



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:28 PM UTC

PDB ID : 2C9O / pdb_00002c9o
Title : 3D Structure of the human RuvB-like helicase RuvBL1
Authors : Matias, P.M.; Gorynia, S.; Donner, P.; Carrondo, M.A.
Deposited on : 2005-12-14
Resolution : 2.20 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

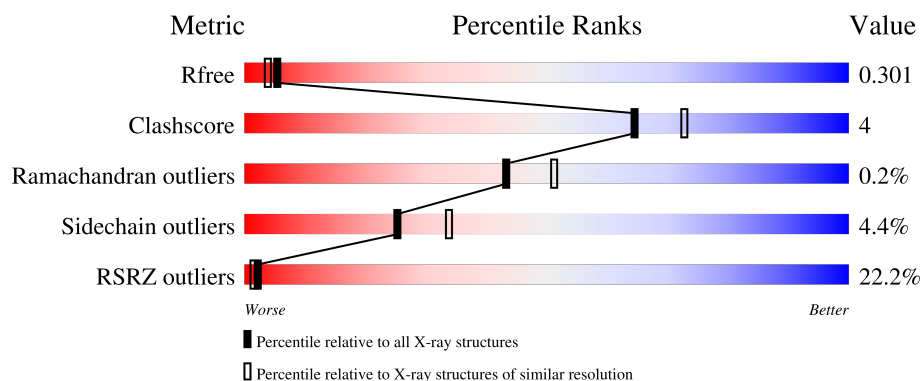
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	456	
1	B	456	
1	C	456	

2 Entry composition [i](#)

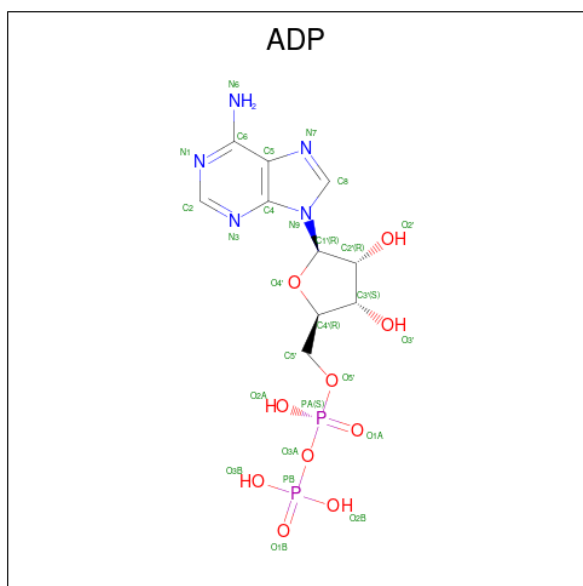
There are 3 unique types of molecules in this entry. The entry contains 8706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RUVB-LIKE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3061	1932	523	593	13			
1	B	393	Total	C	N	O	S	0	0	0
			3026	1912	517	584	13			
1	C	311	Total	C	N	O	S	0	0	0
			2380	1503	411	455	11			

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



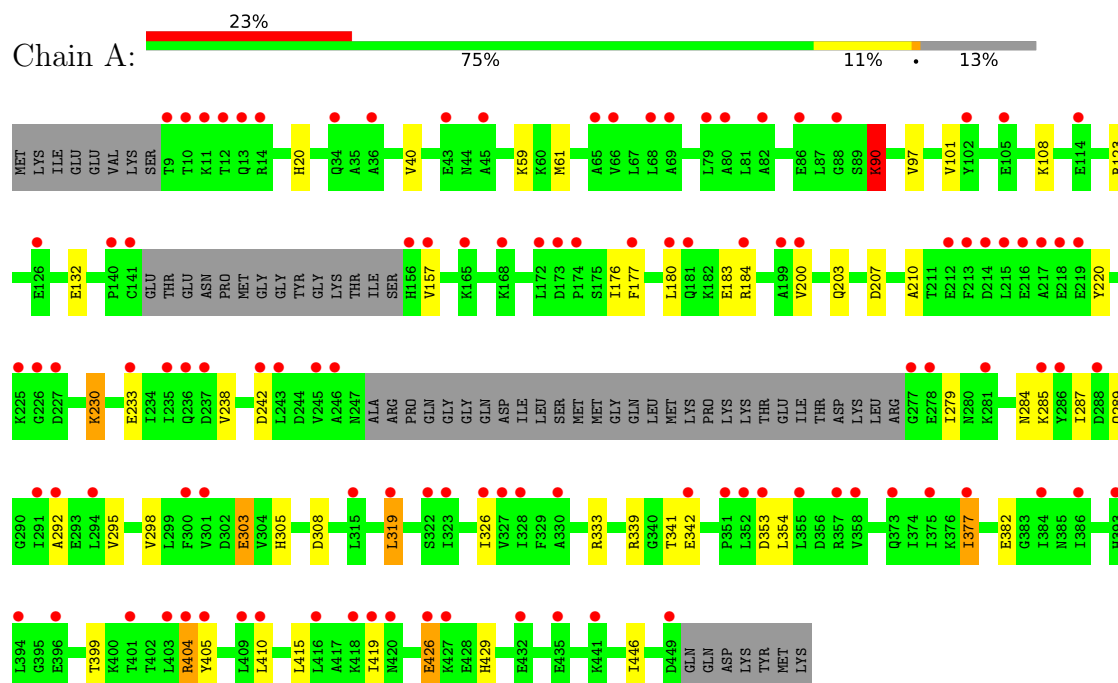
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total 91	O 91	0	0
3	B	45	Total 45	O 45	0	0
3	C	22	Total 22	O 22	0	0

