



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:30 pm BST

PDB ID : 4IOK
Title : N10-formyltetrahydrofolate synthetase from *Moorella thermoacetica* with ADP, XPO
Authors : Stec, B.
Deposited on : 2013-01-08
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

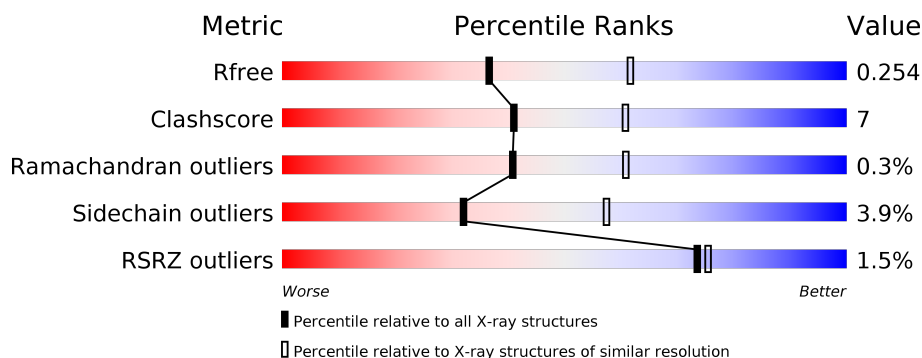
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	559	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	559	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8763 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 Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			
1	B	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



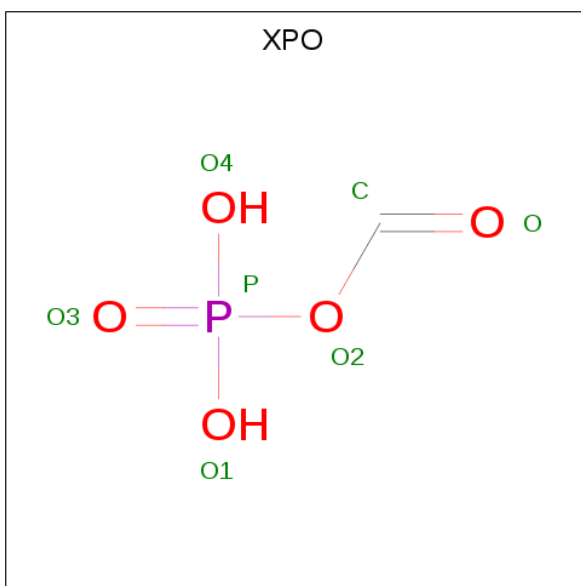
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is formyl phosphate (three-letter code: XPO) (formula: $\text{CH}_3\text{O}_5\text{P}$).

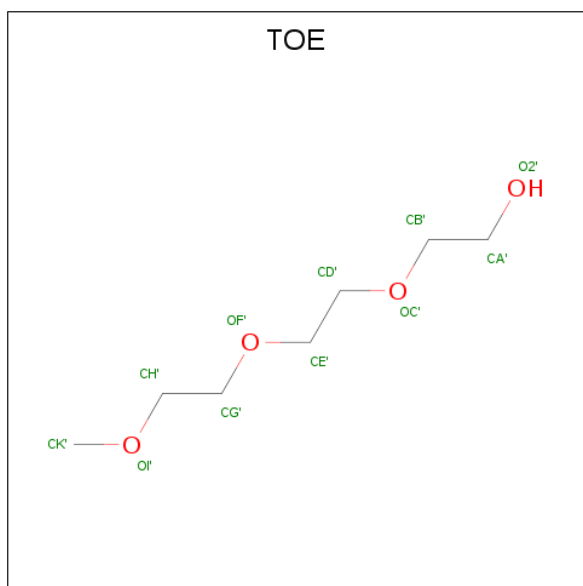


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			7	1	5	1		
4	B	1	Total	C	O	P	0	0
			7	1	5	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: C₇H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		
6	B	1	Total	C	O	0	0
			11	7	4		

