3	1.54	0.44
1:A:198:LEU:O	1:B:142:HIS:HB3	2.18	0.44
3:B:302:B12:H18	3:B:302:B12:H562	1.74	0.44
1:C:178:GLU:HB2	1:C:197:TYR:OH	2.17	0.44
1:A:224:VAL:O	1:A:249:GLN:HG3	2.17	0.44
1:D:131:TRP:CD2	4:D:703:5AD:H3'	2.53	0.44
3:C:302:B12:H531	3:C:302:B12:C55	2.47	0.44
1:A:206:ASP:C	1:A:208:ARG:H	2.24	0.44
1:B:178:GLU:HB2	1:B:197:TYR:OH	2.18	0.44
3:D:702:B12:H531	3:D:702:B12:C55	2.40	0.43
3:A:302:B12:H533	3:A:302:B12:H482	2.00	0.43
3:B:302:B12:H362	3:B:302:B12:H351	1.99	0.43
1:C:178:GLU:HG2	3:C:302:B12:H522	1.84	0.43
1:D:264:MET:HE3	1:D:264:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLU:HB2	1:A:197:TYR:OH	2.18	0.43
1:B:178:GLU:HG2	3:B:302:B12:H522	1.84	0.43
1:B:190:ARG:HD3	2:B:301:BR:BR	2.74	0.43
1:C:162:PRO:HG2	1:C:192:GLY:O	2.18	0.43
1:A:131:TRP:CE3	4:A:303:5AD:H3'	2.54	0.42
1:D:121:LEU:HD21	1:D:183:LEU:CD1	2.44	0.42
1:A:183:LEU:HD12	3:A:302:B12:C3P	2.50	0.41
1:C:121:LEU:HD13	3:C:302:B12:H5R1	2.02	0.41
1:A:241:ALA:HB1	1:A:242:PRO:HD2	2.02	0.41
1:C:132:HIS:ND1	8:C:402:HOH:O	2.37	0.41
1:B:88:LEU:O	1:B:92:LEU:HD13	2.20	0.41
1:A:173:PRO:HG2	1:A:204:LEU:CD1	2.47	0.41
1:D:177:HIS:CE1	3:D:702:B12:N22	2.89	0.41
1:A:173:PRO:CG	1:A:204:LEU:HD13	2.47	0.41
1:B:177:HIS:CD2	3:B:302:B12:C14	3.03	0.41
1:B:239:ASP:OD1	1:B:239:ASP:N	2.53	0.41
1:C:198:LEU:O	1:D:142:HIS:HB3	2.21	0.41
1:D:143:LEU:HD12	8:D:825:HOH:O	2.20	0.40
1:A:235:GLY:HA2	1:A:238:LYS:HG3	2.03	0.40
1:D:232:LEU:HA	1:D:233:PRO:HD3	1.94	0.40
1:A:177:HIS:CE1	3:A:302:B12:N22	2.90	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	191/215 (89%)	185 (97%)	6 (3%)	0	100	100
1	B	196/215 (91%)	191 (97%)	5 (3%)	0	100	100
1	C	195/215 (91%)	191 (98%)	4 (2%)	0	100	100
1	D	193/215 (90%)	189 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	775/860 (90%)	756 (98%)	19 (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	145/161 (90%)	143 (99%)	2 (1%)	59 52
1	B	146/161 (91%)	142 (97%)	4 (3%)	39 27
1	C	146/161 (91%)	146 (100%)	0	100 100
1	D	143/161 (89%)	142 (99%)	1 (1%)	76 73
All	All	580/644 (90%)	573 (99%)	7 (1%)	63 57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ARG
1	A	259	LEU
1	B	105	ARG
1	B	142	HIS
1	B	196	LEU
1	B	238	LYS
1	D	142	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	GLN
1	B	249	GLN
1	C	132	HIS
1	C	153	GLN
1	D	187	HIS

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	B12	C	302	1	93,101,101	1.33	10 (10%)	146,166,166	1.91	33 (22%)
3	B12	A	302	1	93,101,101	1.34	8 (8%)	146,166,166	1.79	23 (15%)
4	5AD	C	303	-	20,20,20	0.31	0	27,30,30	0.71	0
6	PGE	C	305	-	9,9,9	0.21	0	8,8,8	0.13	0
5	IMD	A	304	-	5,5,5	0.45	0	5,5,5	0.54	0
4	5AD	B	303	-	20,20,20	0.23	0	27,30,30	0.75	0
3	B12	B	302	1	93,101,101	1.47	11 (11%)	146,166,166	1.87	32 (21%)
4	5AD	A	303	-	20,20,20	0.43	0	27,30,30	0.87	2 (7%)
7	EDO	D	706	-	3,3,3	0.19	0	2,2,2	0.18	0
7	EDO	D	701	-	3,3,3	0.27	0	2,2,2	0.33	0
7	EDO	D	705	-	3,3,3	1.02	0	2,2,2	0.94	0
7	EDO	D	704	-	3,3,3	0.19	0	2,2,2	0.22	0
3	B12	D	702	1	93,101,101	1.30	14 (15%)	146,166,166	1.83	22 (15%)
4	5AD	D	703	-	20,20,20	0.46	0	27,30,30	0.62	0
5	IMD	C	304	-	5,5,5	0.81	0	5,5,5	0.38	0
7	EDO	C	306	-	3,3,3	0.11	0	2,2,2	0.19	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
3	B12	C	302	1	-	16/56/223/223	0/3/11/11
3	B12	A	302	1	-	13/56/223/223	0/3/11/11
4	5AD	C	303	-	-	0/4/20/20	0/3/3/3
6	PGE	C	305	-	-	6/7/7/7	-
5	IMD	A	304	-	-	-	0/1/1/1
4	5AD	B	303	-	-	0/4/20/20	0/3/3/3
3	B12	B	302	1	1/1/36/38	14/56/223/223	0/3/11/11
4	5AD	A	303	-	-	0/4/20/20	0/3/3/3
7	EDO	D	706	-	-	0/1/1/1	-
7	EDO	D	701	-	-	1/1/1/1	-
7	EDO	D	705	-	-	1/1/1/1	-
7	EDO	D	704	-	-	1/1/1/1	-
3	B12	D	702	1	-	9/56/223/223	0/3/11/11
4	5AD	D	703	-	-	0/4/20/20	0/3/3/3
5	IMD	C	304	-	-	-	0/1/1/1
7	EDO	C	306	-	-	0/1/1/1	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	B12	C19-N24	-6.13	1.37	1.48
3	A	302	B12	C8B-C9B	5.64	1.49	1.40
3	B	302	B12	C14-N23	-5.05	1.28	1.35
3	D	702	B12	C8B-C9B	4.48	1.47	1.40
3	C	302	B12	C8B-C9B	4.46	1.47	1.40
3	D	702	B12	C9-N22	4.42	1.42	1.30
3	B	302	B12	C9-N22	4.32	1.41	1.30
3	B	302	B12	C8B-C9B	4.31	1.47	1.40
3	B	302	B12	C19-N24	-4.12	1.41	1.48
3	C	302	B12	C19-N24	-4.03	1.41	1.48
3	C	302	B12	C6B-C5B	3.84	1.50	1.40
3	B	302	B12	C16-C15	-3.71	1.34	1.44
3	B	302	B12	C8B-N1B	-3.63	1.32	1.39
3	C	302	B12	C9-N22	3.32	1.39	1.30
3	A	302	B12	C2B-N3B	3.29	1.37	1.31
3	A	302	B12	C6B-C5B	3.28	1.49	1.40
3	B	302	B12	C6B-C5B	3.20	1.48	1.40
3	D	702	B12	C16-C15	-3.15	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	B12	C8B-N1B	-3.13	1.33	1.39
3	C	302	B12	C16-C15	-3.01	1.36	1.44
3	B	302	B12	C9B-N3B	-2.87	1.34	1.39
3	C	302	B12	O3-C2P	-2.86	1.38	1.45
3	D	702	B12	C6B-C5B	2.78	1.47	1.40
3	C	302	B12	C2B-N3B	2.59	1.36	1.31
3	C	302	B12	C8B-N1B	-2.49	1.34	1.39
3	D	702	B12	C2B-N3B	2.45	1.36	1.31
3	D	702	B12	C10-C9	2.43	1.46	1.39
3	D	702	B12	C2B-N1B	-2.37	1.33	1.37
3	D	702	B12	O6R-C1R	2.37	1.47	1.42
3	D	702	B12	C7B-C6B	2.33	1.43	1.39
3	A	302	B12	C10-C9	2.33	1.45	1.39
3	D	702	B12	C19-N24	-2.30	1.44	1.48
3	B	302	B12	C10-C9	2.29	1.45	1.39
3	D	702	B12	C8B-N1B	-2.26	1.34	1.39
3	D	702	B12	C1R-N1B	2.24	1.52	1.46
3	A	302	B12	C1-C2	-2.21	1.53	1.58
3	C	302	B12	C14-N23	-2.15	1.32	1.35
3	D	702	B12	P-O2	2.14	1.66	1.60
3	B	302	B12	C1-C2	-2.14	1.53	1.58
3	D	702	B12	C14-C15	2.06	1.47	1.38
3	B	302	B12	C2B-N3B	2.06	1.35	1.31
3	A	302	B12	C35-C5	2.02	1.55	1.50
3	C	302	B12	O34-C32	-2.01	1.17	1.24

