Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2026 – 09:46 AM JST

PDB ID	:	8J2Y / pdb_00008j2y
Title	:	Acidimicrobiaceae bacterium photocobilins protein, dark state
Authors	:	Zhang, S.; Poddar, H.; Levy, W.C.; Leys, D.
Deposited on	:	2023-04-15
Resolution	:	2.30 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:

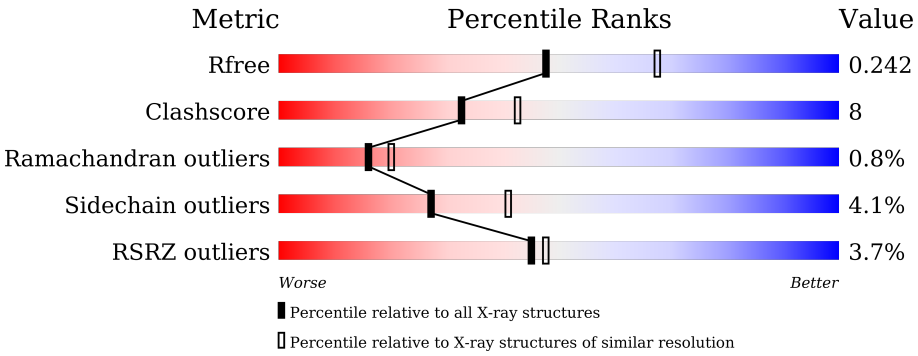
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	352	4% 78% 11% • 7%
1	B	352	3% 79% 11% • 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B12	A	401	X	-	-	-
2	B12	B	401	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5261 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.

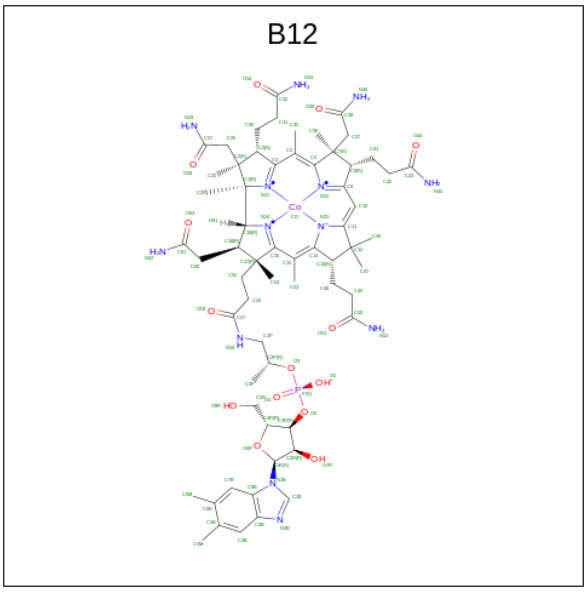
- Molecule 1 is a protein called GGDEF domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	3	0
			2459	1547	434	474	4			
1	B	327	Total	C	N	O	S	0	1	0
			2443	1535	431	473	4			

There are 18 discrepancies between the modelled and reference sequences:

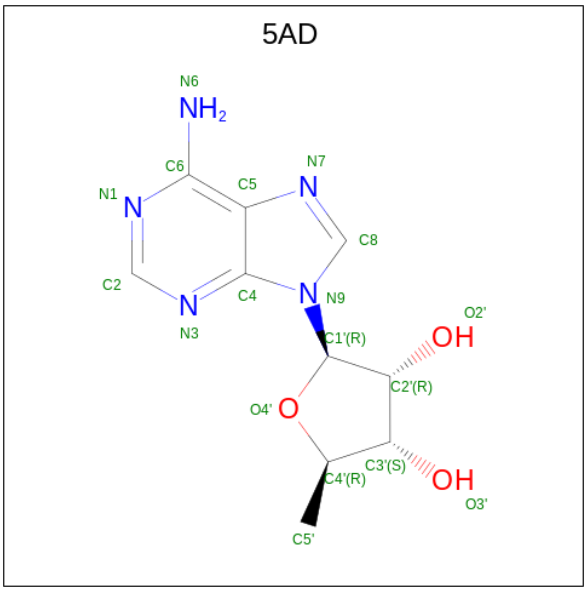
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A349B205
A	345	LEU	-	expression tag	UNP A0A349B205
A	346	GLU	-	expression tag	UNP A0A349B205
A	347	HIS	-	expression tag	UNP A0A349B205
A	348	HIS	-	expression tag	UNP A0A349B205
A	349	HIS	-	expression tag	UNP A0A349B205
A	350	HIS	-	expression tag	UNP A0A349B205
A	351	HIS	-	expression tag	UNP A0A349B205
A	352	HIS	-	expression tag	UNP A0A349B205
B	1	MET	-	initiating methionine	UNP A0A349B205
B	345	LEU	-	expression tag	UNP A0A349B205
B	346	GLU	-	expression tag	UNP A0A349B205
B	347	HIS	-	expression tag	UNP A0A349B205
B	348	HIS	-	expression tag	UNP A0A349B205
B	349	HIS	-	expression tag	UNP A0A349B205
B	350	HIS	-	expression tag	UNP A0A349B205
B	351	HIS	-	expression tag	UNP A0A349B205
B	352	HIS	-	expression tag	UNP A0A349B205

- Molecule 2 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
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



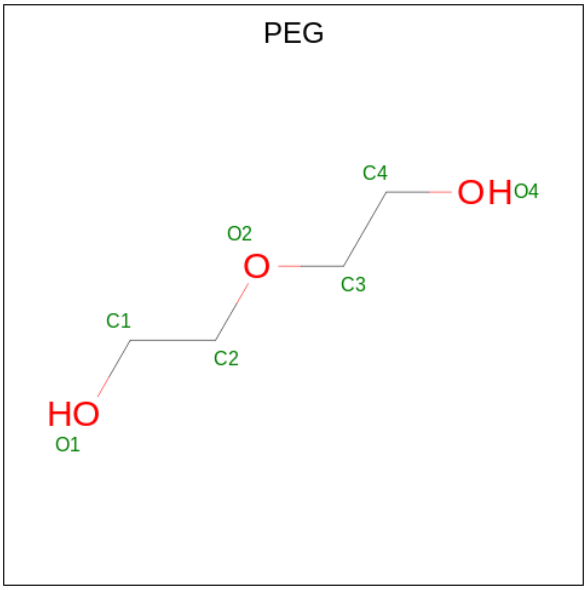
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		

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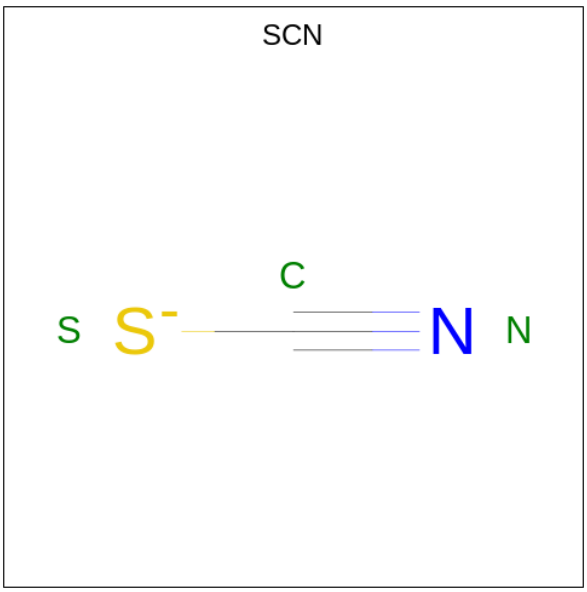
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

- Molecule 6 is water.