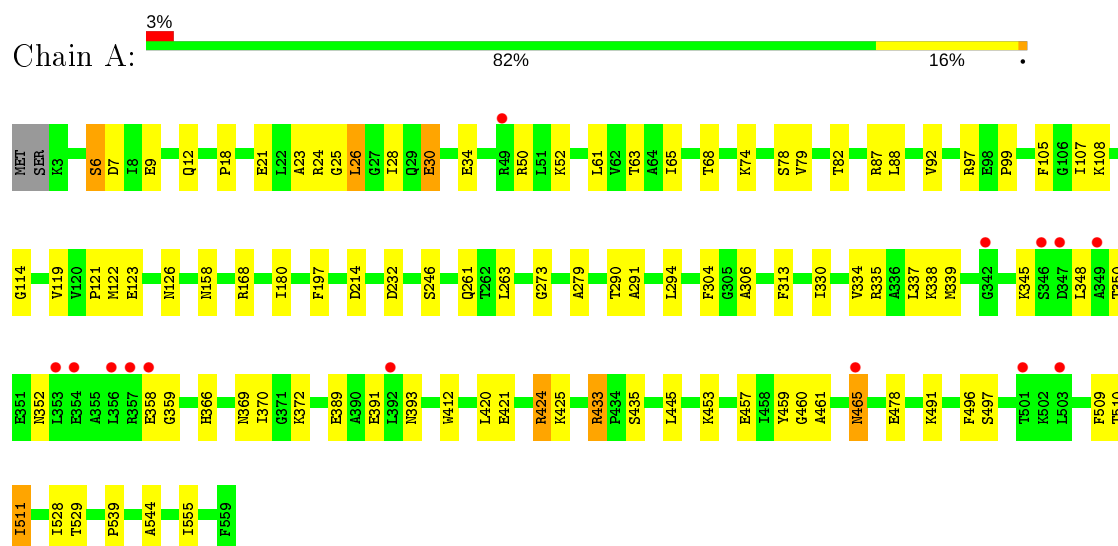
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	130	Total	O	0	0
			130	130		
7	B	130	Total	O	0	0
			130	130		

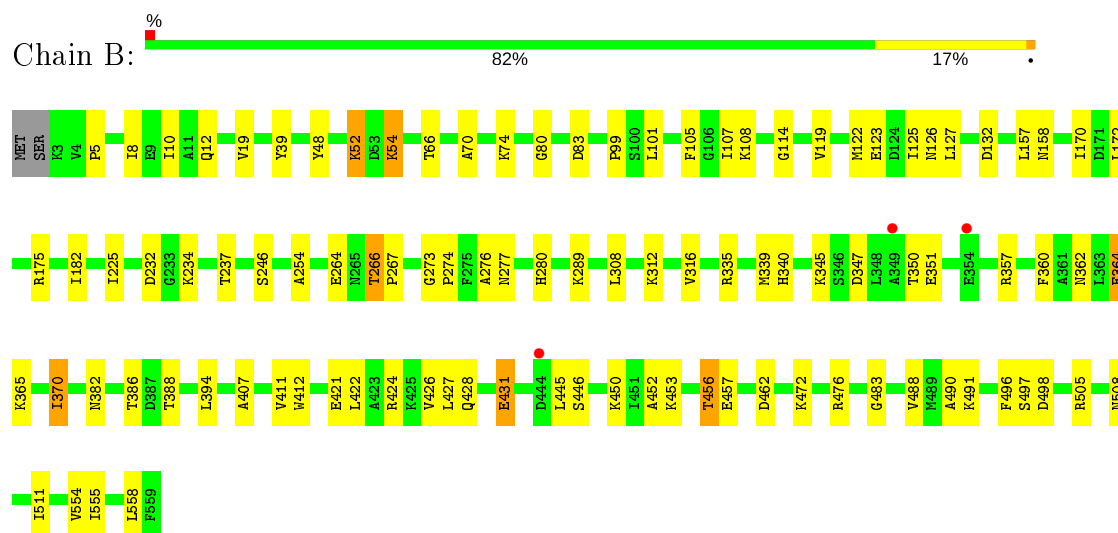
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Formate--tetrahydrofolate ligase



• Molecule 1: Formate--tetrahydrofolate ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	91.17Å 212.98Å 53.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.49 – 2.50 47.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.2 (106.49-2.50) 87.2 (47.77-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.259 0.163 , 0.254	Depositor DCC
R_{free} test set	3396 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	1.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8763	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5183e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, XPO, SO4, ADP, TOE

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	0.60	1/4266 (0.0%)	0.76	1/5778 (0.0%)
1	B	0.62	1/4266 (0.0%)	0.77	0/5778
All	All	0.61	2/8532 (0.0%)	0.77	1/11556 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	TRP	CD2-CE2	5.78	1.48	1.41
1	A	412	TRP	CD2-CE2	5.67	1.48	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

