



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:26 AM UTC

PDB ID : 8CQX / pdb_00008cqx
Title : Ribokinase from T.sp mutant A92G
Authors : Timofeev, V.I.; Shevtsov, M.B.; Abramchik, Y.A.; Kostromina, M.A.; Zayats, E.A.; Kuranova, I.P.; Esipov, R.S.
Deposited on : 2023-03-07
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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

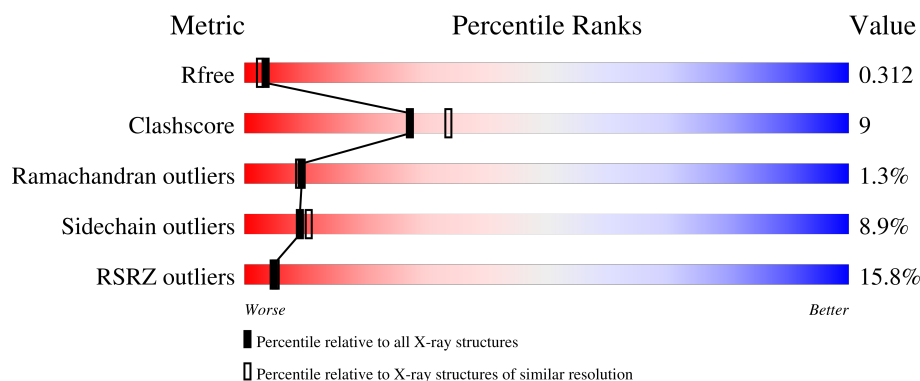
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	300	10% 76% 21% .
1	B	300	2% 85% 13% .
1	C	300	3% 81% 19% .
1	D	300	48% 64% 30% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	D	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9056 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.

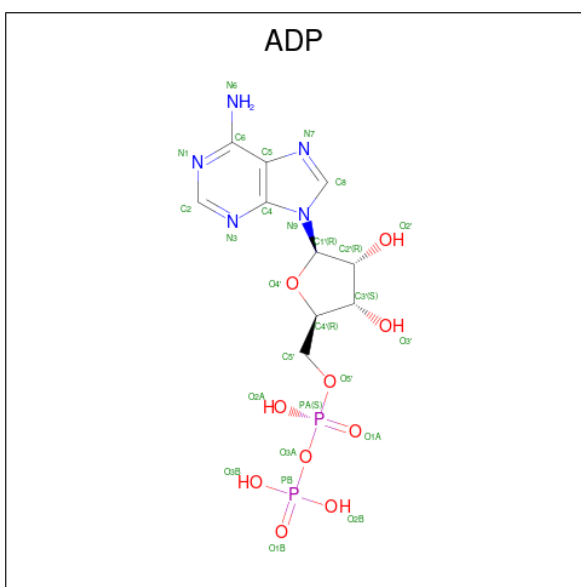
- Molecule 1 is a protein called Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2194	1383	398	409	4			
1	B	300	Total	C	N	O	S	0	0	0
			2183	1377	394	408	4			
1	C	300	Total	C	N	O	S	0	0	0
			2183	1377	394	408	4			
1	D	300	Total	C	N	O	S	0	0	0
			2183	1377	394	408	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75
B	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75
C	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75
D	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: 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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	63	Total	O	0	0
			63	63		

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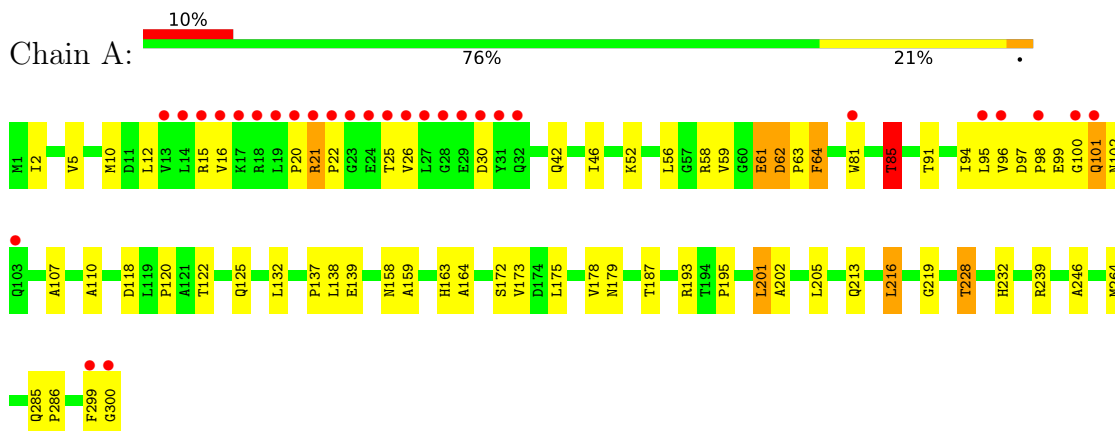
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	68	Total 68	O 68	0	0
4	D	11	Total 11	O 11	0	0

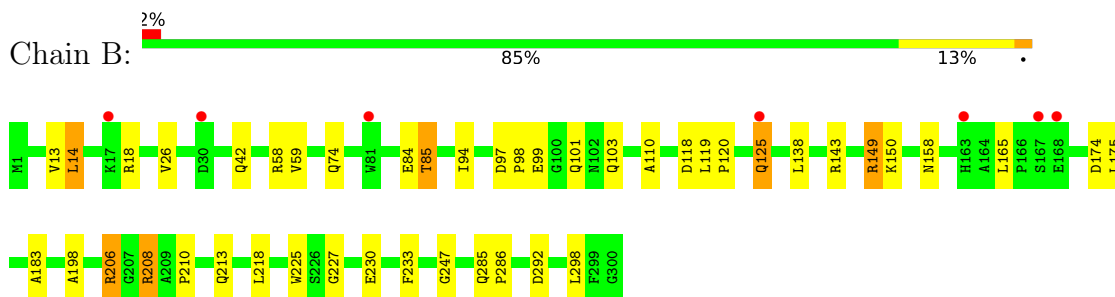
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

