



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:17 PM UTC

PDB ID : 3G15 / pdb_00003g15
Title : Crystal structure of human choline kinase alpha in complex with hemicholinium-3 and ADP
Authors : Hong, B.S.; Tempel, W.; Rabeh, W.M.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.W.; Structural Genomics Consortium (SGC)
Deposited on : 2009-01-29
Resolution : 1.70 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

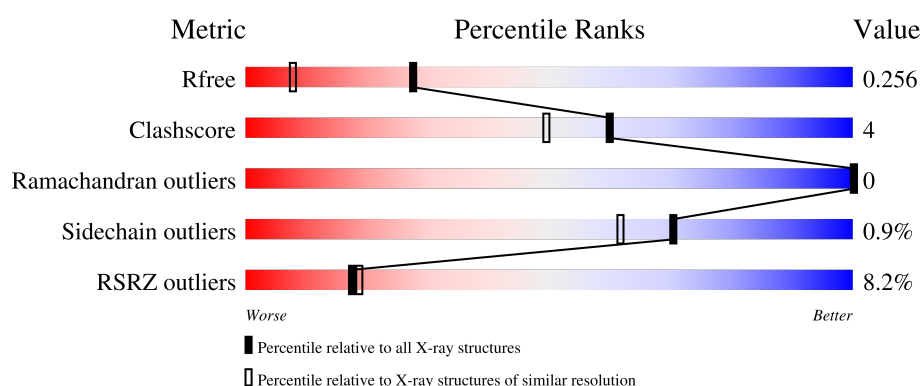
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	401	
1	B	401	

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
6	UNX	A	1	-	-	-	X
6	UNX	A	12	-	-	-	X
6	UNX	A	13	-	-	-	X
6	UNX	A	14	-	-	-	X
6	UNX	A	16	-	-	-	X
6	UNX	A	17	-	-	-	X
6	UNX	A	19	-	-	-	X
6	UNX	A	2	-	-	-	X
6	UNX	A	20	-	-	-	X
6	UNX	A	3	-	-	-	X
6	UNX	A	4	-	-	-	X
6	UNX	A	606	-	-	-	X
6	UNX	B	10	-	-	-	X
6	UNX	B	15	-	-	-	X
6	UNX	B	18	-	-	-	X
6	UNX	B	5	-	-	-	X
6	UNX	B	6	-	-	-	X
6	UNX	B	606	-	-	-	X
6	UNX	B	7	-	-	-	X
6	UNX	B	8	-	-	-	X
6	UNX	B	9	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5861 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 Choline kinase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	2	0
			2858	1861	470	510	17			
1	B	306	Total	C	N	O	S	0	6	0
			2530	1661	403	448	18			

There are 42 discrepancies between the modelled and reference sequences:

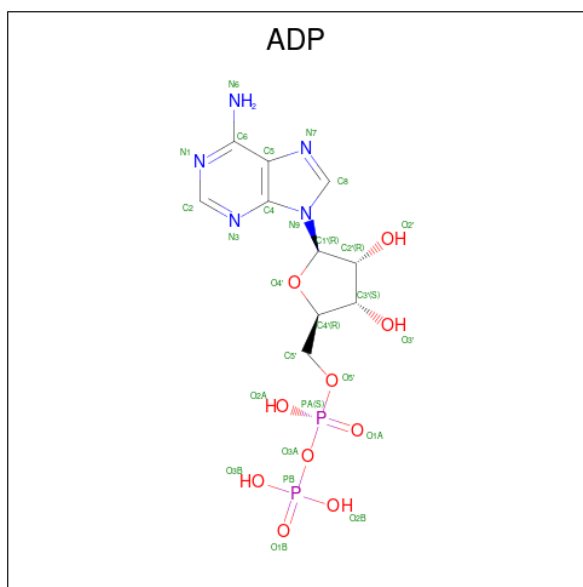
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLY	-	expression tag	UNP P35790
A	58	SER	-	expression tag	UNP P35790
A	59	SER	-	expression tag	UNP P35790
A	60	HIS	-	expression tag	UNP P35790
A	61	HIS	-	expression tag	UNP P35790
A	62	HIS	-	expression tag	UNP P35790
A	63	HIS	-	expression tag	UNP P35790
A	64	HIS	-	expression tag	UNP P35790
A	65	HIS	-	expression tag	UNP P35790
A	66	SER	-	expression tag	UNP P35790
A	67	SER	-	expression tag	UNP P35790
A	68	GLY	-	expression tag	UNP P35790
A	69	LEU	-	expression tag	UNP P35790
A	70	VAL	-	expression tag	UNP P35790
A	71	PRO	-	expression tag	UNP P35790
A	72	ARG	-	expression tag	UNP P35790
A	73	GLY	-	expression tag	UNP P35790
A	74	SER	-	expression tag	UNP P35790
A	154	MET	VAL	variant	UNP P35790
A	220	SER	GLY	variant	UNP P35790
A	422	LEU	GLN	variant	UNP P35790
B	57	GLY	-	expression tag	UNP P35790
B	58	SER	-	expression tag	UNP P35790
B	59	SER	-	expression tag	UNP P35790
B	60	HIS	-	expression tag	UNP P35790

Continued on next page...