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	4195	0	4278	60	0
1	B	4195	0	4278	64	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	5	0
4	A	7	0	2	0	0
4	B	7	0	2	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	0	32	1	0
6	B	11	0	16	0	0
7	A	130	0	0	7	0
7	B	130	0	0	3	0
All	All	8763	0	8632	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (122) 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:A:335:ARG:HH21	1:A:335:ARG:HB3	1.16	1.06
1:B:462:ASP:OD2	1:B:508:ASN:HA	1.77	0.83
1:A:335:ARG:NH2	1:A:335:ARG:HB3	1.94	0.80
1:B:491:LYS:HE3	1:B:496:PHE:O	1.88	0.74
1:A:7:ASP:OD2	1:A:114:GLY:HA2	1.88	0.74
1:A:461:ALA:HB2	1:A:509:PHE:CE1	2.22	0.73
1:B:66:THR:H	1:B:362:ASN:HD21	1.34	0.73
1:B:452:ALA:O	1:B:456:THR:HB	1.89	0.72
1:A:74:LYS:HE2	1:A:304:PHE:O	1.91	0.71
1:A:335:ARG:HH21	1:A:335:ARG:CB	2.00	0.69
1:B:360:PHE:CE1	1:B:364:GLU:HG2	2.32	0.65
1:B:122:MET:CE	1:B:558:LEU:HD23	2.26	0.64
1:A:491:LYS:HE3	1:A:497:SER:O	1.96	0.64
1:A:337:LEU:O	1:A:359:GLY:HA3	1.98	0.63
1:B:99:PRO:HG2	1:B:126:ASN:HD22	1.63	0.63
1:B:450:LYS:NZ	1:B:483:GLY:O	2.32	0.62
1:B:427:LEU:O	1:B:431:GLU:HG2	1.99	0.62
1:B:119:VAL:HG13	1:B:125:ILE:HD13	1.81	0.62
1:B:360:PHE:HE1	1:B:364:GLU:HG2	1.66	0.61
1:A:491:LYS:HB3	1:A:529:THR:OG1	2.02	0.60
1:B:456:THR:HG22	1:B:457:GLU:HG3	1.84	0.59
1:A:330:ILE:HD11	1:A:370:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG21	1:A:370:ILE:HD11	1.85	0.59
1:B:132:ASP:OD2	1:B:254:ALA:HA	2.03	0.58
1:B:422:LEU:O	1:B:426:VAL:HG23	2.04	0.57
1:A:279:ALA:HB1	7:A:736:HOH:O	2.03	0.57
1:B:273:GLY:N	1:B:274:PRO:HD3	2.20	0.56
1:B:5:PRO:HG2	1:B:10:ILE:HG13	1.88	0.56
1:A:24:ARG:HH11	1:A:30:GLU:HB2	1.71	0.55
1:B:382:ASN:HD21	3:B:602:ADP:HN61	1.54	0.55
1:A:99:PRO:HG2	1:A:126:ASN:ND2	2.23	0.54
1:B:175:ARG:HG2	7:B:739:HOH:O	2.06	0.54
1:A:263:LEU:HB2	7:A:812:HOH:O	2.08	0.53
1:B:54:LYS:N	1:B:54:LYS:HD2	2.23	0.53
1:A:99:PRO:HG2	1:A:126:ASN:HD22	1.73	0.53
1:A:335:ARG:HG3	1:A:348:LEU:HB3	1.91	0.53
1:A:180:ILE:HG22	1:B:182:ILE:HA	1.92	0.52
1:B:114:GLY:HA3	3:B:602:ADP:O2'	2.09	0.52
1:B:277:ASN:O	1:B:490:ALA:HA	2.10	0.52
1:A:6:SER:OG	1:A:9:GLU:HG3	2.09	0.52
1:B:99:PRO:HG2	1:B:126:ASN:ND2	2.23	0.52
1:B:12:GLN:HE22	1:B:555:ILE:H	1.59	0.51
1:B:8:ILE:HD13	1:B:122:MET:CE	2.41	0.51
1:A:369:ASN:O	1:A:372:LYS:HB2	2.10	0.51
1:A:82:THR:HG23	1:A:92:VAL:HG22	1.93	0.51
1:A:23:ALA:O	1:A:28:ILE:HB	2.10	0.51
1:B:276:ALA:O	1:B:312:LYS:NZ	2.44	0.50
1:A:421:GLU:HA	1:A:424:ARG:NH1	2.25	0.49
1:B:491:LYS:HE2	1:B:497:SER:O	2.12	0.49
1:B:170:ILE:HD13	1:B:172:LEU:HD12	1.93	0.49
1:B:232:ASP:OD1	1:B:234:LYS:HE3	2.12	0.49
1:A:338:LYS:NZ	1:A:350:THR:O	2.46	0.48
1:A:105:PHE:HB3	1:A:544:ALA:HB2	1.94	0.48
1:B:266:THR:HG22	1:B:267:PRO:HD2	1.95	0.48
1:B:12:GLN:NE2	1:B:555:ILE:H	2.12	0.47
1:A:87:ARG:NH2	6:A:606:TOE:H4	2.29	0.47
1:B:74:LYS:HE3	3:B:602:ADP:O2B	2.13	0.47
1:B:280:HIS:HA	1:B:312:LYS:HD3	1.96	0.47
1:B:446:SER:O	1:B:450:LYS:HG3	2.14	0.47
1:B:52:LYS:HB2	1:B:52:LYS:HE3	1.70	0.46
