



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:15 AM UTC

PDB ID : 9ZOI / pdb_00009zoi
Title : Crystal structure of Phosphoribosylaminoimidazole carboxylase from Burkholderia xenovorans (ATP complex)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-12-15
Resolution : 1.93 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

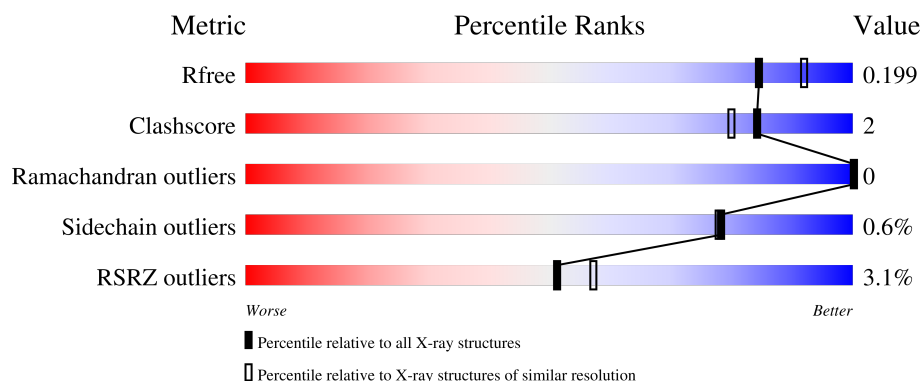
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	397	94%
1	B	397	93%
1	C	397	94%
1	D	397	90%

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	GOL	B	402	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12509 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 N5-carboxyaminoimidazole ribonucleotide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	5	0
			2935	1842	532	543	18			
1	B	385	Total	C	N	O	S	0	7	0
			2919	1834	530	538	17			
1	C	387	Total	C	N	O	S	0	5	0
			2884	1812	517	535	20			
1	D	386	Total	C	N	O	S	0	4	0
			2856	1799	512	526	19			

There are 32 discrepancies between the modelled and reference sequences:

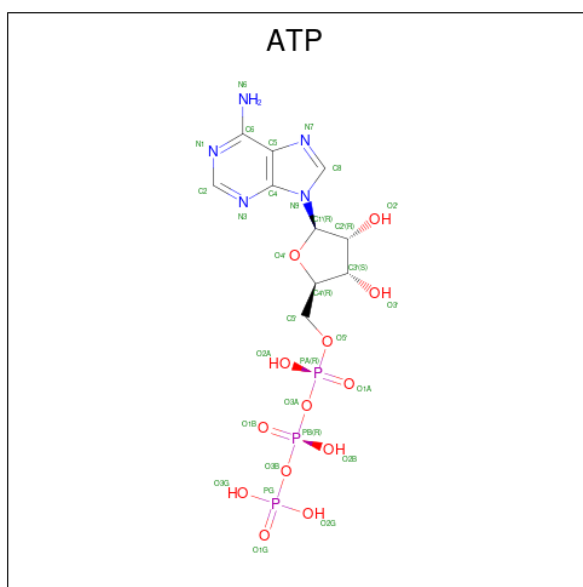
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q13UJ9
A	2	ALA	-	expression tag	UNP Q13UJ9
A	3	HIS	-	expression tag	UNP Q13UJ9
A	4	HIS	-	expression tag	UNP Q13UJ9
A	5	HIS	-	expression tag	UNP Q13UJ9
A	6	HIS	-	expression tag	UNP Q13UJ9
A	7	HIS	-	expression tag	UNP Q13UJ9
A	8	HIS	-	expression tag	UNP Q13UJ9
B	1	MET	-	expression tag	UNP Q13UJ9
B	2	ALA	-	expression tag	UNP Q13UJ9
B	3	HIS	-	expression tag	UNP Q13UJ9
B	4	HIS	-	expression tag	UNP Q13UJ9
B	5	HIS	-	expression tag	UNP Q13UJ9
B	6	HIS	-	expression tag	UNP Q13UJ9
B	7	HIS	-	expression tag	UNP Q13UJ9
B	8	HIS	-	expression tag	UNP Q13UJ9
C	1	MET	-	expression tag	UNP Q13UJ9
C	2	ALA	-	expression tag	UNP Q13UJ9
C	3	HIS	-	expression tag	UNP Q13UJ9
C	4	HIS	-	expression tag	UNP Q13UJ9
C	5	HIS	-	expression tag	UNP Q13UJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	HIS	-	expression tag	UNP Q13UJ9
C	7	HIS	-	expression tag	UNP Q13UJ9
C	8	HIS	-	expression tag	UNP Q13UJ9
D	1	MET	-	expression tag	UNP Q13UJ9
D	2	ALA	-	expression tag	UNP Q13UJ9
D	3	HIS	-	expression tag	UNP Q13UJ9
D	4	HIS	-	expression tag	UNP Q13UJ9
D	5	HIS	-	expression tag	UNP Q13UJ9
D	6	HIS	-	expression tag	UNP Q13UJ9
D	7	HIS	-	expression tag	UNP Q13UJ9
D	8	HIS	-	expression tag	UNP Q13UJ9

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



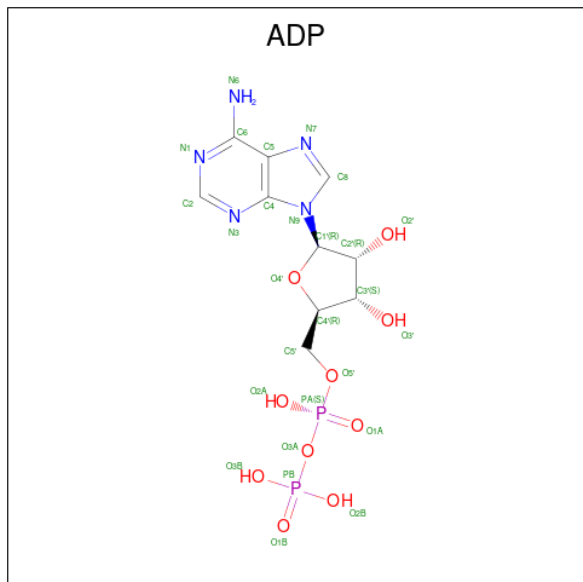
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