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	702	B12	C1-C19-N24	9.70	117.16	106.24
3	C	302	B12	C20-C1-C19	-9.50	100.20	109.36
3	D	702	B12	C20-C1-C19	-9.08	100.60	109.36
3	B	302	B12	C1-C19-N24	8.76	116.09	106.24
3	C	302	B12	C1-C19-N24	8.06	115.31	106.24
3	B	302	B12	C20-C1-C19	-7.92	101.72	109.36
3	A	302	B12	C1-C19-N24	7.64	114.84	106.24
3	A	302	B12	C20-C1-C19	-7.08	102.53	109.36
3	B	302	B12	C18-C19-N24	6.38	112.03	102.31
3	C	302	B12	C2P-C1P-N59	-6.21	103.78	112.93
3	A	302	B12	C1-C19-C18	6.08	131.86	121.88
3	B	302	B12	C1-C19-C18	5.96	131.67	121.88
3	A	302	B12	O3-P-O4	-5.70	88.06	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	B12	C1-C19-C18	5.65	131.15	121.88
3	A	302	B12	C18-C19-N24	5.50	110.68	102.31
3	A	302	B12	O5-P-O4	5.46	139.22	112.24
3	D	702	B12	C18-C19-N24	5.39	110.51	102.31
3	C	302	B12	C18-C19-N24	5.03	109.96	102.31
3	D	702	B12	C1-C19-C18	4.84	129.82	121.88
3	D	702	B12	C2-C1-C19	4.68	125.99	118.60
3	B	302	B12	C8B-C9B-N3B	-4.07	105.47	109.97
3	D	702	B12	C8B-C9B-N3B	-3.88	105.69	109.97
3	D	702	B12	C13-C14-N23	3.75	114.20	109.10
3	D	702	B12	C13-C14-C15	-3.74	118.61	124.32
3	D	702	B12	C2P-C1P-N59	-3.73	107.43	112.93
3	C	302	B12	C8B-N1B-C2B	3.66	109.78	106.37
3	B	302	B12	C17-C16-C15	3.62	131.96	126.26
3	A	302	B12	C12-C11-C10	-3.60	118.69	123.37
3	B	302	B12	C12-C11-C10	-3.39	118.95	123.37
3	A	302	B12	C9B-C8B-N1B	3.39	106.78	105.35
3	B	302	B12	C18-C17-C16	3.35	104.74	100.67
3	B	302	B12	C54-C17-C18	-3.34	108.05	112.98
3	B	302	B12	C9B-N3B-C2B	3.34	108.42	104.44
3	C	302	B12	C41-C8-C9	-3.25	105.46	111.19
3	B	302	B12	C2P-C1P-N59	-3.21	108.20	112.93
3	A	302	B12	C2-C1-C19	3.16	123.58	118.60
3	C	302	B12	C12-C11-C10	-3.15	119.27	123.37
3	B	302	B12	C17-C16-N24	-3.12	106.34	111.15
3	D	702	B12	C17-C16-N24	-3.10	106.37	111.15
3	B	302	B12	C8B-N1B-C2B	3.10	109.26	106.37
3	C	302	B12	C8B-C9B-N3B	-3.03	106.63	109.97
3	B	302	B12	C9B-C8B-N1B	3.01	106.62	105.35
3	A	302	B12	C13-C14-N23	2.97	113.14	109.10
3	C	302	B12	C17-C16-N24	-2.95	106.61	111.15
3	D	702	B12	C8B-N1B-C2B	2.91	109.08	106.37
3	A	302	B12	C17-C16-N24	-2.87	106.73	111.15
3	C	302	B12	C12-C11-N23	2.83	115.77	111.83
3	B	302	B12	C13-C14-N23	2.81	112.92	109.10
3	C	302	B12	C2-C3-C4	2.81	104.82	101.63
3	A	302	B12	C2-C1-N21	2.79	105.66	101.77
3	B	302	B12	C55-C56-C57	-2.79	105.14	111.23
3	D	702	B12	C2R-C3R-C4R	2.78	108.15	103.22
3	C	302	B12	C13-C14-N23	2.75	112.84	109.10
3	A	302	B12	C8B-N1B-C1R	-2.72	120.76	125.39
3	B	302	B12	N1B-C2B-N3B	-2.71	110.21	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	B12	C2-C1-N21	2.70	105.53	101.77
3	B	302	B12	C30-C3-C2	-2.69	113.41	119.09
3	C	302	B12	C55-C17-C18	-2.67	105.98	111.15
3	D	702	B12	C18-C17-C16	2.67	103.91	100.67
3	C	302	B12	C2-C1-C19	2.66	122.80	118.60
3	A	302	B12	C8B-C9B-N3B	-2.65	107.04	109.97
3	C	302	B12	O6R-C1R-N1B	-2.63	102.87	108.06
3	C	302	B12	C9B-N3B-C2B	2.63	107.57	104.44
3	D	702	B12	C55-C17-C18	-2.61	106.10	111.15
3	A	302	B12	C1-C2-C3	-2.60	98.27	101.60
3	B	302	B12	C20-C1-N21	2.60	114.54	110.27
3	B	302	B12	C19-C1-N21	2.59	104.82	102.16
3	C	302	B12	C1-C2-C3	-2.59	98.29	101.60
3	D	702	B12	C9-C10-C11	-2.57	122.25	125.97
3	C	302	B12	C3R-C2R-C1R	2.57	105.58	99.89
3	C	302	B12	N1B-C2B-N3B	-2.55	110.42	113.91
3	C	302	B12	C26-C2-C1	2.51	113.92	110.01
3	C	302	B12	C18-C60-C61	-2.50	107.73	113.97
3	C	302	B12	C13-C14-C15	-2.50	120.50	124.32
3	C	302	B12	C10-C9-N22	2.49	128.59	125.73
3	D	702	B12	P-O2-C3R	-2.49	110.34	119.41
3	B	302	B12	C25-C2-C1	-2.47	110.05	113.78
3	B	302	B12	C9-C10-C11	-2.47	122.40	125.97
3	A	302	B12	C26-C2-C1	2.46	113.83	110.01
3	D	702	B12	C60-C18-C19	2.44	120.99	114.62
3	D	702	B12	C9B-C8B-N1B	2.43	106.38	105.35
3	C	302	B12	C8-C9-N22	-2.41	105.97	110.77
3	B	302	B12	C4B-C9B-N3B	2.40	134.63	130.51
3	B	302	B12	C26-C2-C1	2.38	113.72	110.01
3	A	302	B12	C4B-C9B-N3B	2.38	134.60	130.51
4	A	303	5AD	O4'-C1'-N9	2.38	112.75	108.06
3	B	302	B12	C3R-C2R-C1R	2.38	105.16	99.89
3	B	302	B12	C13-C14-C15	-2.37	120.69	124.32
3	A	302	B12	C48-C13-C14	2.37	114.40	108.49
3	C	302	B12	C3P-C2P-C1P	2.36	115.96	111.39
3	B	302	B12	C8B-N1B-C1R	-2.34	121.40	125.39
3	B	302	B12	C48-C13-C14	2.31	114.25	108.49
3	B	302	B12	C2-C1-C19	2.30	122.23	118.60
3	C	302	B12	C60-C18-C19	2.27	120.56	114.62
3	C	302	B12	C4B-C9B-N3B	2.26	134.39	130.51
3	C	302	B12	O6R-C4R-C5R	-2.26	104.33	109.21
3	B	302	B12	C56-C55-C17	-2.22	111.23	115.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	B12	C17-C16-C15	2.22	129.76	126.26
4	A	303	5AD	C5'-C4'-C3'	-2.19	113.40	115.70
3	D	702	B12	C12-C11-C10	-2.19	120.53	123.37
3	D	702	B12	O63-C61-C60	2.16	125.42	120.87
3	B	302	B12	C5-C6-N22	-2.15	120.59	123.88
3	C	302	B12	O2-C3R-C2R	-2.15	103.90	111.68
3	D	702	B12	O6R-C4R-C5R	2.12	113.80	109.21
3	A	302	B12	C2-C3-C4	2.11	104.03	101.63
3	A	302	B12	C47-C12-C46	-2.08	105.84	109.35
3	D	702	B12	C54-C17-C55	2.08	112.67	109.25
3	A	302	B12	C9-C10-C11	-2.04	123.02	125.97
3	A	302	B12	C13-C14-C15	-2.04	121.21	124.32
3	B	302	B12	C18-C60-C61	-2.02	108.94	113.97
3	C	302	B12	C7-C8-C9	2.01	103.48	100.90
3	A	302	B12	O2-C3R-C4R	-2.01	102.82	110.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	302	B12	C19

