Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 12:56 PM EDT

PDB ID	:	9C3W / pdb_00009c3w
Title	:	Crystal structure of biphenyl synthase from Malus domestica complexed with diketide-CoA mimetics
Authors	:	Re, R.N.; Noel, J.P.; Burkart, M.D.
Deposited on	:	2024-06-02
Resolution	:	1.57 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:

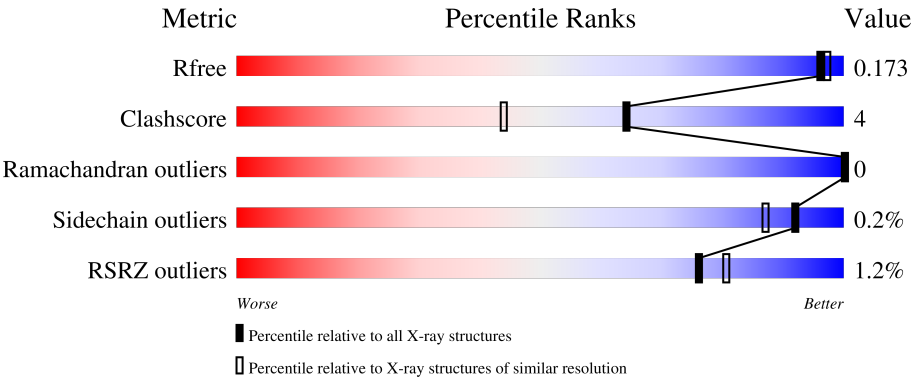
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

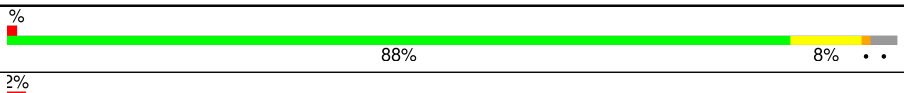
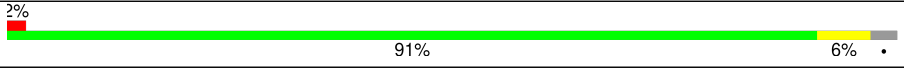
The reported resolution of this entry is 1.57 Å.

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}	164625	7165 (1.60-1.56)
Clashscore	180529	1026 (1.58-1.58)
Ramachandran outliers	177936	1005 (1.58-1.58)
Sidechain outliers	177891	1004 (1.58-1.58)
RSRZ outliers	164620	7163 (1.60-1.56)

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	390	
1	B	390	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13141 atoms, of which 6165 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.

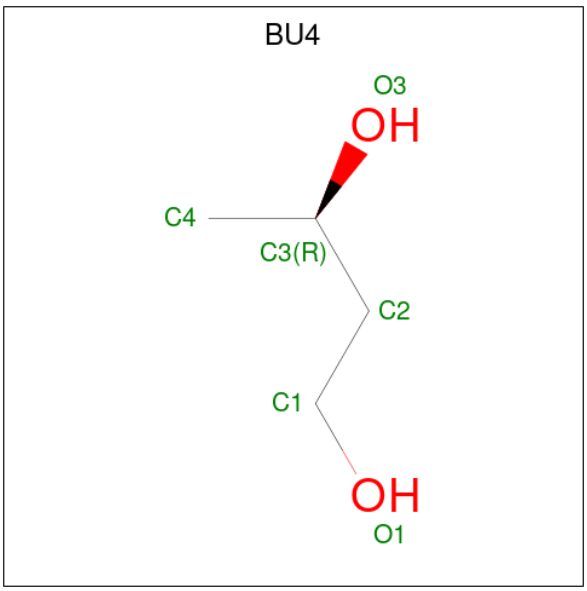
- Molecule 1 is a protein called BIS3 biphenyl synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	H	N	O	S	0	10	0
			6060	1919	3045	521	557	18			
1	B	378	Total	C	H	N	O	S	0	10	0
			6017	1909	3018	517	557	16			

There are 6 discrepancies between the modelled and reference sequences:

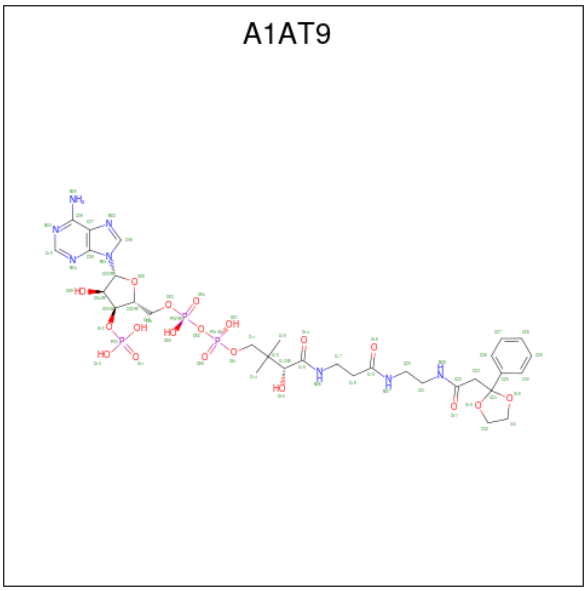
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP K9MST3
A	0	SER	-	expression tag	UNP K9MST3
A	251	VAL	ALA	engineered mutation	UNP K9MST3
B	-1	GLY	-	expression tag	UNP K9MST3
B	0	SER	-	expression tag	UNP K9MST3
B	251	VAL	ALA	engineered mutation	UNP K9MST3

- Molecule 2 is (3R)-butane-1,3-diol (CCD ID: BU4) (formula: $C_4H_{10}O_2$).



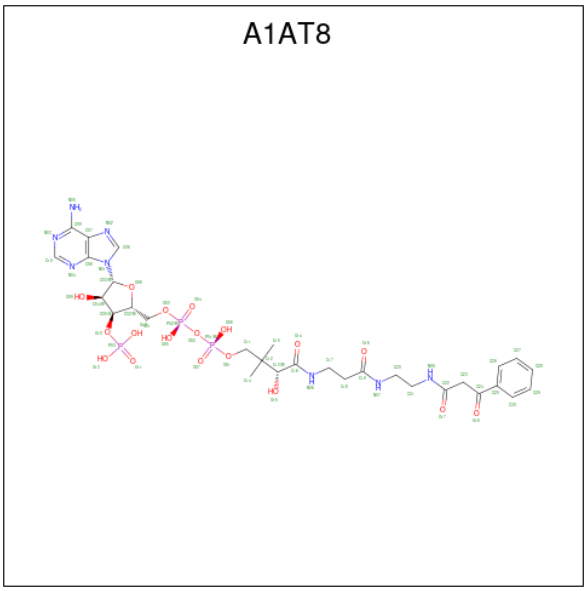
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			16	4	10	2		
2	B	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)oxolan-2-yl]methyl (3R)-3-hydroxy-2,2-dimethyl-4-oxo-4-{[3-oxo-3-({2-[2-(2-phenyl-1,3-dioxolan-2-yl)acetamido]ethyl}amino)propyl]amino}butyl dihydrogen diphosphate (CCD ID: A1AT9) (formula: $C_{32}H_{47}N_8O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			105	32	43	8	19	3		

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)oxolan-2-yl]methyl (3R)-3-hydroxy-2,2-dimethyl-4-oxo-4-[(3-oxo-3-{[2-(3-oxo-3-phenylpropanamido)ethyl]amino}propyl)amino]butyl dihydrogen diphosphate (CCD ID: A1AT8) (formula: $C_{30}H_{43}N_8O_{18}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	0	0
			98	30	39	8	18	3		

- Molecule 5 is water.

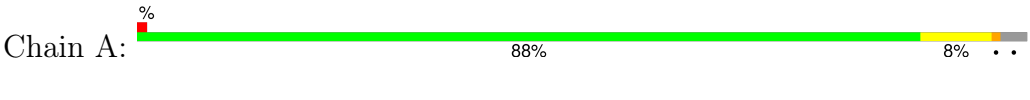
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	412	Total	O	0	0
			412	412		
5	B	417	Total	O	0	0
			417	417		

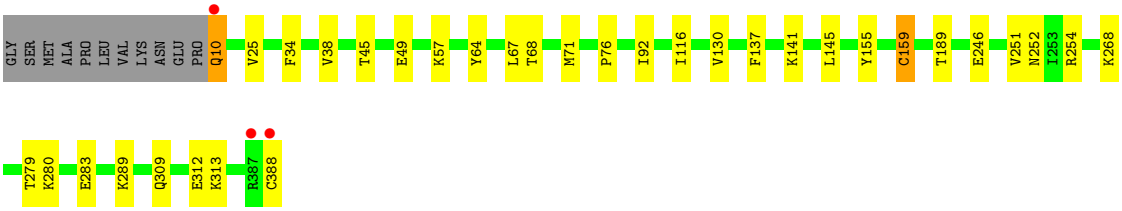
3 Residue-property plots (i)

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: BIS3 biphenyl synthase

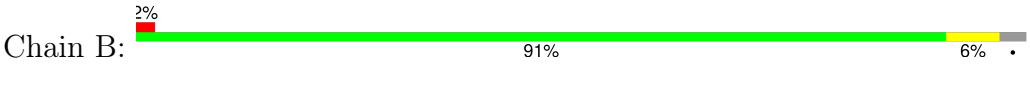
Chain A:

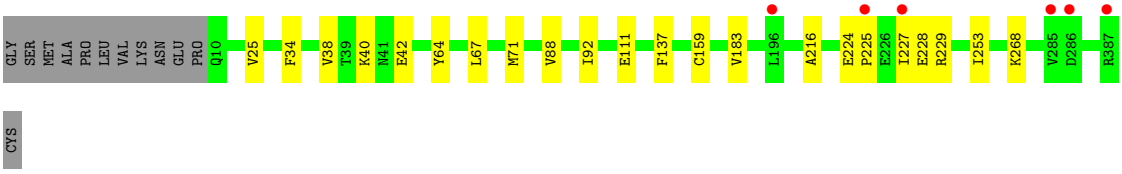




• Molecule 1: BIS3 biphenyl synthase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.25Å 112.52Å 62.71Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	56.26 – 1.57 56.26 – 1.57	Depositor EDS
% Data completeness (in resolution range)	98.8 (56.26-1.57) 96.3 (56.26-1.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 1.57Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.143 , 0.173 0.143 , 0.173	Depositor DCC
R_{free} test set	5174 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	9.0	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13141	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: BU4, A1AT9, CSD, A1AT8

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	0.44	0/3089	0.62	1/4176 (0.0%)
1	B	0.43	0/3076	0.61	0/4163
All	All	0.43	0/6165	0.61	1/8339 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	PRO	N-CD-CG	-5.03	95.65	103.20

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	3015	3045	3056	30	0
1	B	2999	3018	3033	19	0
2	A	6	10	10	1	0
2	B	6	10	10	0	0
3	A	62	43	0	2	0
4	B	59	39	0	0	0
5	A	412	0	0	5	2
5	B	417	0	0	5	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6976	6165	6109	47	2

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 (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HD12	1:B:71:MET:HE2	1.72	0.71
1:A:10:GLN:HE21	1:A:10:GLN:N	1.92	0.68
1:A:71[B]:MET:HE3	1:A:92:ILE:HD13	1.76	0.67
1:B:268:LYS:HD3	5:B:547:HOH:O	1.94	0.67
1:B:225:PRO:O	1:B:227:ILE:HD12	1.94	0.66
1:A:289:LYS:HE2	5:A:504:HOH:O	1.96	0.65
1:A:251:VAL:HG21	3:A:401:A1AT9:C32	2.33	0.58
1:A:312:GLU:OE2	1:A:313:LYS:NZ	2.36	0.58
1:B:268:LYS:HE3	5:B:673:HOH:O	2.03	0.58
1:A:68:THR:OG1	1:A:71[A]:MET:HG3	2.05	0.57
1:B:25[B]:VAL:HG22	1:B:64:TYR:CE2	2.41	0.56
1:A:159[A]:CSD:OD1	3:A:401:A1AT9:C23	2.55	0.55
1:A:279:THR:O	1:A:283:GLU:HG3	2.08	0.54
1:B:88[A]:VAL:HG23	5:B:806:HOH:O	2.08	0.54
1:A:67:LEU:HD12	1:A:71[B]:MET:HE2	1.90	0.53
1:A:283:GLU:HG2	5:A:504:HOH:O	2.09	0.53
1:A:189:THR:HB	2:A:400:BU4:H4B	1.90	0.53
1:A:268:LYS:HE2	1:A:309:GLN:HE22	1.75	0.52
1:A:116:ILE:HG23	1:A:145:LEU:HD23	1.93	0.51
1:A:246[B]:GLU:HG2	1:B:137:PHE:CZ	2.46	0.49
1:A:388:CYS:SG	1:A:388:CYS:O	2.71	0.48
1:B:67:LEU:CD1	1:B:71:MET:HE2	2.42	0.47
1:A:268:LYS:HE2	1:A:309:GLN:NE2	2.30	0.46
1:B:227:ILE:HD12	1:B:227:ILE:N	2.31	0.46
1:A:57:LYS:HE3	5:A:505:HOH:O	2.16	0.45
1:A:34:PHE:O	1:A:38:VAL:HG22	2.17	0.45
1:A:252:ASN:HB3	1:A:254:ARG:HD3	1.99	0.45
1:A:280:LYS:HE3	5:A:774:HOH:O	2.17	0.45
1:B:268:LYS:HD2	1:B:268:LYS:HA	1.71	0.45
1:A:312:GLU:OE2	1:A:313:LYS:HD2	2.18	0.44
1:A:25[B]:VAL:HG22	1:A:64:TYR:CE2	2.53	0.43
1:B:111:GLU:OE2	1:B:229:ARG:NH2	2.51	0.43
1:A:57:LYS:CE	5:A:505:HOH:O	2.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:O	1:B:216:ALA:HA	2.18	0.43
1:A:57:LYS:HE3	1:A:57:LYS:HB3	1.95	0.42
1:B:253:ILE:N	1:B:253:ILE:HD12	2.34	0.42
1:A:137:PHE:CE2	1:A:141[A]:LYS:HD2	2.54	0.42
1:B:71:MET:HE3	1:B:92:ILE:HD13	2.02	0.42
1:B:224:GLU:HG3	1:B:228:GLU:OE1	2.19	0.42
1:B:42:GLU:HG3	5:B:792:HOH:O	2.19	0.41
1:A:45:THR:O	1:A:49:GLU:HG3	2.20	0.41
1:A:246[B]:GLU:HG2	1:B:137:PHE:CE2	2.56	0.41
1:A:130:VAL:HA	1:A:155:TYR:CE1	2.56	0.40
1:B:40:LYS:HE2	5:B:647:HOH:O	2.20	0.40
1:A:268:LYS:CE	1:A:309:GLN:HE22	2.34	0.40
1:B:34:PHE:O	1:B:38:VAL:HG13	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:839:HOH:O	5:B:875:HOH:O[2_655]	2.16	0.04
5:A:763:HOH:O	5:B:827:HOH:O[1_455]	2.18	0.02