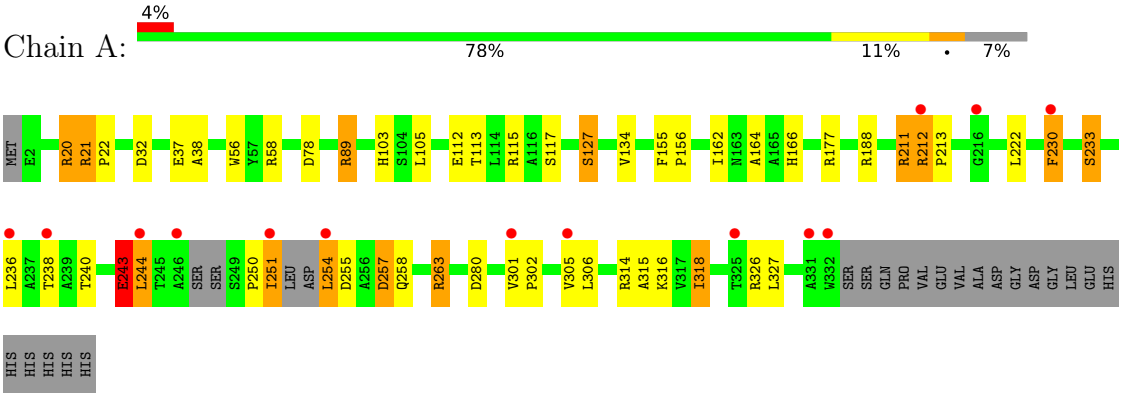
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	64	Total O 64 64	0	0
6	B	64	Total O 64 64	0	0

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.

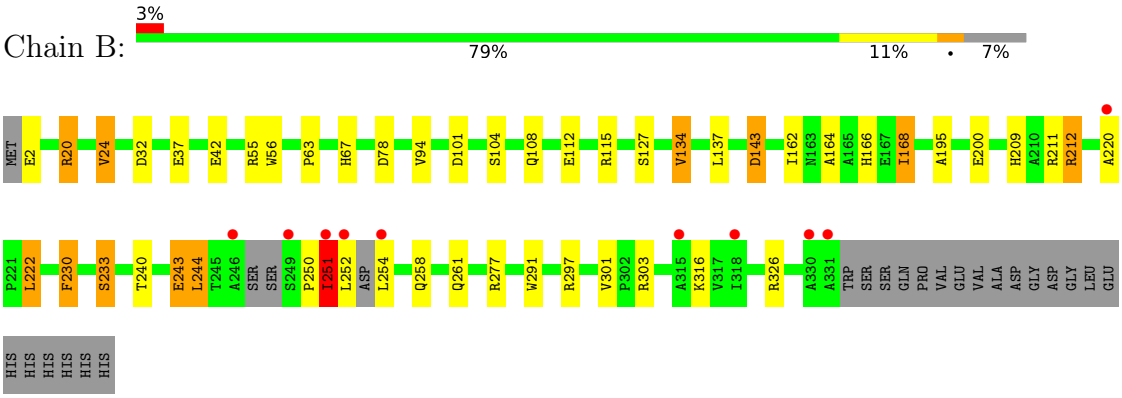
• Molecule 1: GGDEF domain-containing protein

Chain A:



• Molecule 1: GGDEF domain-containing protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	108.77Å 125.84Å 124.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.31 – 2.30 44.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.31-2.30) 100.0 (44.31-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.209 , 0.237 0.212 , 0.242	Depositor DCC
R_{free} test set	1997 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.9	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	0.95	EDS
Total number of atoms	5261	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: B12, PEG, SCN, 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	0.76	1/2518 (0.0%)	1.02	3/3438 (0.1%)
1	B	0.76	1/2488 (0.0%)	1.06	6/3397 (0.2%)
All	All	0.76	2/5006 (0.0%)	1.04	9/6835 (0.1%)

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	10
1	B	0	7
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	ILE	CA-CB	6.29	1.61	1.54
1	A	280	ASP	CG-OD2	5.20	1.35	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	101	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	20	ARG	N-CA-C	5.83	118.11	111.11
1	B	42	GLU	CB-CG-CD	5.36	121.72	112.60
1	A	243	GLU	N-CA-C	-5.26	103.53	110.43
1	B	32	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	143	ASP	CA-CB-CG	5.05	117.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	243	GLU	N-CA-C	-5.04	103.83	110.43

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	20[A]	ARG	Sidechain
1	A	20[B]	ARG	Sidechain
1	A	21	ARG	Sidechain
1	A	211	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	58	ARG	Sidechain
1	A	89	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	211	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	277	ARG	Sidechain
1	B	297	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	55	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	2459	0	2418	36	0
1	B	2443	0	2397	25	0
2	A	91	0	86	15	0
2	B	91	0	86	11	0
3	A	18	0	13	3	0
3	B	18	0	12	2	0
4	A	7	0	10	1	0
5	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	64	0	0	1	0
6	B	64	0	0	0	0
All	All	5261	0	5022	80	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 8.