Continued from previous page...

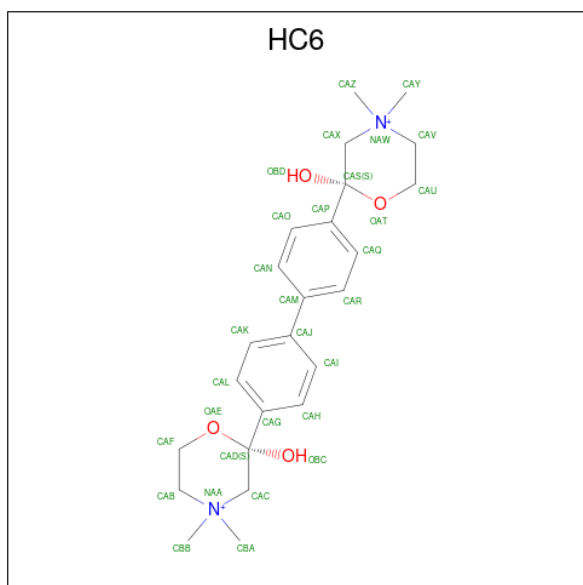
Chain	Residue	Modelled	Actual	Comment	Reference
B	61	HIS	-	expression tag	UNP P35790
B	62	HIS	-	expression tag	UNP P35790
B	63	HIS	-	expression tag	UNP P35790
B	64	HIS	-	expression tag	UNP P35790
B	65	HIS	-	expression tag	UNP P35790
B	66	SER	-	expression tag	UNP P35790
B	67	SER	-	expression tag	UNP P35790
B	68	GLY	-	expression tag	UNP P35790
B	69	LEU	-	expression tag	UNP P35790
B	70	VAL	-	expression tag	UNP P35790
B	71	PRO	-	expression tag	UNP P35790
B	72	ARG	-	expression tag	UNP P35790
B	73	GLY	-	expression tag	UNP P35790
B	74	SER	-	expression tag	UNP P35790
B	154	MET	VAL	variant	UNP P35790
B	220	SER	GLY	variant	UNP P35790
B	422	LEU	GLN	variant	UNP P35790

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is (2S,2'S)-2,2'-biphenyl-4,4'-diylbis(2-hydroxy-4,4-dimethylmorpholin-4-ium) (CCD ID: HC6) (formula: C₂₄H₃₄N₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 30 24 2 4	0	0
4	B	1	Total C N O 30 24 2 4	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	X	0	0
			12	12		
6	B	9	Total	X	0	0
			9	9		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	169	Total	O	0	0
			169	169		
7	B	155	Total	O	0	0
			155	155		