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	385/390 (99%)	378 (98%)	7 (2%)	0	100	100
1	B	384/390 (98%)	379 (99%)	5 (1%)	0	100	100
All	All	769/780 (99%)	757 (98%)	12 (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	329/329 (100%)	328 (100%)	1 (0%)	91 86
1	B	328/329 (100%)	328 (100%)	0	100 100
All	All	657/658 (100%)	656 (100%)	1 (0%)	92 87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN

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

Mol	Chain	Res	Type
1	A	244	ASN
1	A	273	ASN
1	B	11	HIS
1	B	222	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSD	B	159[A]	1	4,7,8	1.96	1 (25%)	1,8,10	2.08	1 (100%)
1	CSD	A	159[A]	1	4,7,8	3.44	1 (25%)	1,8,10	0.85	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
1	CSD	B	159[A]	1	-	0/2/6/8	-
1	CSD	A	159[A]	1	-	0/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159[A]	CSD	OD1-SG	-6.76	1.41	1.47
1	B	159[A]	CSD	OD1-SG	-3.55	1.44	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	159[A]	CSD	OD1-SG-CB	-2.08	101.78	105.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	159[A]	CSD	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BU4	A	400	-	5,5,5	0.32	0	5,5,5	0.83	0
2	BU4	B	400	-	5,5,5	0.25	0	5,5,5	0.52	0
3	A1AT9	A	401	-	60,66,66	3.30	24 (40%)	78,98,98	1.52	8 (10%)
4	A1AT8	B	401	-	56,62,62	4.20	31 (55%)	72,91,91	1.46	9 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BU4	A	400	-	-	2/3/3/3	-
2	BU4	B	400	-	-	3/3/3/3	-
3	A1AT9	A	401	-	-	17/58/87/87	0/5/5/5
4	A1AT8	B	401	-	-	14/55/75/75	0/4/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	A1AT8	O08-C03	11.86	1.56	1.40
4	B	401	A1AT8	C27-C26	10.40	1.56	1.38
4	B	401	A1AT8	C30-C25	10.39	1.55	1.39
3	A	401	A1AT9	O08-C03	9.84	1.53	1.40
4	B	401	A1AT8	P02-O02	8.93	1.69	1.59
3	A	401	A1AT9	C27-C26	8.88	1.54	1.38
3	A	401	A1AT9	C30-C25	8.39	1.53	1.39
4	B	401	A1AT8	P01-O02	8.37	1.68	1.59
4	B	401	A1AT8	C29-C28	8.10	1.56	1.38
4	B	401	A1AT8	C16-N06	7.44	1.51	1.33
3	A	401	A1AT9	C29-C28	6.77	1.53	1.38
4	B	401	A1AT8	C22-N08	6.75	1.49	1.33
4	B	401	A1AT8	C25-C24	6.27	1.58	1.49
3	A	401	A1AT9	P02-O02	6.22	1.66	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	A1AT9	P01-O02	6.13	1.66	1.59
3	A	401	A1AT9	C16-N06	5.94	1.47	1.33
3	A	401	A1AT9	C22-N08	5.72	1.47	1.33