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	B12	C3R-O2-P-O5
3	B	302	B12	C18-C60-C61-O63
3	B	302	B12	C18-C60-C61-N62
3	B	302	B12	C2R-C1R-N1B-C8B
3	B	302	B12	O6R-C1R-N1B-C8B
3	C	302	B12	N59-C1P-C2P-C3P
3	C	302	B12	N59-C1P-C2P-O3
3	C	302	B12	C3R-C4R-C5R-O8R
3	D	702	B12	N59-C1P-C2P-C3P
3	D	702	B12	C2R-C1R-N1B-C8B
3	C	302	B12	O6R-C4R-C5R-O8R
3	A	302	B12	C3R-C4R-C5R-O8R
7	D	705	EDO	O1-C1-C2-O2
3	B	302	B12	C16-C17-C55-C56
3	A	302	B12	C2R-C1R-N1B-C8B
3	A	302	B12	O6R-C1R-N1B-C8B
3	C	302	B12	C2R-C1R-N1B-C8B
3	C	302	B12	O6R-C1R-N1B-C8B

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Mol	Chain	Res	Type	Atoms
3	D	702	B12	O6R-C1R-N1B-C8B
3	A	302	B12	O6R-C4R-C5R-O8R
3	B	302	B12	C2-C3-C30-C31
7	D	701	EDO	O1-C1-C2-O2
6	C	305	PGE	C4-C3-O2-C2
6	C	305	PGE	O1-C1-C2-O2
3	C	302	B12	C2P-O3-P-O2
3	B	302	B12	C4-C3-C30-C31
3	B	302	B12	C48-C49-C50-O51
3	C	302	B12	C30-C31-C32-O34
3	C	302	B12	C30-C31-C32-N33
3	D	702	B12	C2P-O3-P-O4
6	C	305	PGE	O2-C3-C4-O3
3	B	302	B12	C18-C17-C55-C56
7	D	704	EDO	O1-C1-C2-O2
3	C	302	B12	C48-C49-C50-O51
3	C	302	B12	C48-C49-C50-N52
3	D	702	B12	C1P-C2P-O3-P
3	A	302	B12	C3R-O2-P-O3
3	A	302	B12	C48-C49-C50-O51
3	B	302	B12	N59-C1P-C2P-C3P
3	D	702	B12	C17-C18-C60-C61
3	B	302	B12	C48-C49-C50-N52
3	C	302	B12	C3R-O2-P-O3
3	A	302	B12	C48-C49-C50-N52
6	C	305	PGE	C1-C2-O2-C3
3	D	702	B12	C3P-C2P-O3-P
6	C	305	PGE	C6-C5-O3-C4
3	C	302	B12	C55-C56-C57-O58
3	A	302	B12	C2-C26-C27-O28
3	C	302	B12	C3R-O2-P-O5
3	B	302	B12	C19-C18-C60-C61
3	D	702	B12	C19-C18-C60-C61
3	C	302	B12	C55-C56-C57-N59
3	C	302	B12	C42-C41-C8-C9
6	C	305	PGE	C3-C4-O3-C5
3	A	302	B12	C55-C56-C57-N59
3	A	302	B12	C2-C26-C27-N29
3	A	302	B12	C55-C56-C57-O58
3	A	302	B12	C19-C18-C60-C61
3	B	302	B12	C17-C18-C60-C61
3	B	302	B12	C3R-O2-P-O3

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Mol	Chain	Res	Type	Atoms
3	D	702	B12	C2P-C1P-N59-C57

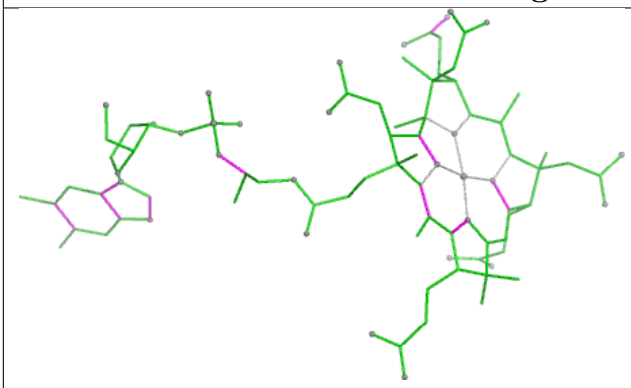
There are no ring outliers.

8 monomers are involved in 48 short contacts:

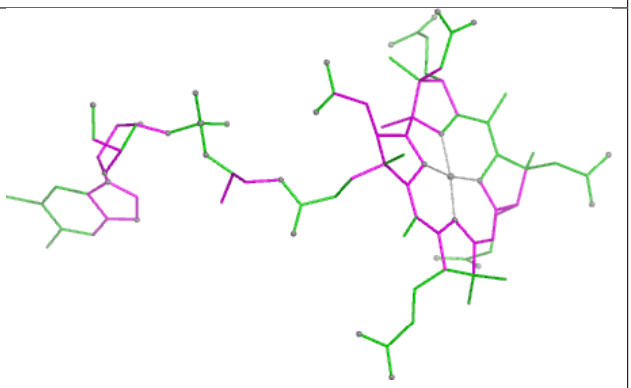
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	B12	10	0
3	A	302	B12	14	0
5	A	304	IMD	2	0
4	B	303	5AD	1	0
3	B	302	B12	12	0
4	A	303	5AD	2	0
3	D	702	B12	6	0
4	D	703	5AD	1	0

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.