All (80) 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:A:401:B12:H362	2:A:401:B12:H351	1.35	1.06
2:B:401:B12:H351	2:B:401:B12:H362	1.53	0.90
1:A:238:THR:HG22	1:A:263:ARG:HD2	1.57	0.85
1:A:78:ASP:OD1	1:B:20:ARG:NH1	2.11	0.82
2:A:401:B12:H531	2:A:401:B12:H543	1.66	0.78
2:A:401:B12:H362	2:A:401:B12:C35	2.15	0.74
1:A:105:LEU:H	2:A:401:B12:H522	1.38	0.72
1:A:243:GLU:O	1:A:244:LEU:HB2	1.90	0.71
2:A:401:B12:H351	2:A:401:B12:C36	2.18	0.70
1:B:243:GLU:O	1:B:244:LEU:HB2	1.90	0.69
1:A:103:HIS:CD2	2:A:401:B12:H451	2.13	0.66
1:B:291:TRP:HE1	2:B:401:B12:H292	1.45	0.65
2:B:401:B12:H531	2:B:401:B12:H543	1.79	0.64
1:A:56:TRP:CD2	3:A:402:5AD:H3'	2.32	0.63
1:B:104:SER:HB3	1:B:108:GLN:HE21	1.65	0.62
1:B:104:SER:HB3	1:B:108:GLN:NE2	2.15	0.61
1:A:38:ALA:HA	1:A:113:THR:HG22	1.83	0.60
1:A:236:LEU:HD22	1:A:316:LYS:HB3	1.82	0.60
1:A:211:ARG:NH1	1:A:212:ARG:O	2.39	0.56
1:B:56:TRP:CD2	3:B:402:5AD:H3'	2.41	0.55
2:B:401:B12:H401	2:B:401:B12:H8	1.71	0.55
1:A:89:ARG:NH1	1:A:117:SER:O	2.39	0.55
1:B:134:VAL:HG11	1:B:164:ALA:HB1	1.88	0.55
1:B:220:ALA:O	1:B:222:LEU:HD22	2.07	0.54
1:A:255:ASP:OD1	1:A:257:ASP:HB2	2.08	0.53
1:B:63:PRO:O	1:B:67:HIS:CD2	2.62	0.53
1:A:302:PRO:O	1:A:305:VAL:HG22	2.08	0.53
2:B:401:B12:N24	3:B:402:5AD:H5'3	2.22	0.53
1:A:37:GLU:OE2	1:A:112:GLU:HG3	2.08	0.52
1:A:134:VAL:HG21	1:A:164:ALA:HB1	1.90	0.52
1:A:254:LEU:HD22	1:A:258:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:OE2	1:B:112:GLU:HG3	2.10	0.51
1:B:254:LEU:HD22	1:B:258:GLN:HB3	1.92	0.51
2:A:401:B12:N21	3:A:402:5AD:H5'1	2.26	0.51
2:A:401:B12:H492	2:A:401:B12:H471	1.93	0.50
1:A:188:ARG:HH12	1:A:222:LEU:HD23	1.78	0.48
1:A:315:ALA:O	1:A:318:ILE:HD13	2.13	0.48
1:A:89:ARG:HH21	4:A:403:PEG:H12	1.78	0.48
1:A:103:HIS:CE1	2:A:401:B12:H202	2.49	0.47
1:A:230:PHE:O	1:A:233:SER:OG	2.29	0.47
1:A:38:ALA:HB2	5:A:404:SCN:C	2.44	0.47
2:B:401:B12:H351	2:B:401:B12:C36	2.33	0.47
1:A:20[A]:ARG:NH1	1:B:78:ASP:OD1	2.40	0.47
1:B:240:THR:O	1:B:244:LEU:HD13	2.15	0.46
1:A:211:ARG:NH1	1:A:213:PRO:HA	2.30	0.46
1:A:251:ILE:HG23	1:A:254:LEU:HG	1.97	0.46
2:B:401:B12:H362	2:B:401:B12:C35	2.37	0.46
2:A:401:B12:H401	2:A:401:B12:H8	1.80	0.45
1:A:115:ARG:NH1	6:A:501:HOH:O	2.20	0.45
2:A:401:B12:N22	3:A:402:5AD:H5'1	2.31	0.45
1:B:195:ALA:HB1	1:B:200[B]:GLU:HB3	1.99	0.45
1:A:162:ILE:HG23	1:A:166:HIS:CE1	2.52	0.45
1:B:143:ASP:O	1:B:212:ARG:NH1	2.50	0.45
1:A:127:SER:O	1:B:67:HIS:HE1	2.01	0.44
1:B:20:ARG:O	1:B:24:VAL:HG13	2.17	0.44
2:B:401:B12:H601	2:B:401:B12:H262	1.99	0.44
1:A:244:LEU:HA	1:A:250:PRO:HG2	1.99	0.44
1:B:162:ILE:CG2	1:B:166:HIS:CE1	3.01	0.44
1:A:240:THR:O	1:A:244:LEU:HD13	2.18	0.43
1:B:143:ASP:OD2	1:B:209:HIS:HD2	2.01	0.43
2:B:401:B12:H8	2:B:401:B12:N40	2.32	0.43
2:A:401:B12:H531	2:A:401:B12:C54	2.37	0.43
1:B:230:PHE:O	1:B:233:SER:OG	2.30	0.43
2:A:401:B12:C53	2:A:401:B12:H551	2.49	0.43
1:A:134:VAL:HG21	1:A:164:ALA:CB	2.48	0.43
1:A:155:PHE:N	1:A:156:PRO:CD	2.82	0.42
2:B:401:B12:H3	2:B:401:B12:H291	1.85	0.42
2:A:401:B12:C35	2:A:401:B12:C36	2.86	0.42
1:B:261:GLN:NE2	1:B:261:GLN:HA	2.34	0.42
1:A:162:ILE:CG2	1:A:166:HIS:CE1	3.03	0.42
1:A:211:ARG:HH11	1:A:213:PRO:HA	1.83	0.41
1:B:250:PRO:O	1:B:251:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:B12:H533	2:A:401:B12:H482	2.03	0.41
1:B:94:VAL:HG21	1:B:137:LEU:HD23	2.03	0.41
1:B:162:ILE:HG23	1:B:166:HIS:CE1	2.55	0.41
1:A:21:ARG:N	1:A:22:PRO:HD2	2.36	0.41
1:A:305:VAL:HG23	1:A:306:LEU:N	2.37	0.40
2:B:401:B12:H531	2:B:401:B12:C56	2.52	0.40
1:A:314:ARG:O	1:A:318:ILE:HG23	2.21	0.40
1:B:195:ALA:HB1	1:B:200[A]:GLU:HB2	2.04	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	325/352 (92%)	318 (98%)	5 (2%)	2 (1%)	21	27
1	B	322/352 (92%)	311 (97%)	8 (2%)	3 (1%)	14	17
All	All	647/704 (92%)	629 (97%)	13 (2%)	5 (1%)	16	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	B	127	SER
1	A	244	LEU
1	B	244	LEU
1	B	251	ILE

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	247/265 (93%)	239 (97%)	8 (3%)	34 51
1	B	244/265 (92%)	232 (95%)	12 (5%)	22 34
All	All	491/530 (93%)	471 (96%)	20 (4%)	27 41

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

Mol	Chain	Res	Type
1	A	230	PHE
1	A	233	SER
1	A	243	GLU
1	A	251	ILE
1	A	254	LEU
1	A	301	VAL
1	A	318	ILE
1	A	327	LEU
1	B	2	GLU
1	B	24	VAL
1	B	134	VAL
1	B	168	ILE
1	B	222	LEU
1	B	230	PHE
1	B	233	SER
1	B	251	ILE
1	B	252	LEU
1	B	301	VAL
1	B	303	ARG
1	B	316	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	265	HIS
1	B	67	HIS
1	B	108	GLN
1	B	209	HIS
1	B	261	GLN

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

7 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	5AD	B	402	-	20,20,20	0.39	0	27,30,30	0.98	1 (3%)
2	B12	A	401	-	93,101,101	1.37	13 (13%)	146,166,166	2.31	35 (23%)
3	5AD	A	402	-	20,20,20	0.37	0	27,30,30	1.03	2 (7%)
5	SCN	A	405	-	1,2,2	0.30	0	0,1,1	-	-
5	SCN	A	404	-	1,2,2	0.26	0	0,1,1	-	-
4	PEG	A	403	-	6,6,6	0.17	0	5,5,5	0.11	0
2	B12	B	401	1	93,101,101	1.44	9 (9%)	146,166,166	2.48	36 (24%)

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	5AD	B	402	-	-	0/4/20/20	0/3/3/3
2	B12	A	401	-	1/1/36/38	27/56/223/223	0/3/11/11
3	5AD	A	402	-	-	0/4/20/20	0/3/3/3
4	PEG	A	403	-	-	3/4/4/4	-
2	B12	B	401	1	1/1/36/38	19/56/223/223	0/3/11/11