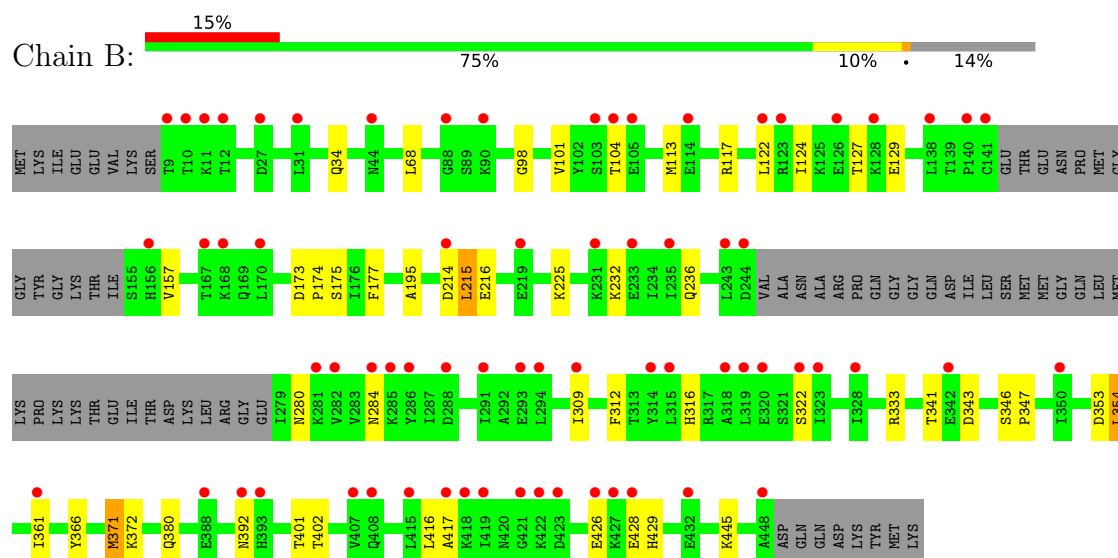
3 Residue-property plots

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

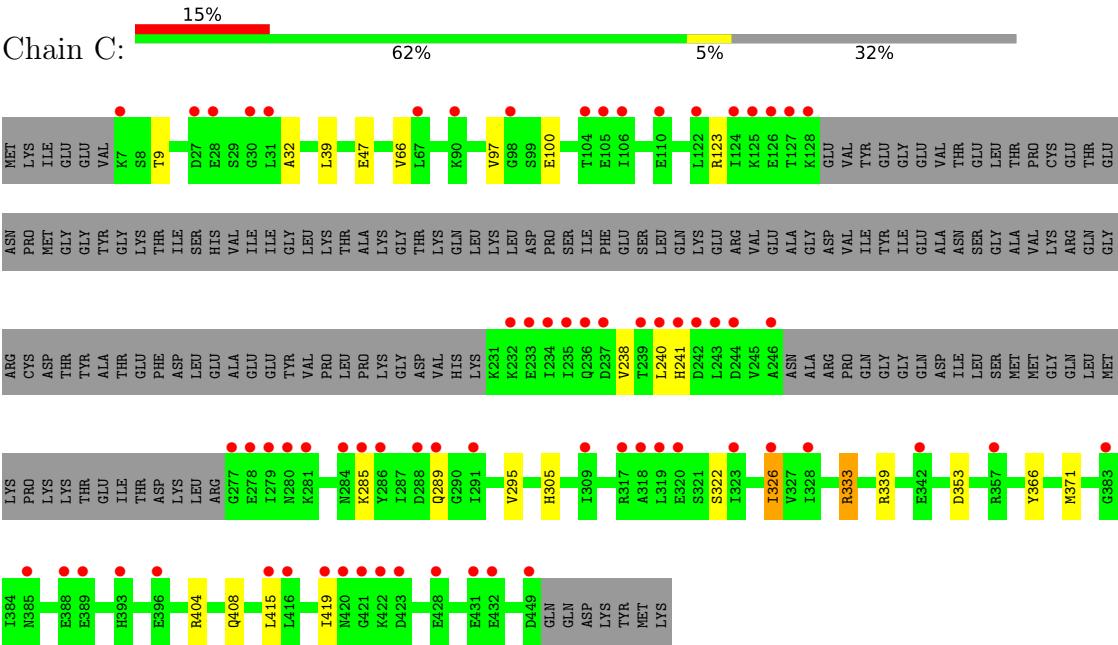
• Molecule 1: RUVB-LIKE 1



• Molecule 1: RUVB-LIKE 1



● Molecule 1: RUVB-LIKE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	207.08Å 207.08Å 60.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	179.61 – 2.20 179.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (179.61-2.20) 97.1 (179.61-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.257 (Not available) , 0.301	Depositor DCC
R_{free} test set	3705 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 22.93 % 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 5.1589e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ADP

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	0.99	1/3100 (0.0%)	0.99	4/4182 (0.1%)
1	B	0.83	0/3065	0.91	0/4134
1	C	0.76	0/2407	0.86	0/3243
All	All	0.87	1/8572 (0.0%)	0.92	4/11559 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	ILE	CG1-CD1	-5.32	1.30	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ILE	CB-CA-C	-8.09	101.22	112.14
1	A	90	LYS	N-CA-C	7.29	120.09	111.71
1	A	404	ARG	CB-CG-CD	5.26	123.41	111.30
1	A	410	LEU	N-CA-C	5.01	117.12	111.11

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	3061	0	3151	31	0
1	B	3026	0	3123	23	0
1	C	2380	0	2480	14	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
3	A	91	0	0	2	0
3	B	45	0	0	0	0
3	C	22	0	0	0	0
All	All	8706	0	8790	66	0