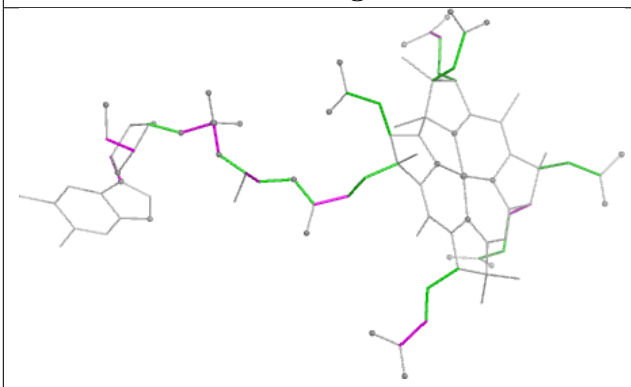
Ligand B12 C 302



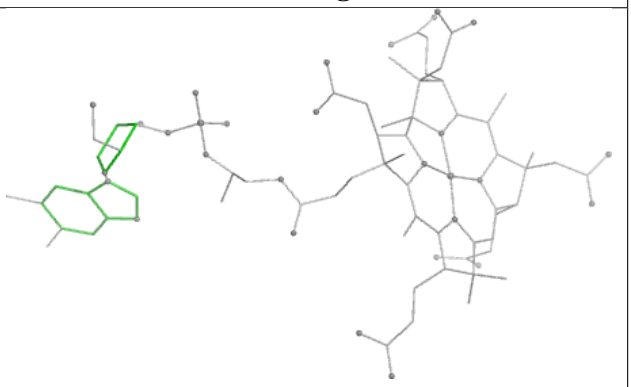
Bond lengths



Bond angles

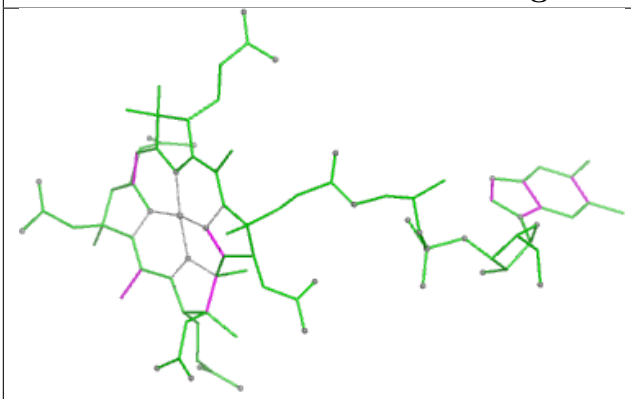


Torsions

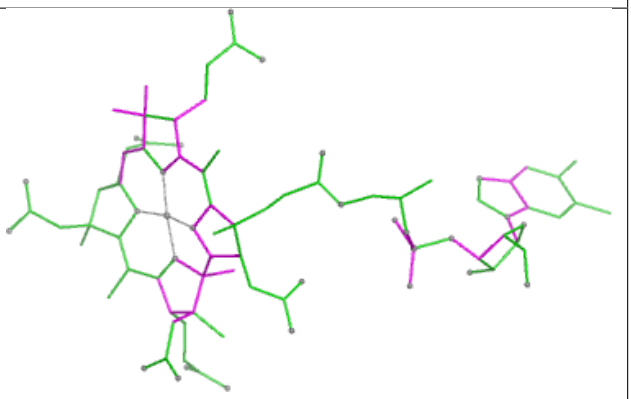


Rings

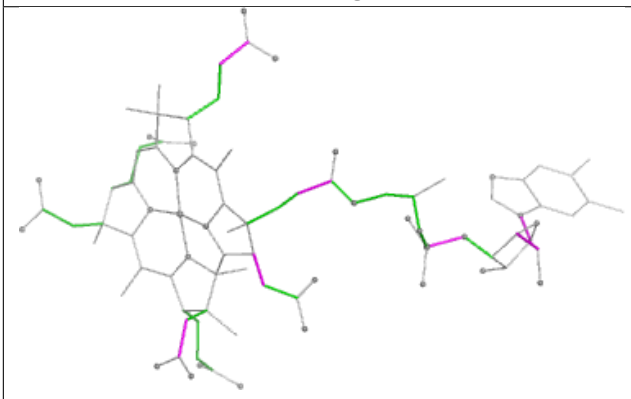
Ligand B12 A 302



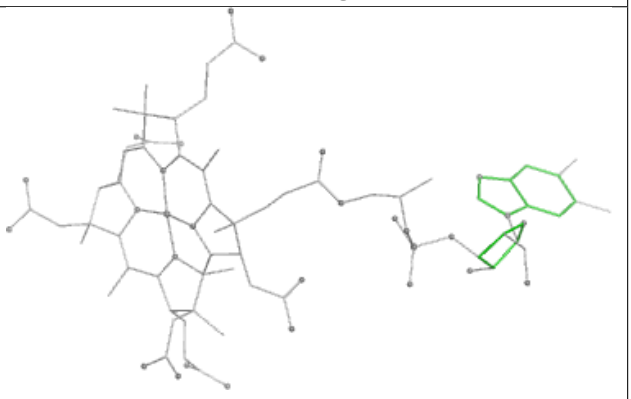
Bond lengths



Bond angles

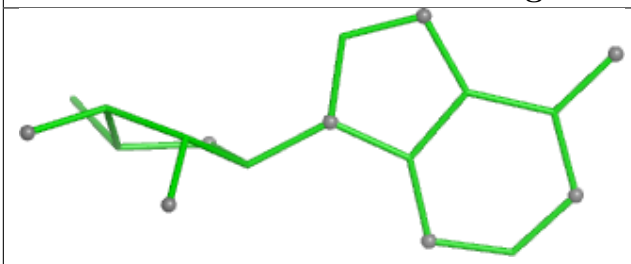


Torsions

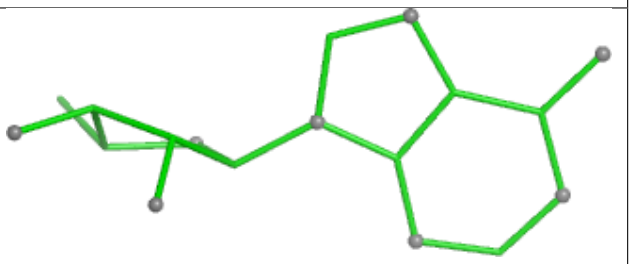


Rings

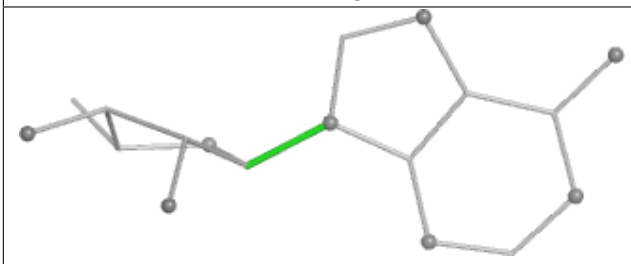
Ligand 5AD C 303



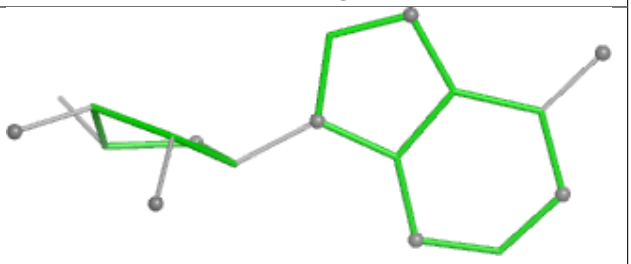
Bond lengths



Bond angles

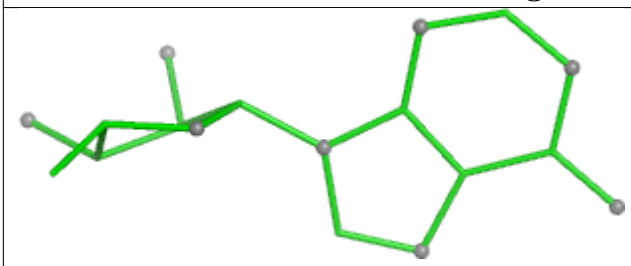


Torsions

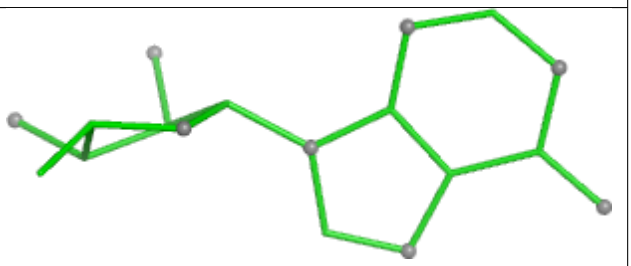


Rings

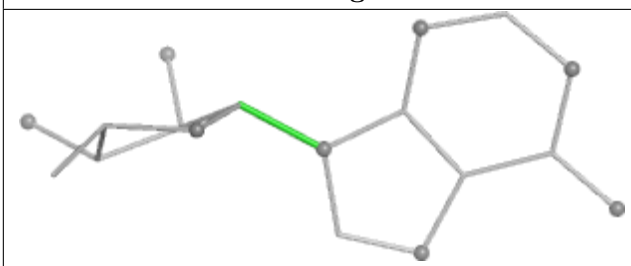
Ligand 5AD B 303



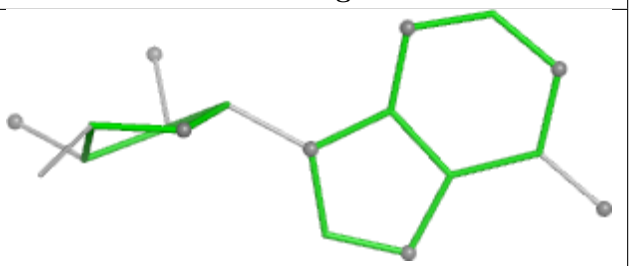
Bond lengths



Bond angles

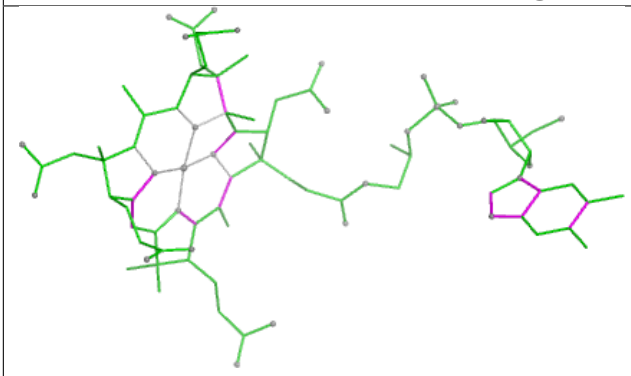


Torsions

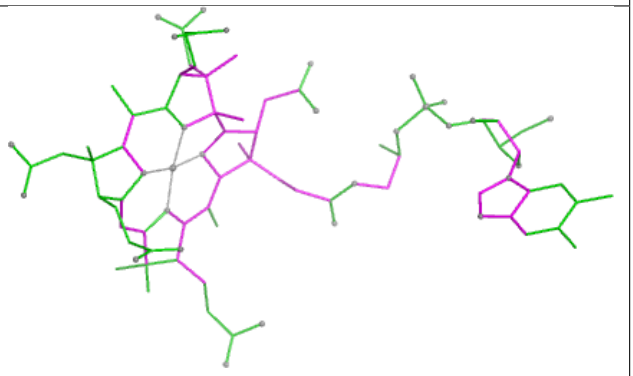


Rings

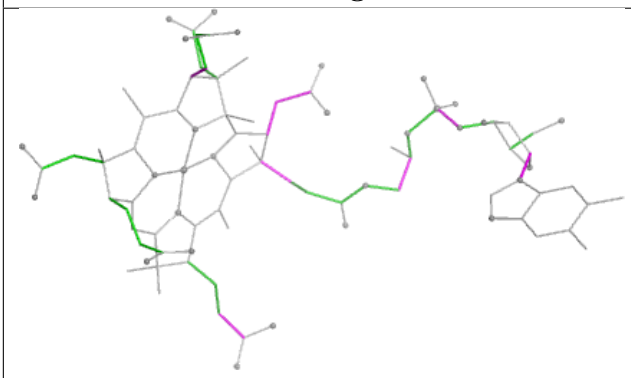
Ligand B12 B 302



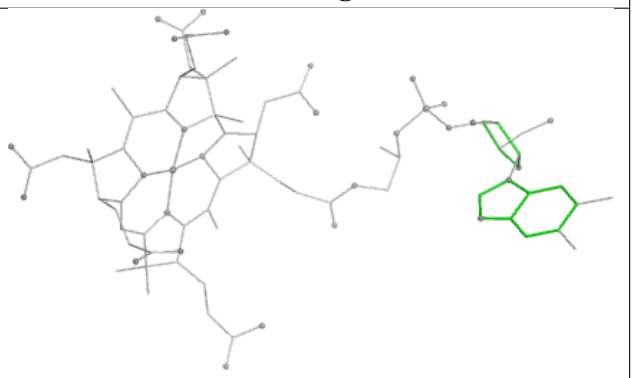
Bond lengths



Bond angles

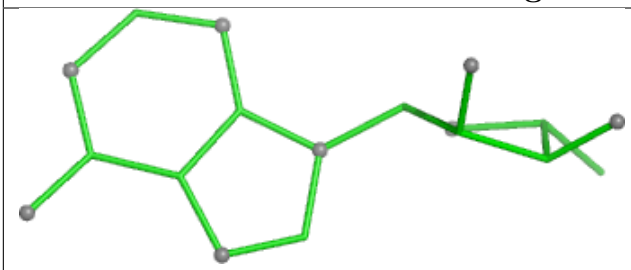


Torsions

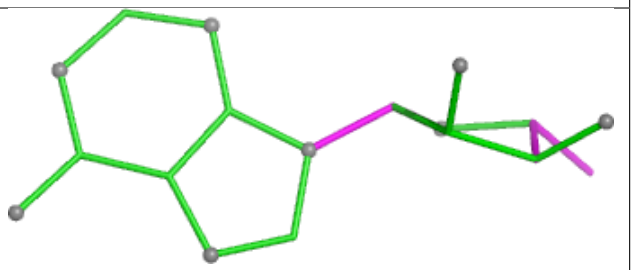


Rings

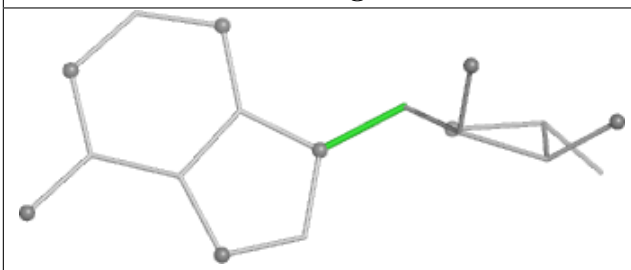
Ligand 5AD A 303



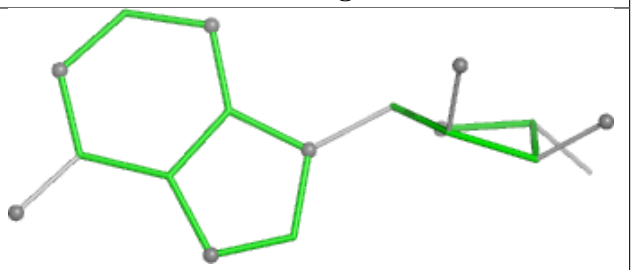
Bond lengths



Bond angles

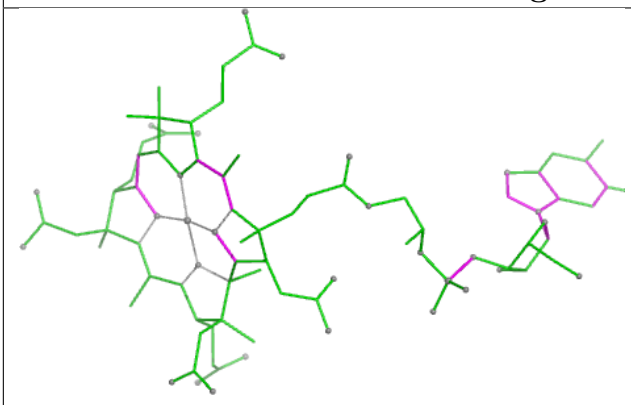


Torsions

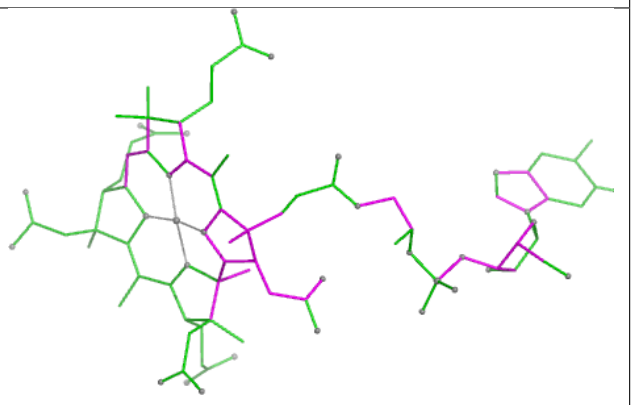


Rings

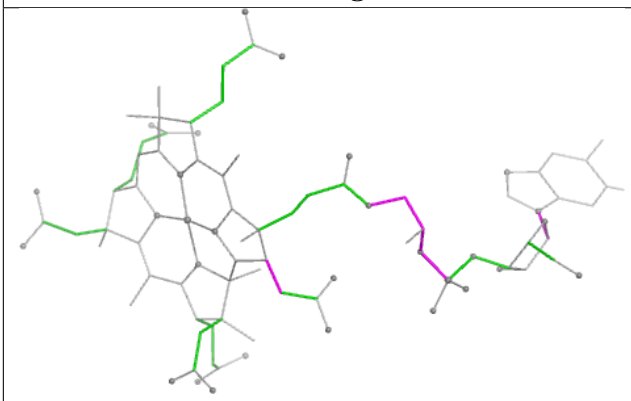
Ligand B12 D 702



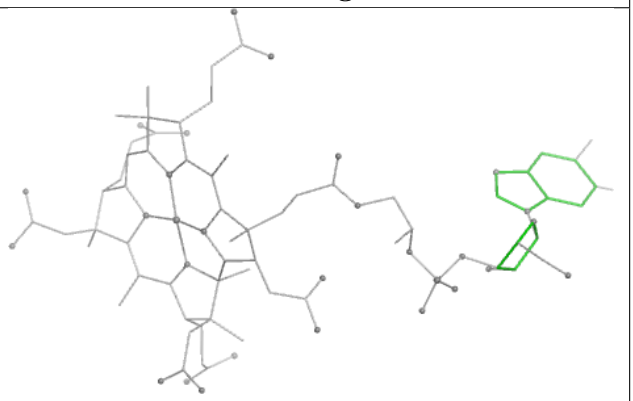
Bond lengths



Bond angles