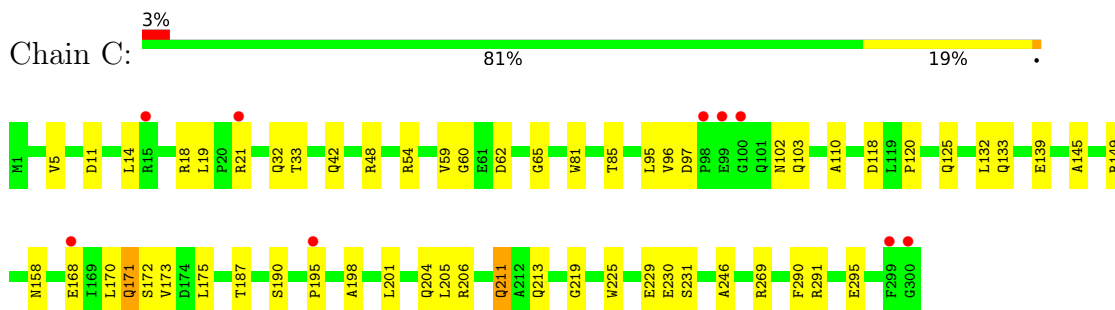
- Molecule 1: Ribokinase



- Molecule 1: Ribokinase

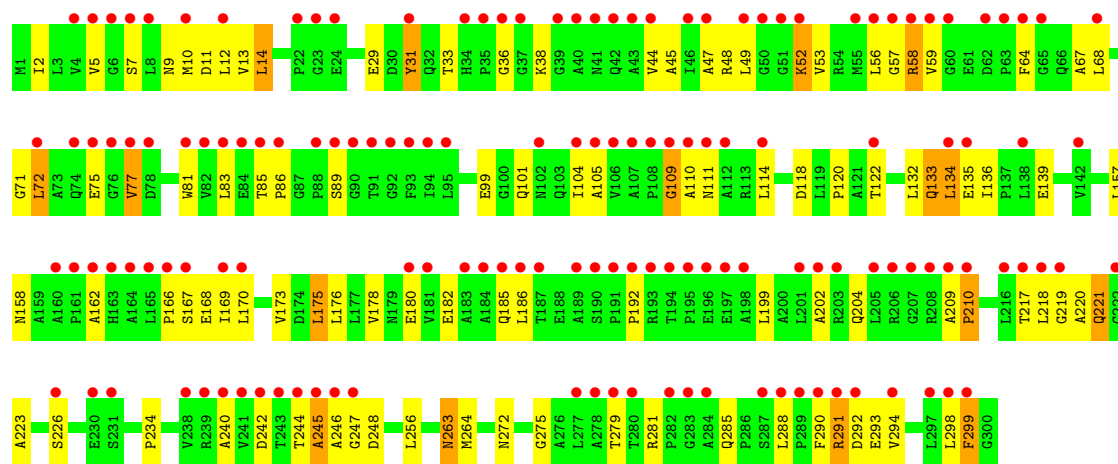


- Molecule 1: Ribokinase



- Molecule 1: Ribokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.31Å 155.61Å 82.92Å 90.00° 96.37° 90.00°	Depositor
Resolution (Å)	29.52 – 2.27 29.52 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.52-2.27) 99.3 (29.52-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.229 , 0.311 0.233 , 0.312	Depositor DCC
R_{free} test set	2481 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9056	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: ADP, 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	1.12	0/2232	1.49	12/3043 (0.4%)
1	B	1.13	0/2221	1.51	5/3029 (0.2%)
1	C	1.10	0/2221	1.48	7/3029 (0.2%)
1	D	1.15	0/2221	1.55	8/3029 (0.3%)
All	All	1.13	0/8895	1.51	32/12130 (0.3%)

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	0	1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASP	CA-CB-CG	7.30	119.90	112.60
1	D	264	MET	CA-C-N	6.15	128.84	120.54
1	D	264	MET	C-N-CA	6.15	128.84	120.54
1	B	74	GLN	CB-CA-C	-5.95	99.61	110.63
1	C	171	GLN	CB-CA-C	-5.93	100.76	110.85
1	A	202	ALA	CA-C-N	5.66	127.86	120.28
1	A	202	ALA	C-N-CA	5.66	127.86	120.28
1	C	170	LEU	CA-C-N	5.59	128.23	120.29
1	C	170	LEU	C-N-CA	5.59	128.23	120.29
1	B	233	PHE	CB-CA-C	5.55	117.56	110.13
1	C	62	ASP	CB-CA-C	5.54	117.55	109.08
1	A	179	ASN	CA-C-N	5.47	127.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASN	C-N-CA	5.47	127.61	120.28
1	C	97	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	85	THR	CB-CA-C	5.32	117.17	109.45
1	D	58	ARG	CB-CA-C	5.27	117.94	110.24
1	A	246	ALA	CA-C-N	5.26	125.82	119.98
1	A	246	ALA	C-N-CA	5.26	125.82	119.98
1	A	137	PRO	CA-C-N	5.23	127.29	120.28
1	A	137	PRO	C-N-CA	5.23	127.29	120.28
1	D	109	GLY	CA-C-N	5.17	128.88	120.60
1	D	109	GLY	C-N-CA	5.17	128.88	120.60
1	B	183	ALA	CA-C-N	5.16	127.45	120.38
1	B	183	ALA	C-N-CA	5.16	127.45	120.38
1	A	139	GLU	CB-CG-CD	5.13	121.31	112.60
1	D	299	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	64	PHE	CA-C-N	5.06	125.71	119.99
1	A	64	PHE	C-N-CA	5.06	125.71	119.99
1	C	246	ALA	CA-C-N	5.06	126.64	120.22
1	C	246	ALA	C-N-CA	5.06	126.64	120.22
1	D	167	SER	CA-C-N	5.04	127.35	120.54
1	D	167	SER	C-N-CA	5.04	127.35	120.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	247	GLY	Peptide

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	2194	0	2244	42	0
1	B	2183	0	2232	27	0
1	C	2183	0	2232	26	0
1	D	2183	0	2232	71	0
2	A	27	0	12	0	0
2	B	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	0	0
2	D	27	0	12	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	60	0	0	1	0
4	B	63	0	0	0	0
4	C	68	0	0	0	0
4	D	11	0	0	2	0
All	All	9056	0	8988	163	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 9.