1:B:382:ASN:ND2	3:B:602:ADP:HN61	2.13	0.46
1:B:157:LEU:O	1:B:158:ASN:CB	2.62	0.46
1:A:457:GLU:HA	1:A:457:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:C	1:A:26:LEU:H	2.19	0.46
1:B:70:ALA:HB3	1:B:335:ARG:HH22	1.80	0.46
1:B:351:GLU:HB2	1:B:388:THR:HG21	1.98	0.45
1:B:365:LYS:HB2	1:B:505:ARG:HD2	1.97	0.45
1:A:18:PRO:O	1:A:21:GLU:HB2	2.16	0.45
1:B:308:LEU:HD12	7:B:732:HOH:O	2.15	0.45
1:A:107:ILE:HD13	7:A:794:HOH:O	2.17	0.45
1:A:214:ASP:OD1	1:A:214:ASP:C	2.54	0.45
1:B:122:MET:HE3	1:B:558:LEU:HD23	1.97	0.45
1:B:339:MET:HE2	1:B:345:LYS:HG2	1.98	0.45
1:A:334:VAL:HG11	1:A:391:GLU:HB3	1.99	0.45
1:A:330:ILE:CD1	1:A:370:ILE:HD13	2.45	0.44
1:A:78:SER:O	1:A:82:THR:OG1	2.30	0.44
1:A:28:ILE:HD11	1:A:294:LEU:HD13	2.00	0.44
1:A:491:LYS:CE	1:A:497:SER:O	2.63	0.44
1:A:65:ILE:HA	1:A:366:HIS:CD2	2.53	0.44
1:B:80:GLY:HA3	1:B:411:VAL:HG21	2.00	0.43
1:B:8:ILE:HD13	1:B:122:MET:HE1	2.00	0.43
1:A:97:ARG:HB3	1:A:273:GLY:HA2	2.01	0.43
1:A:306:ALA:HB3	1:A:366:HIS:HD1	1.83	0.43
1:B:66:THR:HB	1:B:340:HIS:HE2	1.84	0.43
1:B:424:ARG:O	1:B:428:GLN:HG3	2.19	0.43
1:B:19:VAL:HG13	1:B:39:TYR:HA	2.00	0.43
1:A:79:VAL:HG21	1:A:119:VAL:HG23	2.01	0.42
1:A:433:ARG:HD2	7:A:716:HOH:O	2.19	0.42
1:A:453:LYS:O	1:A:457:GLU:HB2	2.19	0.42
1:A:459:TYR:HB3	1:A:496:PHE:O	2.19	0.42
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.83	0.42
1:A:539:PRO:HB2	7:A:793:HOH:O	2.19	0.42
1:A:126:ASN:HA	1:A:126:ASN:HD22	1.61	0.42
1:B:12:GLN:HE22	1:B:554:VAL:HA	1.83	0.42
1:B:370:ILE:HD12	1:B:370:ILE:HA	1.88	0.42
1:A:168:ARG:O	1:A:197:PHE:HA	2.19	0.42
1:B:123:GLU:O	1:B:127:LEU:HG	2.20	0.42
1:B:48:TYR:CD1	1:B:289:LYS:HG3	2.54	0.42
1:B:498:ASP:HB3	1:B:511:ILE:HD12	2.01	0.42
1:A:338:LYS:HD2	1:A:352:ASN:HB3	2.01	0.41
1:A:465:ASN:N	1:A:511:ILE:O	2.48	0.41
1:B:101:LEU:HD23	1:B:101:LEU:C	2.40	0.41
1:A:105:PHE:CE2	1:B:246:SER:HB3	2.56	0.41
3:B:602:ADP:O3B	4:B:603:XPO:H1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HG23	1:B:108:LYS:N	2.35	0.41
1:A:12:GLN:HE22	1:A:555:ILE:H	1.69	0.41
1:A:290:THR:O	1:A:291:ALA:C	2.57	0.41
1:A:389:GLU:O	1:A:393:ASN:ND2	2.53	0.41
1:A:88:LEU:HD21	1:A:420:LEU:HD22	2.02	0.41
1:A:460:GLY:HA2	7:A:711:HOH:O	2.21	0.41
1:A:61:LEU:HD22	1:A:313:PHE:CD2	2.56	0.41
1:B:312:LYS:HE2	1:B:488:VAL:HG13	2.03	0.40
1:A:107:ILE:CD1	7:A:794:HOH:O	2.69	0.40
1:B:472:LYS:CE	1:B:476:ARG:HH21	2.34	0.40
1:B:407:ALA:HB1	1:B:421:GLU:HG2	2.03	0.40
1:A:246:SER:HB3	1:B:105:PHE:CE2	2.57	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.98	0.40
1:A:68:THR:HG22	1:A:339:MET:SD	2.62	0.40
1:B:225:ILE:O	1:B:237:THR:HA	2.22	0.40
1:B:83:ASP:HB3	1:B:264:GLU:OE1	2.21	0.40
1:B:357:ARG:HH21	1:B:394:LEU:HD11	1.87	0.40
1:B:428:GLN:NE2	7:B:751:HOH:O	2.54	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	555/559 (99%)	515 (93%)	38 (7%)	2 (0%)	34	54
1	B	555/559 (99%)	524 (94%)	30 (5%)	1 (0%)	47	68
All	All	1110/1118 (99%)	1039 (94%)	68 (6%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	LEU
1	A	25	GLY
1	B	445	LEU