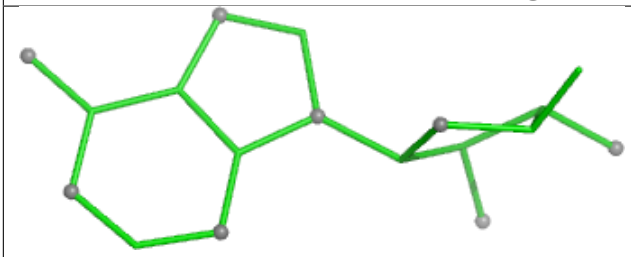


Torsions

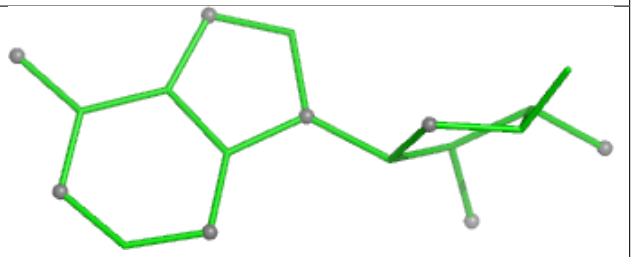


Rings

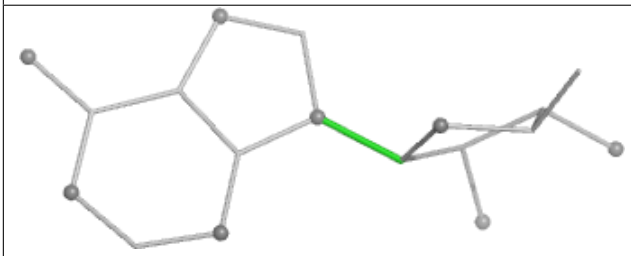
Ligand 5AD D 703



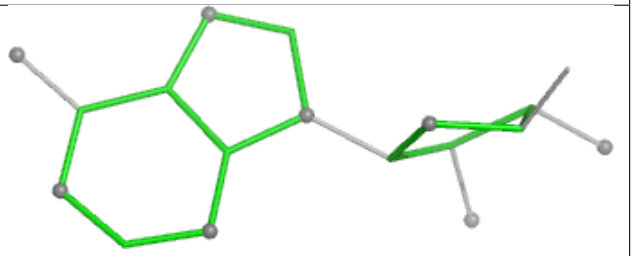
Bond lengths



Bond angles



Torsions



Rings

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

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	194/215 (90%)	0.67	26 (13%) 7 5	23, 44, 84, 92	1 (0%)
1	B	198/215 (92%)	0.53	13 (6%) 24 23	27, 46, 80, 101	0
1	C	197/215 (91%)	0.05	4 (2%) 65 65	26, 39, 66, 92	0
1	D	194/215 (90%)	0.12	6 (3%) 51 51	20, 38, 59, 80	1 (0%)
All	All	783/860 (91%)	0.34	49 (6%) 26 24	20, 41, 75, 101	2 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	TRP	7.2
1	A	241	ALA	5.3
1	C	274	LEU	4.7
1	A	204	LEU	4.6
1	A	274	LEU	4.5
1	A	208	ARG	4.5
1	A	209	ALA	4.2
1	A	214	LEU	4.2
1	A	207	LEU	4.1
1	B	109	PHE	4.0
1	D	274	LEU	3.9
1	A	213	ARG	3.8
1	B	275	TRP	3.3
1	A	78	VAL	3.3
1	C	78	VAL	3.1
1	B	82	ASP	3.0
1	D	83	LEU	3.0
1	C	160	GLY	3.0
1	B	110	TRP	2.9
1	B	131	TRP	2.8
1	D	112	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	2.6
1	A	257	ARG	2.5
1	B	138	VAL	2.5
1	B	277	PRO	2.5
1	A	263	TYR	2.4
1	A	215	GLY	2.4
1	B	279	GLY	2.3
1	D	267	LEU	2.3
1	A	237	LEU	2.3
1	B	274	LEU	2.3
1	A	264	MET	2.3
1	A	273	ALA	2.2
1	A	161	PHE	2.2
1	D	109	PHE	2.2
1	B	254	GLU	2.1
1	A	216	ALA	2.1
1	C	268	LYS	2.1
1	A	259	LEU	2.1
1	A	270	LEU	2.1
1	B	83	LEU	2.1
1	B	85	THR	2.0
1	B	276	LEU	2.0
1	A	230	ARG	2.0
1	A	236	ALA	2.0
1	A	254	GLU	2.0
1	A	245	PHE	2.0
1	A	235	GLY	2.0
1	A	252	GLY	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,