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

All (66) 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:C:97:VAL:O	1:C:100:GLU:HG2	1.84	0.76
1:C:285:LYS:O	1:C:289:GLN:HG2	1.95	0.67
1:B:372:LYS:NZ	1:B:392:ASN:OD1	2.27	0.65
1:B:113:MET:HE2	1:B:117:ARG:HG3	1.80	0.64
1:B:117:ARG:HH12	1:B:280:ASN:HD21	1.46	0.63
1:A:405:TYR:OH	3:A:2081:HOH:O	2.15	0.61
1:A:238:VAL:HG22	1:A:242:ASP:HB2	1.82	0.60
1:A:426:GLU:H	1:A:429:HIS:HD2	1.51	0.59
1:A:203:GLN:HA	1:A:203:GLN:HE21	1.68	0.59
1:C:238:VAL:HG22	1:C:241:HIS:CG	2.38	0.58
1:C:238:VAL:HG22	1:C:241:HIS:ND1	2.21	0.56
1:B:309:ILE:HD11	1:B:341:THR:CG2	2.36	0.56
1:A:298:VAL:HG22	1:A:326:ILE:CG2	2.36	0.55
1:C:9:THR:H	1:C:241:HIS:CE1	2.25	0.55
1:B:68:LEU:HD23	1:B:361:ILE:HB	1.89	0.55
1:A:285:LYS:HE2	1:A:289:GLN:HE22	1.72	0.55
1:B:366:TYR:HB2	1:B:371:MET:HE3	1.89	0.54
1:B:122:LEU:HD23	1:B:124:ILE:HD11	1.91	0.53
1:C:66:VAL:HG23	1:C:326:ILE:HD11	1.89	0.53
1:A:319:LEU:C	1:A:319:LEU:HD12	2.36	0.51
1:B:215:LEU:C	1:B:215:LEU:HD23	2.35	0.51
1:B:366:TYR:HB2	1:B:371:MET:CE	2.41	0.50
1:A:20:HIS:CD2	1:A:377:ILE:HG21	2.47	0.50
1:A:90:LYS:H	1:A:90:LYS:CD	2.24	0.49
1:A:238:VAL:CG2	1:A:242:ASP:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:CE	1:A:326:ILE:HD11	2.43	0.49
1:B:127:THR:HA	1:B:232:LYS:O	2.13	0.49
1:A:210:ALA:HB2	1:A:220:TYR:CD2	2.49	0.48
1:A:101:VAL:HB	1:A:108:LYS:HB2	1.96	0.48
1:A:90:LYS:H	1:A:90:LYS:HD3	1.80	0.46
1:C:305:HIS:CE1	1:C:333:ARG:HD3	2.50	0.46
1:A:308:ASP:HB3	1:A:339:ARG:HG2	1.97	0.46
1:A:97:VAL:HG13	1:A:303:GLU:HB2	1.96	0.46
1:A:341:THR:O	1:A:342:GLU:HB2	2.15	0.46
1:A:157:VAL:HG21	1:A:177:PHE:CG	2.51	0.46
1:B:129:GLU:HG2	1:B:195:ALA:HB3	1.97	0.46
1:B:417:ALA:HA	1:B:429:HIS:CE1	2.52	0.45
1:C:32:ALA:HB2	1:C:47:GLU:HG3	1.98	0.45
1:A:285:LYS:HG2	1:A:289:GLN:HE22	1.81	0.44
1:C:238:VAL:HG23	1:C:241:HIS:H	1.82	0.44
1:A:426:GLU:H	1:A:429:HIS:CD2	2.32	0.44
1:A:183:GLU:O	1:A:184:ARG:HG3	2.17	0.44
1:A:305:HIS:CD2	1:A:333:ARG:HD2	2.53	0.43
1:A:415:LEU:O	1:A:419:ILE:HG12	2.19	0.43
1:C:366:TYR:HB2	1:C:371:MET:HG3	2.00	0.43
1:B:173:ASP:HB2	1:B:174:PRO:HD2	2.01	0.42
1:B:426:GLU:H	1:B:429:HIS:CD2	2.37	0.42
1:C:404:ARG:O	1:C:408:GLN:HG2	2.19	0.42
1:B:343:ASP:OD1	1:C:339:ARG:NH2	2.52	0.42
1:B:98:GLY:O	1:B:101:VAL:HG22	2.20	0.42
1:B:157:VAL:HG11	1:B:177:PHE:CD1	2.55	0.42
1:A:132:GLU:OE1	1:A:230:LYS:NZ	2.50	0.42
1:A:285:LYS:HG2	1:A:289:GLN:NE2	2.34	0.42
1:B:129:GLU:HG2	1:B:195:ALA:CB	2.50	0.42
1:B:312:PHE:CD1	1:B:354:LEU:HD12	2.54	0.42
1:A:298:VAL:HG22	1:A:326:ILE:HG22	2.02	0.41
1:B:346:SER:HB2	1:B:347:PRO:HD2	2.01	0.41
1:C:39:LEU:HA	2:C:1450:ADP:N1	2.36	0.41
1:C:123:ARG:HG3	1:C:295:VAL:HG21	2.02	0.41
1:A:59:LYS:HA	3:A:2013:HOH:O	2.21	0.41
1:A:180:LEU:HA	1:A:200:VAL:HG11	2.03	0.41
1:A:287:ILE:HA	1:A:292:ALA:O	2.22	0.40
1:B:113:MET:HE2	1:B:117:ARG:CG	2.50	0.40
1:A:176:ILE:HD12	1:B:214:ASP:O	2.21	0.40
1:A:180:LEU:HD23	1:A:180:LEU:C	2.47	0.40
1:B:401:THR:OG1	1:B:402:THR:N	2.53	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	392/456 (86%)	382 (97%)	9 (2%)	1 (0%)	36	42
1	B	387/456 (85%)	380 (98%)	6 (2%)	1 (0%)	36	42
1	C	305/456 (67%)	301 (99%)	4 (1%)	0	100	100
All	All	1084/1368 (79%)	1063 (98%)	19 (2%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	B	34	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/387 (87%)	319 (95%)	17 (5%)	21	27
1	B	333/387 (86%)	316 (95%)	17 (5%)	21	27
1	C	262/387 (68%)	255 (97%)	7 (3%)	39	53
All	All	931/1161 (80%)	890 (96%)	41 (4%)	25	34