All (163) 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:D:217:THR:HG22	2:D:401:ADP:N3	1.61	1.15
1:C:85:THR:HG21	1:C:110:ALA:HB1	1.46	0.96
1:D:242:ASP:O	1:D:279:THR:HA	1.72	0.90
1:A:81:TRP:CZ3	1:A:120:PRO:HG2	2.07	0.90
1:C:85:THR:HG21	1:C:110:ALA:CB	2.02	0.89
1:D:9:ASN:OD1	1:D:111:ASN:ND2	2.10	0.85
1:D:133:GLN:C	1:D:134:LEU:HD23	2.05	0.81
1:D:219:GLY:O	1:D:221:GLN:N	2.15	0.78
1:C:59:VAL:O	1:C:85:THR:HG22	1.85	0.77
1:D:217:THR:CG2	2:D:401:ADP:N3	2.46	0.74
1:D:275:GLY:HA3	2:D:401:ADP:O2'	1.92	0.70
1:D:105:ALA:HB2	4:D:504:HOH:O	1.92	0.70
1:C:42:GLN:HE22	1:C:158:ASN:HD22	1.41	0.69
1:B:149:ARG:NH2	1:B:174:ASP:OD1	2.28	0.67
1:D:219:GLY:HA2	2:D:401:ADP:O5'	1.96	0.65
1:D:217:THR:HG22	2:D:401:ADP:C2	2.30	0.65
1:A:42:GLN:HE22	1:A:158:ASN:HD22	1.44	0.64
1:A:213:GLN:HE22	1:A:228:THR:CG2	2.11	0.64
1:D:2:ILE:HD11	1:D:256:LEU:HA	1.80	0.64
1:D:281:ARG:NH1	1:D:293:GLU:OE2	2.33	0.62
1:A:15:ARG:HA	1:A:96:VAL:O	2.00	0.62
1:D:263:ASN:HD22	1:D:263:ASN:H	1.49	0.61
1:C:54:ARG:HD3	1:C:81:TRP:CZ3	2.36	0.61
1:B:42:GLN:HE22	1:B:158:ASN:HD22	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:O	1:A:101:GLN:O	2.20	0.60
1:B:58:ARG:HB3	1:B:85:THR:HG21	1.83	0.60
1:D:52:LYS:N	1:D:52:LYS:HD2	2.16	0.59
1:B:149:ARG:HH22	1:B:174:ASP:CG	2.11	0.59
1:B:118:ASP:O	1:B:120:PRO:HD3	2.03	0.59
1:D:133:GLN:HA	1:D:158:ASN:O	2.02	0.58
1:D:217:THR:HG22	2:D:401:ADP:C4	2.36	0.58
1:B:59:VAL:O	1:B:85:THR:HG23	2.03	0.58
1:C:85:THR:CG2	1:C:110:ALA:CB	2.81	0.58
1:D:48:ARG:NH1	1:D:285:GLN:O	2.37	0.58
1:D:57:GLY:HA2	1:D:114:LEU:HD22	1.86	0.58
1:D:245:ALA:CB	1:D:288:LEU:HD21	2.33	0.58
1:D:134:LEU:HD23	1:D:134:LEU:N	2.18	0.58
1:A:81:TRP:CE3	1:A:120:PRO:HG2	2.38	0.57
1:D:202:ALA:HB1	1:D:226:SER:HB3	1.85	0.57
1:A:59:VAL:O	1:A:85:THR:HG23	2.05	0.57
1:A:163:HIS:HD2	1:A:164:ALA:O	1.88	0.57
1:D:219:GLY:C	1:D:221:GLN:H	2.10	0.56
1:D:175:LEU:HD12	1:D:176:LEU:N	2.20	0.55
1:A:58:ARG:HB3	1:A:85:THR:HG21	1.89	0.55
1:D:217:THR:O	2:D:401:ADP:H2	1.90	0.55
1:C:95:LEU:O	1:C:102:ASN:HA	2.07	0.55
1:D:56:LEU:HD23	1:D:56:LEU:C	2.31	0.55
1:A:5:VAL:HB	1:A:132:LEU:CD2	2.37	0.55
1:A:213:GLN:HE22	1:A:228:THR:HG23	1.71	0.55
1:D:9:ASN:O	1:D:36:GLY:N	2.37	0.54
1:A:25:THR:HG23	1:D:104:ILE:HG21	1.90	0.54
1:C:85:THR:CG2	1:C:110:ALA:HB1	2.30	0.54
1:C:206:ARG:NH1	1:C:230:GLU:OE1	2.37	0.54
1:D:71:GLY:O	1:D:75:GLU:HG2	2.08	0.54
1:C:171:GLN:HA	1:C:211:GLN:NE2	2.23	0.54
1:D:49:LEU:O	1:D:291:ARG:NH1	2.41	0.52
1:B:175:LEU:HA	1:B:213:GLN:O	2.10	0.52
1:A:25:THR:HA	1:D:104:ILE:HB	1.92	0.52
1:D:118:ASP:O	1:D:120:PRO:HD3	2.09	0.52
2:D:401:ADP:H3'	2:D:401:ADP:O2A	2.10	0.51
1:D:13:VAL:O	1:D:31:TYR:HA	2.10	0.51
1:B:97:ASP:HB2	1:B:98:PRO:CD	2.40	0.51
1:D:38:LYS:HG3	1:D:135:GLU:OE2	2.11	0.51
1:D:169:ILE:O	1:D:170:LEU:HD23	2.10	0.51
1:A:118:ASP:O	1:A:120:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:VAL:O	1:D:85:THR:HG22	2.11	0.50
1:A:187:THR:HG21	1:A:201:LEU:HD23	1.94	0.50
1:D:81:TRP:CZ3	1:D:120:PRO:HG2	2.46	0.50
1:B:85:THR:CG2	1:B:110:ALA:HB1	2.42	0.50
1:C:133:GLN:HA	1:C:158:ASN:O	2.12	0.50
1:C:195:PRO:O	1:C:198:ALA:HB3	2.12	0.50
1:B:125:GLN:HE21	1:B:125:GLN:HA	1.76	0.50
1:C:149:ARG:NH1	1:C:172:SER:O	2.41	0.50
1:A:95:LEU:O	1:A:102:ASN:HA	2.12	0.49
1:B:208:ARG:HH11	1:B:208:ARG:HB3	1.77	0.49
1:D:134:LEU:HD21	1:D:157:LEU:HD11	1.93	0.49
1:C:60:GLY:HA2	1:C:85:THR:HG22	1.95	0.49
1:B:13:VAL:HG22	1:B:94:ILE:HB	1.95	0.49
1:B:59:VAL:O	1:B:85:THR:CG2	2.61	0.49
1:D:294:VAL:HG12	1:D:298:LEU:HD12	1.93	0.49
1:D:44:VAL:HG22	1:D:75:GLU:HG3	1.95	0.49
1:D:11:ASP:OD2	1:D:36:GLY:HA3	2.13	0.48
1:B:247:GLY:CA	2:B:401:ADP:O2B	2.62	0.48
1:D:132:LEU:O	1:D:158:ASN:N	2.46	0.48
1:A:187:THR:HG21	1:A:201:LEU:CD2	2.44	0.48
1:D:166:PRO:O	1:D:169:ILE:HG22	2.14	0.48
1:D:202:ALA:HB1	1:D:226:SER:CB	2.44	0.48
1:C:48:ARG:O	1:C:290:PHE:HA	2.14	0.47
1:A:2:ILE:HG21	1:A:46:ILE:HD13	1.96	0.47
1:D:11:ASP:O	1:D:33:THR:HA	2.15	0.47
1:D:58:ARG:HG3	1:D:83:LEU:O	2.15	0.47
1:C:19:LEU:HD13	1:C:103:GLN:HG3	1.95	0.46
1:A:26:VAL:O	1:D:105:ALA:HA	2.16	0.46
1:C:118:ASP:O	1:C:120:PRO:HD3	2.15	0.46
1:B:85:THR:HG21	1:B:110:ALA:HB1	1.97	0.46
1:C:59:VAL:C	1:C:85:THR:HG22	2.41	0.46
1:D:64:PHE:O	1:D:68:LEU:HG	2.15	0.46
1:B:198:ALA:CB	1:B:218:LEU:HD11	2.46	0.45
1:D:170:LEU:HB3	1:D:209:ALA:HB2	1.98	0.45
1:A:21:ARG:HB3	1:A:22:PRO:CD	2.46	0.45
1:D:272:ASN:HA	2:D:401:ADP:O3'	2.16	0.45
1:B:206:ARG:O	1:B:210:PRO:HA	2.16	0.45
1:A:96:VAL:HA	1:A:101:GLN:O	2.16	0.45
1:A:299:PHE:O	1:A:300:GLY:C	2.60	0.45
1:A:62:ASP:HB2	1:A:63:PRO:CD	2.47	0.45
1:A:81:TRP:CZ2	1:A:122:THR:OG1	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:NH1	1:B:85:THR:HB	2.32	0.44
1:C:187:THR:HB	1:C:204:GLN:NE2	2.32	0.44
1:D:180:GLU:HG3	1:D:192:PRO:HG2	1.99	0.44
1:B:285:GLN:N	1:B:286:PRO:CD	2.80	0.44
1:D:10:MET:HB2	1:D:68:LEU:HD21	1.99	0.44
1:D:47:ALA:HB2	1:D:77:VAL:HG12	1.99	0.44
1:A:10:MET:HG2	1:A:64:PHE:CD1	2.53	0.44
1:B:14:LEU:HA	1:B:14:LEU:HD13	1.82	0.44
1:B:208:ARG:HH11	1:B:208:ARG:CB	2.30	0.44
1:A:58:ARG:NH1	1:A:85:THR:HB	2.32	0.44
1:A:61:GLU:O	1:A:62:ASP:O	2.35	0.44
1:D:132:LEU:O	1:D:157:LEU:HD12	2.16	0.44
1:D:290:PHE:HB2	1:D:292:ASP:OD1	2.17	0.44
1:C:145:ALA:O	1:C:149:ARG:HG3	2.18	0.44
1:D:14:LEU:CD1	1:D:29:GLU:O	2.66	0.44
1:A:81:TRP:CZ3	1:A:120:PRO:CG	2.90	0.44
1:D:132:LEU:HB2	1:D:157:LEU:HD13	1.99	0.43
1:A:20:PRO:HD3	4:D:504:HOH:O	2.18	0.43
1:C:5:VAL:HB	1:C:132:LEU:CD2	2.48	0.43
1:D:48:ARG:HD2	1:D:288:LEU:O	2.18	0.43
1:D:52:LYS:HD2	1:D:52:LYS:H	1.82	0.43
1:B:97:ASP:HB2	1:B:98:PRO:HD2	2.00	0.43
1:A:91:THR:OG1	1:A:107:ALA:HB3	2.19	0.43
1:D:45:ALA:O	1:D:49:LEU:HG	2.19	0.42
1:A:285:GLN:N	1:A:286:PRO:CD	2.83	0.42
1:B:119:LEU:HD12	1:B:143:ARG:HB3	2.01	0.42
1:D:175:LEU:HD12	1:D:175:LEU:C	2.45	0.42
1:D:178:VAL:HA	1:D:182:GLU:OE2	2.19	0.42
1:A:97:ASP:CB	1:A:98:PRO:CD	2.96	0.42
1:B:225:TRP:O	1:B:230:GLU:HA	2.20	0.42
1:C:171:GLN:HA	1:C:211:GLN:HE22	1.83	0.42
1:C:225:TRP:CZ3	1:C:229:GLU:CG	3.02	0.42
1:D:209:ALA:O	1:D:210:PRO:C	2.62	0.42
1:A:125:GLN:HG2	4:A:559:HOH:O	2.20	0.42
1:D:58:ARG:HA	1:D:83:LEU:O	2.20	0.42
1:D:68:LEU:O	1:D:72:LEU:HD12	2.19	0.42
1:D:85:THR:CG2	1:D:110:ALA:HB1	2.49	0.42
1:A:195:PRO:HB3	1:A:232:HIS:CD2	2.55	0.41
1:A:122:THR:HG22	1:A:125:GLN:NE2	2.34	0.41
1:C:59:VAL:HB	1:C:65:GLY:HA2	2.01	0.41
1:C:175:LEU:HA	1:C:213:GLN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TRP:CH2	1:A:122:THR:OG1	2.73	0.41
1:B:213:GLN:OE1	1:B:227:GLY:HA3	2.20	0.41
1:A:5:VAL:HB	1:A:132:LEU:HD23	2.01	0.41
1:A:85:THR:HG21	1:A:110:ALA:HB1	2.03	0.41
1:B:58:ARG:HH11	1:B:85:THR:HB	1.85	0.41
1:D:5:VAL:HB	1:D:132:LEU:HD23	2.03	0.41
1:D:162:ALA:HB1	1:D:186:LEU:HG	2.02	0.41
1:A:264:MET:HE2	1:A:264:MET:HB2	1.66	0.41
1:D:218:LEU:CD2	1:D:223:ALA:HA	2.51	0.41
1:A:159:ALA:HB3	1:A:178:VAL:HG12	2.04	0.40
1:D:7:SER:HB3	1:D:135:GLU:O	2.21	0.40
1:A:178:VAL:HG23	1:A:216:LEU:HG	2.03	0.40
1:D:67:ALA:O	1:D:68:LEU:C	2.63	0.40
1:A:25:THR:HG23	1:D:104:ILE:CG2	2.51	0.40
1:B:247:GLY:HA3	2:B:401:ADP:O2B	2.20	0.40
1:C:11:ASP:O	1:C:33:THR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/300 (100%)	278 (93%)	17 (6%)	4 (1%)	9	9
1	B	298/300 (99%)	288 (97%)	10 (3%)	0	100	100
1	C	298/300 (99%)	282 (95%)	14 (5%)	2 (1%)	18	21
1	D	298/300 (99%)	256 (86%)	33 (11%)	9 (3%)	3	2
All	All	1193/1200 (99%)	1104 (92%)	74 (6%)	15 (1%)	9	9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	D	220	ALA
1	C	219	GLY
1	D	89	SER
1	D	240	ALA
1	D	210	PRO
1	D	246	ALA
1	A	30	ASP
1	A	62	ASP
1	C	168	GLU
1	D	245	ALA
1	A	219	GLY
1	D	234	PRO
1	D	109	GLY
1	D	86	PRO

