



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2024 – 04:31 AM EDT

PDB ID : 1WUU
Title : crystal structure of human galactokinase complexed with MgAMPPNP and galactose
Authors : Thoden, J.B.; Timson, D.J.; Reece, R.J.; Holden, H.M.
Deposited on : 2004-12-08
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

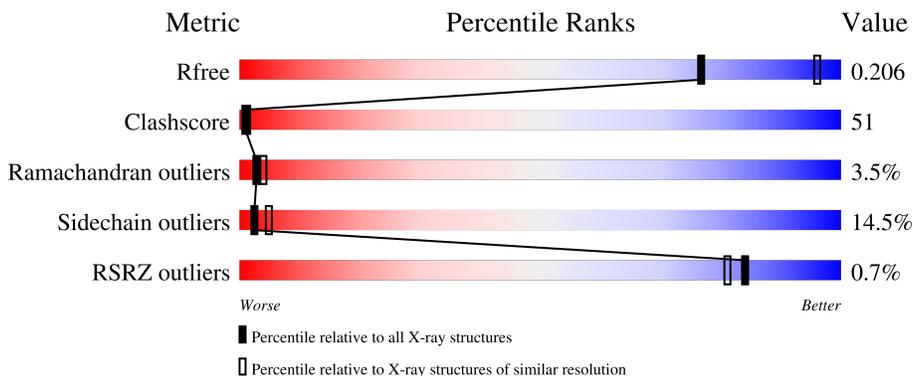
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

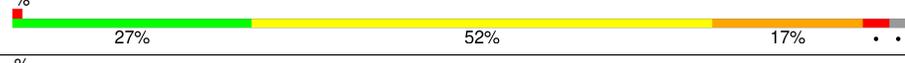
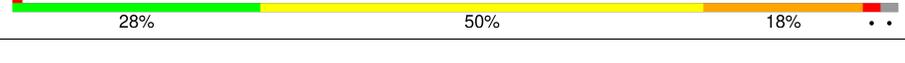
The reported resolution of this entry is 2.50 Å.

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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 $\leq 5\%$. 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	399	 28% 55% 13% . .
1	B	399	 27% 52% 17% . .
1	C	399	 29% 55% 11% . .
1	D	399	 28% 50% 18% . .

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12358 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 Galactokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	391	2960	1847	538	559	8	8	0	0	0
1	B	390	2942	1838	530	558	8	8	0	0	0
1	C	390	2944	1838	532	558	8	8	0	0	0
1	D	390	2952	1842	535	559	8	8	0	1	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MSE	-	expression tag	UNP P51570
A	-5	ALA	-	expression tag	UNP P51570
A	-4	HIS	-	expression tag	UNP P51570
A	-3	HIS	-	expression tag	UNP P51570
A	-2	HIS	-	expression tag	UNP P51570
A	-1	HIS	-	expression tag	UNP P51570
A	0	HIS	-	expression tag	UNP P51570
A	1	HIS	-	expression tag	UNP P51570
A	55	MSE	MET	modified residue	UNP P51570
A	60	MSE	MET	modified residue	UNP P51570
A	180	MSE	MET	modified residue	UNP P51570
A	185	MSE	MET	modified residue	UNP P51570
A	192	MSE	MET	modified residue	UNP P51570
A	307	MSE	MET	modified residue	UNP P51570
A	343	MSE	MET	modified residue	UNP P51570
A	365	MSE	MET	modified residue	UNP P51570
B	-6	MSE	-	expression tag	UNP P51570
B	-5	ALA	-	expression tag	UNP P51570
B	-4	HIS	-	expression tag	UNP P51570
B	-3	HIS	-	expression tag	UNP P51570
B	-2	HIS	-	expression tag	UNP P51570

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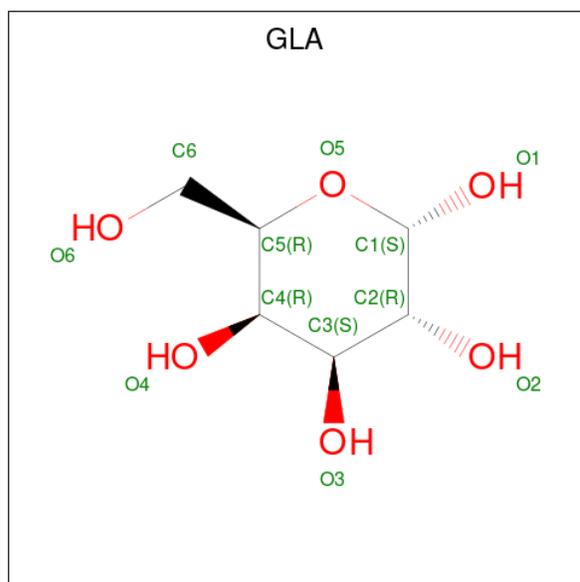
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP P51570
B	0	HIS	-	expression tag	UNP P51570
B	1	HIS	-	expression tag	UNP P51570
B	55	MSE	MET	modified residue	UNP P51570
B	60	MSE	MET	modified residue	UNP P51570
B	180	MSE	MET	modified residue	UNP P51570
B	185	MSE	MET	modified residue	UNP P51570
B	192	MSE	MET	modified residue	UNP P51570
B	307	MSE	MET	modified residue	UNP P51570
B	343	MSE	MET	modified residue	UNP P51570
B	365	MSE	MET	modified residue	UNP P51570
C	-6	MSE	-	expression tag	UNP P51570
C	-5	ALA	-	expression tag	UNP P51570
C	-4	HIS	-	expression tag	UNP P51570
C	-3	HIS	-	expression tag	UNP P51570
C	-2	HIS	-	expression tag	UNP P51570
C	-1	HIS	-	expression tag	UNP P51570
C	0	HIS	-	expression tag	UNP P51570
C	1	HIS	-	expression tag	UNP P51570
C	55	MSE	MET	modified residue	UNP P51570
C	60	MSE	MET	modified residue	UNP P51570
C	180	MSE	MET	modified residue	UNP P51570
C	185	MSE	MET	modified residue	UNP P51570
C	192	MSE	MET	modified residue	UNP P51570
C	307	MSE	MET	modified residue	UNP P51570
C	343	MSE	MET	modified residue	UNP P51570
C	365	MSE	MET	modified residue	UNP P51570
D	-6	MSE	-	expression tag	UNP P51570
D	-5	ALA	-	expression tag	UNP P51570
D	-4	HIS	-	expression tag	UNP P51570
D	-3	HIS	-	expression tag	UNP P51570
D	-2	HIS	-	expression tag	UNP P51570
D	-1	HIS	-	expression tag	UNP P51570
D	0	HIS	-	expression tag	UNP P51570
D	1	HIS	-	expression tag	UNP P51570
D	55	MSE	MET	modified residue	UNP P51570
D	60	MSE	MET	modified residue	UNP P51570
D	180	MSE	MET	modified residue	UNP P51570
D	185	MSE	MET	modified residue	UNP P51570
D	192	MSE	MET	modified residue	UNP P51570
D	307	MSE	MET	modified residue	UNP P51570
D	343	MSE	MET	modified residue	UNP P51570

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Chain	Residue	Modelled	Actual	Comment	Reference
D	365	MSE	MET	modified residue	UNP P51570

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C₆H₁₂O₆).