4	B	401	A1AT8	C19-N07	5.71	1.46	1.33
3	A	401	A1AT9	C19-N07	5.55	1.46	1.33
4	B	401	A1AT8	C10-N03	-4.96	1.25	1.33
4	B	401	A1AT8	O08-C02	4.42	1.54	1.45
4	B	401	A1AT8	P03-O10	4.42	1.67	1.59
3	A	401	A1AT9	C29-C30	-4.00	1.32	1.38
4	B	401	A1AT8	C06-N02	3.85	1.41	1.34
4	B	401	A1AT8	C23-C22	3.84	1.57	1.51
3	A	401	A1AT9	C26-C25	-3.82	1.33	1.39
3	A	401	A1AT9	C10-N04	3.77	1.37	1.32
3	A	401	A1AT9	O08-C02	3.67	1.53	1.45
4	B	401	A1AT8	C09-N05	3.62	1.47	1.34
3	A	401	A1AT9	P03-O10	3.54	1.65	1.59
4	B	401	A1AT8	C11-C12	3.49	1.58	1.52
3	A	401	A1AT9	C04-C05	-3.37	1.45	1.53
4	B	401	A1AT8	C18-C19	3.34	1.58	1.51
4	B	401	A1AT8	C26-C25	-3.33	1.34	1.39
3	A	401	A1AT9	C09-N05	3.31	1.45	1.34
3	A	401	A1AT9	C03-N01	-3.30	1.41	1.49
4	B	401	A1AT8	O14-C16	-3.10	1.17	1.23
4	B	401	A1AT8	C04-C05	-2.88	1.46	1.53
4	B	401	A1AT8	C29-C30	-2.85	1.34	1.38
4	B	401	A1AT8	C28-C27	-2.75	1.32	1.38
4	B	401	A1AT8	P01-O01	2.70	1.69	1.59
4	B	401	A1AT8	C09-N03	-2.60	1.26	1.36
3	A	401	A1AT9	C09-C07	-2.46	1.34	1.43
3	A	401	A1AT9	C10-N03	2.43	1.38	1.33
3	A	401	A1AT9	O14-C16	-2.42	1.18	1.23
3	A	401	A1AT9	C28-C27	-2.41	1.32	1.38
3	A	401	A1AT9	C08-N04	-2.39	1.32	1.35
4	B	401	A1AT8	C03-N01	-2.33	1.44	1.49
4	B	401	A1AT8	O15-C13	-2.31	1.38	1.42
3	A	401	A1AT9	O17-C22	-2.23	1.18	1.23
4	B	401	A1AT8	C05-C02	-2.17	1.47	1.52
4	B	401	A1AT8	O17-C22	-2.15	1.19	1.23
3	A	401	A1AT9	C07-N02	2.12	1.47	1.39
4	B	401	A1AT8	P02-O03	2.11	1.67	1.59
4	B	401	A1AT8	O16-C19	-2.01	1.19	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	A1AT8	C02-O08-C03	-7.14	103.39	109.92
3	A	401	A1AT9	C02-O08-C03	-6.60	103.88	109.92
3	A	401	A1AT9	N04-C10-N03	-6.18	120.29	128.67
4	B	401	A1AT8	C23-C22-N08	5.03	122.85	116.25
3	A	401	A1AT9	O19-C24-C25	-3.82	105.83	110.38
3	A	401	A1AT9	O19-C24-O18	3.52	110.09	105.92
4	B	401	A1AT8	C05-C04-C03	3.01	106.51	99.89
4	B	401	A1AT8	C18-C19-N07	2.76	121.36	116.34
3	A	401	A1AT9	C13-C16-N06	2.71	121.62	116.48
4	B	401	A1AT8	O17-C22-N08	-2.70	117.73	123.03
4	B	401	A1AT8	C13-C16-N06	2.54	121.31	116.48
3	A	401	A1AT9	C03-N01-C08	-2.40	122.43	126.64
3	A	401	A1AT9	C18-C19-N07	2.21	120.38	116.34
4	B	401	A1AT8	C15-C12-C13	2.19	112.51	108.77
4	B	401	A1AT8	O16-C19-N07	-2.13	118.85	123.03
3	A	401	A1AT9	C05-C04-C03	2.06	104.42	99.89
4	B	401	A1AT8	C04-C05-C02	2.06	106.84	103.24