- Molecule 1: Choline kinase alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.80Å 118.99Å 131.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-1.70) 96.6 (30.00-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.220 , 0.257 0.222 , 0.256	Depositor DCC
R_{free} test set	2122 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5861	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HC6, SO4, ADP, UNX, 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	0.93	0/2940	0.88	0/3972
1	B	0.93	0/2611	0.89	0/3518
All	All	0.93	0/5551	0.88	0/7490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2858	0	2768	14	0
1	B	2530	0	2451	28	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	30	0	34	5	0
4	B	30	0	34	3	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	0	0
7	A	169	0	0	1	0
7	B	155	0	0	1	0
All	All	5861	0	5311	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (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:192:LEU:HD22	1:B:238[B]:MET:CE	1.12	1.56
1:B:192:LEU:CD2	1:B:238[B]:MET:CE	1.98	1.40
1:B:192:LEU:CD2	1:B:238[B]:MET:HE2	1.55	1.33
1:A:192:LEU:HD22	1:A:238[B]:MET:HE2	1.28	1.16
1:B:192:LEU:HD22	1:B:238[B]:MET:HE1	1.01	0.99
1:A:192:LEU:HD22	1:A:238[B]:MET:CE	1.94	0.98
1:B:192:LEU:HD22	1:B:238[B]:MET:HE2	0.98	0.97
1:A:192:LEU:CD2	1:A:238[B]:MET:HE2	1.95	0.96
1:B:235:PHE:HA	1:B:238[B]:MET:HE3	1.53	0.90
1:B:192:LEU:CD2	1:B:238[B]:MET:HE1	1.88	0.79
1:A:235:PHE:HA	1:A:238[B]:MET:HE3	1.70	0.73
1:B:192:LEU:HD21	1:B:238[B]:MET:HE2	1.64	0.73
4:B:603:HC6:HBAB	4:B:603:HC6:OBC	1.96	0.65
4:A:603:HC6:HAZB	4:A:603:HC6:OBD	1.99	0.62
1:B:146:ARG:O	1:B:203:GLY:CA	2.47	0.62
1:B:91:ALA:HA	1:B:94:TRP:CE3	2.35	0.61
4:A:603:HC6:HBAB	4:A:603:HC6:OBC	2.04	0.58
1:B:91:ALA:HA	1:B:94:TRP:HE3	1.70	0.57
1:B:424[B]:SER:OG	1:B:440:TYR:HD2	1.89	0.54
1:B:94:TRP:CZ2	1:B:202:GLN:HB2	2.43	0.53
1:A:235:PHE:HA	1:A:238[B]:MET:CE	2.36	0.53
1:B:146:ARG:O	1:B:203:GLY:HA3	2.08	0.53
1:A:420:TRP:CE3	4:A:603:HC6:HABA	2.44	0.53
1:A:180:GLU:HG3	7:A:534:HOH:O	2.10	0.52
1:B:187:LEU:CD2	1:B:238[B]:MET:SD	2.99	0.51
1:A:116:ILE:HD12	1:A:144:LEU:CD1	2.40	0.51
1:B:192:LEU:HD21	1:B:238[B]:MET:CE	2.20	0.50
1:B:147:LEU:HA	1:B:202:GLN:O	2.13	0.49
1:B:254[B]:GLU:OE2	1:B:290:ARG:NH2	2.47	0.47
1:B:256:TYR:O	1:B:260:VAL:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:NH1	7:B:533:HOH:O	2.47	0.47
1:A:117:ARG:NH2	2:A:601:ADP:O3B	2.48	0.47
1:A:181:SER:HB3	1:A:199:ILE:CD1	2.45	0.47
1:B:343:ILE:CD1	1:B:405:MET:CE	2.94	0.46
1:B:420:TRP:CD2	4:B:603:HC6:HABA	2.51	0.46
1:B:146:ARG:O	1:B:203:GLY:HA2	2.16	0.46
4:A:603:HC6:OBD	4:A:603:HC6:CAZ	2.64	0.45
1:B:187:LEU:HD21	1:B:238[B]:MET:SD	2.58	0.44
1:B:303:CYS:SG	1:B:337:ASN:HB3	2.58	0.43
1:A:277:LEU:HD13	1:A:425:ILE:HD11	2.01	0.43
4:B:603:HC6:OBC	4:B:603:HC6:CBA	2.66	0.42
1:A:269:SER:O	1:A:273:LYS:HG3	2.20	0.42
1:A:179:LEU:HD22	1:A:242:PHE:CE1	2.54	0.42
4:A:603:HC6:OBC	4:A:603:HC6:CBA	2.67	0.41
1:B:99:LEU:HD11	1:B:143:VAL:HG21	2.02	0.40
1:A:178:VAL:HG22	1:B:178:VAL:HG22	2.03	0.40
1:B:94:TRP:CH2	1:B:202:GLN:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	352/401 (88%)	346 (98%)	6 (2%)	0	100	100
1	B	302/401 (75%)	292 (97%)	10 (3%)	0	100	100
All	All	654/802 (82%)	638 (98%)	16 (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	296/357 (83%)	294 (99%)	2 (1%)	76	69
1	B	265/357 (74%)	262 (99%)	3 (1%)	65	54
All	All	561/714 (79%)	556 (99%)	5 (1%)	70	62

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	387	GLN
1	B	143	VAL
1	B	192	LEU
1	B	199	ILE