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	90	LYS
1	A	123	ARG
1	A	230	LYS
1	A	233	GLU
1	A	279	ILE
1	A	284	ASN
1	A	295	VAL
1	A	303	GLU
1	A	319	LEU
1	A	353	ASP
1	A	354	LEU
1	A	382	GLU
1	A	399	THR
1	A	404	ARG
1	A	426	GLU
1	A	446	ILE
1	B	104	THR
1	B	175	SER
1	B	215	LEU
1	B	216	GLU
1	B	225	LYS
1	B	236	GLN
1	B	284	ASN
1	B	316	HIS
1	B	322	SER
1	B	333	ARG
1	B	353	ASP
1	B	354	LEU
1	B	371	MET
1	B	380	GLN
1	B	416	LEU
1	B	428	GLU
1	B	445	LYS
1	C	240	LEU
1	C	322	SER
1	C	326	ILE
1	C	333	ARG
1	C	353	ASP
1	C	415	LEU
1	C	419	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	203	GLN
1	A	289	GLN
1	A	305	HIS
1	A	393	HIS
1	A	429	HIS
1	B	34	GLN
1	B	169	GLN
1	B	181	GLN
1	B	236	GLN
1	B	280	ASN
1	B	284	ASN
1	B	335	ASN
1	B	373	GLN
1	B	393	HIS
1	B	429	HIS
1	C	34	GLN
1	C	280	ASN
1	C	289	GLN
1	C	373	GLN
1	C	380	GLN
1	C	393	HIS
1	C	408	GLN
1	C	420	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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	1449	-	28,29,29	1.35	4 (14%)	43,45,45	2.12	11 (25%)
2	ADP	A	1450	-	28,29,29	1.51	8 (28%)	43,45,45	1.89	11 (25%)
2	ADP	C	1450	-	28,29,29	1.50	6 (21%)	43,45,45	1.87	11 (25%)

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	1449	-	-	3/16/32/32	0/3/3/3
2	ADP	A	1450	-	-	5/16/32/32	0/3/3/3
2	ADP	C	1450	-	-	4/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1450	ADP	C5-C4	4.16	1.46	1.39
2	A	1450	ADP	PA-O3A	3.53	1.63	1.59
2	C	1450	ADP	PA-O3A	3.49	1.63	1.59
2	B	1449	ADP	C5-C4	3.43	1.45	1.39
2	B	1449	ADP	C5-C6	3.05	1.49	1.41
2	C	1450	ADP	C5-C6	2.66	1.48	1.41
2	A	1450	ADP	C5-C4	2.61	1.43	1.39
2	A	1450	ADP	C8-N9	-2.53	1.33	1.37
2	A	1450	ADP	O4'-C1'	2.45	1.47	1.42
2	A	1450	ADP	C5-C6	2.37	1.47	1.41
2	C	1450	ADP	C5-N7	-2.32	1.34	1.39
2	C	1450	ADP	C4-N9	-2.29	1.32	1.37
2	B	1449	ADP	C5-N7	-2.22	1.35	1.39
2	A	1450	ADP	C5-N7	-2.16	1.35	1.39
2	B	1449	ADP	PA-O3A	2.15	1.61	1.59
2	A	1450	ADP	C2'-C1'	-2.06	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1450	ADP	C8-N7	2.02	1.35	1.31