5.3.2 Protein sidechains ⓘ

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	439/441 (100%)	417 (95%)	22 (5%)	24	46
1	B	439/441 (100%)	427 (97%)	12 (3%)	44	71
All	All	878/882 (100%)	844 (96%)	34 (4%)	32	57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	30	GLU
1	A	34	GLU
1	A	52	LYS
1	A	108	LYS
1	A	121	PRO
1	A	122	MET
1	A	123	GLU
1	A	158	ASN
1	A	232	ASP
1	A	261	GLN
1	A	345	LYS
1	A	358	GLU
1	A	424	ARG
1	A	425	LYS
1	A	433	ARG
1	A	435	SER
1	A	465	ASN
1	A	478	GLU
1	A	510	THR
1	A	511	ILE

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Mol	Chain	Res	Type
1	A	528	ILE
1	B	52	LYS
1	B	54	LYS
1	B	266	THR
1	B	316	VAL
1	B	347	ASP
1	B	350	THR
1	B	364	GLU
1	B	370	ILE
1	B	386	THR
1	B	431	GLU
1	B	453	LYS
1	B	456	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	126	ASN
1	A	393	ASN
1	A	428	GLN
1	A	465	ASN
1	B	12	GLN
1	B	126	ASN
1	B	265	ASN
1	B	362	ASN
1	B	382	ASN
1	B	442	ASN
1	B	475	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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$
6	TOE	B	605	-	10,10,10	0.71	0	9,9,9	0.52	0
2	SO4	A	601	-	4,4,4	0.46	0	6,6,6	0.31	0
2	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.43	0
4	XPO	B	603	5	5,6,6	3.57	2 (40%)	6,8,8	0.84	0
6	TOE	A	606	-	10,10,10	0.83	0	9,9,9	0.61	0
4	XPO	A	603	5	5,6,6	3.36	2 (40%)	6,8,8	1.38	1 (16%)
6	TOE	A	605	-	10,10,10	0.62	0	9,9,9	0.43	0
3	ADP	A	602	5	24,29,29	1.07	2 (8%)	29,45,45	1.36	4 (13%)
3	ADP	B	602	5	24,29,29	1.10	2 (8%)	29,45,45	1.50	4 (13%)