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	442	GLN
1	B	377	HIS
1	B	427	GLN
1	B	442	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 31 ligands modelled in this entry, 4 are monoatomic and 21 are unknown - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HC6	A	603	-	31,33,33	2.38	12 (38%)	42,52,52	1.09	4 (9%)
4	HC6	B	603	-	31,33,33	1.95	9 (29%)	42,52,52	1.37	4 (9%)
5	SO4	A	604	3	4,4,4	0.33	0	6,6,6	0.65	0
2	ADP	A	601	3	28,29,29	1.52	4 (14%)	43,45,45	1.77	8 (18%)
2	ADP	B	601	3	28,29,29	1.46	5 (17%)	43,45,45	1.78	9 (20%)
5	SO4	B	604	3	4,4,4	0.61	0	6,6,6	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HC6	B	603	-	-	0/16/44/44	0/4/4/4
2	ADP	B	601	3	-	5/16/32/32	0/3/3/3
4	HC6	A	603	-	-	0/16/44/44	0/4/4/4
2	ADP	A	601	3	-	4/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	HC6	OAT-CAS	5.82	1.48	1.42
4	A	603	HC6	CAS-CAP	-5.44	1.47	1.52
4	B	603	HC6	OBD-CAS	5.05	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	4.61	1.47	1.39
4	A	603	HC6	CAD-CAG	-4.31	1.48	1.52
2	A	601	ADP	C5-C4	4.21	1.46	1.39
2	A	601	ADP	PA-O3A	3.96	1.63	1.59
4	A	603	HC6	CAX-NAW	-3.48	1.48	1.51
4	B	603	HC6	OBC-CAD	3.47	1.44	1.39
4	B	603	HC6	OAE-CAD	3.38	1.46	1.42
4	A	603	HC6	OBD-CAS	3.35	1.44	1.39
4	A	603	HC6	OBC-CAD	3.20	1.44	1.39
2	B	601	ADP	C5-N7	-2.98	1.33	1.39
4	A	603	HC6	OAE-CAF	2.96	1.48	1.44
4	B	603	HC6	CAS-CAP	-2.87	1.49	1.52
4	A	603	HC6	CAM-CAJ	-2.87	1.42	1.49
2	B	601	ADP	PA-O3A	2.81	1.62	1.59
4	B	603	HC6	OAT-CAS	2.62	1.45	1.42
4	A	603	HC6	OAE-CAD	2.59	1.45	1.42
4	B	603	HC6	CAM-CAJ	-2.55	1.43	1.49
2	A	601	ADP	C5-N7	-2.54	1.34	1.39
4	B	603	HC6	CAD-CAG	-2.46	1.50	1.52
4	B	603	HC6	CAQ-CAR	2.40	1.42	1.38
4	A	603	HC6	OAT-CAU	2.37	1.47	1.44
4	A	603	HC6	CAB-NAA	-2.33	1.45	1.51
4	A	603	HC6	CAC-NAA	-2.33	1.49	1.51
4	B	603	HC6	CAC-NAA	-2.27	1.49	1.51
2	A	601	ADP	C8-N7	2.26	1.36	1.31
2	B	601	ADP	C5-C6	2.13	1.46	1.41
2	B	601	ADP	C4-N9	-2.13	1.33	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-5.84	118.67	126.72
2	A	601	ADP	C5-C4-N3	-5.52	119.12	126.72
2	A	601	ADP	N3-C4-N9	4.86	135.43	127.17
2	B	601	ADP	N3-C4-N9	4.80	135.34	127.17
4	B	603	HC6	CAB-NAA-CAC	4.62	112.87	108.30
2	B	601	ADP	C2-N3-C4	3.68	120.83	111.83
2	B	601	ADP	N3-C2-N1	-3.67	123.02	128.58
2	A	601	ADP	N3-C2-N1	-3.65	123.06	128.58
4	B	603	HC6	CAV-NAW-CAX	3.65	111.90	108.30
2	A	601	ADP	C2-N3-C4	3.54	120.48	111.83
4	B	603	HC6	OAE-CAF-CAB	-3.36	109.03	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	HC6	CAF-OAE-CAD	-3.15	109.86	113.16
2	B	601	ADP	C4-C5-N7	-3.06	107.09	110.58
4	A	603	HC6	CAU-OAT-CAS	-2.98	110.04	113.16
2	A	601	ADP	C4-N9-C8	2.50	108.37	105.74
2	B	601	ADP	C2-N1-C6	2.39	122.65	118.73
2	B	601	ADP	O2A-PA-O3A	2.35	113.63	107.27
4	A	603	HC6	CBB-NAA-CBA	2.34	112.72	107.68
2	B	601	ADP	C5-N7-C8	2.34	107.12	103.45
2	A	601	ADP	N6-C6-N1	2.32	123.54	118.38
4	A	603	HC6	OAT-CAU-CAV	2.30	112.71	111.21
2	B	601	ADP	C4-N9-C8	2.30	108.15	105.74
2	A	601	ADP	C4-C5-N7	-2.11	108.17	110.58
2	A	601	ADP	C2-N1-C6	2.09	122.16	118.73
4	A	603	HC6	CBB-NAA-CAC	-2.05	104.48	110.14