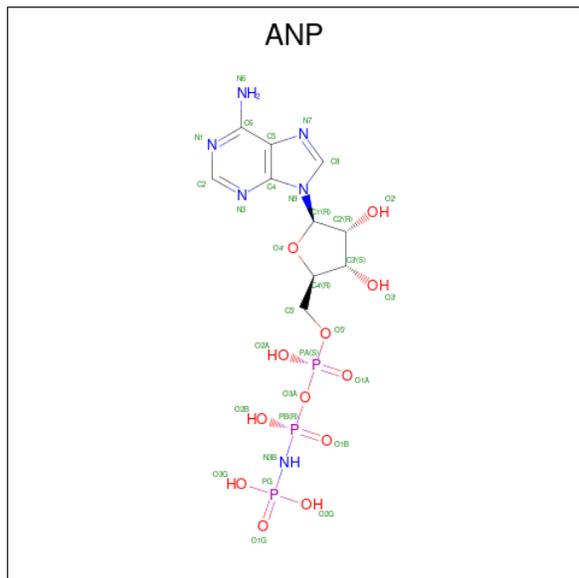


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

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

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

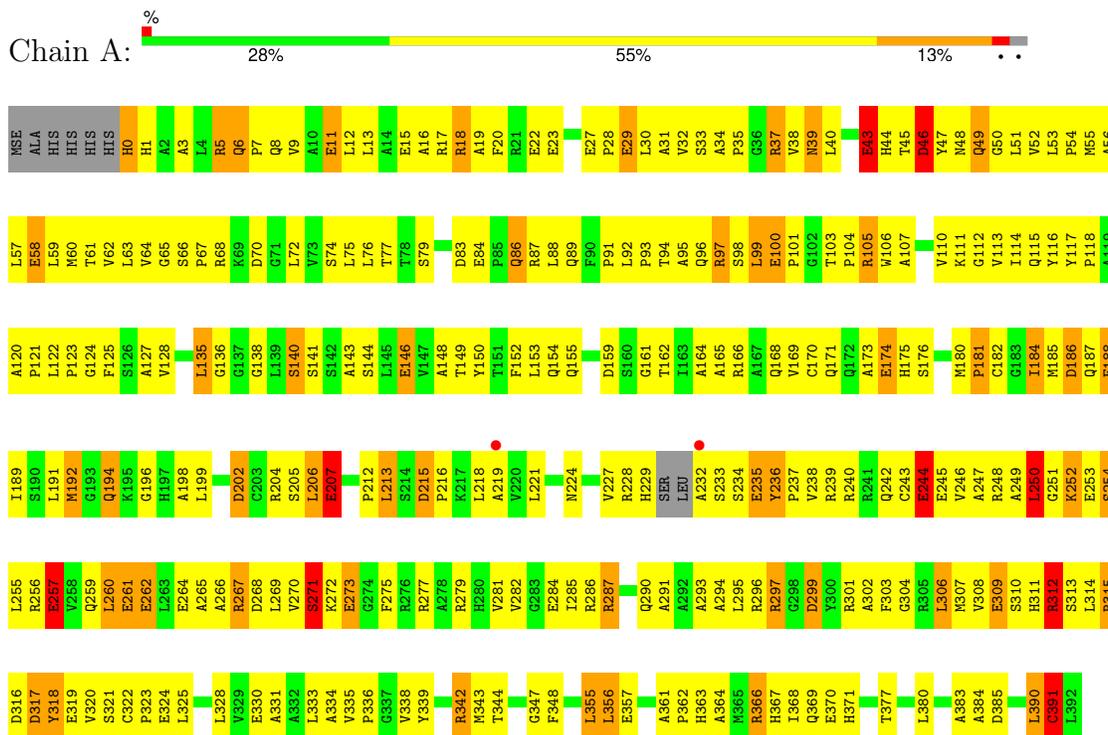
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	94	Total	O	0	0
			94	94		
5	B	89	Total	O	0	0
			89	89		
5	C	105	Total	O	0	0
			105	105		
5	D	96	Total	O	0	0
			96	96		