2	A	1450	ADP	C4-N3	2.00	1.38	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1449	ADP	C5-C4-N3	-5.03	119.79	126.72
2	B	1449	ADP	N3-C4-N9	4.90	135.50	127.17
2	B	1449	ADP	C4-N9-C8	4.73	110.71	105.74
2	A	1450	ADP	N3-C2-N1	-4.53	121.73	128.58
2	A	1450	ADP	N3-C4-N9	4.51	134.83	127.17
2	C	1450	ADP	C5-C4-N3	-4.48	120.54	126.72
2	A	1450	ADP	C5-C4-N3	-4.31	120.79	126.72
2	C	1450	ADP	C4-N9-C8	3.94	109.88	105.74
2	B	1449	ADP	N3-C2-N1	-3.93	122.64	128.58
2	C	1450	ADP	N3-C4-N9	3.87	133.75	127.17
2	A	1450	ADP	C4-N9-C8	3.68	109.60	105.74
2	B	1449	ADP	N9-C8-N7	-3.60	108.83	113.94
2	A	1450	ADP	C2-N3-C4	3.58	120.58	111.83
2	C	1450	ADP	N3-C2-N1	-3.58	123.17	128.58
2	B	1449	ADP	O4'-C1'-N9	-3.55	101.28	108.09
2	B	1449	ADP	C2-N3-C4	3.51	120.40	111.83
2	C	1450	ADP	C2-N3-C4	3.33	119.97	111.83
2	C	1450	ADP	C4-C5-N7	-3.33	106.78	110.58
2	B	1449	ADP	C5-N7-C8	3.33	108.68	103.45
2	C	1450	ADP	N9-C8-N7	-3.25	109.33	113.94
2	B	1449	ADP	C4-C5-N7	-3.10	107.04	110.58
2	C	1450	ADP	C5-N7-C8	3.08	108.29	103.45
2	A	1450	ADP	C2-N1-C6	2.81	123.35	118.73
2	B	1449	ADP	C2-N1-C6	2.62	123.03	118.73
2	C	1450	ADP	O3A-PA-O1A	2.44	118.05	110.70
2	C	1450	ADP	C6-C5-N7	2.43	136.78	132.09
2	A	1450	ADP	C2'-C1'-N9	2.42	119.33	113.30
2	A	1450	ADP	C4-N9-C1'	-2.29	121.27	126.63
2	C	1450	ADP	C2-N1-C6	2.28	122.48	118.73
2	B	1449	ADP	C6-C5-N7	2.28	136.48	132.09
2	A	1450	ADP	N6-C6-N1	2.17	123.22	118.38
2	A	1450	ADP	C6-C5-N7	2.05	136.05	132.09
2	A	1450	ADP	O4'-C1'-N9	-2.05	104.16	108.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1450	ADP	PA-O3A-PB-O2B
2	A	1450	ADP	C5'-O5'-PA-O2A
2	B	1449	ADP	C5'-O5'-PA-O2A
2	C	1450	ADP	C5'-O5'-PA-O2A
2	A	1450	ADP	C5'-O5'-PA-O1A
2	A	1450	ADP	C5'-O5'-PA-O3A
2	B	1449	ADP	C5'-O5'-PA-O1A
2	B	1449	ADP	C5'-O5'-PA-O3A
2	C	1450	ADP	C5'-O5'-PA-O1A
2	C	1450	ADP	C5'-O5'-PA-O3A
2	C	1450	ADP	PA-O3A-PB-O2B
2	A	1450	ADP	C4'-C5'-O5'-PA