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
6	TOE	B	605	-	-	6/8/8/8	-
4	XPO	B	603	5	-	0/0/4/4	-
6	TOE	A	606	-	-	8/8/8/8	-
4	XPO	A	603	5	-	0/0/4/4	-
6	TOE	A	605	-	-	4/8/8/8	-
3	ADP	A	602	5	-	1/12/32/32	0/3/3/3
3	ADP	B	602	5	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	XPO	P-O2	6.67	1.69	1.59
4	A	603	XPO	P-O2	6.44	1.69	1.59
4	B	603	XPO	P-O3	3.55	1.62	1.50
3	A	602	ADP	O4'-C1'	3.27	1.45	1.41
4	A	603	XPO	P-O3	3.17	1.60	1.50
3	B	602	ADP	O4'-C1'	3.09	1.45	1.41
3	A	602	ADP	C5-C4	2.49	1.47	1.40
3	B	602	ADP	C5-C4	2.12	1.46	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ADP	N3-C2-N1	-4.21	122.11	128.68
3	B	602	ADP	PA-O3A-PB	-3.91	119.42	132.83
3	A	602	ADP	N3-C2-N1	-3.47	123.25	128.68
4	A	603	XPO	O1-P-O2	3.00	114.62	105.24
3	A	602	ADP	C2-N1-C6	2.79	123.53	118.75
3	A	602	ADP	PA-O3A-PB	-2.33	124.85	132.83
3	B	602	ADP	C4-C5-N7	-2.17	107.14	109.40
3	B	602	ADP	C2-N1-C6	2.12	122.38	118.75
3	A	602	ADP	O3'-C3'-C4'	-2.05	105.11	111.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	605	TOE	OC'-CD'-CE'-OF'
6	A	605	TOE	OF'-CG'-CH'-OI'
6	A	605	TOE	OC'-CD'-CE'-OF'
6	B	605	TOE	O2'-CA'-CB'-OC'
6	A	605	TOE	O2'-CA'-CB'-OC'
6	A	606	TOE	O2'-CA'-CB'-OC'
6	A	606	TOE	OC'-CD'-CE'-OF'
6	A	606	TOE	OF'-CG'-CH'-OI'
6	B	605	TOE	CE'-CD'-OC'-CB'
6	A	605	TOE	CA'-CB'-OC'-CD'
6	A	606	TOE	CD'-CE'-OF'-CG'
6	A	606	TOE	CA'-CB'-OC'-CD'
6	A	606	TOE	CH'-CG'-OF'-CE'
6	A	606	TOE	CG'-CH'-OI'-CK'
6	A	606	TOE	CE'-CD'-OC'-CB'
6	B	605	TOE	CD'-CE'-OF'-CG'

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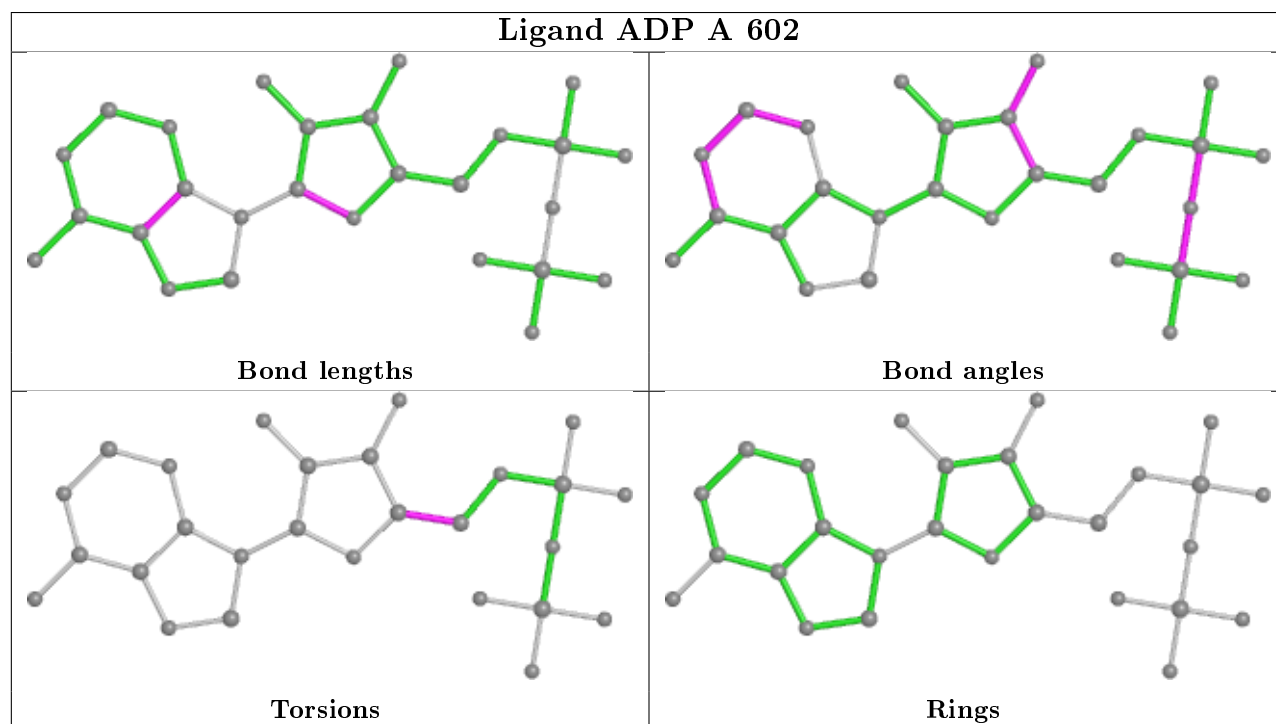
Mol	Chain	Res	Type	Atoms
3	A	602	ADP	O4'-C4'-C5'-O5'
6	B	605	TOE	CH'-CG'-OF'-CE'
6	B	605	TOE	OF'-CG'-CH'-OI'