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	218/217 (100%)	199 (91%)	19 (9%)	9	11
1	B	217/217 (100%)	201 (93%)	16 (7%)	13	15
1	C	217/217 (100%)	201 (93%)	16 (7%)	13	15
1	D	217/217 (100%)	191 (88%)	26 (12%)	5	5
All	All	869/868 (100%)	792 (91%)	77 (9%)	9	10

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	16	VAL
1	A	21	ARG
1	A	52	LYS
1	A	56	LEU
1	A	61	GLU
1	A	85	THR

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Mol	Chain	Res	Type
1	A	94	ILE
1	A	99	GLU
1	A	138	LEU
1	A	172	SER
1	A	173	VAL
1	A	175	LEU
1	A	193	ARG
1	A	201	LEU
1	A	205	LEU
1	A	216	LEU
1	A	228	THR
1	A	239	ARG
1	B	14	LEU
1	B	18	ARG
1	B	26	VAL
1	B	84	GLU
1	B	85	THR
1	B	99	GLU
1	B	101	GLN
1	B	103	GLN
1	B	125	GLN
1	B	138	LEU
1	B	149	ARG
1	B	150	LYS
1	B	165	LEU
1	B	206	ARG
1	B	208	ARG
1	B	298	LEU
1	C	14	LEU
1	C	18	ARG
1	C	21	ARG
1	C	32	GLN
1	C	96	VAL
1	C	125	GLN
1	C	139	GLU
1	C	173	VAL
1	C	190	SER
1	C	201	LEU
1	C	205	LEU
1	C	211	GLN
1	C	231	SER
1	C	269	ARG

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Mol	Chain	Res	Type
1	C	291	ARG
1	C	295	GLU
1	D	12	LEU
1	D	14	LEU
1	D	31	TYR
1	D	52	LYS
1	D	53	VAL
1	D	72	LEU
1	D	77	VAL
1	D	99	GLU
1	D	101	GLN
1	D	122	THR
1	D	133	GLN
1	D	134	LEU
1	D	136	ILE
1	D	139	GLU
1	D	168	GLU
1	D	173	VAL
1	D	175	LEU
1	D	185	GLN
1	D	199	LEU
1	D	204	GLN
1	D	221	GLN
1	D	244	THR
1	D	248	ASP
1	D	263	ASN
1	D	291	ARG
1	D	299	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	125	GLN
1	A	158	ASN
1	A	163	HIS
1	A	185	GLN
1	A	213	GLN
1	B	34	HIS
1	B	101	GLN
1	B	125	GLN
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	163	HIS
1	B	204	GLN
1	C	34	HIS
1	C	42	GLN
1	C	103	GLN
1	C	133	GLN
1	C	204	GLN
1	C	211	GLN
1	C	221	GLN
1	D	34	HIS
1	D	42	GLN
1	D	103	GLN
1	D	133	GLN
1	D	211	GLN
1	D	221	GLN
1	D	263	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](#)