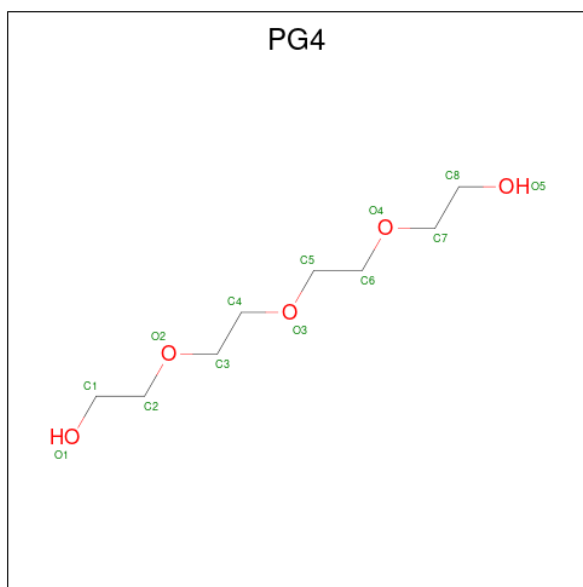
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		

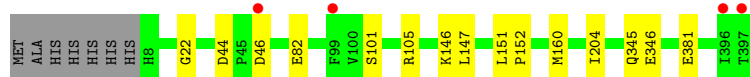
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	228	Total	O	0	0
			228	228		
9	B	215	Total	O	0	0
			215	215		
9	C	170	Total	O	0	0
			170	170		
9	D	117	Total	O	0	0
			117	117		

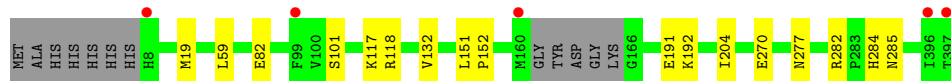
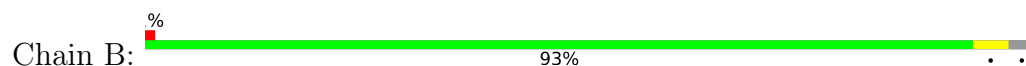
3 Residue-property plots [i](#)

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: N5-carboxyaminoimidazole ribonucleotide synthase



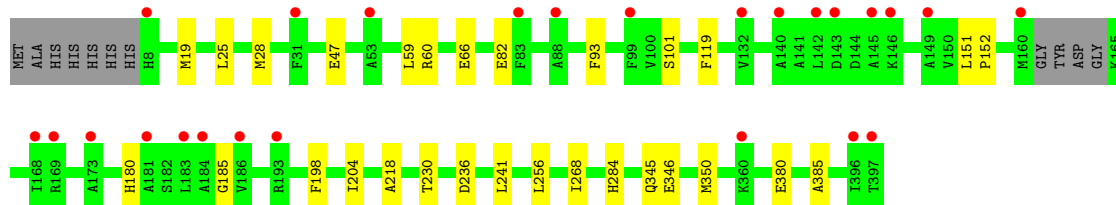
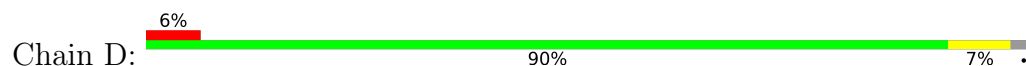
- Molecule 1: N5-carboxyaminoimidazole ribonucleotide synthase



- Molecule 1: N5-carboxyaminoimidazole ribonucleotide synthase



- Molecule 1: N5-carboxyaminoimidazole ribonucleotide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.01Å 170.44Å 170.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.81 – 1.93 44.81 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.81-1.93) 99.5 (44.81-1.93)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.94Å)	Xtriage
Refinement program	PHENIX (2.0_5765: ???)	Depositor
R, R_{free}	0.169 , 0.196 0.174 , 0.199	Depositor DCC
R_{free} test set	7286 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12509	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: ATP, PEG, PGE, ADP, PG4, GOL, 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	0.44	0/3010	0.59	0/4095
1	B	0.43	0/2999	0.59	0/4080
1	C	0.40	0/2956	0.56	0/4023
1	D	0.33	0/2927	0.52	0/3989
All	All	0.41	0/11892	0.57	0/16187

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 [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	2935	0	2935	10	0
1	B	2919	0	2927	14	0
1	C	2884	0	2859	9	0
1	D	2856	0	2824	22	0
2	A	31	0	12	0	0
2	C	31	0	12	0	0
3	A	7	0	10	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	10	0	14	0	0
6	B	6	0	8	5	0
6	C	6	0	8	2	0
6	D	6	0	8	2	0
7	B	27	0	12	0	0
7	D	27	0	12	0	0
8	B	13	0	18	0	0
8	D	13	0	18	1	0
9	A	228	0	0	3	0
9	B	215	0	0	2	0
9	C	170	0	0	0	0
9	D	117	0	0	1	0
All	All	12509	0	11677	55	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 2.