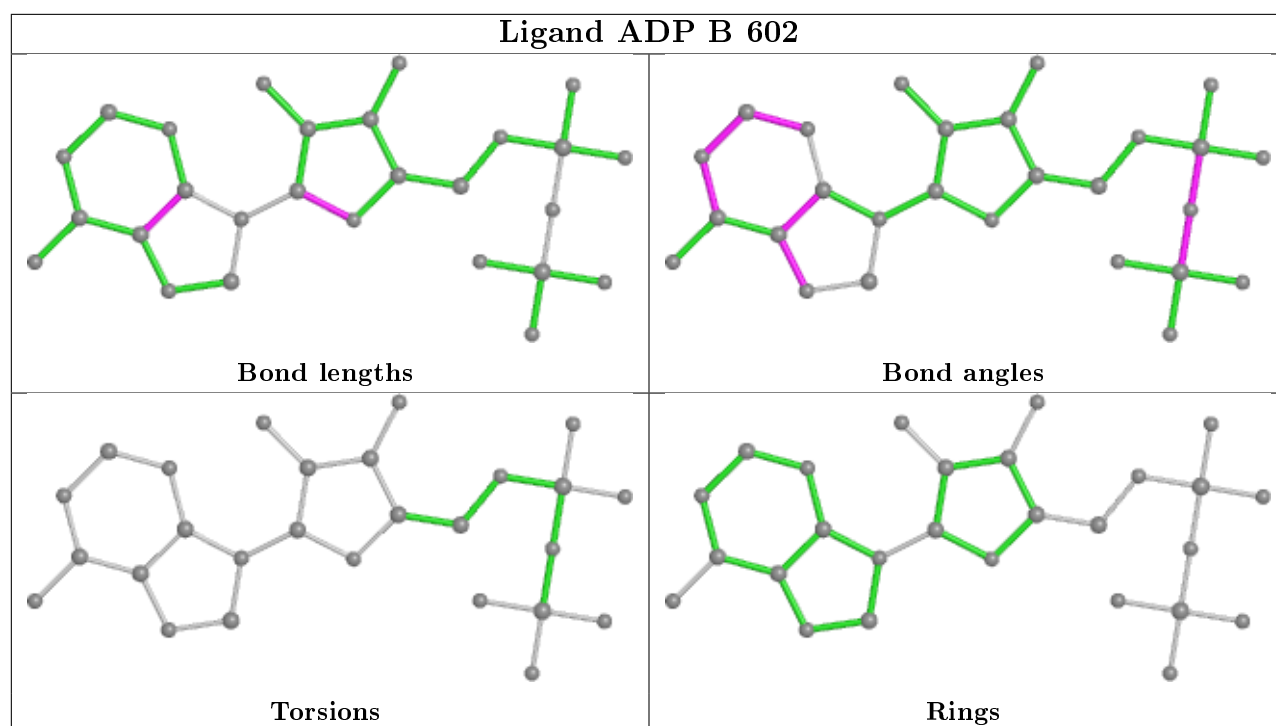
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	XPO	1	0
6	A	606	TOE	1	0
3	B	602	ADP	5	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	557/559 (99%)	-0.17	14 (2%) 57 61	17, 35, 66, 82	0
1	B	557/559 (99%)	-0.29	3 (0%) 91 91	16, 32, 57, 73	0
All	All	1114/1118 (99%)	-0.23	17 (1%) 73 75	16, 33, 60, 82	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	SER	3.8
1	A	503	LEU	2.9
1	A	501	THR	2.7
1	B	349	ALA	2.7
1	B	444	ASP	2.6
1	A	354	GLU	2.5
1	A	358	GLU	2.4
1	A	349	ALA	2.4
1	A	356	LEU	2.3
1	A	49	ARG	2.3
1	A	465	ASN	2.2
1	A	357	ARG	2.2
1	A	353	LEU	2.2
1	B	354	GLU	2.1
1	A	342	GLY	2.1
1	A	392	LEU	2.0
1	A	347	ASP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