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	B12	C16-C15	-4.85	1.31	1.44
2	A	401	B12	C14-N23	-4.61	1.29	1.35
2	B	401	B12	C9-N22	4.41	1.42	1.30
2	A	401	B12	C6B-C5B	4.29	1.51	1.40
2	A	401	B12	C8B-C9B	4.27	1.47	1.40
2	B	401	B12	C14-N23	-4.27	1.29	1.35
2	B	401	B12	C8B-C9B	3.95	1.47	1.40
2	B	401	B12	C2B-N1B	-3.42	1.31	1.37
2	B	401	B12	C9B-N3B	-3.32	1.33	1.39
2	B	401	B12	C18-C19	-3.18	1.46	1.53
2	A	401	B12	C19-N24	-3.18	1.42	1.48
2	A	401	B12	C16-C15	-2.98	1.36	1.44
2	A	401	B12	C10-C9	2.93	1.47	1.39
2	A	401	B12	C8B-N1B	-2.71	1.33	1.39
2	B	401	B12	C19-N24	-2.42	1.44	1.48
2	A	401	B12	C9-N22	2.35	1.36	1.30
2	B	401	B12	C1-C19	-2.34	1.50	1.55
2	A	401	B12	C1P-C2P	2.26	1.57	1.51
2	A	401	B12	C1-C2	-2.26	1.53	1.58
2	A	401	B12	C2B-N3B	2.12	1.35	1.31
2	A	401	B12	C9B-N3B	-2.07	1.35	1.39
2	A	401	B12	C17-C16	-2.04	1.49	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	B12	C54-C17-C55	10.64	126.79	109.25
2	B	401	B12	C54-C17-C55	10.37	126.36	109.25
2	B	401	B12	C1-C19-N24	10.25	117.77	106.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	B12	C18-C19-N24	9.40	116.62	102.31
2	A	401	B12	C1-C19-N24	9.03	116.40	106.24
2	A	401	B12	C55-C17-C16	-8.92	99.03	116.65
2	B	401	B12	C8B-C9B-N3B	-7.47	101.72	109.97
2	B	401	B12	C9B-N3B-C2B	7.18	113.00	104.44
2	A	401	B12	C20-C1-C19	-6.68	102.92	109.36
2	B	401	B12	C18-C19-N24	6.63	112.40	102.31
2	B	401	B12	C9B-C8B-N1B	6.45	108.07	105.35
2	B	401	B12	O58-C57-C56	-6.27	110.54	122.02
2	B	401	B12	C55-C17-C18	-6.21	99.15	111.15
2	B	401	B12	C56-C57-N59	5.54	125.76	116.42
2	A	401	B12	C18-C17-C16	5.15	106.93	100.67
2	B	401	B12	C55-C17-C16	-5.12	106.54	116.65
2	A	401	B12	C56-C55-C17	-4.94	105.99	115.52
2	A	401	B12	O58-C57-C56	-4.52	113.75	122.02
2	B	401	B12	C18-C17-C16	4.16	105.72	100.67
2	B	401	B12	C7B-C8B-C9B	-4.04	117.73	122.52
2	B	401	B12	C1-C19-C18	4.00	128.45	121.88
2	B	401	B12	C20-C1-C19	-3.96	105.54	109.36
2	B	401	B12	C4B-C9B-N3B	3.93	137.25	130.51
2	A	401	B12	C17-C18-C19	-3.91	96.39	102.36
2	B	401	B12	C13-C14-N23	3.87	114.36	109.10
2	B	401	B12	C13-C14-C15	-3.86	118.42	124.32
3	B	402	5AD	C5'-C4'-C3'	-3.83	111.68	115.70
2	B	401	B12	N1B-C2B-N3B	-3.71	108.84	113.91
2	A	401	B12	C9-C10-C11	-3.70	120.62	125.97
2	A	401	B12	C8B-N1B-C2B	3.68	109.80	106.37
2	B	401	B12	C60-C18-C19	3.51	123.78	114.62
2	A	401	B12	C26-C2-C1	3.50	115.46	110.01
2	B	401	B12	C9-C10-C11	-3.43	121.00	125.97
2	A	401	B12	C56-C57-N59	3.42	122.17	116.42
2	A	401	B12	C13-C14-N23	3.40	113.73	109.10
2	B	401	B12	O6R-C4R-C5R	-3.37	101.92	109.21
2	A	401	B12	C41-C8-C9	-3.28	105.41	111.19
3	A	402	5AD	C5'-C4'-C3'	-3.21	112.33	115.70
2	A	401	B12	C3P-C2P-C1P	3.10	117.41	111.39
2	A	401	B12	C60-C18-C19	3.10	122.70	114.62
2	A	401	B12	O3-P-O4	-3.02	98.13	109.47
2	B	401	B12	O7R-C2R-C3R	2.84	119.24	111.17
2	B	401	B12	O6R-C1R-N1B	-2.78	102.58	108.06
2	A	401	B12	C1-C19-C18	2.70	126.32	121.88
2	B	401	B12	C2-C3-C4	2.69	104.69	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	B12	C2-C1-N21	2.68	105.50	101.77
2	A	401	B12	N1B-C2B-N3B	-2.63	110.32	113.91
2	A	401	B12	C13-C14-C15	-2.54	120.44	124.32
2	A	401	B12	C20-C1-C2	2.53	117.52	113.28
2	B	401	B12	C13-C12-C11	2.49	103.79	100.97
2	B	401	B12	C26-C27-N29	2.49	124.41	116.52
2	A	401	B12	C1P-N59-C57	-2.44	117.36	122.69
2	B	401	B12	C31-C30-C3	-2.43	107.72	114.73
2	A	401	B12	C12-C11-C10	-2.38	120.27	123.37
2	A	401	B12	C9B-N3B-C2B	2.36	107.24	104.44
2	B	401	B12	C55-C56-C57	2.35	116.37	111.23
2	A	401	B12	C54-C17-C18	-2.28	109.62	112.98
2	B	401	B12	C37-C7-C8	2.26	114.43	108.39
2	A	401	B12	O6R-C1R-N1B	-2.26	103.61	108.06
2	A	401	B12	C7-C6-C5	-2.22	124.58	128.07
2	B	401	B12	C17-C16-N24	-2.22	107.73	111.15
2	B	401	B12	C1-C2-C3	-2.19	98.80	101.60
2	A	401	B12	C37-C38-N40	2.19	123.45	116.52
2	B	401	B12	C8B-N1B-C2B	2.13	108.35	106.37
3	A	402	5AD	O3'-C3'-C4'	-2.12	105.27	110.47
2	A	401	B12	C55-C17-C18	-2.12	107.05	111.15
2	A	401	B12	C8B-C9B-N3B	-2.12	107.63	109.97
2	B	401	B12	C26-C2-C1	2.11	113.30	110.01
2	B	401	B12	C25-C2-C26	-2.09	105.49	109.71
2	A	401	B12	C8B-N1B-C1R	-2.09	121.84	125.39
2	B	401	B12	C1P-N59-C57	-2.08	118.15	122.69
2	A	401	B12	C3-C4-C5	2.08	127.31	123.81
2	A	401	B12	O5-P-O3	2.07	114.96	106.78
2	A	401	B12	C7-C6-N22	2.03	111.64	107.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	B12	C19
2	B	401	B12	C19