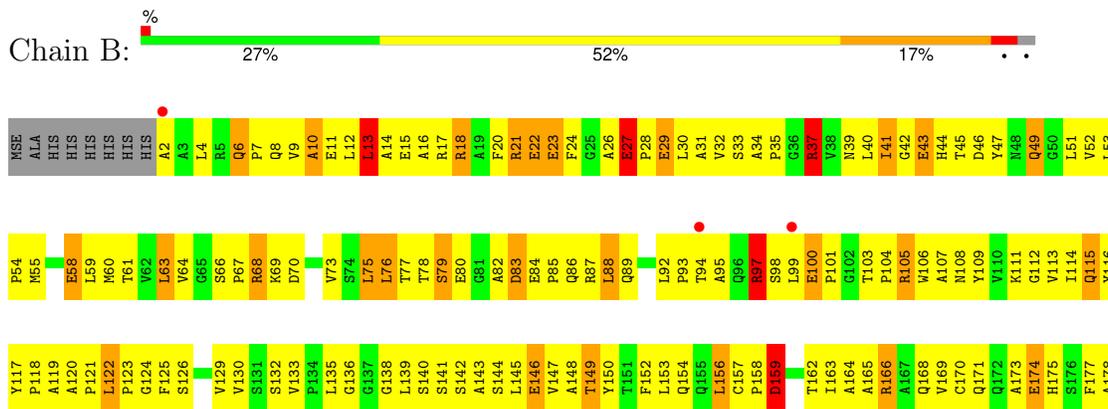
3 Residue-property plots

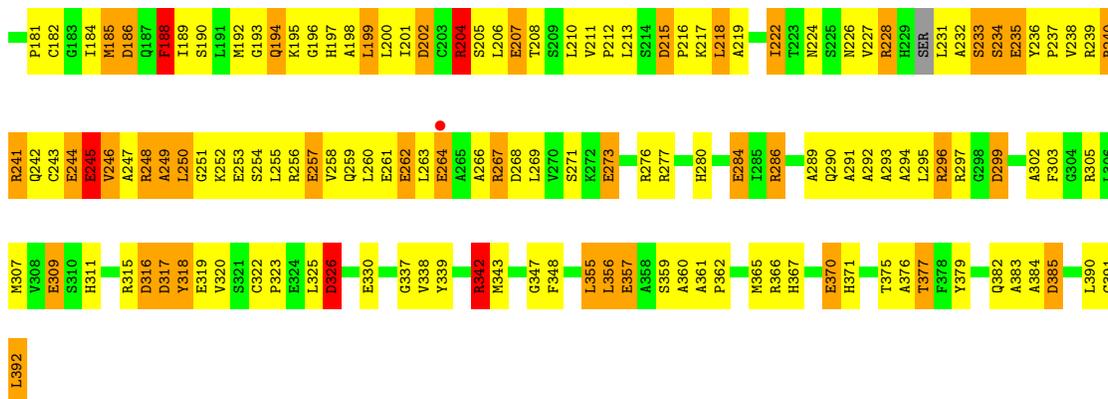
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Galactokinase

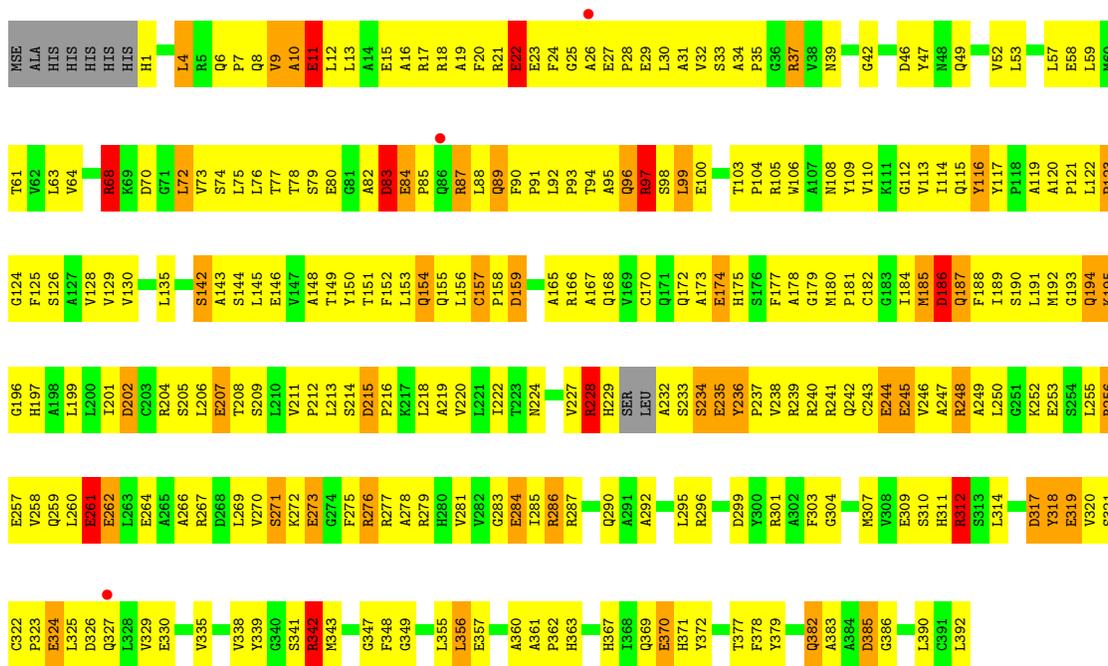


- Molecule 1: Galactokinase

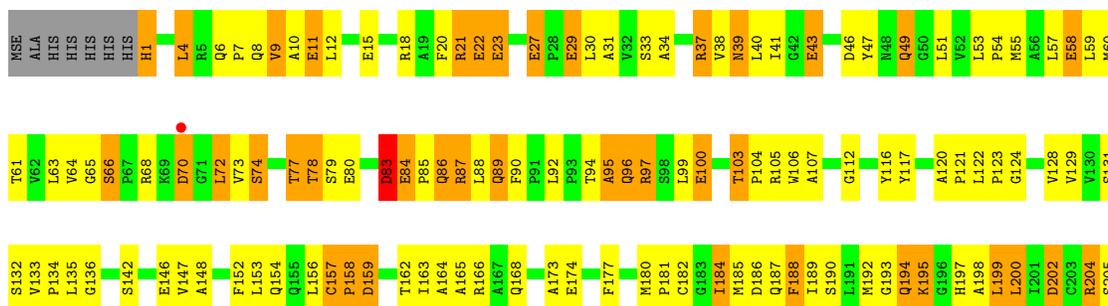




• Molecule 1: Galactokinase



• Molecule 1: Galactokinase



L206	A266	R326
E207	R267	Q327
T208	D268	L328
S209	L269	V329
L210	V270	E330
V211	S271	A331
P212	K272	A332
L213	E273	L333
S214	G274	A334
D215	F275	V335
P216	R276	
K217	R277	Y339
L218	A278	G340
A219	R279	S341
V220	H280	R342
L221	V281	M343
I222	V282	T344
T223	G283	G345
M224	E284	G346
S225	I285	G347
M226	R286	F348
V227	R287	G349
R228	T288	G350
H229	A289	C351
S230	Q290	T352
LEU	A291	R353
ALA	A292	T354
S233	A293	L355
S234	A294	L356
E235	L295	E357
Y236	R296	A358
P237	R297	S359
V238	G298	A360
R239	D299	A361
R240	Y300	P362
R241	R301	H363
Q242	A302	A364
C243	F303	M365
E244	G304	R366
E245	R305	H367
V246	L306	T368
A247	M307	Q369
R248	V308	E370
A249	E309	H371
L250	S310	Y372
K252	H311	G373
G251	R312	G374
E253	S313	T375
L255	L314	A376
R256	R315	T377
E257	D316	F378
V258	D317	Y379
Q259	Y318	L380
L260	E319	S381
E261	V320	Q382
E262	S321	
L263	G322	D385
E264	P323	
A265	E324	L392
	L325	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.20Å 109.60Å 115.80Å 90.00° 95.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.50) 97.7 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.50Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.201 , 0.258 0.201 , 0.206	Depositor DCC
R_{free} test set	6099 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtrriage
Anisotropy	0.546	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 151.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12358	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, GLA, MG

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	1.05	24/3007 (0.8%)	1.32	28/4062 (0.7%)
1	B	1.02	28/2987 (0.9%)	1.39	38/4036 (0.9%)
1	C	1.05	29/2990 (1.0%)	1.31	31/4040 (0.8%)
1	D	1.05	26/3002 (0.9%)	1.33	32/4055 (0.8%)
All	All	1.04	107/11986 (0.9%)	1.34	129/16193 (0.8%)