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	PB-O3A-PA-O1A
2	A	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PA-O3A-PB-O3B
2	A	601	ADP	PB-O3A-PA-O2A
2	B	601	ADP	PA-O3A-PB-O1B
2	B	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	PB-O3A-PA-O1A
2	B	601	ADP	PB-O3A-PA-O2A

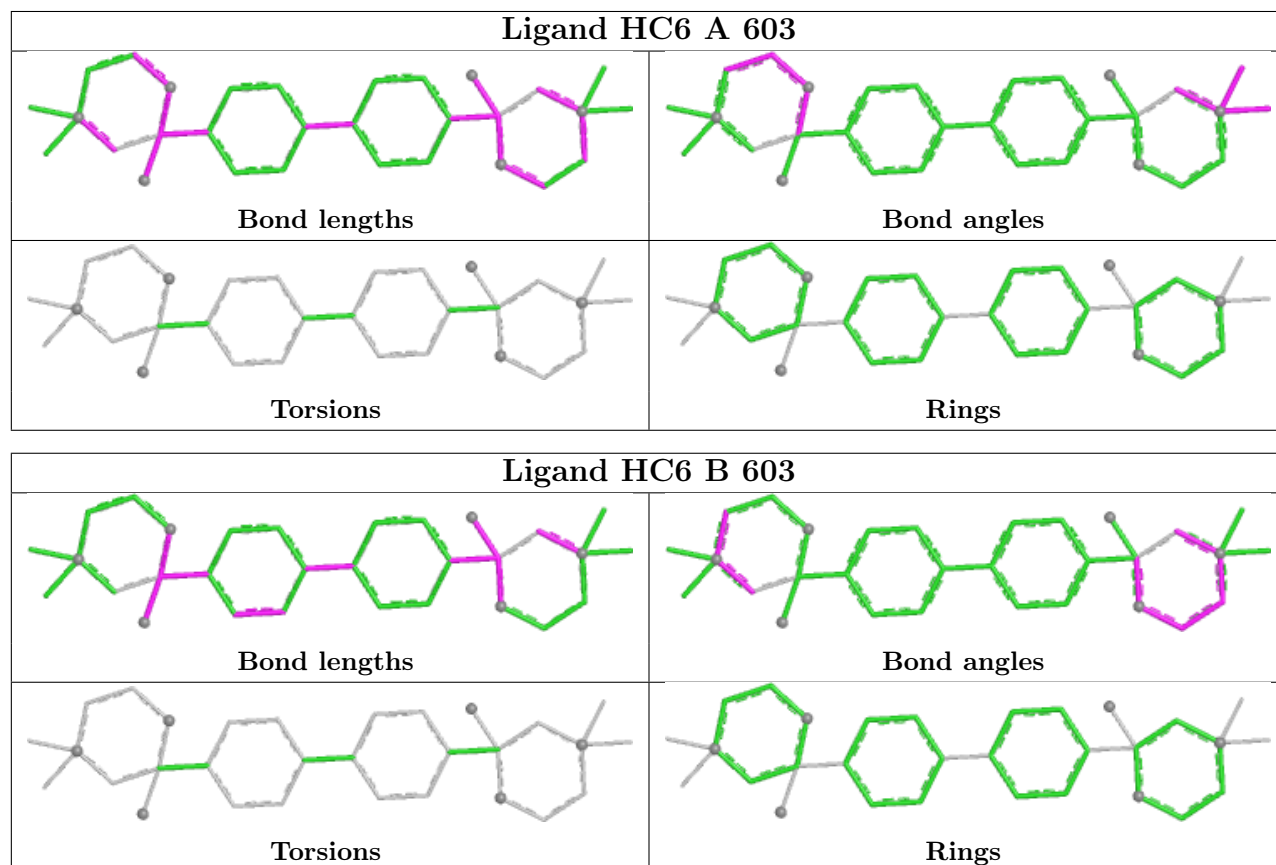
There are no ring outliers.