All (55) 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:25:LEU:HA	1:D:28:MET:HE3	1.82	0.62
1:B:284:HIS:CD2	6:B:402:GOL:H31	2.35	0.62
1:B:117:LYS:HD3	9:B:573:HOH:O	2.04	0.58
1:D:47:GLU:CG	1:D:60:ARG:CZ	2.82	0.57
1:B:19:MET:SD	1:B:82[A]:GLU:HG2	2.43	0.57
1:C:284:HIS:CD2	6:C:402:GOL:H12	2.41	0.55
1:A:160:MET:HA	1:A:160:MET:HE2	1.89	0.54
1:B:204:ILE:C	1:B:204:ILE:HD12	2.33	0.53
1:D:19:MET:SD	1:D:82[A]:GLU:HG2	2.48	0.53
1:D:47:GLU:HG2	1:D:60:ARG:NH1	2.24	0.53
1:B:117:LYS:HE2	1:B:191:GLU:OE2	2.09	0.53
1:D:47:GLU:HG3	1:D:60:ARG:NH2	2.24	0.53
1:D:284:HIS:CD2	6:D:401:GOL:H31	2.45	0.52
1:D:47:GLU:HG3	1:D:60:ARG:CZ	2.41	0.51
1:B:59:LEU:HD12	1:B:59:LEU:N	2.26	0.50
1:B:284:HIS:CD2	6:B:402:GOL:C3	2.94	0.50
1:D:47:GLU:HG2	1:D:60:ARG:CZ	2.41	0.50
1:B:192:LYS:HE2	9:B:521:HOH:O	2.11	0.49
1:D:59:LEU:HD12	1:D:59:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:HIS:CE1	1:D:185:GLY:HA2	2.48	0.49
1:A:146:LYS:HD2	9:A:629:HOH:O	2.13	0.49
1:D:204:ILE:C	1:D:204:ILE:HD12	2.38	0.49
1:C:204:ILE:HD12	1:C:204:ILE:C	2.38	0.48
1:D:151:LEU:HA	1:D:152:PRO:C	2.39	0.48
1:A:105:ARG:NH2	9:A:501:HOH:O	2.47	0.48
1:C:30[A]:CYS:SG	1:C:40:VAL:HG11	2.55	0.47
1:A:204:ILE:C	1:A:204:ILE:HD12	2.39	0.47
1:B:285:ASN:H	6:B:402:GOL:H32	1.80	0.47
1:A:46:ASP:HB2	9:A:688:HOH:O	2.15	0.46
1:A:22:GLY:HA3	1:A:44:ASP:OD2	2.15	0.46
1:A:151:LEU:HA	1:A:152:PRO:C	2.41	0.45
1:D:66:GLU:HG3	1:D:93:PHE:CZ	2.52	0.45
1:C:119:PHE:CE2	1:C:256:LEU:HD13	2.52	0.44
1:B:117:LYS:HE3	1:B:277:ASN:O	2.18	0.44
1:C:151:LEU:HA	1:C:152:PRO:C	2.42	0.44
1:C:19:MET:SD	1:C:82[A]:GLU:HG2	2.58	0.43
1:D:241:LEU:HD21	1:D:268:ILE:CD1	2.49	0.43
1:B:285:ASN:H	6:B:402:GOL:C3	2.31	0.43
1:D:241:LEU:HD21	1:D:268:ILE:HD12	2.00	0.43
1:D:345:GLN:HE21	1:D:346:GLU:HG3	1.83	0.43
1:A:345:GLN:HE21	1:A:346:GLU:HG3	1.84	0.42
1:B:282:ARG:HH12	6:B:402:GOL:H31	1.84	0.42
1:B:151:LEU:HA	1:B:152:PRO:C	2.44	0.42
1:A:147:LEU:O	1:A:151:LEU:HG	2.20	0.42
1:D:198:PHE:CE2	1:D:268:ILE:HG13	2.56	0.41
1:B:118[A]:ARG:CZ	1:B:132:VAL:HG21	2.50	0.41
1:C:284:HIS:CD2	6:C:402:GOL:C1	3.04	0.41
1:C:57:ARG:HG2	1:C:59:LEU:HD12	2.02	0.41
1:D:218:ALA:HB1	1:D:230:THR:HG23	2.02	0.41
1:D:284:HIS:CE1	6:D:401:GOL:H32	2.55	0.41
1:D:350:MET:HE1	1:D:385:ALA:O	2.20	0.41
8:D:403:PG4:C8	9:D:560:HOH:O	2.68	0.41
1:A:381:GLU:OE2	1:D:236:ASP:CG	2.63	0.41
1:C:345[A]:GLN:NE2	1:C:346:GLU:HG3	2.36	0.41
1:D:119:PHE:CE2	1:D:256:LEU:HD13	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	393/397 (99%)	388 (99%)	5 (1%)	0	100	100
1	B	388/397 (98%)	384 (99%)	4 (1%)	0	100	100
1	C	388/397 (98%)	382 (98%)	6 (2%)	0	100	100
1	D	386/397 (97%)	381 (99%)	5 (1%)	0	100	100
All	All	1555/1588 (98%)	1535 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	301/305 (99%)	299 (99%)	2 (1%)	76	74
1	B	301/305 (99%)	299 (99%)	2 (1%)	76	74
1	C	293/305 (96%)	292 (100%)	1 (0%)	86	86
1	D	288/305 (94%)	286 (99%)	2 (1%)	76	74
All	All	1183/1220 (97%)	1176 (99%)	7 (1%)	78	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	A	101	SER