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	BU4	O1-C1-C2-C3
3	A	401	A1AT9	O15-C13-C16-N06
3	A	401	A1AT9	C22-C23-C24-C25
3	A	401	A1AT9	C22-C23-C24-O18
3	A	401	A1AT9	C22-C23-C24-O19
3	A	401	A1AT9	C01-O03-P02-O02
3	A	401	A1AT9	C01-O03-P02-O04
3	A	401	A1AT9	C01-O03-P02-O05
3	A	401	A1AT9	N07-C20-C21-N08
4	B	401	A1AT8	C23-C22-N08-C21
4	B	401	A1AT8	O17-C22-N08-C21
4	B	401	A1AT8	N07-C20-C21-N08
3	A	401	A1AT9	O03-C01-C02-C05
3	A	401	A1AT9	O03-C01-C02-O08
3	A	401	A1AT9	O18-C24-C25-C26
2	B	400	BU4	C1-C2-C3-O3
2	A	400	BU4	O1-C1-C2-C3
3	A	401	A1AT9	O18-C24-C25-C30
4	B	401	A1AT8	P02-O02-P01-O01
4	B	401	A1AT8	O18-C24-C25-C26
4	B	401	A1AT8	O18-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	401	A1AT9	P02-O02-P01-O07
3	A	401	A1AT9	P01-O02-P02-O05
2	B	400	BU4	C1-C2-C3-C4
3	A	401	A1AT9	O15-C13-C16-O14
4	B	401	A1AT8	C12-C11-O01-P01
4	B	401	A1AT8	C01-O03-P02-O05
4	B	401	A1AT8	C23-C24-C25-C30
4	B	401	A1AT8	C23-C24-C25-C26
4	B	401	A1AT8	C02-C01-O03-P02
4	B	401	A1AT8	C02-C05-O10-P03
3	A	401	A1AT9	P02-O02-P01-O06
2	A	400	BU4	C1-C2-C3-O3
3	A	401	A1AT9	C12-C11-O01-P01
4	B	401	A1AT8	O01-C11-C12-C15
4	B	401	A1AT8	O15-C13-C16-N06

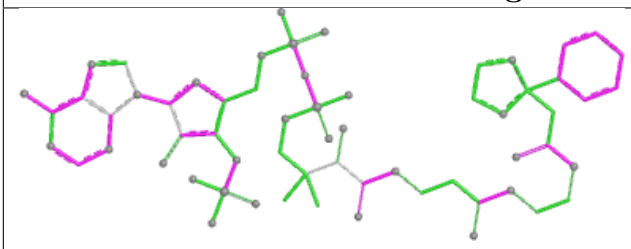
There are no ring outliers.

2 monomers are involved in 3 short contacts:

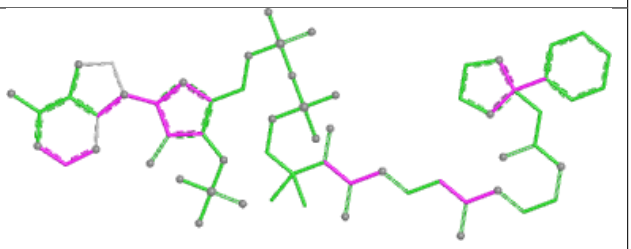
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	BU4	1	0
3	A	401	A1AT9	2	0

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.