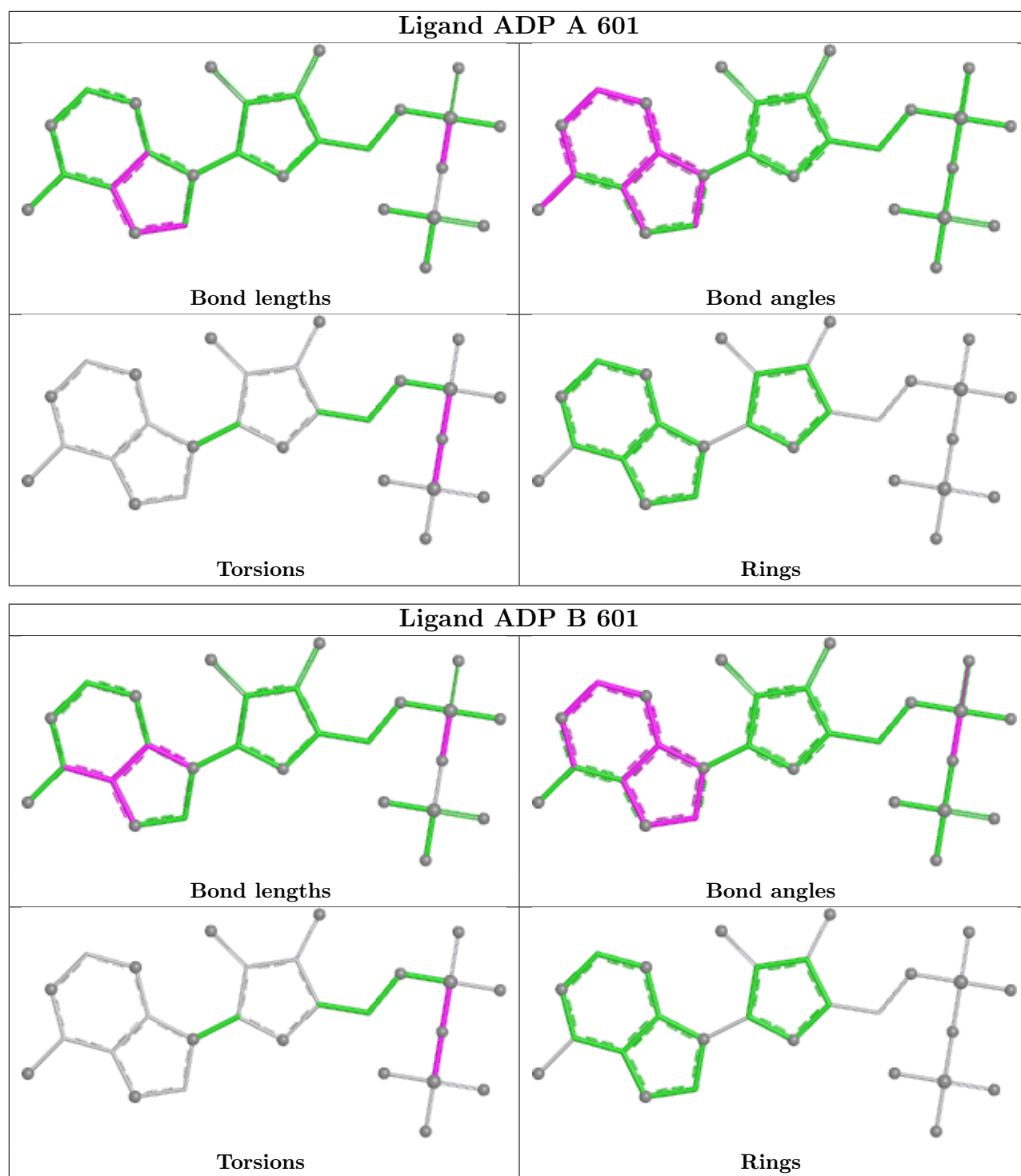
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	HC6	5	0
4	B	603	HC6	3	0
2	A	601	ADP	1	0

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

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, 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	354/401 (88%)	0.41	20 (5%)	30 33	14, 25, 46, 61	2 (0%)
1	B	306/401 (76%)	0.58	34 (11%)	10 10	11, 24, 49, 67	6 (1%)
All	All	660/802 (82%)	0.49	54 (8%)	17 19	11, 24, 48, 67	8 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	TRP	6.7
1	B	124	LEU	5.1
1	B	100	PRO	5.1
1	B	125	PHE	5.0
1	B	127	CYS	4.7
1	B	102	ALA	4.6
1	B	144	LEU	4.5
1	B	143	VAL	4.4
1	B	123	MET	4.4
1	B	145	LEU	4.0
1	B	126	GLN	3.8
1	B	93	LEU	3.5
1	A	457	VAL	3.5
1	B	88	ARG	3.4
1	A	150	ALA	3.2
1	A	122	ASN	3.2
1	B	94	TRP	3.1
1	B	201	PRO	3.1
1	B	92	TYR	3.1
1	B	200	PHE	3.0
1	B	266	THR	2.9
1	A	320	ASN	2.9
1	B	389	ASP	2.8
1	B	267	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	121	SER	2.8
1	B	388	ASN	2.7
1	A	456	GLY	2.7
1	B	91	ALA	2.7
1	B	203	GLY	2.7
1	B	89	ARG	2.6
1	A	120	LEU	2.6
1	B	90	ARG	2.6
1	A	386	PHE	2.5
1	A	174	ALA	2.5
1	B	199	ILE	2.5
1	A	192	LEU	2.4
1	B	202	GLN	2.4
1	A	81	GLU	2.3
1	A	175	GLU	2.3
1	A	319	GLU	2.3
1	B	259	GLU	2.3
1	A	318	ARG	2.3
1	B	318	ARG	2.3
1	B	95	CYS	2.3
1	A	275	HIS	2.2
1	A	453	ARG	2.2
1	A	268	GLU	2.2
1	B	147	LEU	2.2
1	B	258	LYS	2.1
1	A	324	GLN	2.1
1	A	389	ASP	2.1
1	A	115	VAL	2.1
1	B	395	THR	2.1
1	B	433	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 ⓘ