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	B12	C16-C17-C55-C56
2	A	401	B12	C54-C17-C55-C56
2	A	401	B12	C18-C17-C55-C56

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Mol	Chain	Res	Type	Atoms
2	A	401	B12	C18-C60-C61-O63
2	A	401	B12	C18-C60-C61-N62
2	A	401	B12	N59-C1P-C2P-C3P
2	A	401	B12	C3P-C2P-O3-P
2	A	401	B12	C2P-O3-P-O5
2	B	401	B12	C16-C17-C55-C56
2	B	401	B12	C54-C17-C55-C56
2	B	401	B12	C18-C60-C61-O63
2	B	401	B12	C18-C60-C61-N62
2	B	401	B12	N59-C1P-C2P-C3P
2	B	401	B12	C3P-C2P-O3-P
2	A	401	B12	C7-C37-C38-N40
2	A	401	B12	C56-C57-N59-C1P
4	A	403	PEG	O2-C3-C4-O4
2	A	401	B12	C55-C56-C57-O58
2	B	401	B12	C55-C56-C57-N59
2	A	401	B12	C48-C49-C50-N52
2	A	401	B12	C7-C37-C38-O39
2	B	401	B12	C7-C37-C38-N40
2	B	401	B12	C55-C56-C57-O58
2	A	401	B12	C48-C49-C50-O51
2	A	401	B12	C1P-C2P-O3-P
2	B	401	B12	C1P-C2P-O3-P
2	B	401	B12	C7-C37-C38-O39
4	A	403	PEG	O1-C1-C2-O2
2	A	401	B12	C2P-O3-P-O2
2	A	401	B12	C2P-O3-P-O4
2	A	401	B12	C3R-O2-P-O4
2	A	401	B12	C4-C3-C30-C31
2	A	401	B12	C55-C56-C57-N59
2	A	401	B12	N59-C1P-C2P-O3
2	A	401	B12	C2R-C1R-N1B-C2B
2	A	401	B12	C2-C3-C30-C31
4	A	403	PEG	C4-C3-O2-C2
2	A	401	B12	C2R-C1R-N1B-C8B
2	A	401	B12	O6R-C1R-N1B-C8B
2	B	401	B12	C2R-C1R-N1B-C8B
2	B	401	B12	O6R-C1R-N1B-C8B
2	A	401	B12	O58-C57-N59-C1P
2	B	401	B12	C18-C17-C55-C56
2	B	401	B12	C2R-C1R-N1B-C2B
2	B	401	B12	C2R-C3R-O2-P

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Mol	Chain	Res	Type	Atoms
2	B	401	B12	C30-C31-C32-N33
2	B	401	B12	C4-C3-C30-C31
2	A	401	B12	C19-C18-C60-C61
2	B	401	B12	C30-C31-C32-O34

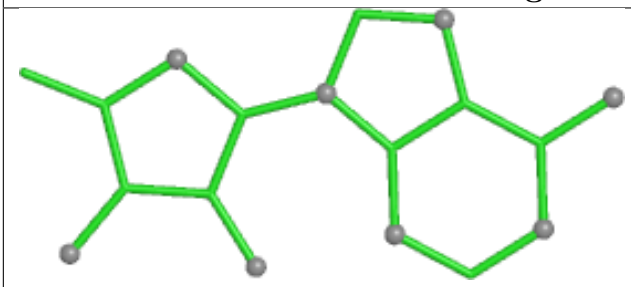
There are no ring outliers.

6 monomers are involved in 30 short contacts:

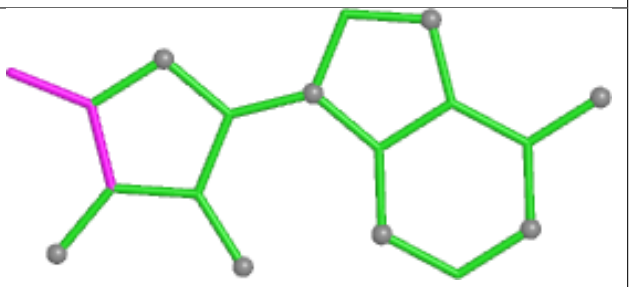
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	5AD	2	0
2	A	401	B12	15	0
3	A	402	5AD	3	0
5	A	404	SCN	1	0
4	A	403	PEG	1	0
2	B	401	B12	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