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	ADP	B	401	-	28,29,29	0.88	1 (3%)	43,45,45	0.60	0
2	ADP	C	401	-	28,29,29	0.55	1 (3%)	43,45,45	0.63	1 (2%)
2	ADP	D	401	-	28,29,29	0.56	0	43,45,45	0.80	0
2	ADP	A	401	-	28,29,29	0.48	0	43,45,45	0.66	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
2	ADP	B	401	-	-	2/16/32/32	0/3/3/3
2	ADP	C	401	-	-	3/16/32/32	0/3/3/3
2	ADP	D	401	-	-	5/16/32/32	0/3/3/3
2	ADP	A	401	-	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ADP	PA-O3A	3.87	1.63	1.59
2	C	401	ADP	PA-O3A	2.17	1.61	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ADP	O2A-PA-O1A	2.12	122.28	112.44

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	PA-O3A-PB-O2B
2	A	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	PA-O3A-PB-O2B
2	D	401	ADP	C2'-C1'-N9-C8
2	C	401	ADP	C5'-O5'-PA-O1A
2	D	401	ADP	C4'-C5'-O5'-PA
2	C	401	ADP	PB-O3A-PA-O2A
2	D	401	ADP	C2'-C1'-N9-C4
2	D	401	ADP	O4'-C1'-N9-C4

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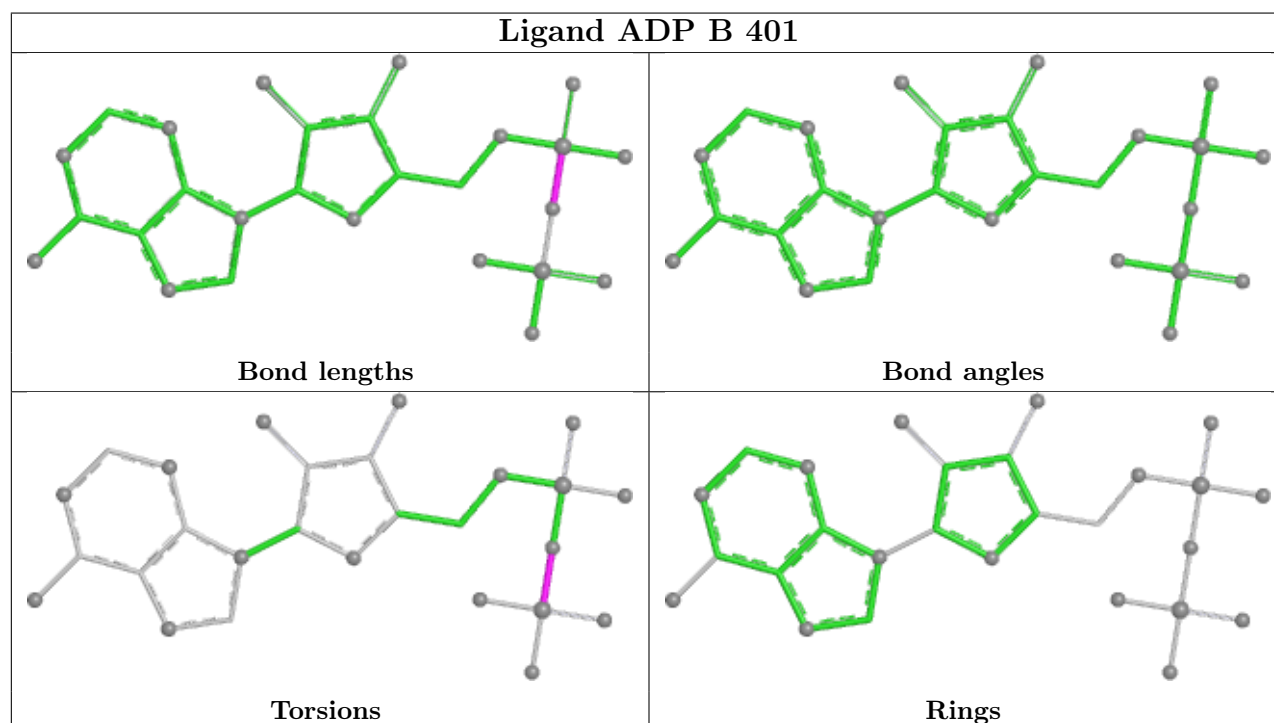
Mol	Chain	Res	Type	Atoms
2	D	401	ADP	O4'-C1'-N9-C8
2	B	401	ADP	PA-O3A-PB-O1B
2	C	401	ADP	PB-O3A-PA-O1A