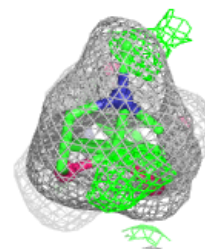
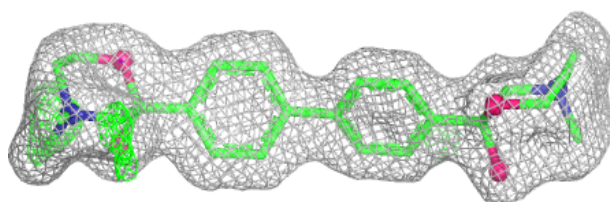
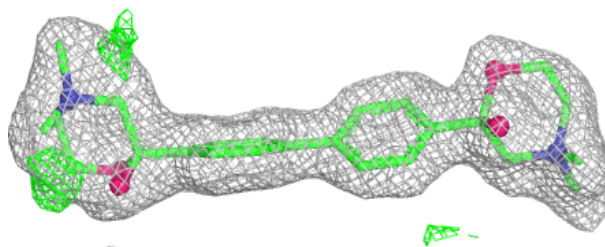
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	UNX	B	10	1/1	-0.38	1.46	2,2,2,2	1
6	UNX	B	15	1/1	-0.35	1.32	2,2,2,2	1
6	UNX	B	18	1/1	-0.35	1.43	2,2,2,2	1
6	UNX	A	4	1/1	-0.23	1.70	2,2,2,2	1
6	UNX	A	19	1/1	0.01	1.28	2,2,2,2	1
6	UNX	A	3	1/1	0.01	1.20	2,2,2,2	1
6	UNX	A	17	1/1	0.03	1.36	2,2,2,2	1
6	UNX	A	606	1/1	0.05	1.34	2,2,2,2	1
6	UNX	A	12	1/1	0.09	1.44	2,2,2,2	1
6	UNX	A	1	1/1	0.09	1.25	2,2,2,2	1
6	UNX	B	7	1/1	0.10	1.42	2,2,2,2	1
6	UNX	A	13	1/1	0.12	1.59	2,2,2,2	1
6	UNX	B	5	1/1	0.12	1.33	2,2,2,2	1
6	UNX	B	606	1/1	0.13	1.36	2,2,2,2	1
6	UNX	A	16	1/1	0.15	1.59	2,2,2,2	1
6	UNX	A	14	1/1	0.22	1.22	2,2,2,2	1
6	UNX	B	9	1/1	0.24	1.17	2,2,2,2	1
6	UNX	B	8	1/1	0.27	1.15	2,2,2,2	1
6	UNX	A	20	1/1	0.34	1.23	2,2,2,2	1
6	UNX	B	6	1/1	0.40	1.31	2,2,2,2	1
6	UNX	A	2	1/1	0.43	1.69	2,2,2,2	1
5	SO4	A	604	5/5	0.82	0.26	28,28,35,38	0
4	HC6	A	603	30/30	0.89	0.10	22,29,32,33	0
2	ADP	A	601	27/27	0.90	0.10	28,32,37,40	0
5	SO4	B	604	5/5	0.91	0.18	24,24,29,32	0
4	HC6	B	603	30/30	0.92	0.09	23,28,32,34	0
3	MG	A	605	1/1	0.95	0.22	33,33,33,33	0
2	ADP	B	601	27/27	0.95	0.07	24,30,33,34	0
3	MG	B	602	1/1	0.97	0.07	25,25,25,25	0
3	MG	A	602	1/1	0.98	0.18	27,27,27,27	0
3	MG	B	605	1/1	0.99	0.16	24,24,24,24	0