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	D	1	0

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	GLU	CD-OE2	7.87	1.34	1.25
1	A	194	GLN	CA-CB	-7.86	1.36	1.53
1	A	84	GLU	CD-OE2	7.60	1.34	1.25
1	C	261	GLU	CD-OE2	7.42	1.33	1.25
1	D	174	GLU	CD-OE2	7.38	1.33	1.25

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ASP	N-CA-CB	-13.51	86.29	110.60
1	B	70	ASP	CB-CA-C	13.23	136.85	110.40
1	D	157	CYS	C-N-CD	-12.20	93.76	120.60
1	B	46	ASP	CB-CG-OD2	-8.62	110.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ARG	NE-CZ-NH1	8.53	124.57	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	229	HIS	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2960	0	2947	286	0
1	B	2942	0	2930	328	0
1	C	2944	0	2929	302	0
1	D	2952	0	2939	311	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	13	6	0
4	B	31	0	13	7	0
4	C	31	0	13	8	0
4	D	31	0	13	3	0
5	A	94	0	0	6	0
5	B	89	0	0	7	0
5	C	105	0	0	9	0
5	D	96	0	0	14	0
All	All	12358	0	11845	1220	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 51.

The worst 5 of 1220 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:201:ILE:HG23	1:B:208:THR:HG22	1.24	1.18
1:B:250:LEU:HD21	1:B:266:ALA:HB2	1.20	1.16
1:A:266:ALA:HB1	1:A:269:LEU:HB2	1.29	1.14
1:A:307:MSE:HE1	1:A:355:LEU:HB2	1.30	1.13
1:A:246:VAL:HG22	1:A:270:VAL:HG11	1.27	1.12

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	387/399 (97%)	326 (84%)	52 (13%)	9 (2%)	5	8
1	B	386/399 (97%)	320 (83%)	50 (13%)	16 (4%)	2	3
1	C	386/399 (97%)	331 (86%)	42 (11%)	13 (3%)	3	4
1	D	387/399 (97%)	319 (82%)	52 (13%)	16 (4%)	2	3
All	All	1546/1596 (97%)	1296 (84%)	196 (13%)	54 (4%)	3	4

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	271	SER
1	B	18	ARG
1	B	115	GLN
1	B	158	PRO

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	309/308 (100%)	261 (84%)	48 (16%)	2	4
1	B	307/308 (100%)	260 (85%)	47 (15%)	2	4
1	C	307/308 (100%)	276 (90%)	31 (10%)	6	12
1	D	309/308 (100%)	257 (83%)	52 (17%)	1	3
All	All	1232/1232 (100%)	1054 (86%)	178 (14%)	2	5

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	248	ARG
1	D	100	GLU
1	C	271	SER
1	D	39	ASN
1	D	195	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	371	HIS
1	D	197	HIS
1	C	382	GLN
1	D	154	GLN
1	D	259	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
2	GLA	A	393	-	12,12,12	0.66	0	17,17,17	1.08	0
4	ANP	A	395	3	29,33,33	1.43	8 (27%)	31,52,52	1.88	8 (25%)
4	ANP	D	395	3	29,33,33	1.33	4 (13%)	31,52,52	1.67	4 (12%)
4	ANP	B	395	3	29,33,33	1.51	6 (20%)	31,52,52	1.84	9 (29%)
4	ANP	C	395	3	29,33,33	1.45	6 (20%)	31,52,52	1.80	7 (22%)
2	GLA	B	393	-	12,12,12	0.55	0	17,17,17	1.44	4 (23%)
2	GLA	D	393	-	12,12,12	0.52	0	17,17,17	1.04	0
2	GLA	C	393	-	12,12,12	0.54	0	17,17,17	1.09	1 (5%)

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	GLA	A	393	-	-	1/2/22/22	0/1/1/1
4	ANP	A	395	3	-	10/14/38/38	0/3/3/3
4	ANP	D	395	3	-	8/14/38/38	0/3/3/3
4	ANP	B	395	3	-	6/14/38/38	0/3/3/3
4	ANP	C	395	3	-	8/14/38/38	0/3/3/3
2	GLA	B	393	-	-	1/2/22/22	0/1/1/1
2	GLA	D	393	-	-	1/2/22/22	0/1/1/1
2	GLA	C	393	-	-	1/2/22/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	395	ANP	O4'-C1'	-3.69	1.36	1.40
4	C	395	ANP	PG-O2G	-3.26	1.48	1.56
4	C	395	ANP	PB-O2B	-3.23	1.48	1.56
4	B	395	ANP	PB-O1B	3.15	1.51	1.46
4	D	395	ANP	PG-O1G	3.04	1.50	1.46

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	395	ANP	C5-C6-N6	4.96	127.87	120.31
4	D	395	ANP	C5-C6-N6	4.74	127.53	120.31
4	A	395	ANP	O1B-PB-N3B	-4.43	105.25	111.77
4	A	395	ANP	C5-C6-N1	-4.26	110.08	120.23
4	C	395	ANP	C5-C6-N1	-4.22	110.17	120.23

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	395	ANP	PB-N3B-PG-O1G
4	A	395	ANP	PA-O3A-PB-O2B
4	A	395	ANP	C5'-O5'-PA-O2A
4	A	395	ANP	O4'-C4'-C5'-O5'
4	B	395	ANP	C5'-O5'-PA-O2A