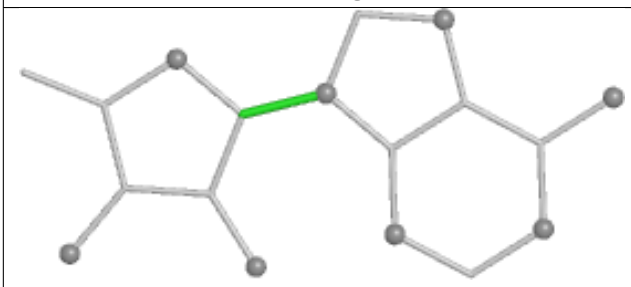
Ligand 5AD B 402



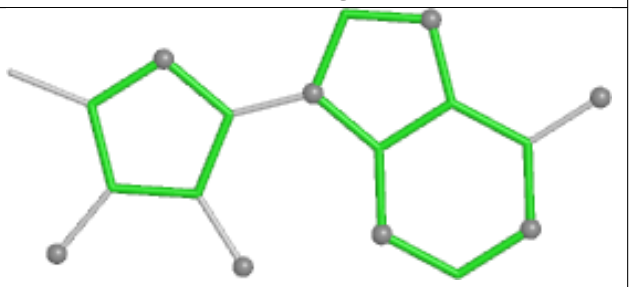
Bond lengths



Bond angles

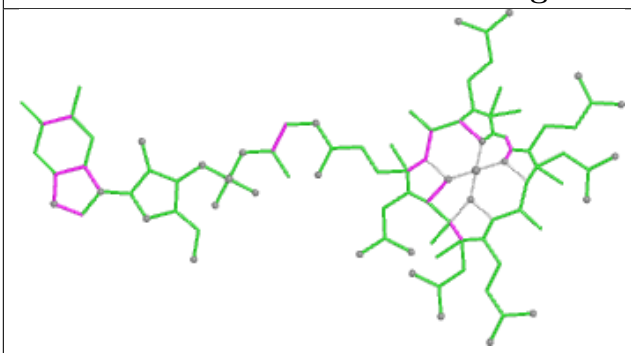


Torsions

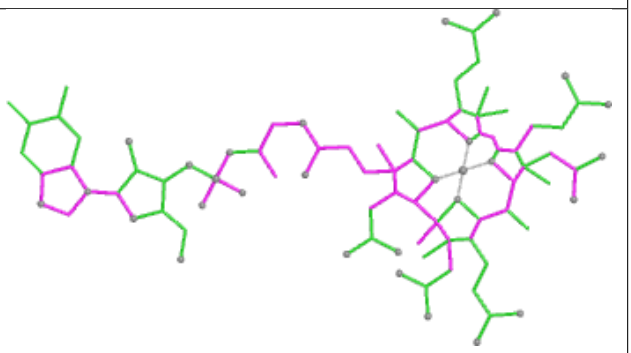


Rings

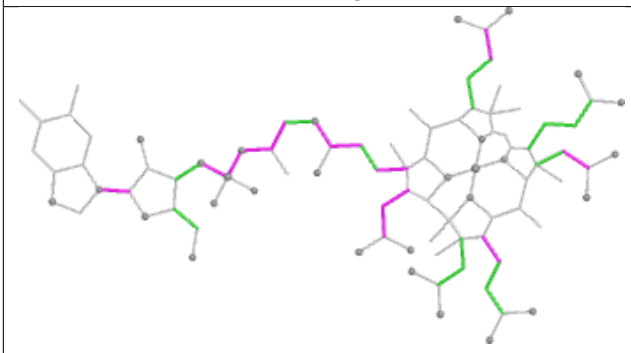
Ligand B12 A 401



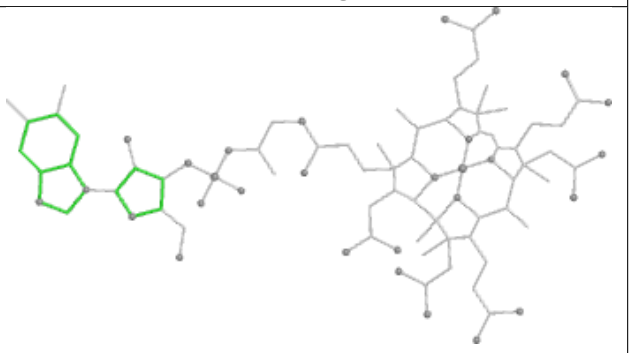
Bond lengths



Bond angles

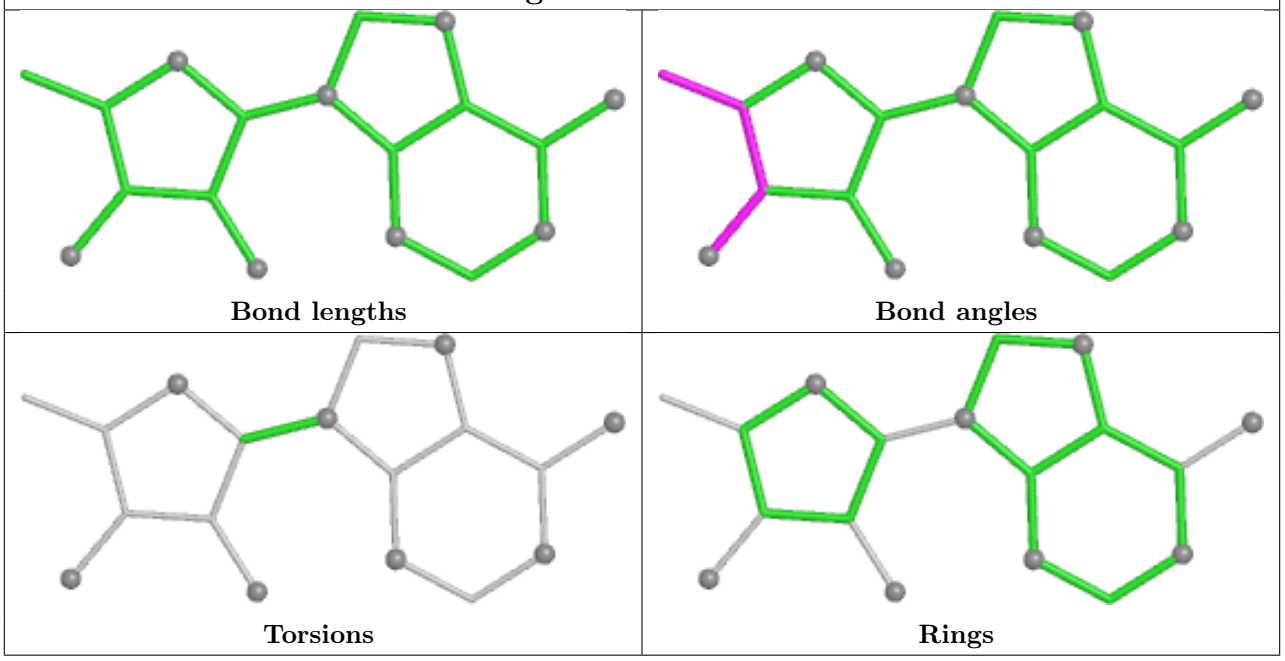


Torsions

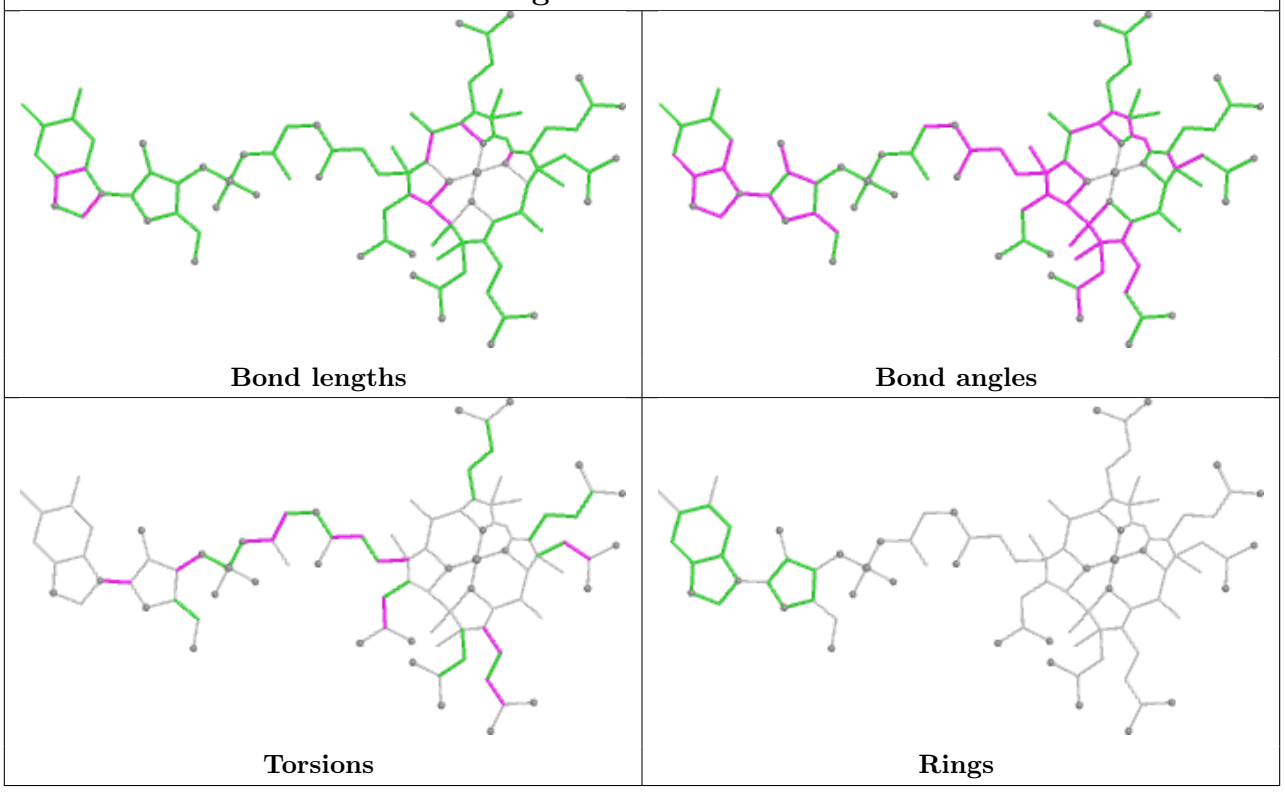


Rings

Ligand 5AD A 402



Ligand B12 B 401



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	327/352 (92%)	0.40	14 (4%)	40	41	28, 58, 122, 176	3 (0%)
1	B	327/352 (92%)	0.32	10 (3%)	51	53	31, 58, 102, 133	1 (0%)
All	All	654/704 (92%)	0.36	24 (3%)	45	48	28, 58, 115, 176	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	ALA	6.2
1	B	246	ALA	5.7
1	A	332	TRP	4.9
1	B	252	LEU	4.4
1	B	330	ALA	3.8
1	A	331	ALA	3.8
1	A	301	VAL	3.6
1	B	254	LEU	3.4
1	A	251	ILE	3.3
1	B	315	ALA	3.2
1	A	246	ALA	3.2
1	B	249	SER	3.1
1	A	238	THR	2.7
1	A	230	PHE	2.6