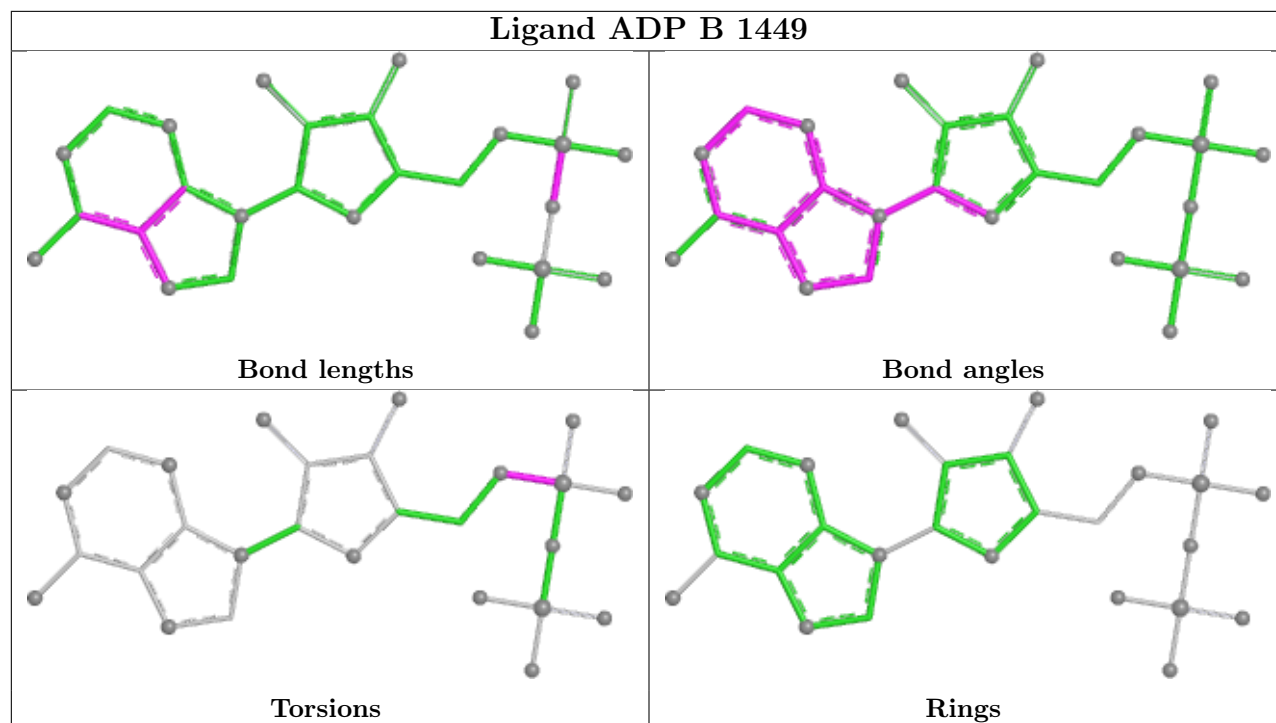
There are no ring outliers.