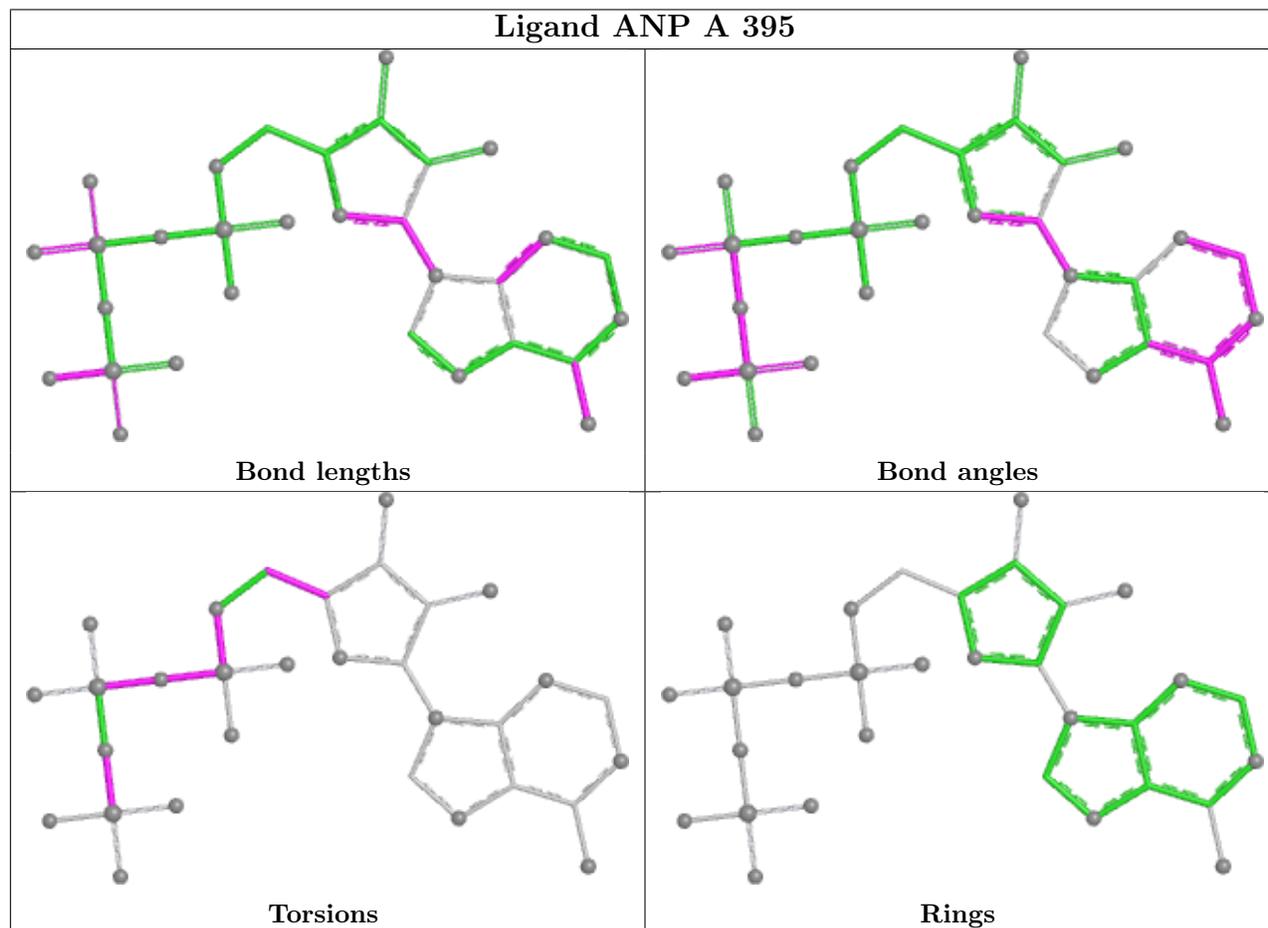
There are no ring outliers.

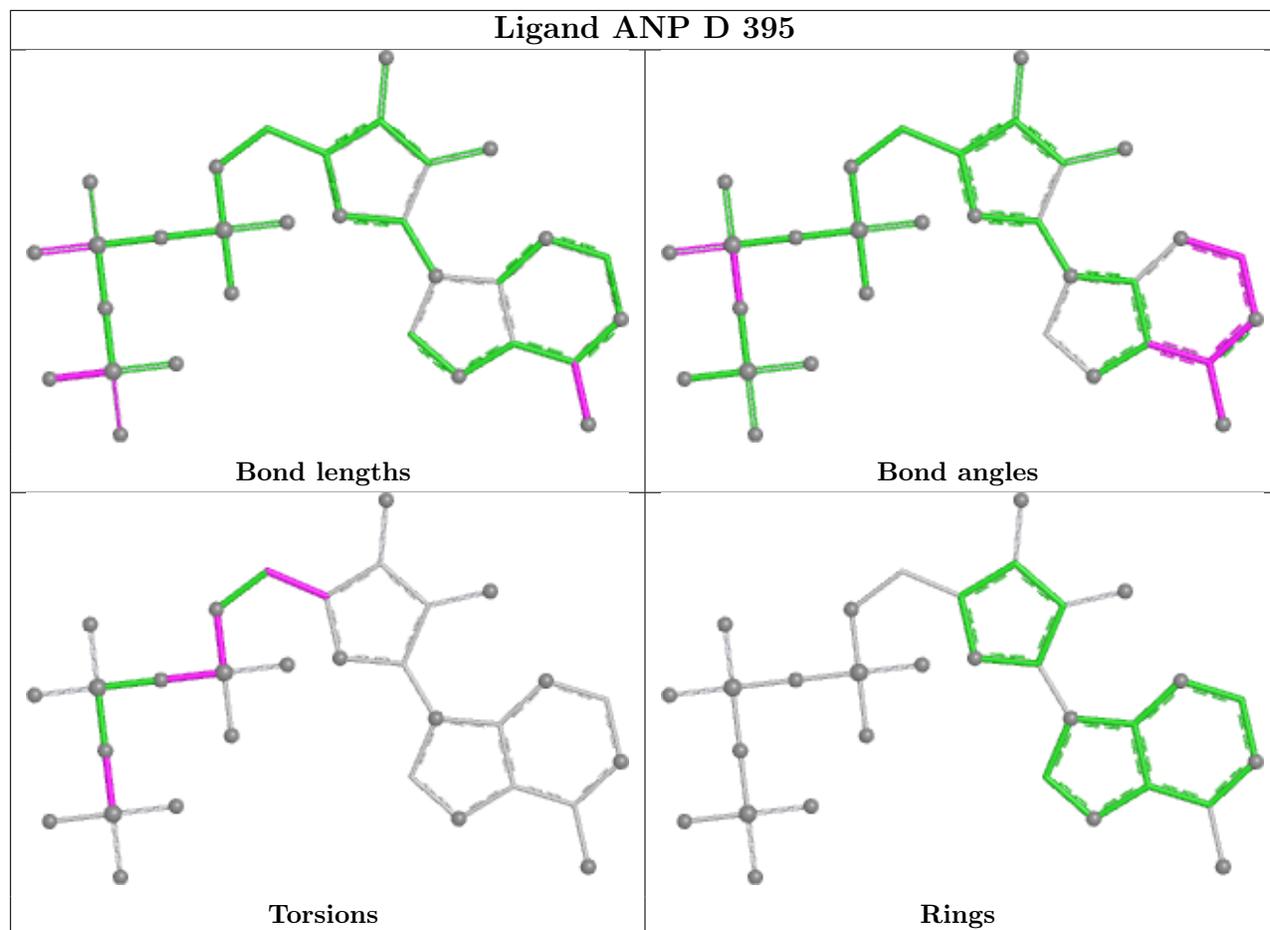
5 monomers are involved in 25 short contacts:

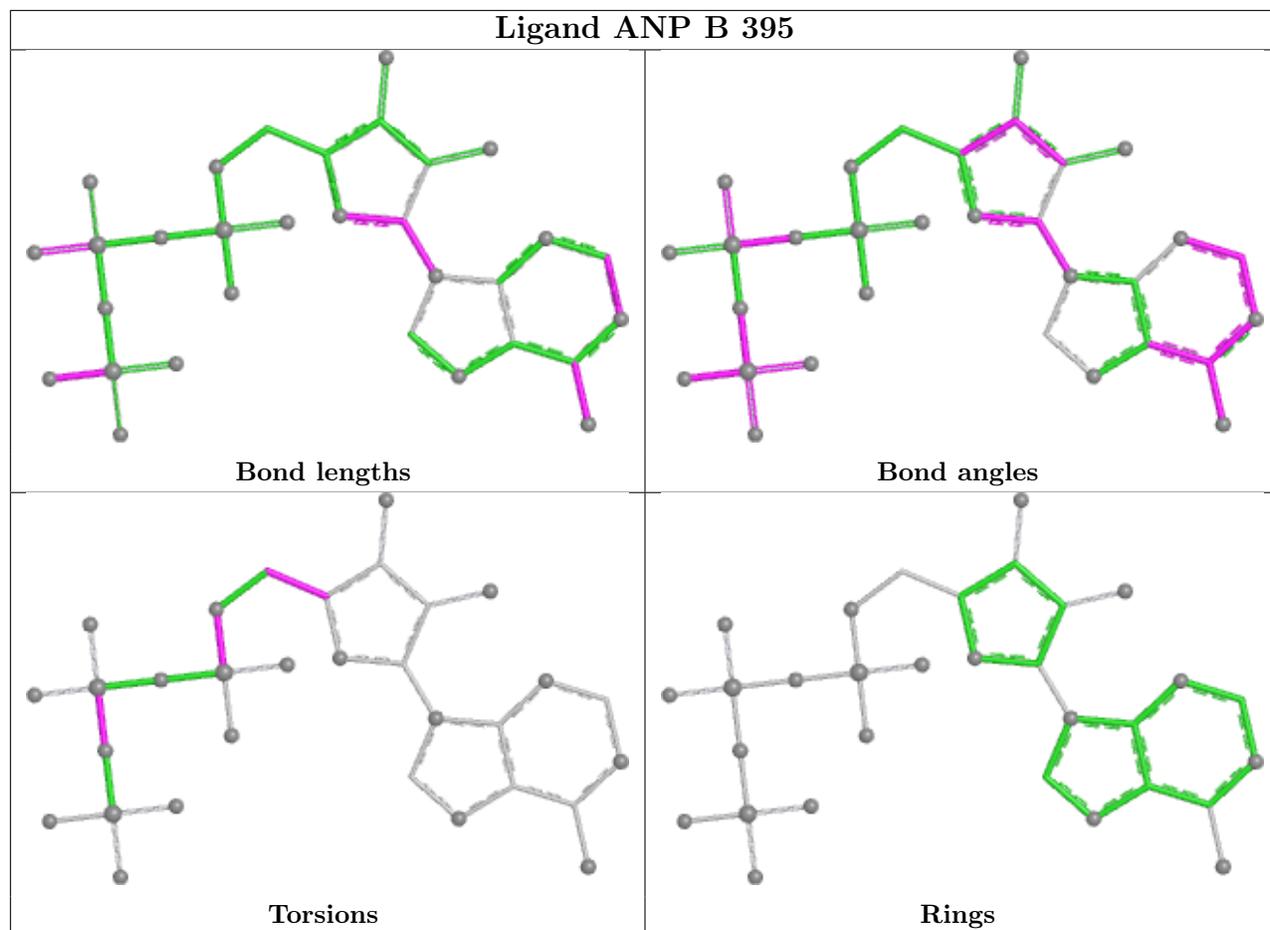
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	393	GLA	1	0
4	A	395	ANP	6	0
4	D	395	ANP	3	0
4	B	395	ANP	7	0
4	C	395	ANP	8	0

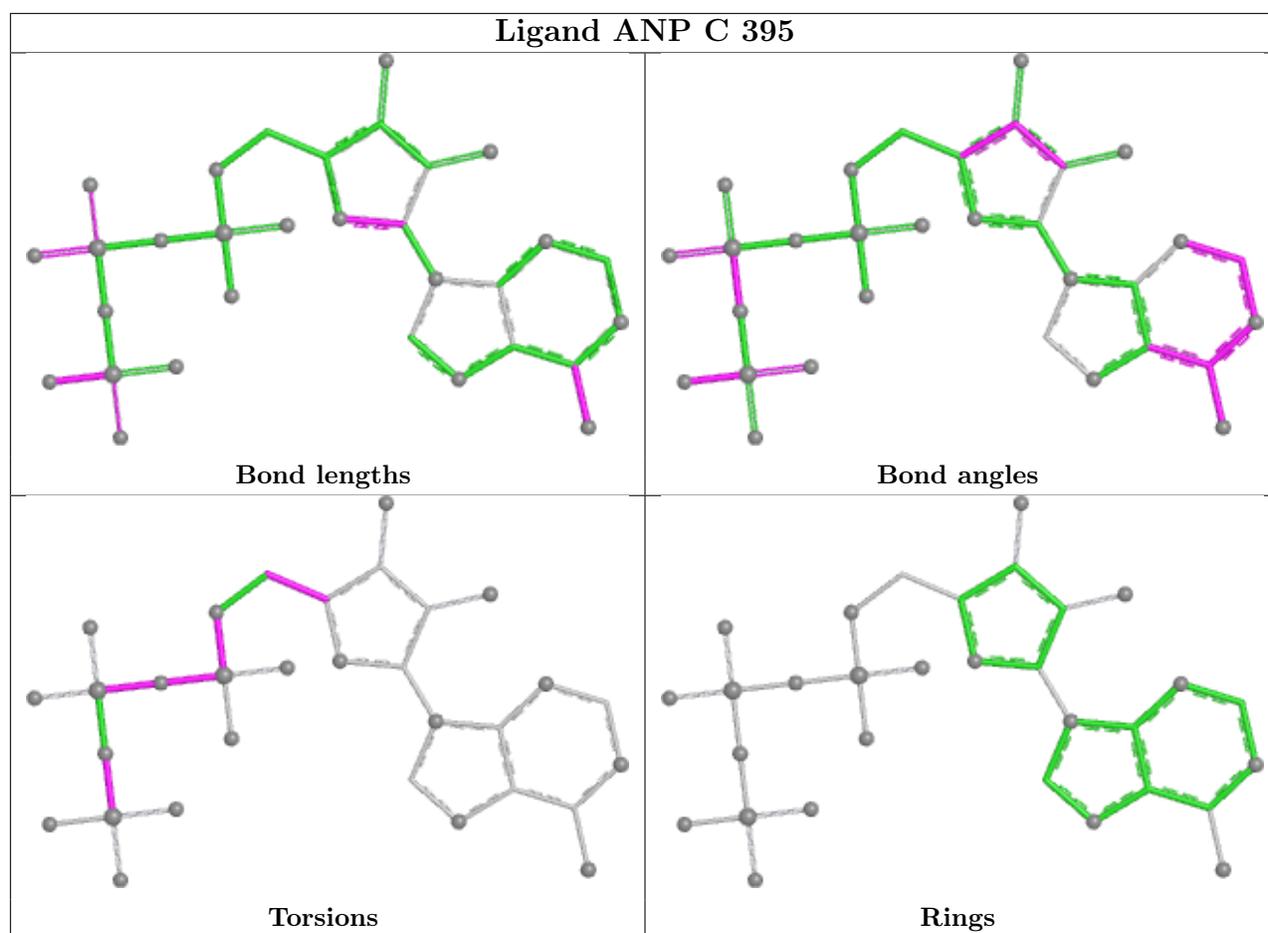
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/399 (95%)	-0.24	2 (0%) 87 85	22, 41, 69, 84	0
1	B	382/399 (95%)	-0.04	4 (1%) 79 76	19, 48, 76, 93	0
1	C	382/399 (95%)	-0.26	3 (0%) 82 79	15, 40, 73, 90	0
1	D	382/399 (95%)	-0.23	2 (0%) 87 85	21, 41, 68, 88	1 (0%)
All	All	1529/1596 (95%)	-0.19	11 (0%) 84 81	15, 43, 73, 93	1 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	3.9
1	C	26	ALA	3.1
1	B	94	THR	3.0
1	C	86	GLN	2.7
1	D	245	GLU	2.6