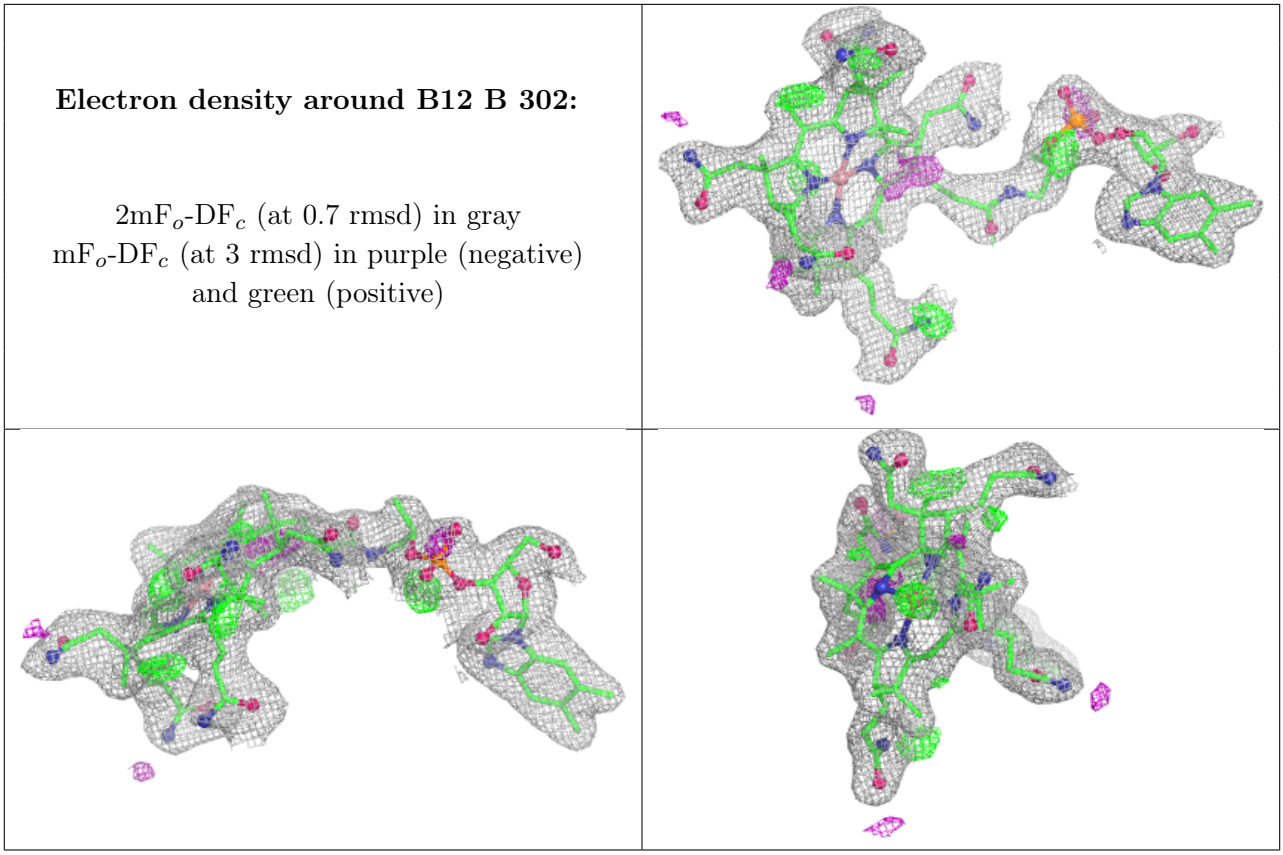
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IMD	A	304	5/5	0.63	0.25	73,74,77,79	0
6	PGE	C	305	10/10	0.78	0.19	64,84,90,90	0
7	EDO	C	306	4/4	0.78	0.17	65,73,74,74	0
7	EDO	D	706	4/4	0.79	0.20	62,70,75,78	0
5	IMD	C	304	5/5	0.82	0.24	64,74,75,81	0
7	EDO	D	704	4/4	0.84	0.14	71,72,73,74	0
7	EDO	D	701	4/4	0.84	0.17	57,63,63,66	0
7	EDO	D	705	4/4	0.87	0.14	39,48,50,54	0
3	B12	B	302	91/91	0.94	0.10	34,48,63,69	0
4	5AD	B	303	18/18	0.94	0.09	46,50,54,56	0
4	5AD	D	703	18/18	0.96	0.07	34,36,39,40	0
4	5AD	A	303	18/18	0.96	0.06	30,31,33,33	0
4	5AD	C	303	18/18	0.96	0.06	26,30,32,32	0
3	B12	A	302	91/91	0.97	0.07	28,37,55,64	0
2	BR	B	301	1/1	0.97	0.10	69,69,69,69	0
3	B12	C	302	91/91	0.97	0.07	24,33,59,77	0
3	B12	D	702	91/91	0.97	0.07	26,35,48,56	0
2	BR	A	301	1/1	0.99	0.05	45,45,45,45	0
2	BR	C	301	1/1	0.99	0.08	49,49,49,49	0

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

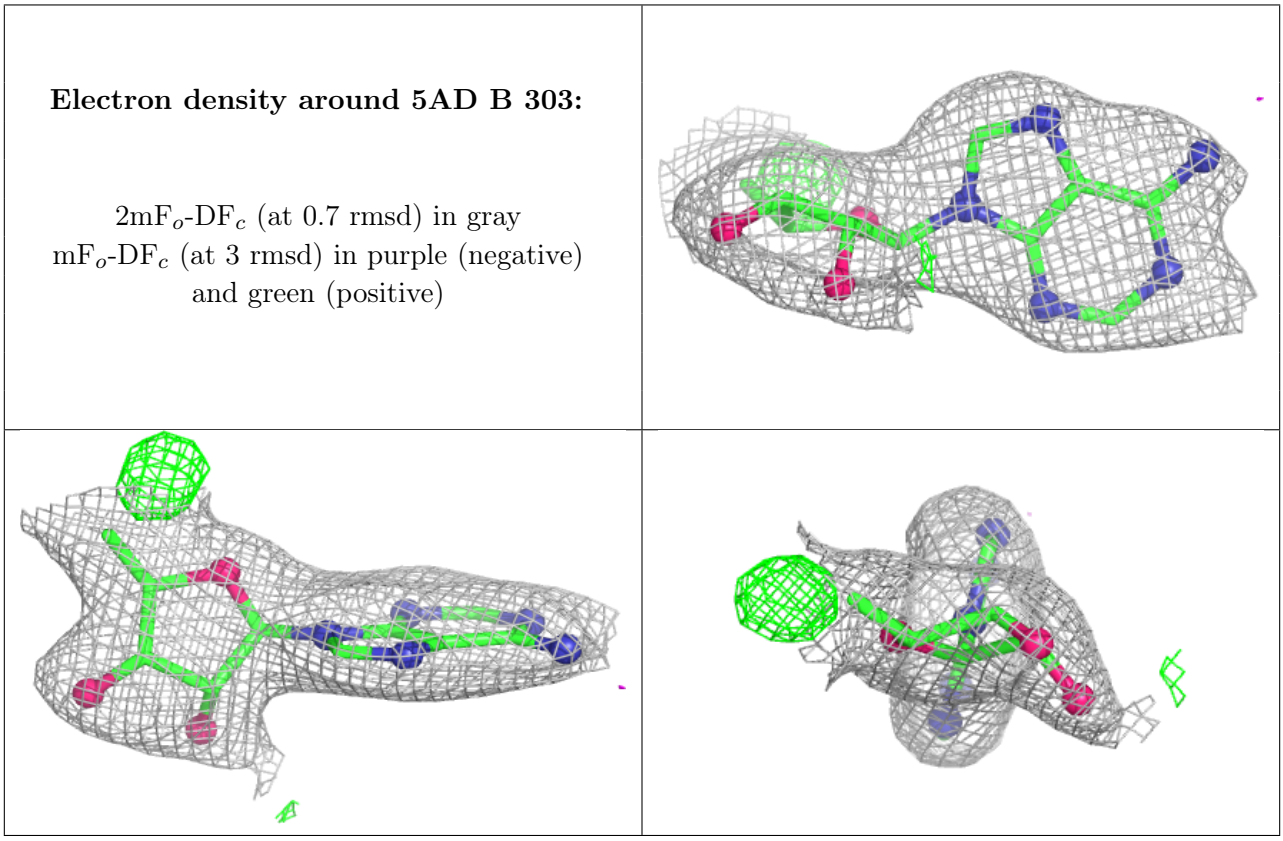
Electron density around B12 B 302:

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



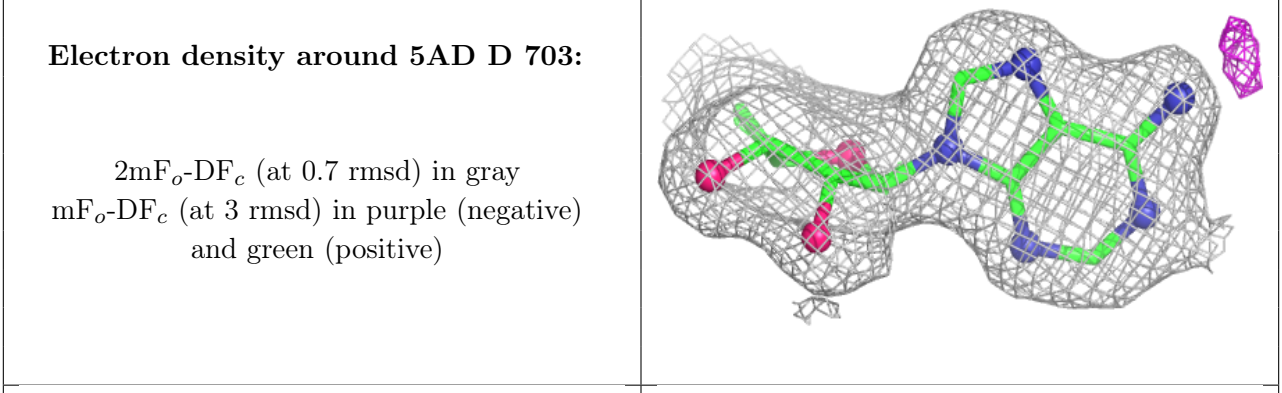
Electron density around 5AD B 303:

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



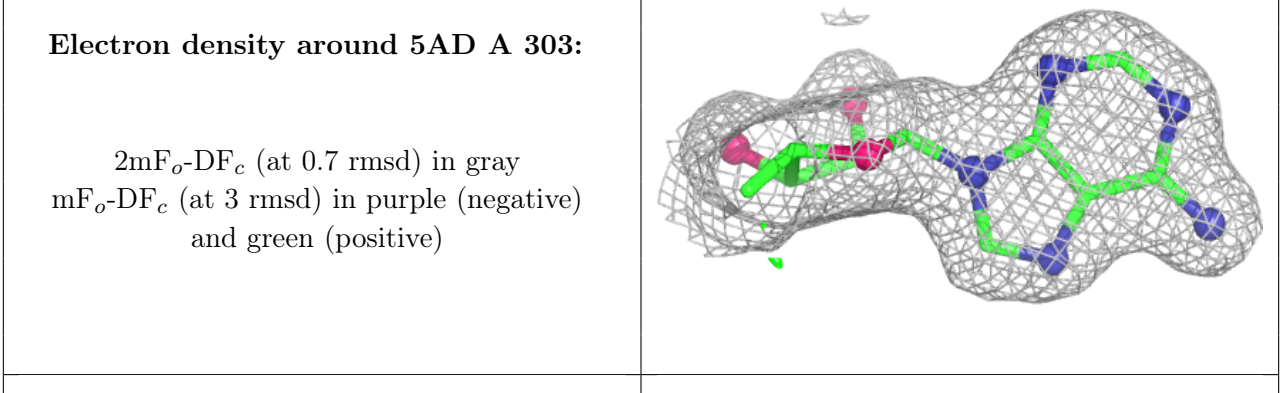
Electron density around 5AD D 703:

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



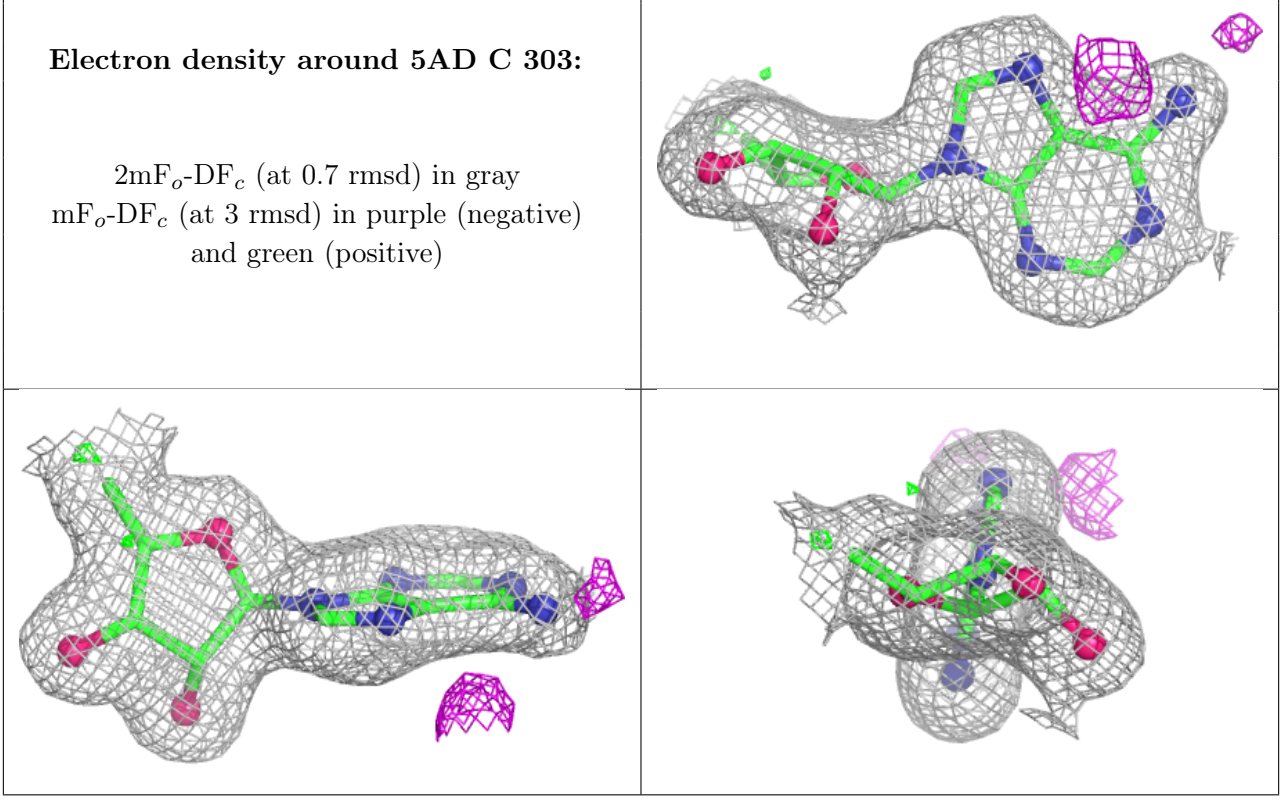
Electron density around 5AD A 303:

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



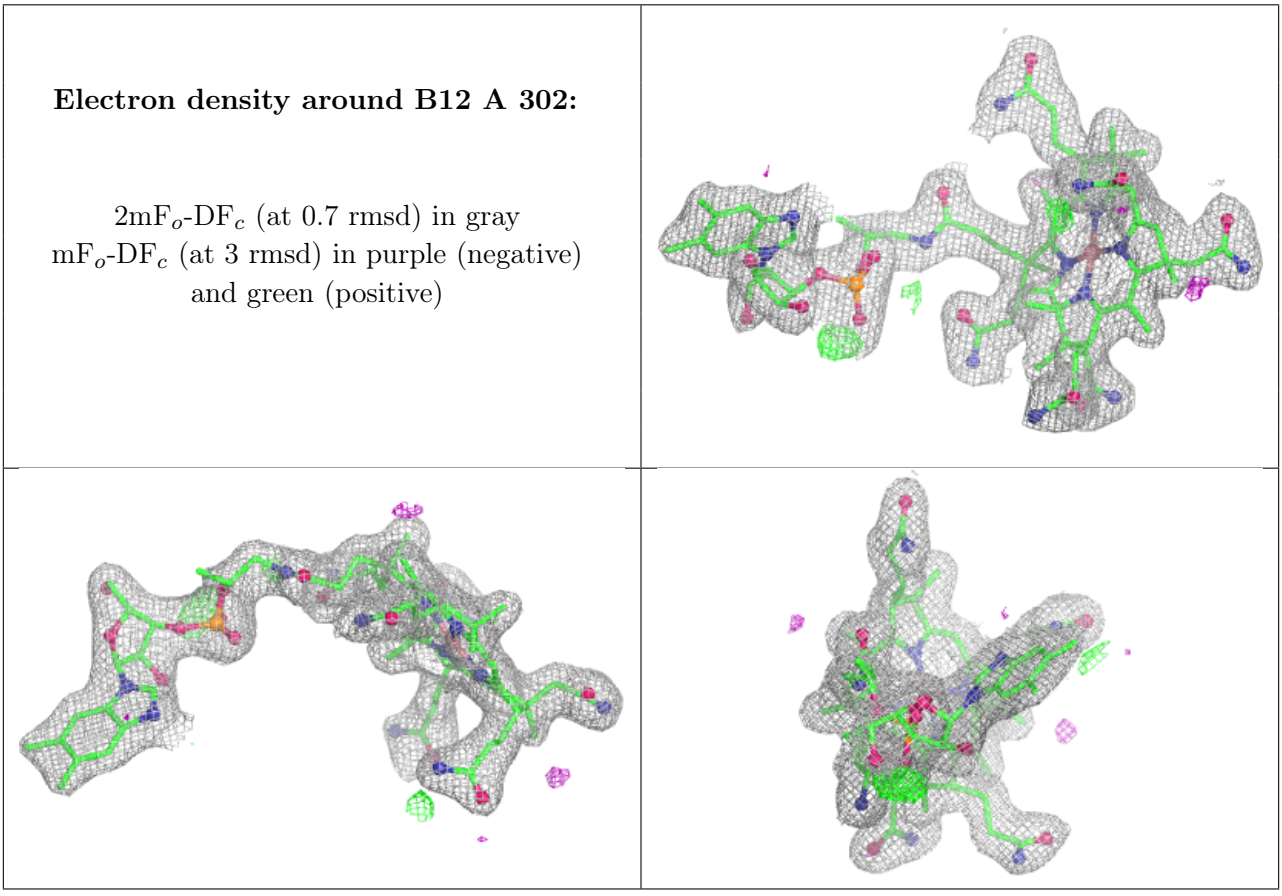
Electron density around 5AD C 303:

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



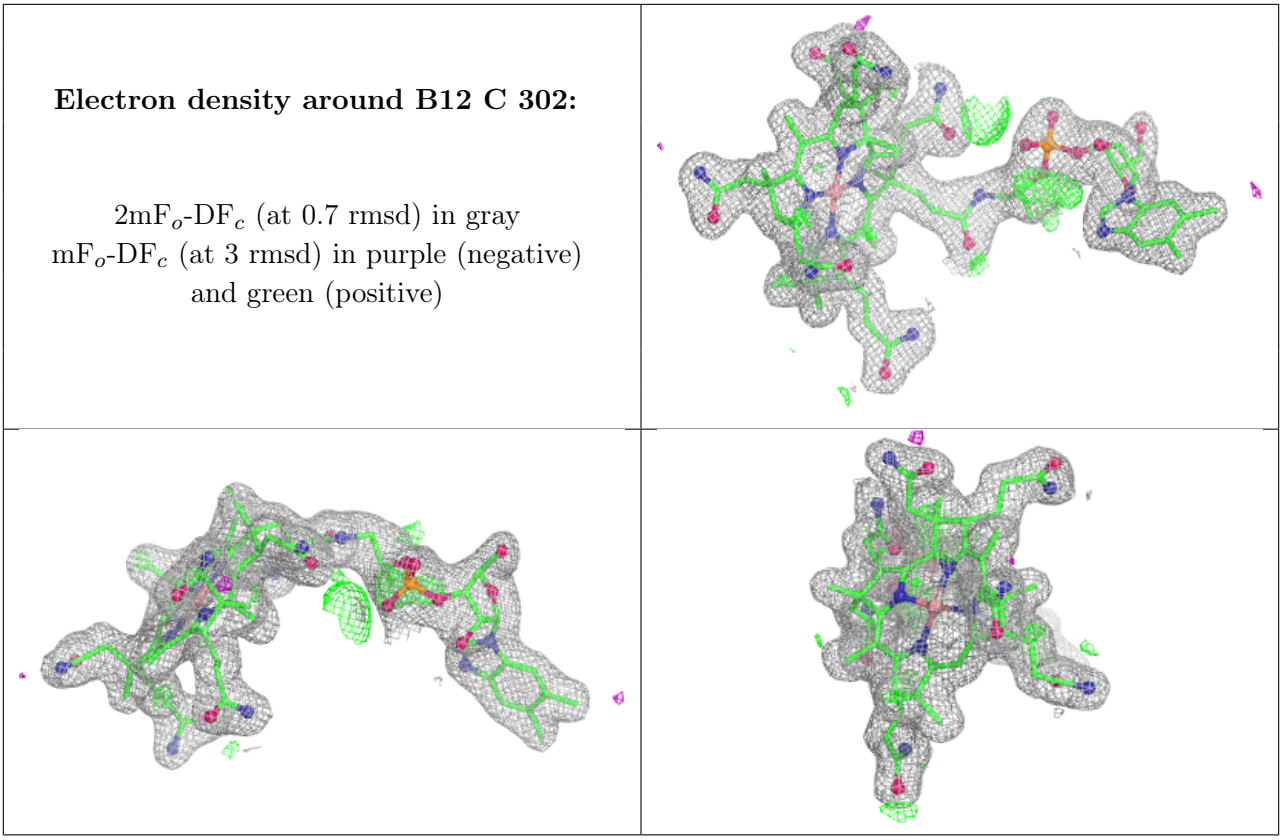
Electron density around B12 A 302:

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



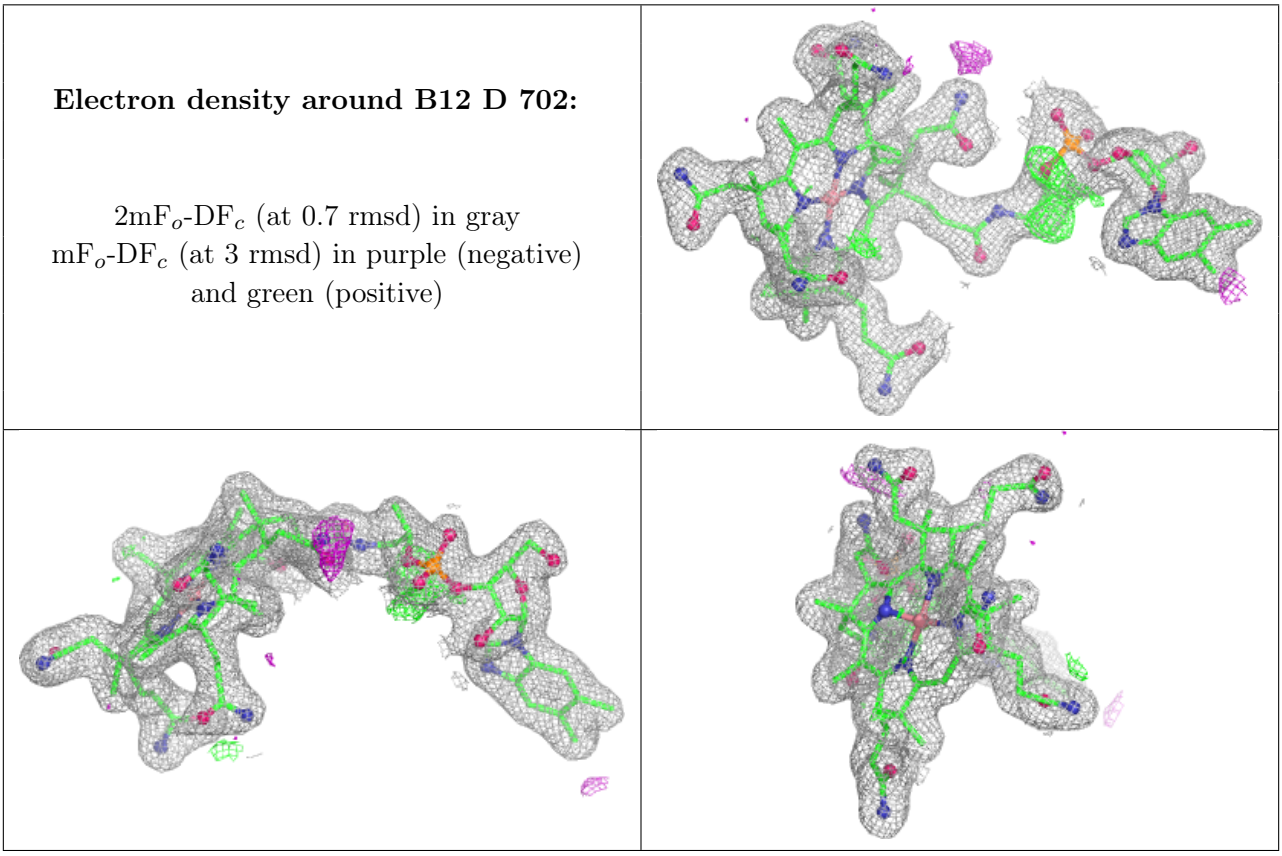
Electron density around B12 C 302:

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



Electron density around B12 D 702:

$2mF_o$-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.