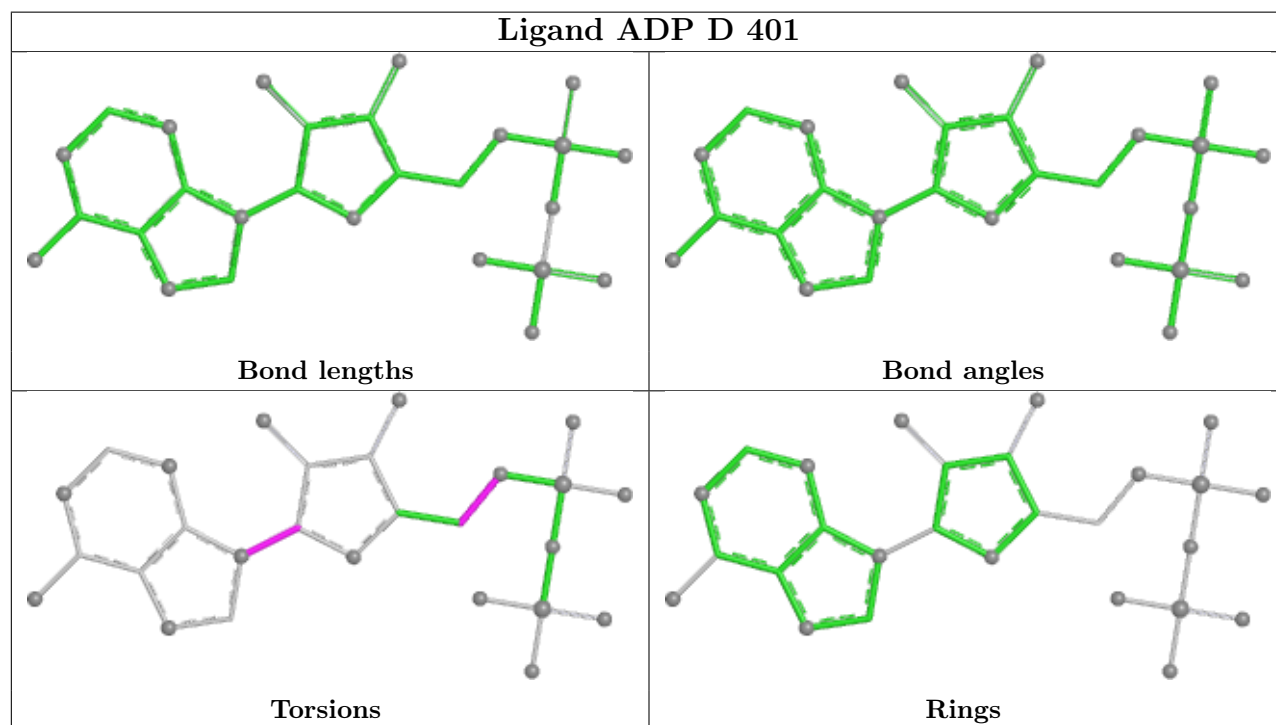
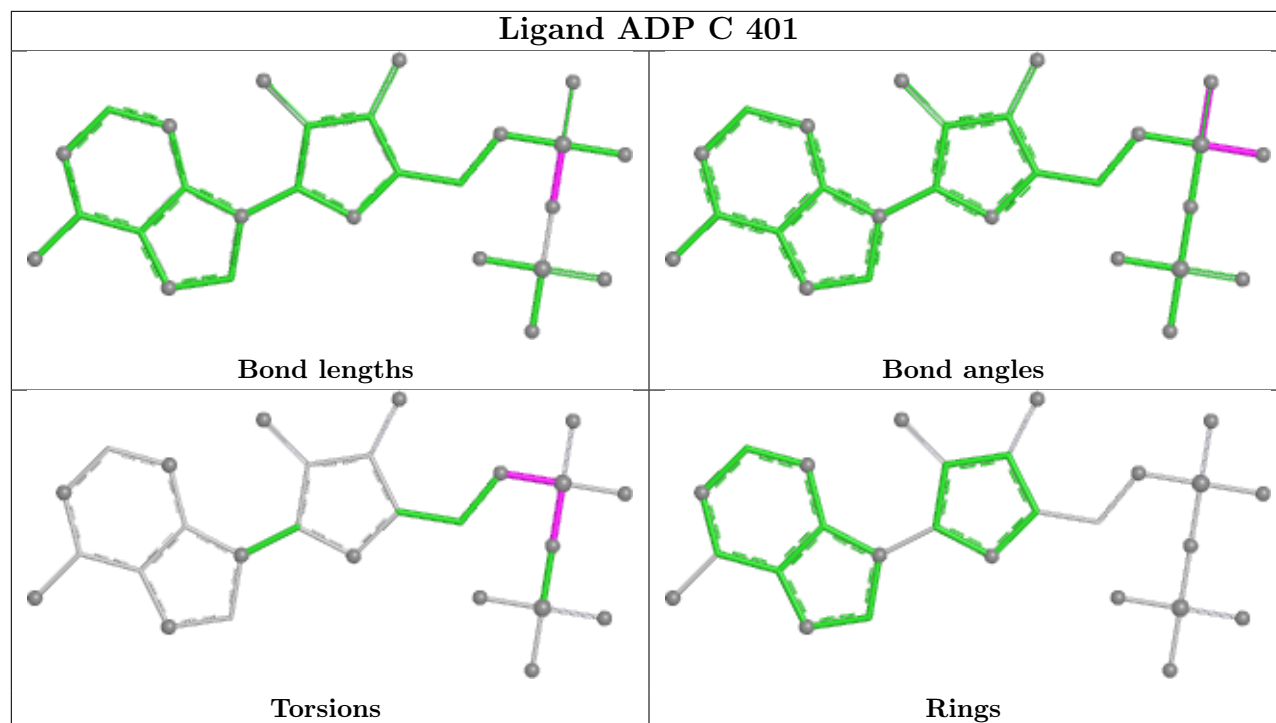
There are no ring outliers.