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

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

6.3 Carbohydrates [i](#)

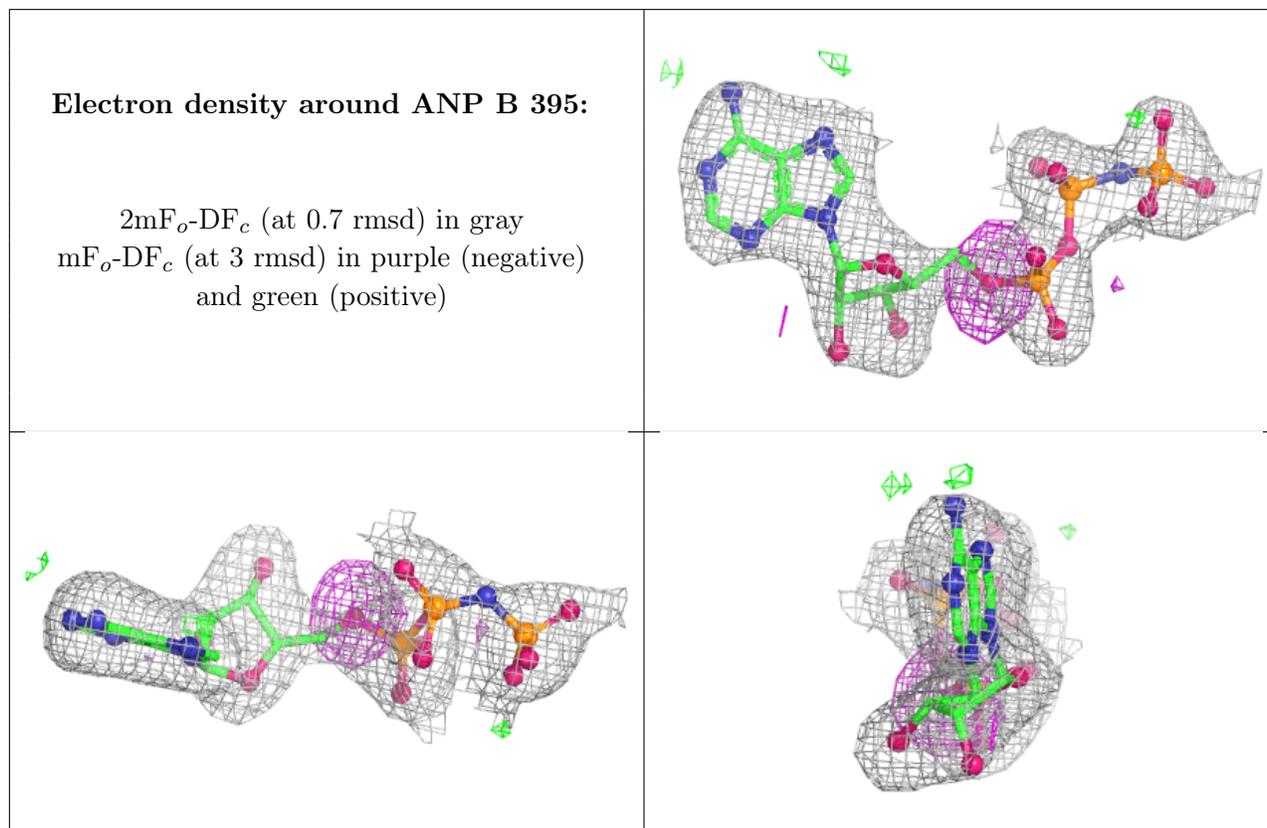
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