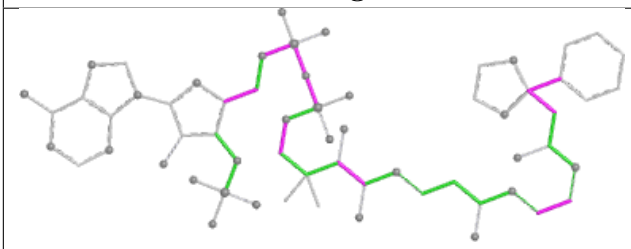
Ligand A1AT9 A 401



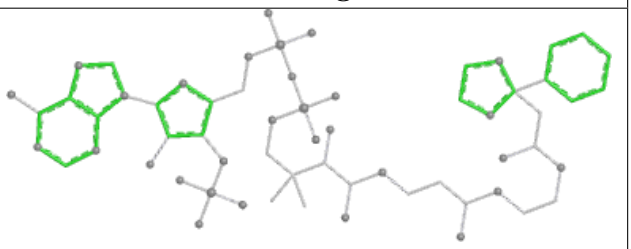
Bond lengths



Bond angles

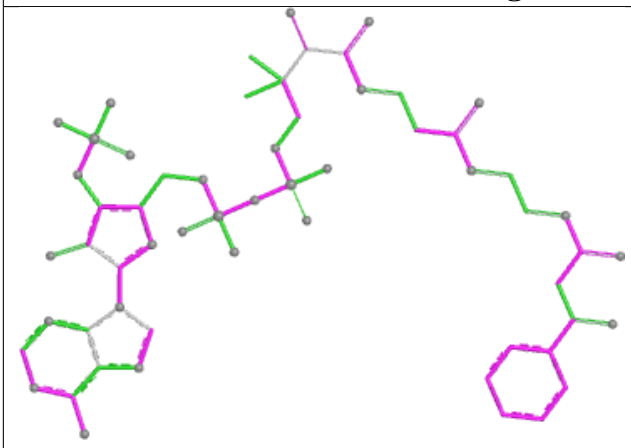


Torsions

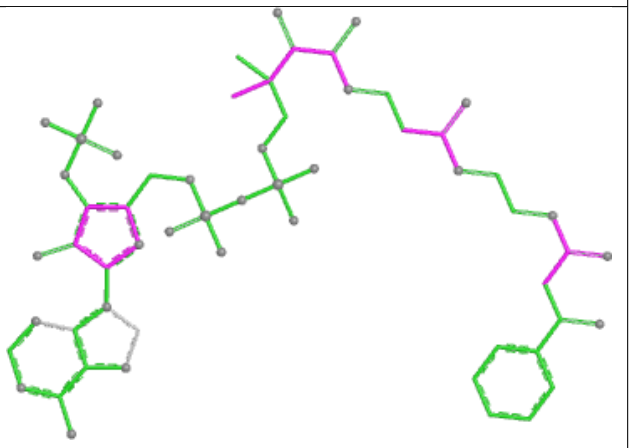


Rings

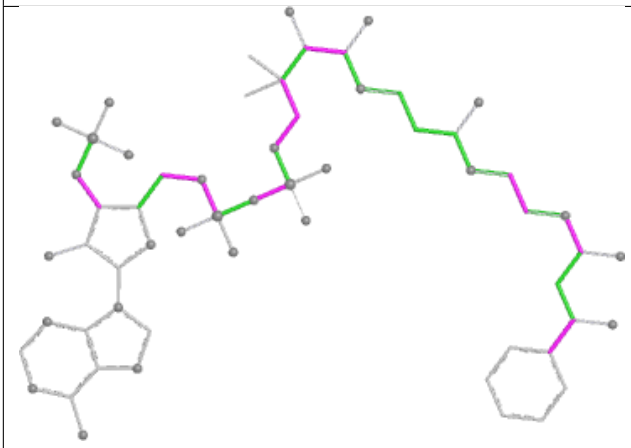
Ligand A1AT8 B 401



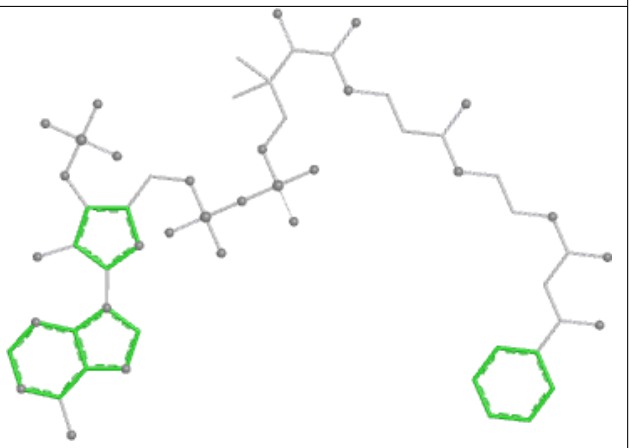
Bond lengths



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	378/390 (96%)	-0.46	3 (0%)	82	86	4, 11, 29, 66	9 (2%)
1	B	377/390 (96%)	-0.36	6 (1%)	70	74	5, 11, 36, 55	9 (2%)
All	All	755/780 (96%)	-0.41	9 (1%)	76	80	4, 11, 32, 66	18 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	CYS	6.4
1	B	387	ARG	3.4
1	B	225	PRO	2.7
1	A	387	ARG	2.5
1	B	227	ILE	2.5
1	B	196	LEU	2.4
1	A	10	GLN	2.1
1	B	286	ASP	2.1
1	B	285	VAL	2.0

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

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
1	CSD	A	159[A]	8/9	0.97	0.06	6,9,16,23	0
1	CSD	B	159[A]	8/9	0.98	0.04	7,8,12,20	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

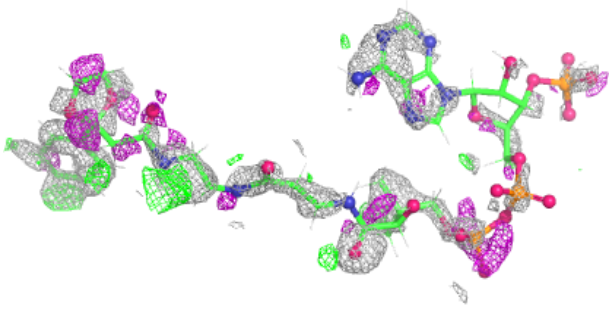
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