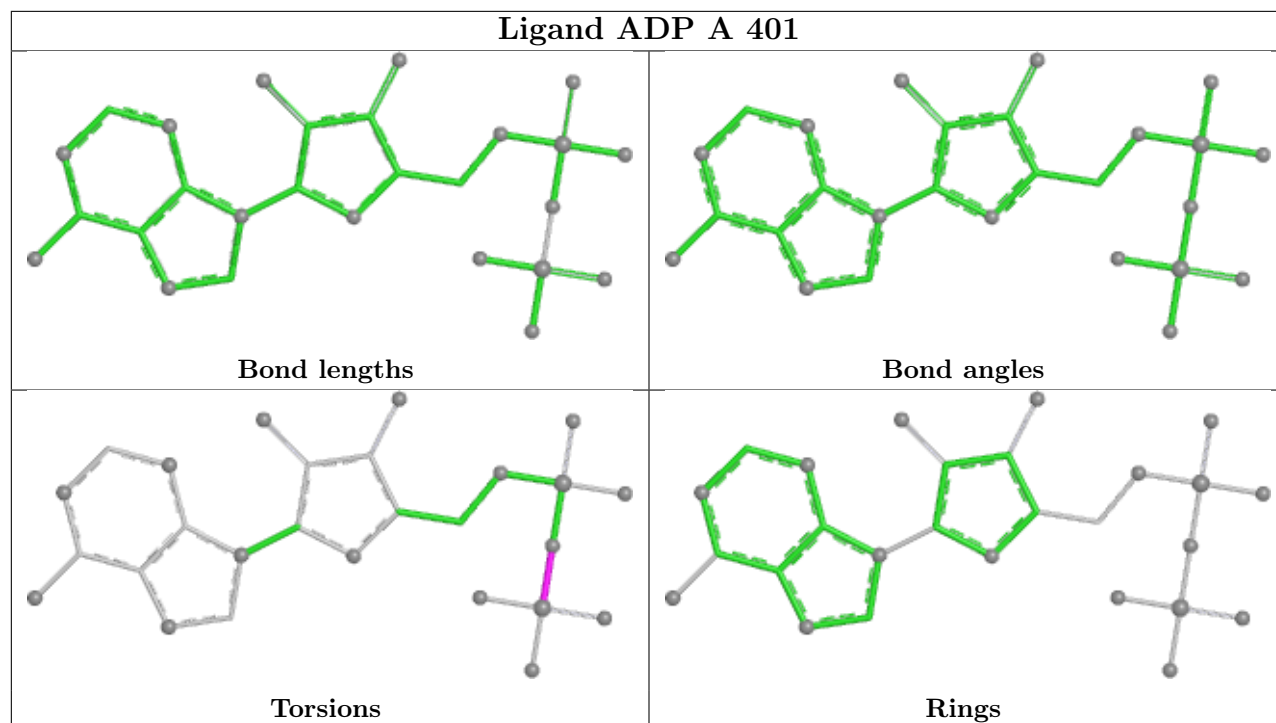
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ADP	2	0
2	D	401	ADP	9	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	300/300 (100%)	0.39	29 (9%) 13 14	11, 27, 88, 164	1 (0%)
1	B	300/300 (100%)	0.10	7 (2%) 61 63	16, 27, 56, 80	0
1	C	300/300 (100%)	0.19	9 (3%) 52 54	16, 28, 61, 96	0
1	D	300/300 (100%)	2.05	145 (48%) 0 0	27, 62, 98, 127	0
All	All	1200/1200 (100%)	0.68	190 (15%) 5 5	11, 32, 84, 164	1 (0%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	GLY	8.3
1	D	245	ALA	6.7
1	D	246	ALA	6.4
1	A	24	GLU	6.3
1	D	205	LEU	5.9
1	A	16	VAL	5.9
1	A	19	LEU	5.8
1	D	207	GLY	5.5
1	A	26	VAL	5.4
1	A	25	THR	5.2
1	A	22	PRO	5.0
1	D	8	LEU	5.0
1	D	6	GLY	4.8
1	A	20	PRO	4.7
1	D	83	LEU	4.7
1	D	169	ILE	4.7
1	A	18	ARG	4.6
1	D	77	VAL	4.5
1	D	284	ALA	4.4
1	C	100	GLY	4.4
1	D	72	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	37	GLY	4.3
1	D	186	LEU	4.3
1	D	114	LEU	4.2
1	D	91	THR	4.2
1	B	167	SER	4.1
1	D	201	LEU	4.1
1	D	93	PHE	4.1
1	D	162	ALA	4.0
1	A	96	VAL	4.0
1	D	39	GLY	4.0
1	D	81	TRP	4.0
1	D	247	GLY	3.9
1	D	289	PRO	3.9
1	D	90	GLY	3.9
1	D	243	THR	3.9
1	A	103	GLN	3.8
1	A	299	PHE	3.8
1	D	164	ALA	3.8
1	D	202	ALA	3.8
1	D	240	ALA	3.8
1	A	17	LYS	3.8
1	D	22	PRO	3.7
1	D	191	PRO	3.7
1	D	244	THR	3.7
1	D	192	PRO	3.7
1	C	299	PHE	3.6
1	D	161	PRO	3.6
1	D	7	SER	3.6
1	C	300	GLY	3.6
1	D	196	GLU	3.5
1	D	183	ALA	3.5
1	D	60	GLY	3.5
1	A	27	LEU	3.4
1	D	63	PRO	3.4
1	D	194	THR	3.4
1	D	160	ALA	3.4
1	D	57	GLY	3.4
1	D	92	GLY	3.4
1	D	166	PRO	3.4
1	D	195	PRO	3.4
1	D	82	VAL	3.3
1	D	299	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	106	VAL	3.3
1	A	100	GLY	3.3
1	A	98	PRO	3.3
1	D	206	ARG	3.3
1	D	165	LEU	3.3
1	D	5	VAL	3.3
1	D	59	VAL	3.2
1	D	290	PHE	3.2
1	D	238	VAL	3.2
1	D	209	ALA	3.2
1	D	62	ASP	3.2
1	D	78	ASP	3.2
1	D	187	THR	3.2
1	D	278	ALA	3.1
1	D	42	GLN	3.1
1	D	88	PRO	3.1
1	D	193	ARG	3.1
1	C	195	PRO	3.1
1	A	101	GLN	3.0
1	D	189	ALA	3.0
1	A	300	GLY	3.0
1	D	44	VAL	3.0
1	D	277	LEU	3.0
1	D	86	PRO	3.0
1	D	170	LEU	3.0
1	D	23	GLY	3.0
1	D	95	LEU	2.9
1	D	190	SER	2.9
1	A	28	GLY	2.9
1	D	40	ALA	2.9
1	A	29	GLU	2.9
1	D	210	PRO	2.9
1	D	12	LEU	2.9
1	D	55	MET	2.9
1	D	288	LEU	2.8
1	D	280	THR	2.8
1	A	14	LEU	2.8
1	D	167	SER	2.8
1	D	283	GLY	2.8
1	D	35	PRO	2.8
1	D	226	SER	2.7
1	B	168	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	15	ARG	2.7
1	D	242	ASP	2.7
1	D	217	THR	2.7
1	D	76	GLY	2.7
1	D	135	GLU	2.7
1	D	49	LEU	2.7
1	D	107	ALA	2.7
1	C	99	GLU	2.6
1	D	46	ILE	2.6
1	D	163	HIS	2.6
1	D	31	TYR	2.6
1	D	241	VAL	2.6
1	D	298	LEU	2.6
1	D	94	ILE	2.6
1	D	64	PHE	2.5
1	D	56	LEU	2.5
1	D	138	LEU	2.5
1	D	111	ASN	2.5
1	D	142	VAL	2.5
1	D	287	SER	2.5
1	B	17	LYS	2.5
1	D	43	ALA	2.5
1	D	34	HIS	2.5
1	A	21	ARG	2.4
1	D	84	GLU	2.4
1	D	122	THR	2.4
1	D	230	GLU	2.4
1	D	181	VAL	2.4
1	D	10	MET	2.4
1	B	30	ASP	2.4
1	D	75	GLU	2.4
1	D	105	ALA	2.4
1	D	231	SER	2.4
1	D	108	PRO	2.4
1	C	15	ARG	2.4
1	D	41	ASN	2.3
1	D	282	PRO	2.3
1	D	65	GLY	2.3
1	A	32	GLN	2.3
1	A	95	LEU	2.3
1	D	184	ALA	2.3
1	D	109	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	21	ARG	2.3
1	D	104	ILE	2.3
1	D	52	LYS	2.3
1	D	68	LEU	2.3
1	D	297	LEU	2.3
1	D	50	GLY	2.3
1	D	219	GLY	2.3
1	D	85	THR	2.3
1	D	74	GLN	2.3
1	D	4	VAL	2.3
1	A	30	ASP	2.2
1	D	208	ARG	2.2
1	D	112	ALA	2.2
1	D	89	SER	2.2
1	D	294	VAL	2.2
1	D	102	ASN	2.2
1	D	47	ALA	2.2
1	A	31	TYR	2.2
1	A	81	TRP	2.2
1	D	134	LEU	2.2
1	A	13	VAL	2.2
1	D	292	ASP	2.2
1	D	197	GLU	2.2
1	D	198	ALA	2.2
1	D	185	GLN	2.1
1	D	216	LEU	2.1
1	D	218	LEU	2.1
1	D	180	GLU	2.1
1	C	98	PRO	2.1
1	D	222	GLY	2.1
1	D	239	ARG	2.1
1	D	110	ALA	2.1
1	D	291	ARG	2.1
1	D	279	THR	2.1
1	D	24	GLU	2.1
1	B	125	GLN	2.1
1	B	163	HIS	2.1
1	D	36	GLY	2.1
1	D	51	GLY	2.1
1	B	81	TRP	2.1
1	D	58	ARG	2.1
1	C	168	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	203	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