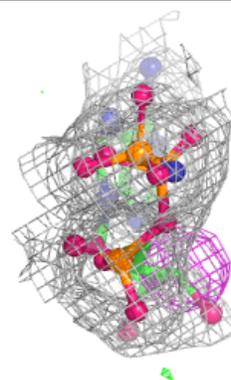
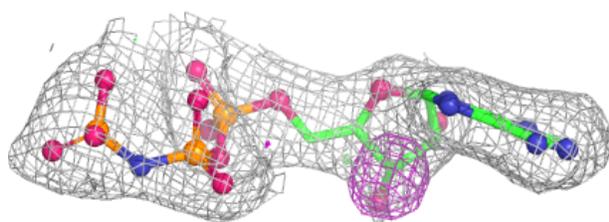
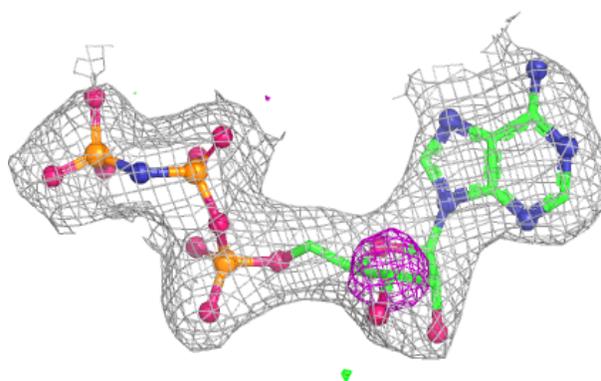
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ANP	B	395	31/31	0.89	0.10	0,44,81,94	0
3	MG	B	394	1/1	0.92	0.05	41,41,41,41	0
2	GLA	A	393	12/12	0.95	0.08	22,33,49,66	0
2	GLA	B	393	12/12	0.96	0.08	22,34,54,71	0
4	ANP	C	395	31/31	0.96	0.08	0,36,57,92	0
3	MG	D	394	1/1	0.97	0.06	27,27,27,27	0
4	ANP	A	395	31/31	0.97	0.06	19,34,50,66	0
3	MG	A	394	1/1	0.97	0.07	38,38,38,38	0
2	GLA	D	393	12/12	0.97	0.06	2,22,31,55	0
4	ANP	D	395	31/31	0.98	0.06	12,26,51,80	0
3	MG	C	394	1/1	0.99	0.04	26,26,26,26	0
2	GLA	C	393	12/12	0.99	0.06	6,19,58,80	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.

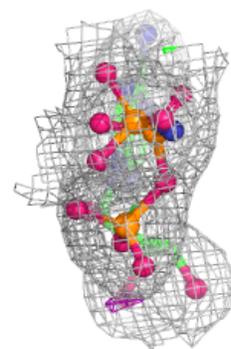
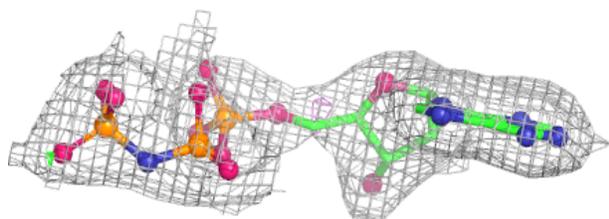
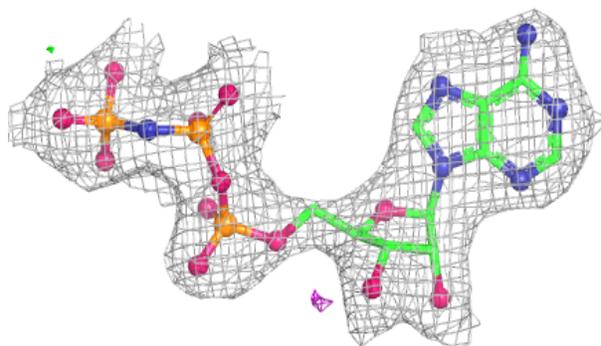


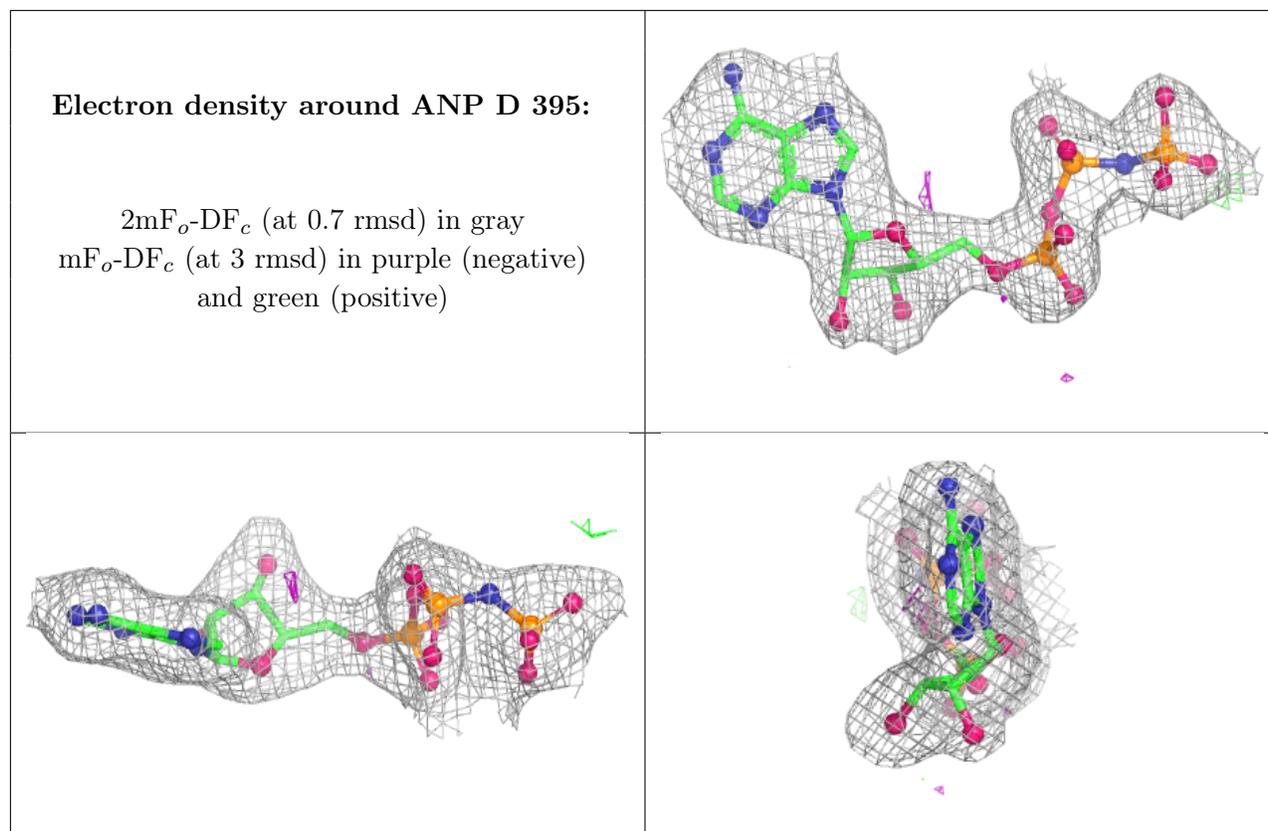
Electron density around ANP C 395:

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

**Electron density around ANP A 395:**

$2mF_o-DF_c$ (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.