1 monomer is involved in 1 short contact:

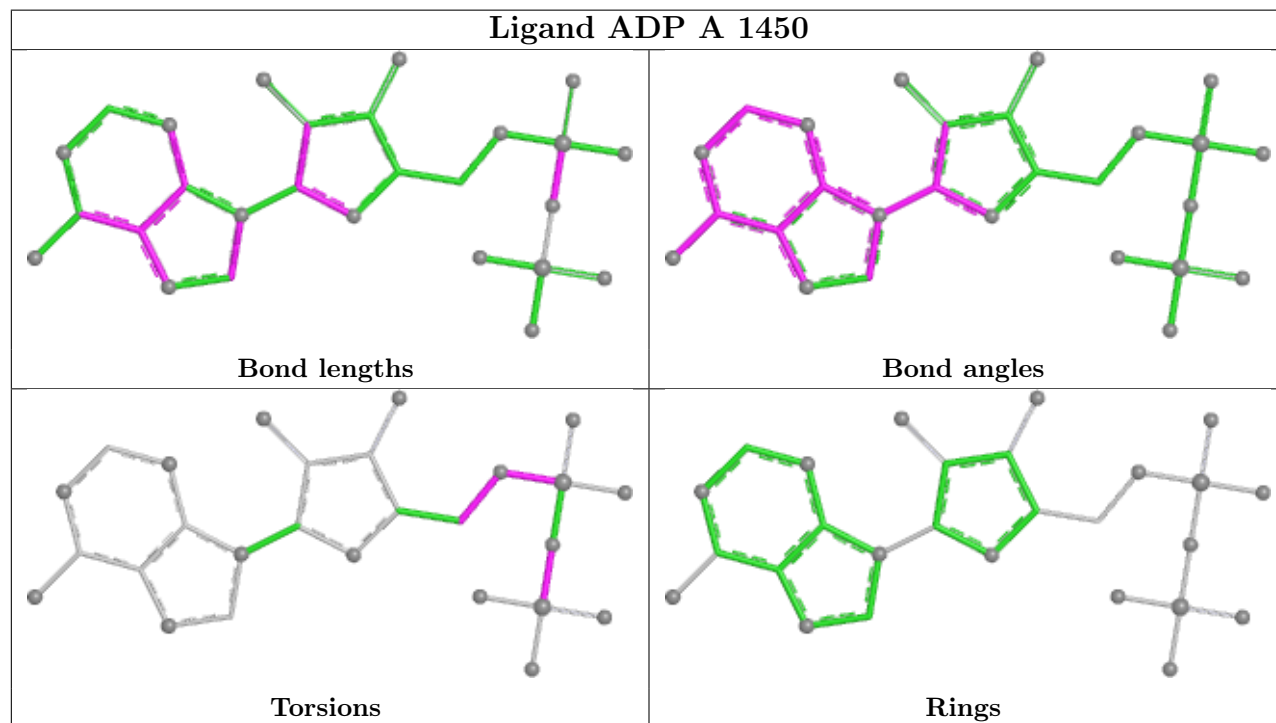
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1450	ADP	1	0

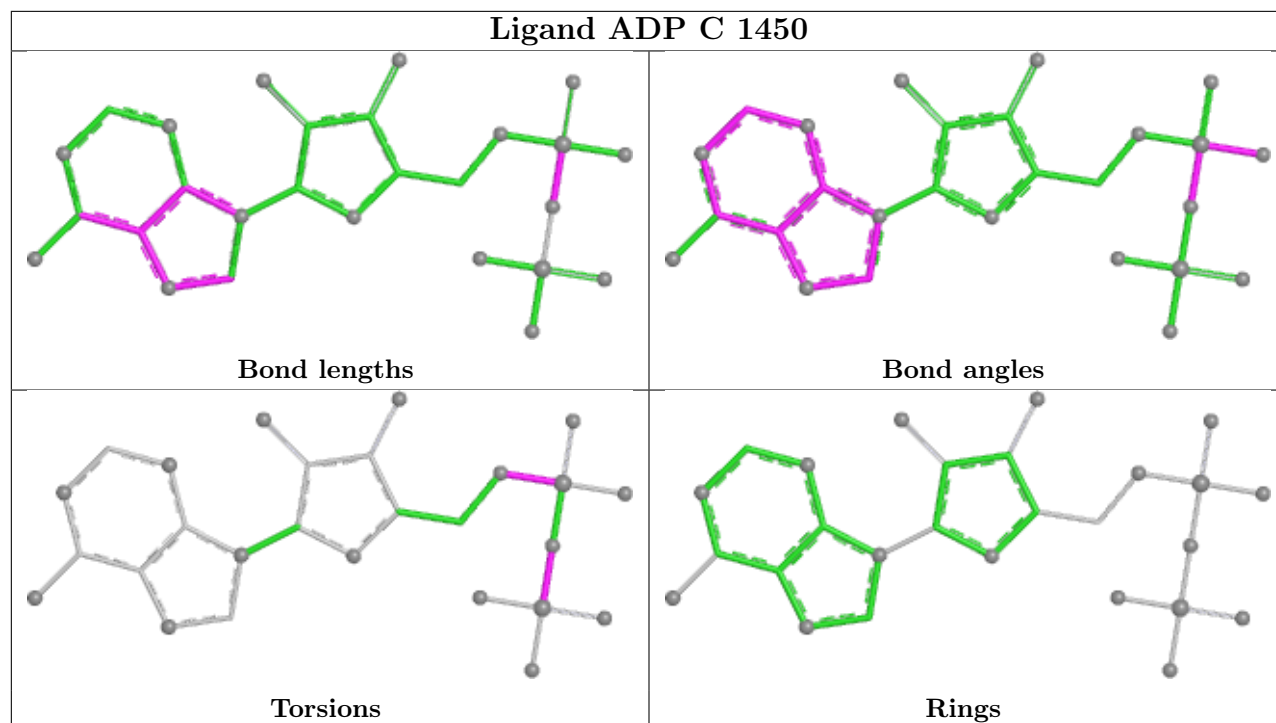
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP B 1449