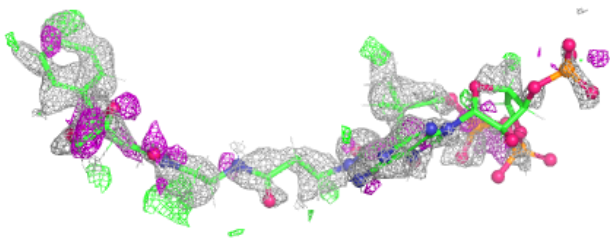
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1AT9	A	401	62/62	0.59	0.19	24,56,93,107	0
4	A1AT8	B	401	59/59	0.62	0.20	19,56,91,117	0
2	BU4	A	400	6/6	0.91	0.10	14,21,26,31	0
2	BU4	B	400	6/6	0.92	0.11	14,24,29,33	0

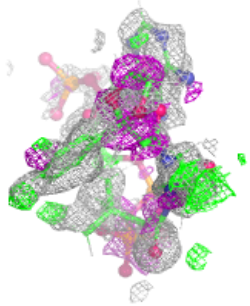
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AT9 A 401:

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

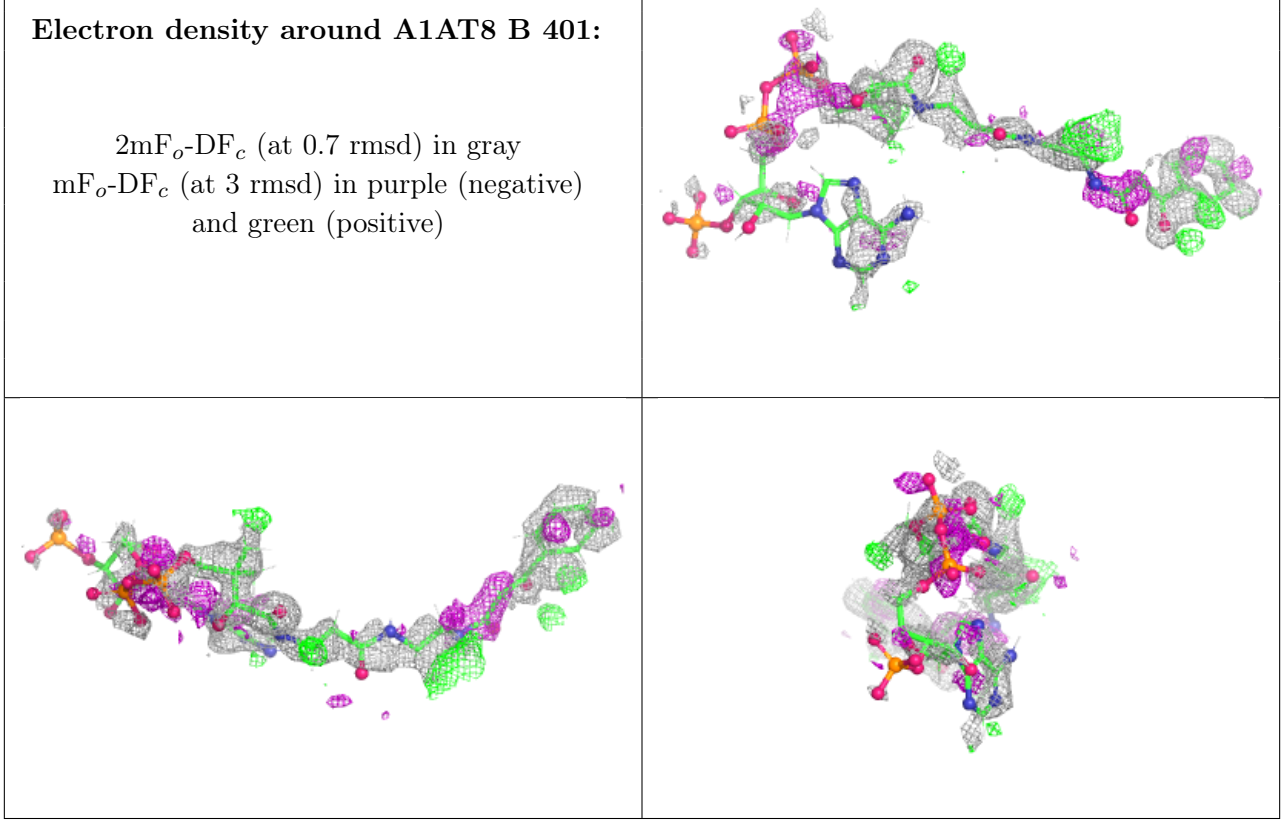






Electron density around A1AT8 B 401:

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



6.5 Other polymers

There are no such residues in this entry.