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Mol	Chain	Res	Type
1	B	101	SER
1	B	270	GLU
1	C	105	ARG
1	D	101	SER
1	D	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	B	243	GLN
1	B	247	GLN
1	B	251	GLN
1	B	302	GLN
1	D	111	GLN
1	D	243	GLN
1	D	247	GLN
1	D	251	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 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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
7	ADP	B	403	4	28,29,29	1.34	5 (17%)	43,45,45	1.86	12 (27%)
3	PEG	A	402	-	6,6,6	0.30	0	5,5,5	0.77	0
7	ADP	D	402	4	28,29,29	1.42	5 (17%)	43,45,45	1.85	11 (25%)
8	PG4	D	403	-	12,12,12	0.32	0	11,11,11	0.36	0
2	ATP	A	401	4	32,33,33	0.71	1 (3%)	48,52,52	0.69	1 (2%)
8	PG4	B	404	-	12,12,12	0.27	0	11,11,11	0.36	0
2	ATP	C	401	4	32,33,33	0.41	0	48,52,52	0.70	0
6	GOL	D	401	-	5,5,5	0.34	0	5,5,5	0.50	0
5	PGE	B	401	-	9,9,9	0.34	0	8,8,8	0.75	0
6	GOL	C	402	-	5,5,5	0.37	0	5,5,5	1.18	0
6	GOL	B	402	-	5,5,5	0.29	0	5,5,5	1.00	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
7	ADP	B	403	4	-	0/16/32/32	0/3/3/3
3	PEG	A	402	-	-	4/4/4/4	-
7	ADP	D	402	4	-	1/16/32/32	0/3/3/3
8	PG4	D	403	-	-	5/10/10/10	-
2	ATP	A	401	4	-	1/22/38/38	0/3/3/3
8	PG4	B	404	-	-	3/10/10/10	-
2	ATP	C	401	4	-	2/22/38/38	0/3/3/3
6	GOL	D	401	-	-	2/4/4/4	-
5	PGE	B	401	-	-	6/7/7/7	-
6	GOL	C	402	-	-	2/4/4/4	-
6	GOL	B	402	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	402	ADP	C5-C4	4.78	1.47	1.39
7	B	403	ADP	C5-C4	4.72	1.47	1.39
2	A	401	ATP	PB-O3B	-3.48	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	403	ADP	C8-N7	2.66	1.36	1.31
7	D	402	ADP	C5-N7	-2.61	1.34	1.39
7	D	402	ADP	PA-O3A	2.44	1.62	1.59
7	B	403	ADP	C5-N7	-2.31	1.34	1.39
7	D	402	ADP	C5-C6	2.23	1.47	1.41
7	B	403	ADP	C5-C6	2.23	1.47	1.41
7	B	403	ADP	C4-N9	-2.21	1.33	1.37
7	D	402	ADP	C8-N7	2.17	1.35	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	402	ADP	C5-C4-N3	-5.77	118.77	126.72
7	B	403	ADP	C5-C4-N3	-5.36	119.34	126.72
7	D	402	ADP	N3-C4-N9	5.27	136.13	127.17
7	B	403	ADP	N3-C4-N9	4.17	134.25	127.17
7	B	403	ADP	N3-C2-N1	-3.85	122.75	128.58
7	B	403	ADP	C2-N3-C4	3.85	121.23	111.83
7	D	402	ADP	N3-C2-N1	-3.60	123.12	128.58
7	D	402	ADP	C2-N3-C4	3.54	120.48	111.83
7	B	403	ADP	C4-C5-N7	-2.98	107.17	110.58
7	D	402	ADP	C4-N9-C8	2.84	108.72	105.74
7	B	403	ADP	C4-N9-C8	2.58	108.45	105.74
7	B	403	ADP	O2A-PA-O3A	-2.55	100.38	107.27
7	D	402	ADP	C2-N1-C6	2.34	122.58	118.73
7	B	403	ADP	C6-C5-N7	2.28	136.49	132.09
7	D	402	ADP	N6-C6-N1	2.23	123.34	118.38
7	B	403	ADP	C5-N7-C8	2.15	106.83	103.45
7	D	402	ADP	C4-C5-N7	-2.15	108.13	110.58
7	B	403	ADP	O3A-PB-O1B	-2.11	99.96	111.04
7	B	403	ADP	C2-N1-C6	2.10	122.19	118.73
2	A	401	ATP	C2'-C1'-N9	-2.08	108.14	113.30
7	D	402	ADP	O3B-PB-O2B	2.06	115.54	107.80
7	D	402	ADP	O2A-PA-O1A	2.05	121.97	112.44
7	B	403	ADP	C2'-C1'-N9	-2.05	108.22	113.30
7	D	402	ADP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
6	B	402	GOL	O1-C1-C2-C3
5	B	401	PGE	O2-C3-C4-O3
6	B	402	GOL	O1-C1-C2-O2
8	D	403	PG4	O3-C5-C6-O4
5	B	401	PGE	O3-C5-C6-O4
6	C	402	GOL	C1-C2-C3-O3
6	D	401	GOL	O1-C1-C2-C3
3	A	402	PEG	O1-C1-C2-O2
8	B	404	PG4	O1-C1-C2-O2
6	C	402	GOL	O2-C2-C3-O3
6	D	401	GOL	O1-C1-C2-O2
5	B	401	PGE	C6-C5-O3-C4
8	B	404	PG4	C4-C3-O2-C2
8	D	403	PG4	C8-C7-O4-C6
2	A	401	ATP	PB-O3B-PG-O2G
8	D	403	PG4	C5-C6-O4-C7
3	A	402	PEG	O2-C3-C4-O4
5	B	401	PGE	C1-C2-O2-C3
5	B	401	PGE	C3-C4-O3-C5
2	C	401	ATP	PB-O3B-PG-O1G
8	D	403	PG4	O4-C7-C8-O5
5	B	401	PGE	C4-C3-O2-C2
8	B	404	PG4	C6-C5-O3-C4
8	D	403	PG4	C6-C5-O3-C4
3	A	402	PEG	C1-C2-O2-C3
7	D	402	ADP	PB-O3A-PA-O1A
3	A	402	PEG	C4-C3-O2-C2