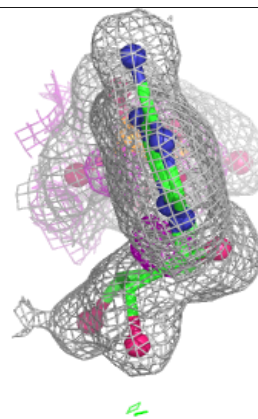
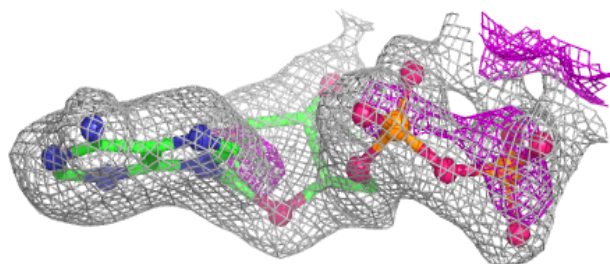
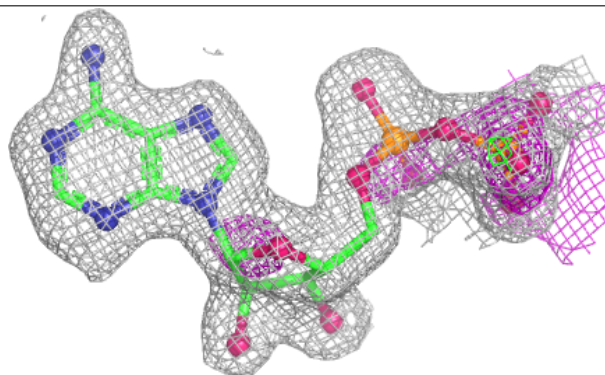
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HC6 A 603:

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

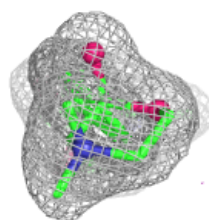
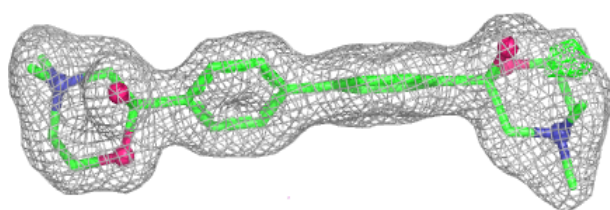
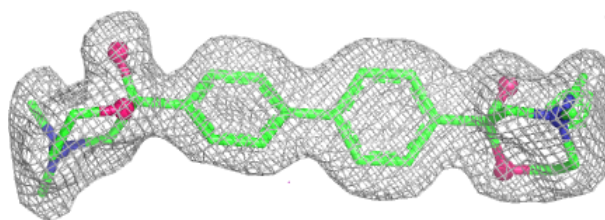
**Electron density around ADP A 601:**

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

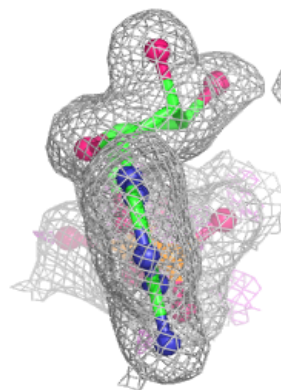
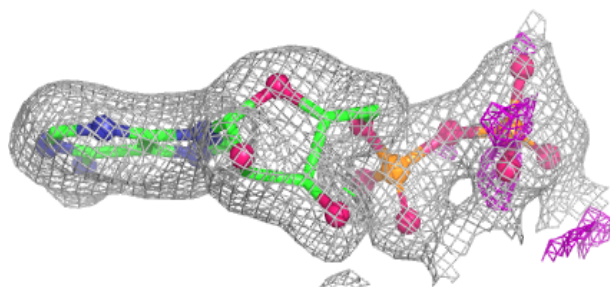
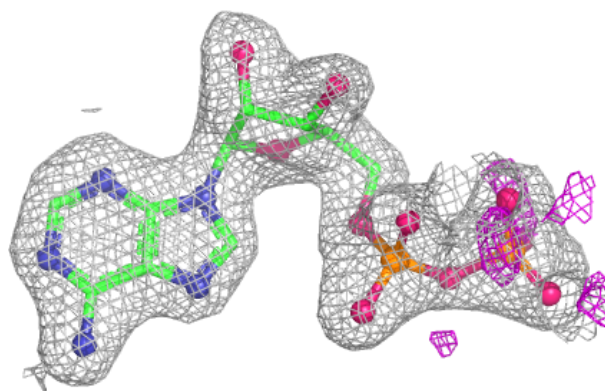


Electron density around HC6 B 603:

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

**Electron density around ADP B 601:**

$2mF_o-DF_c$ (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.