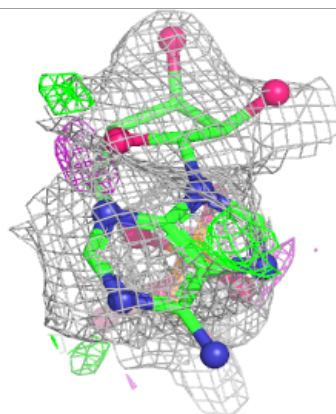
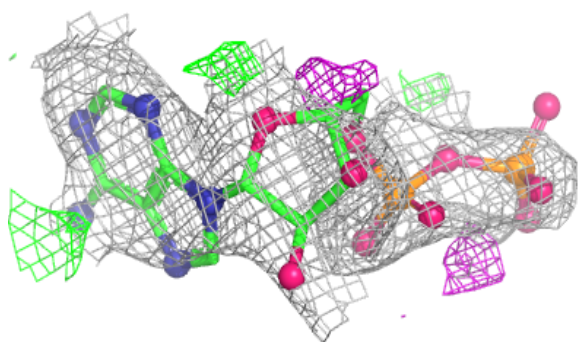
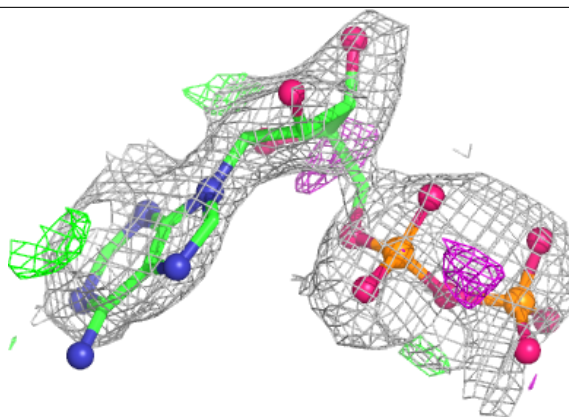
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	D	401	27/27	0.68	0.20	60,72,112,123	0
2	ADP	C	401	27/27	0.89	0.10	28,32,60,74	0
2	ADP	B	401	27/27	0.89	0.11	24,28,68,78	0
2	ADP	A	401	27/27	0.90	0.10	20,24,49,56	0
3	MG	A	402	1/1	0.97	0.07	23,23,23,23	0
3	MG	B	402	1/1	0.98	0.05	9,9,9,9	0
3	MG	C	402	1/1	0.99	0.04	20,20,20,20	0

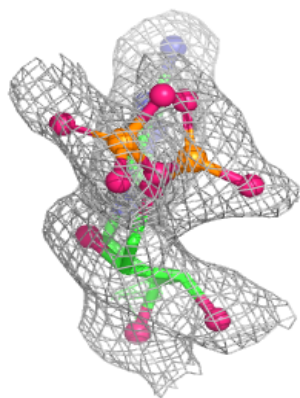
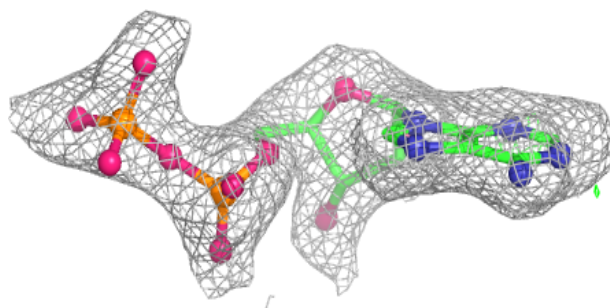
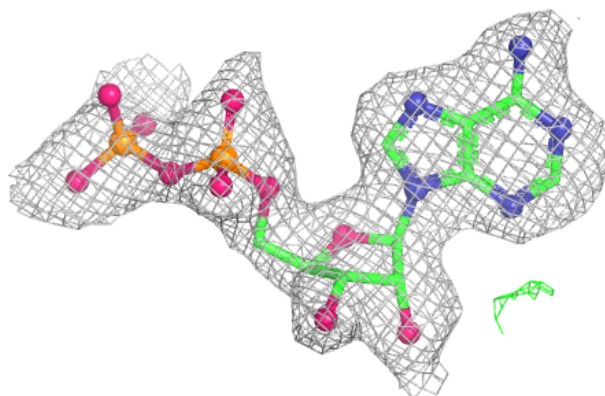
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 401:

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

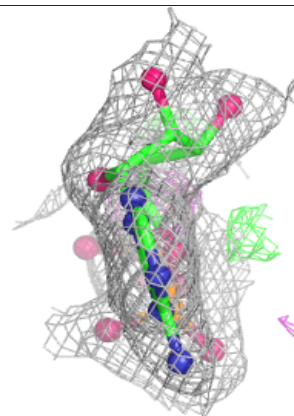
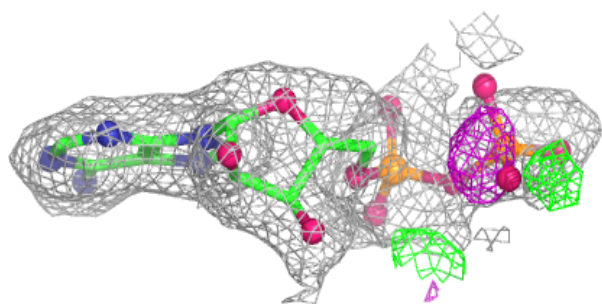
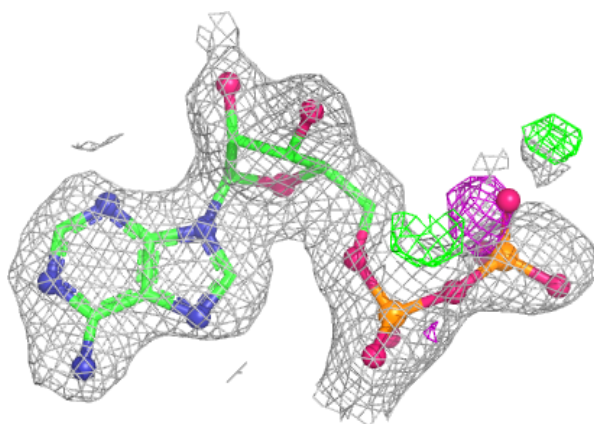
**Electron density around ADP C 401:**

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

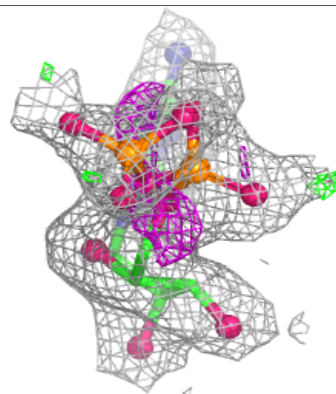
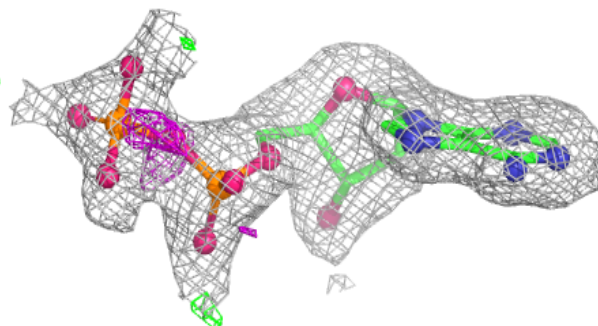
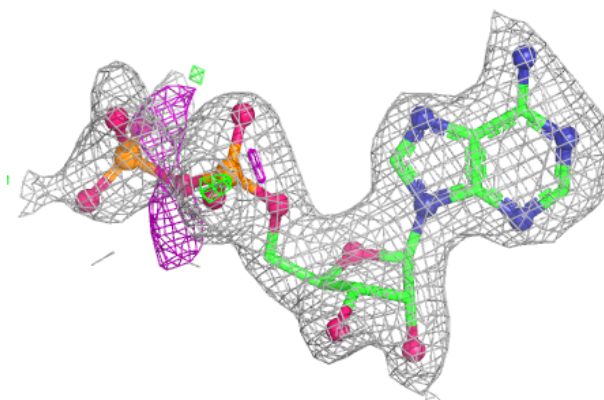


Electron density around ADP B 401:

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

**Electron density around ADP A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.