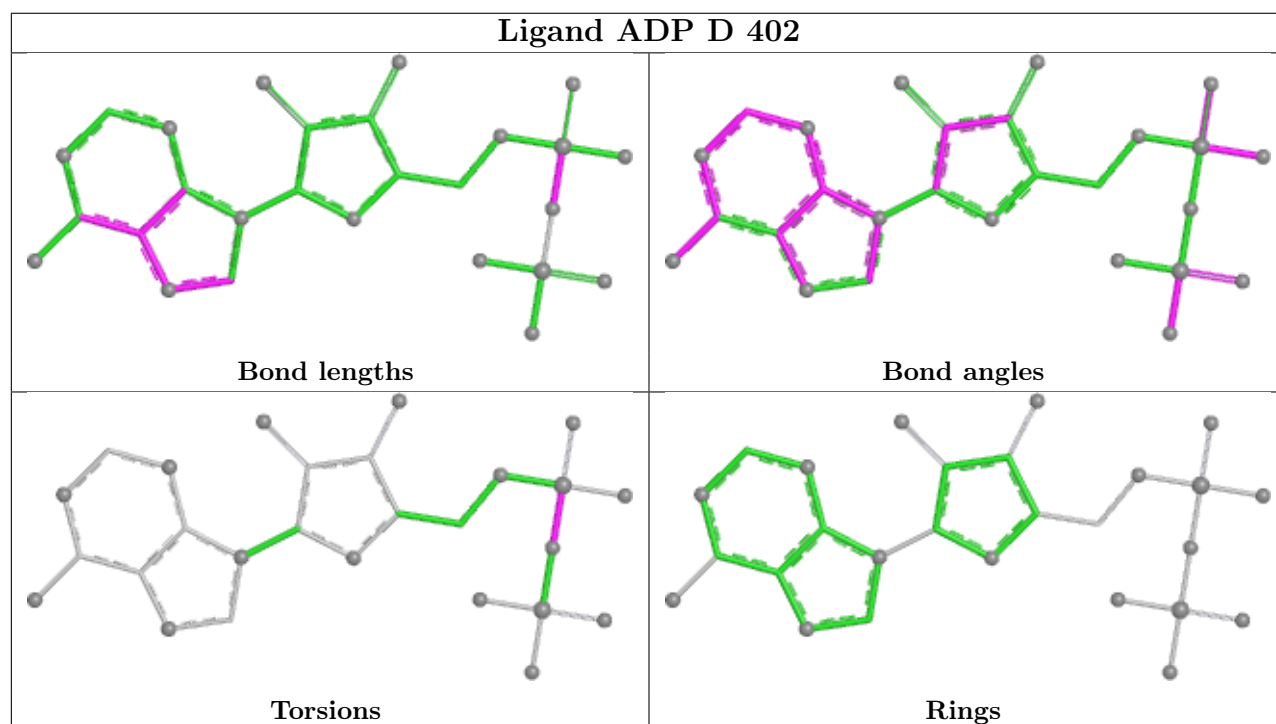
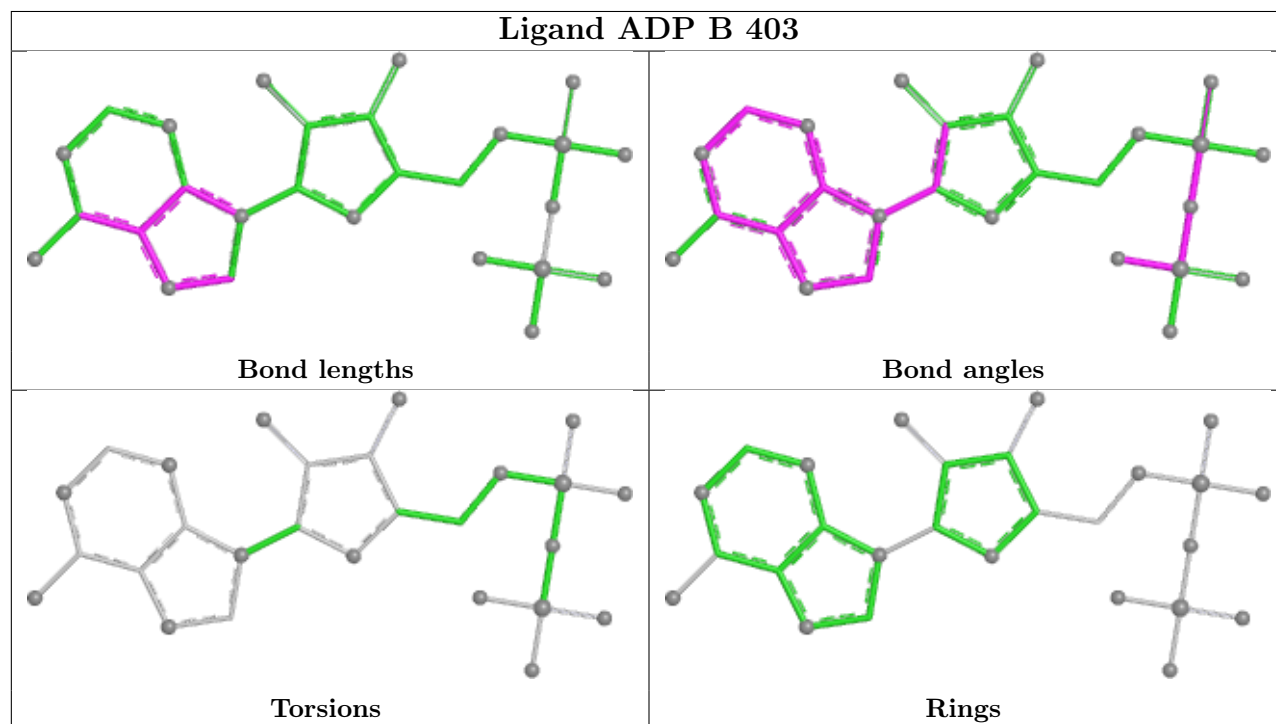
There are no ring outliers.