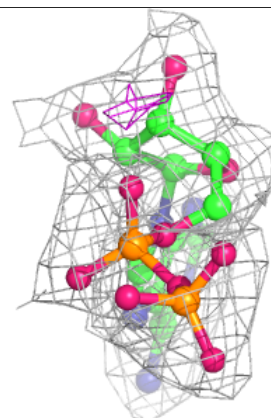
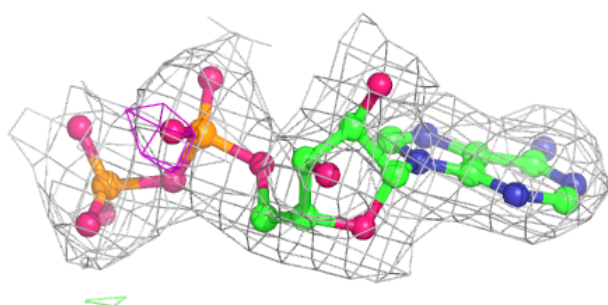
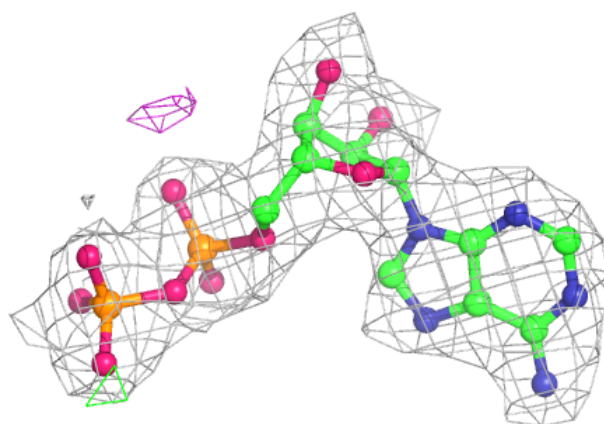
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	TOE	A	606	11/11	0.81	0.18	44,48,51,53	0
6	TOE	B	605	11/11	0.91	0.18	21,30,47,49	0
6	TOE	A	605	11/11	0.93	0.14	28,30,43,43	0
2	SO4	B	601	5/5	0.95	0.13	45,51,53,54	0
5	MG	A	604	1/1	0.96	0.09	34,34,34,34	0
4	XPO	A	603	7/7	0.96	0.16	39,41,45,47	0
2	SO4	A	601	5/5	0.96	0.11	41,44,45,47	0
5	MG	B	604	1/1	0.98	0.08	34,34,34,34	0
4	XPO	B	603	7/7	0.98	0.12	37,39,43,46	0
3	ADP	A	602	27/27	0.98	0.09	27,31,33,34	0
3	ADP	B	602	27/27	0.98	0.09	27,32,36,36	0

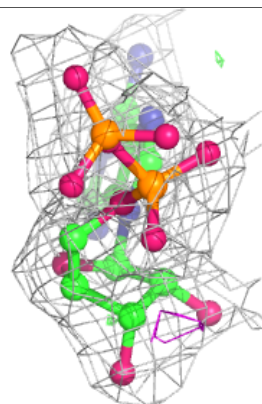
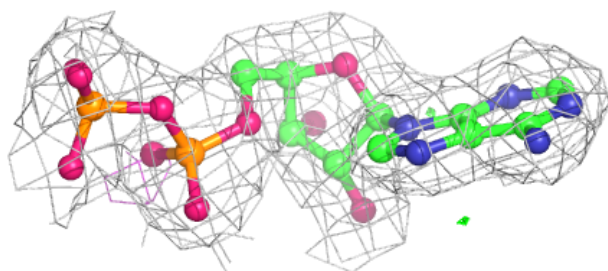
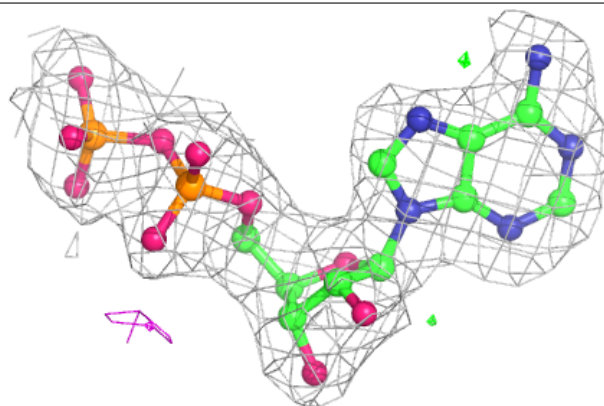
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 602:

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

**Electron density around ADP B 602:**

$2mF_o-DF_c$ (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.