1	B	251	ILE	2.6
1	A	216	GLY	2.4
1	A	212	ARG	2.3
1	B	220	ALA	2.3
1	A	236	LEU	2.2
1	A	305	VAL	2.2
1	A	244	LEU	2.2
1	A	254	LEU	2.2
1	A	325	THR	2.1
1	B	318	ILE	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)

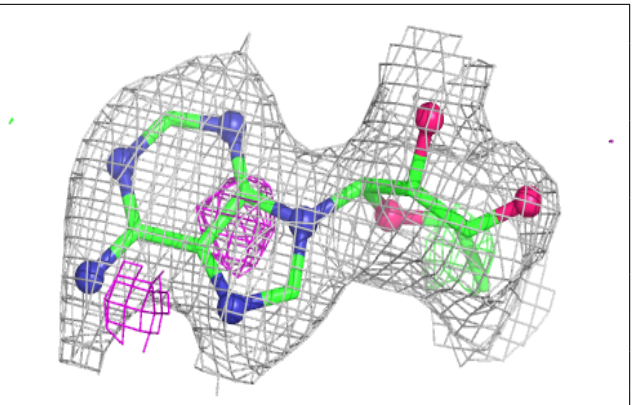
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

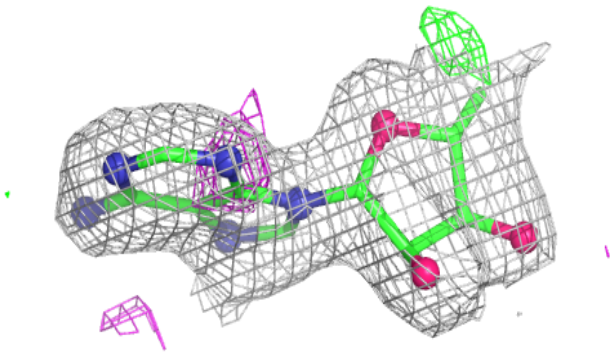
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SCN	A	404	3/3	0.82	0.18	89,89,98,102	0
4	PEG	A	403	7/7	0.91	0.10	67,69,72,74	0
5	SCN	A	405	3/3	0.92	0.11	55,55,56,70	0
3	5AD	B	402	18/18	0.93	0.07	39,40,42,42	0
3	5AD	A	402	18/18	0.93	0.09	48,54,56,56	0
2	B12	B	401	91/91	0.97	0.07	33,37,47,61	0
2	B12	A	401	91/91	0.97	0.08	32,38,48,53	0

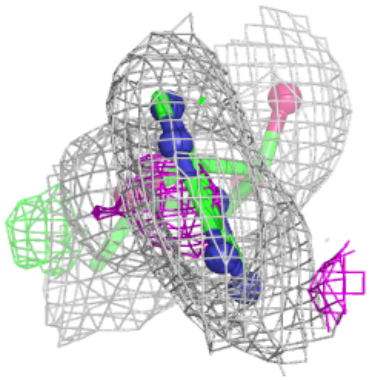
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD B 402:

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

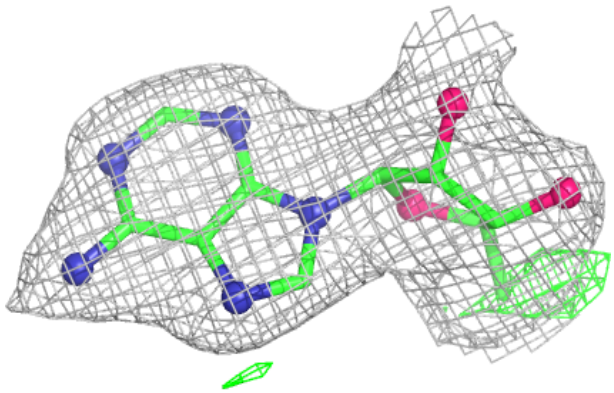


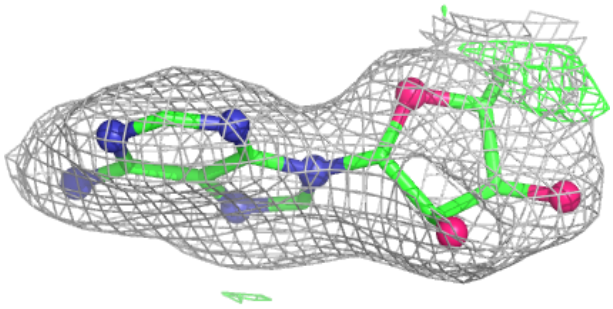


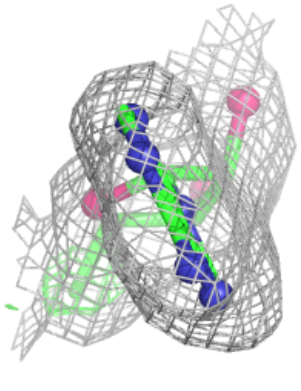


Electron density around 5AD A 402:

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

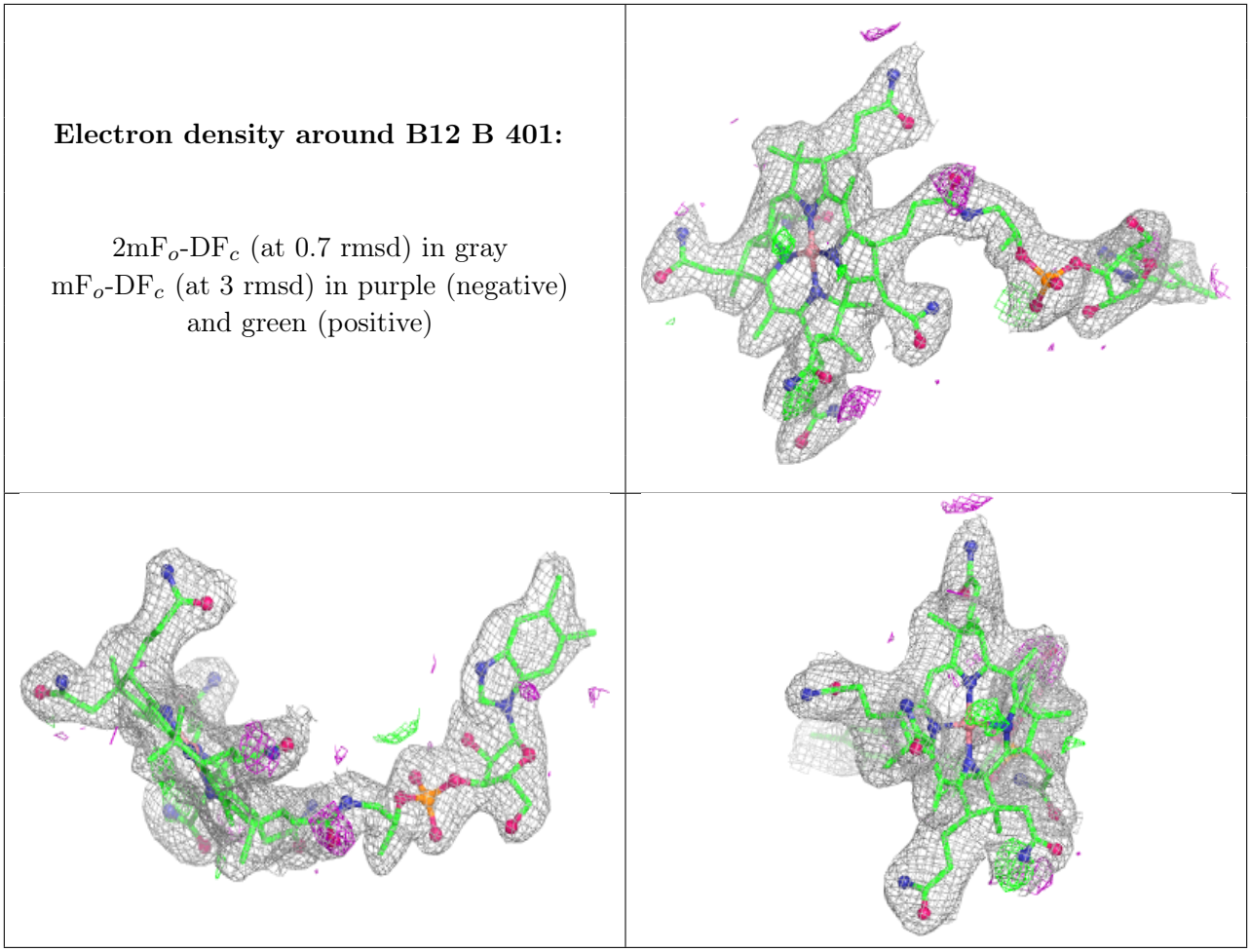






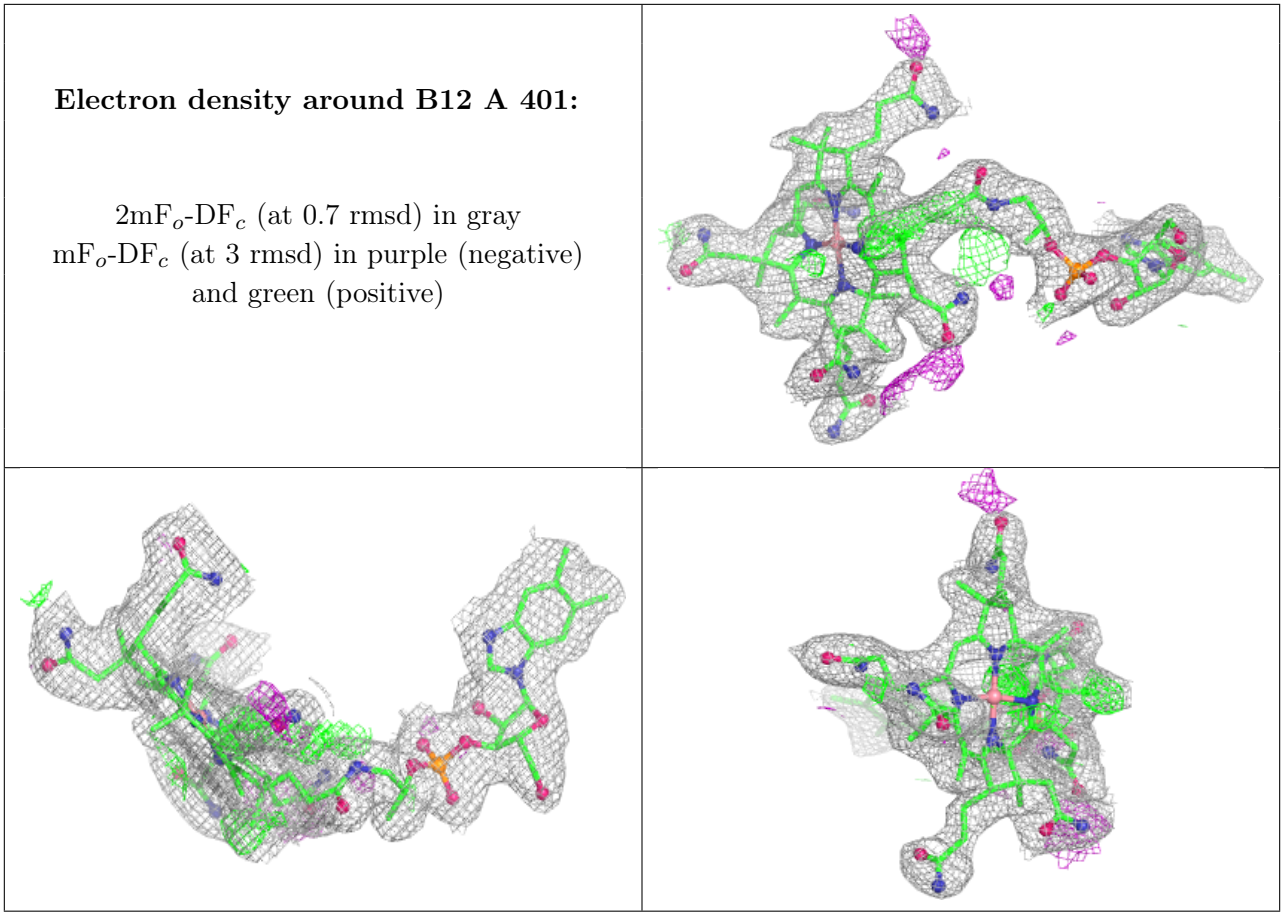
Electron density around B12 B 401:

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



Electron density around B12 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)



6.5 Other polymers

There are no such residues in this entry.