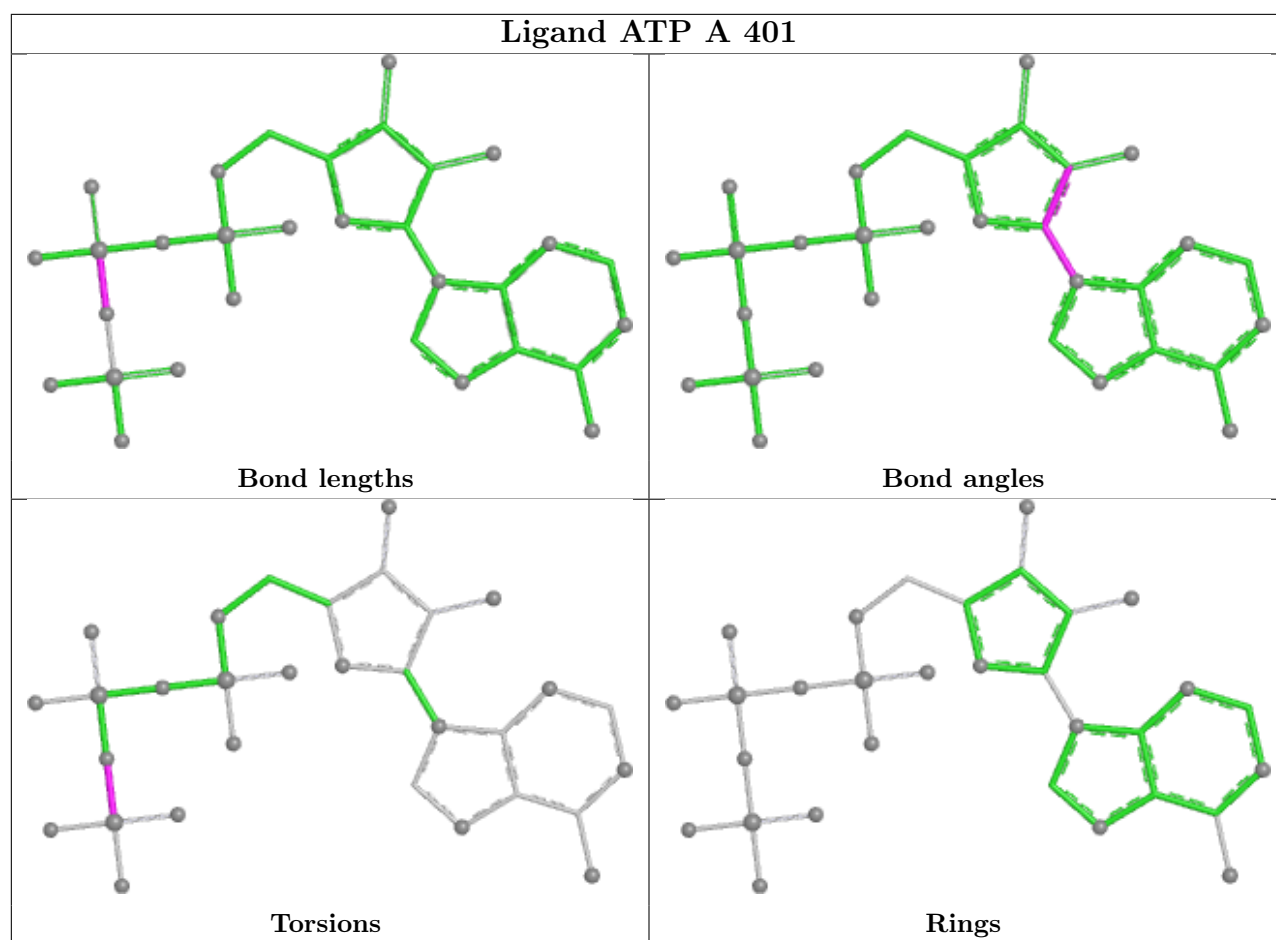
4 monomers are involved in 10 short contacts:

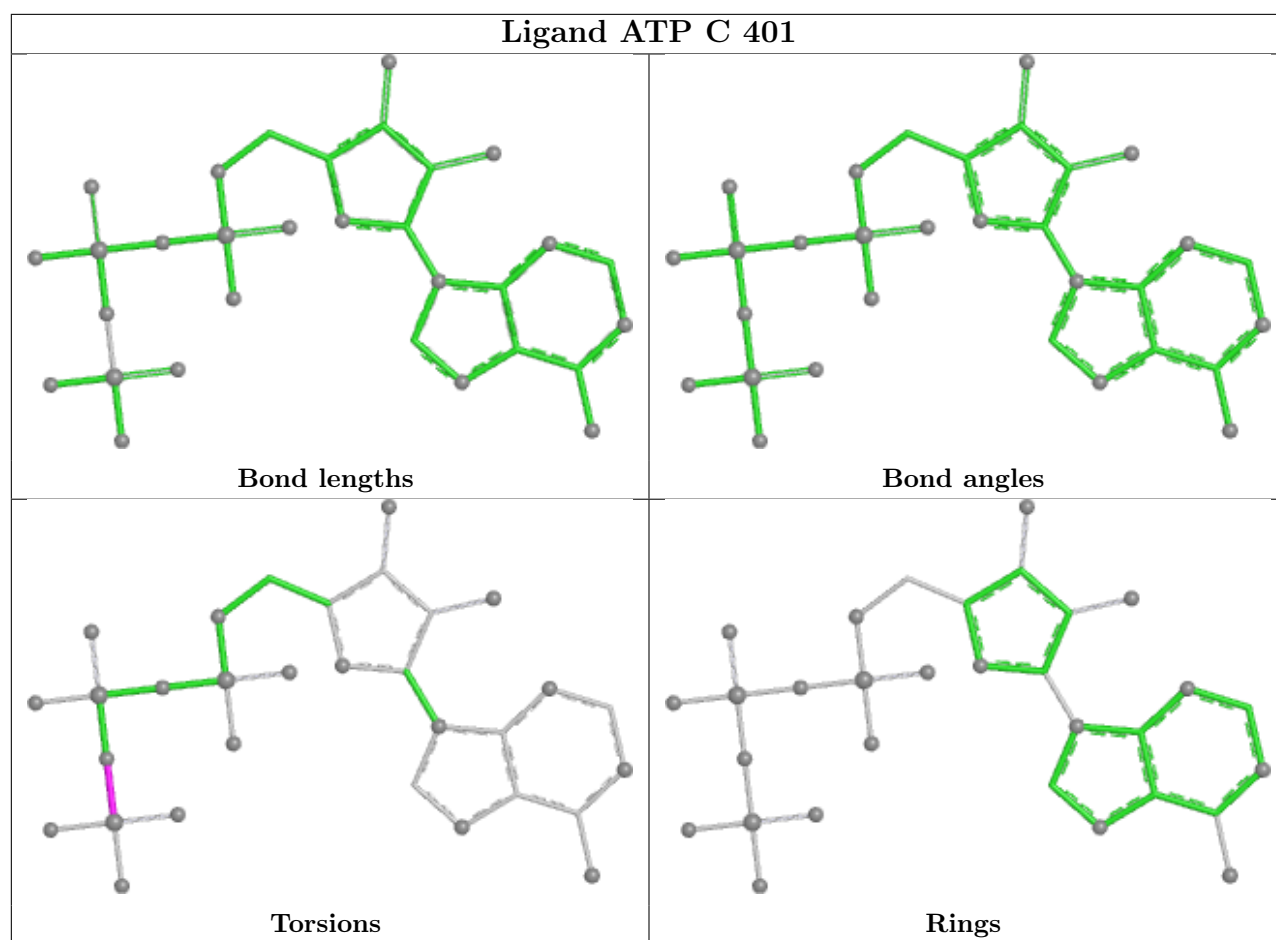
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	403	PG4	1	0
6	D	401	GOL	2	0
6	C	402	GOL	2	0
6	B	402	GOL	5	0

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 ⓘ

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	390/397 (98%)	-0.07	4 (1%)	79 84	21, 33, 53, 84	5 (1%)
1	B	385/397 (96%)	-0.01	5 (1%)	75 80	19, 33, 55, 89	7 (1%)
1	C	387/397 (97%)	0.17	14 (3%)	46 52	20, 37, 71, 114	5 (1%)
1	D	386/397 (97%)	0.54	25 (6%)	25 28	21, 49, 101, 127	4 (1%)
All	All	1548/1588 (97%)	0.16	48 (3%)	51 57	19, 36, 78, 127	21 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	ALA	4.6
1	D	8	HIS	4.5
1	C	359	GLY	4.4
1	D	99[A]	PHE	4.4
1	B	99[A]	PHE	4.2
1	D	396	ILE	4.0
1	C	396	ILE	4.0
1	C	333	ASP	3.8
1	B	8	HIS	3.8
1	B	160	MET	3.7
1	D	160	MET	3.5
1	A	397	THR	3.5
1	B	397	THR	3.5
1	A	396	ILE	3.3
1	D	145	ALA	3.3
1	C	360	LYS	3.2
1	D	143	ASP	3.0
1	C	355	LEU	2.8
1	D	168	ILE	2.8
1	D	140	ALA	2.7
1	D	83	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	338	PRO	2.6
1	D	142	LEU	2.6
1	D	186	VAL	2.6
1	D	193	ARG	2.6
1	D	181	ALA	2.6
1	C	339	ALA	2.5
1	D	132	VAL	2.5
1	D	184	ALA	2.5
1	D	31	PHE	2.4
1	D	360	LYS	2.4
1	D	397	THR	2.4
1	B	396	ILE	2.4
1	C	83	PHE	2.3
1	A	46	ASP	2.3
1	D	183	LEU	2.3
1	D	149	ALA	2.3
1	C	364	ARG	2.3
1	C	394	HIS	2.3
1	C	8	HIS	2.2
1	C	334	GLY	2.2
1	A	99	PHE	2.2
1	D	146	LYS	2.2
1	D	53	ALA	2.2
1	C	143	ASP	2.1
1	D	169	ARG	2.1
1	D	88	ALA	2.0
1	D	173	ALA	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,

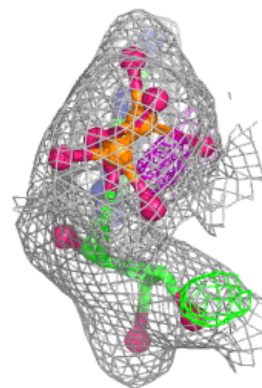
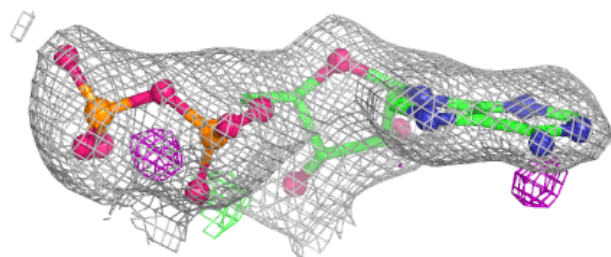
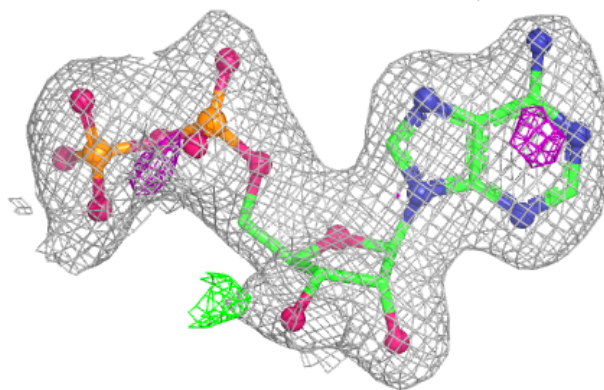
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	405	1/1	0.75	0.21	67,67,67,67	0
8	PG4	D	403	13/13	0.76	0.21	53,70,78,86	0
4	MG	D	404	1/1	0.79	0.12	65,65,65,65	0
6	GOL	D	401	6/6	0.80	0.14	48,59,60,67	0
6	GOL	C	402	6/6	0.81	0.18	31,54,63,72	0
5	PGE	B	401	10/10	0.82	0.16	48,60,66,72	0
8	PG4	B	404	13/13	0.86	0.14	46,53,61,62	0
6	GOL	B	402	6/6	0.87	0.12	34,43,55,57	0
4	MG	D	405	1/1	0.90	0.09	52,52,52,52	0
3	PEG	A	402	7/7	0.91	0.13	48,55,57,63	0
7	ADP	D	402	27/27	0.91	0.09	58,63,74,80	0
4	MG	A	403	1/1	0.93	0.06	40,40,40,40	0
7	ADP	B	403	27/27	0.94	0.07	33,44,68,69	0
4	MG	B	406	1/1	0.96	0.14	33,33,33,33	0
2	ATP	C	401	31/31	0.97	0.07	32,35,56,147	0
4	MG	C	403	1/1	0.97	0.15	39,39,39,39	0
2	ATP	A	401	31/31	0.97	0.06	30,33,48,73	0
4	MG	C	404	1/1	0.98	0.08	38,38,38,38	0
4	MG	A	404	1/1	0.99	0.08	35,35,35,35	0

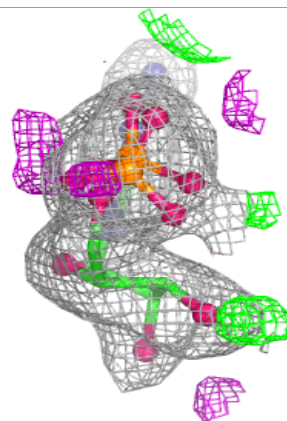
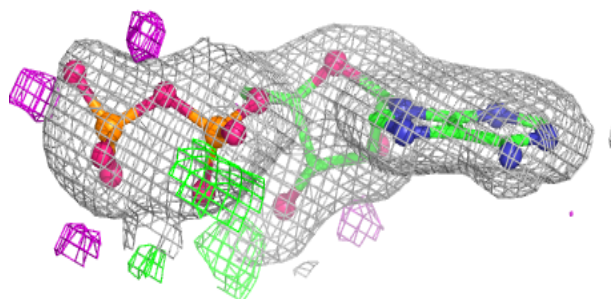
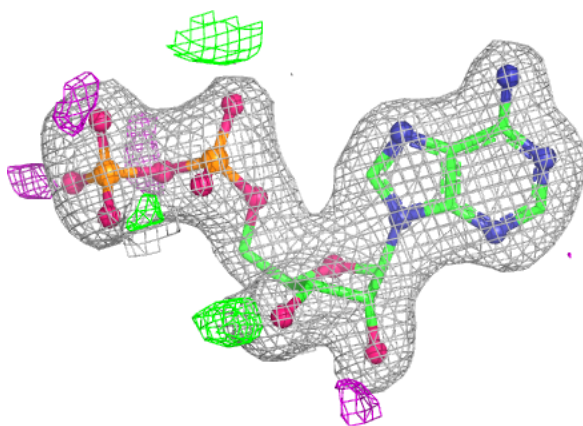
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 402:

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

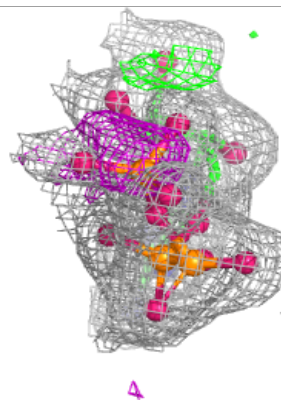
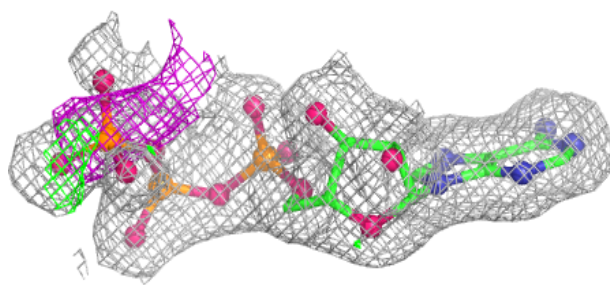
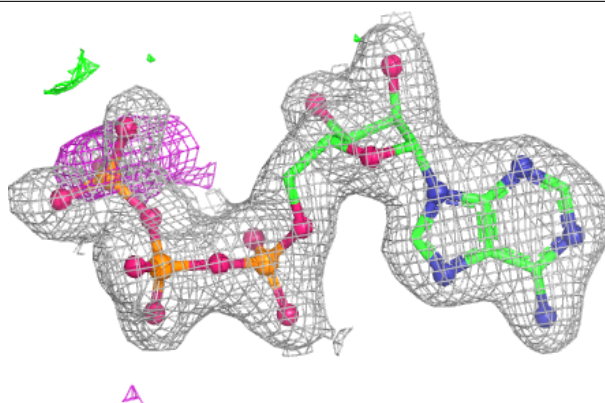
**Electron density around ADP B 403:**

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

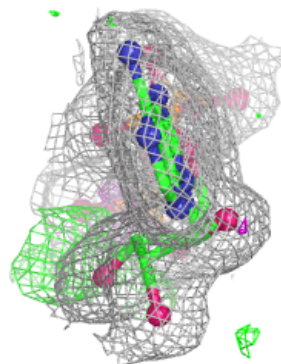
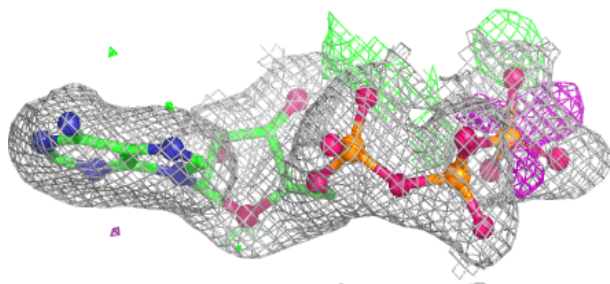
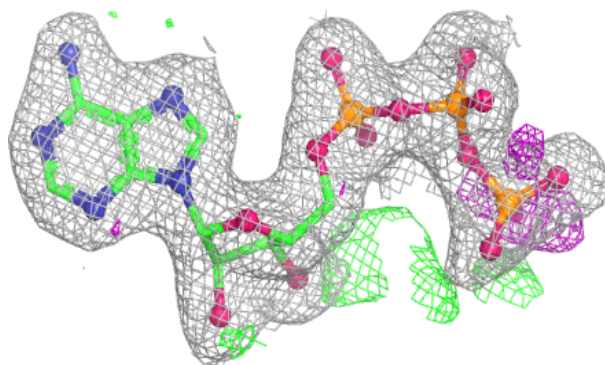


Electron density around ATP C 401:

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

**Electron density around ATP 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.