Ligand ADP A 1450





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	398/456 (87%)	1.60	107 (26%) 1 1	31, 48, 59, 74	14 (3%)
1	B	393/456 (86%)	1.32	69 (17%) 4 3	26, 48, 58, 72	18 (4%)
1	C	311/456 (68%)	1.49	69 (22%) 2 1	19, 46, 54, 67	32 (10%)
All	All	1102/1368 (80%)	1.47	245 (22%) 2 1	19, 48, 58, 74	64 (5%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	8.0
1	B	11	LYS	7.7
1	C	317	ARG	7.6
1	C	423	ASP	7.4
1	C	288	ASP	6.8
1	B	285	LYS	6.4
1	C	422	LYS	6.4
1	C	388	GLU	6.1
1	B	90	LYS	6.1
1	B	281	LYS	6.0
1	C	7	LYS	6.0
1	B	288	ASP	5.9
1	C	105	GLU	5.9
1	C	285	LYS	5.8
1	C	125	LYS	5.6
1	B	291	ILE	5.5
1	C	127	THR	5.4
1	A	10	THR	5.4
1	A	217	ALA	5.3
1	A	281	LYS	5.3
1	C	431	GLU	5.2
1	C	232	LYS	5.1
1	C	428	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	236	GLN	5.0
1	C	244	ASP	4.9
1	A	278	GLU	4.9
1	C	28	GLU	4.7
1	C	236	GLN	4.7
1	B	342	GLU	4.7
1	A	9	THR	4.6
1	A	88	GLY	4.6
1	C	342	GLU	4.6
1	C	383	GLY	4.6
1	C	126	GLU	4.5
1	C	234	ILE	4.4
1	C	233	GLU	4.3
1	C	396	GLU	4.3
1	A	173	ASP	4.1
1	A	288	ASP	4.1
1	B	141	CYS	4.1
1	C	291	ILE	4.0
1	A	177	PHE	4.0
1	A	242	ASP	3.9
1	C	246	ALA	3.9
1	B	322	SER	3.8
1	C	289	GLN	3.8
1	A	286	TYR	3.8
1	C	237	ASP	3.8
1	B	10	THR	3.8
1	C	277	GLY	3.8
1	B	421	GLY	3.7
1	B	9	THR	3.7
1	C	284	ASN	3.6
1	A	418	LYS	3.6
1	B	323	ILE	3.6
1	A	277	GLY	3.6
1	C	243	LEU	3.6
1	B	423	ASP	3.6
1	A	218	GLU	3.6
1	C	241	HIS	3.5
1	B	282	VAL	3.5
1	B	419	ILE	3.5
1	A	419	ILE	3.5
1	B	432	GLU	3.4
1	C	281	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	318	ALA	3.3
1	C	235	ILE	3.3
1	B	114	GLU	3.2
1	B	417	ALA	3.2
1	A	212	GLU	3.2
1	B	392	ASN	3.2
1	A	174	PRO	3.2
1	C	278	GLU	3.1
1	B	284	ASN	3.1
1	A	226	GLY	3.1
1	C	242	ASP	3.1
1	A	358	VAL	3.1
1	A	319	LEU	3.1
1	B	138	LEU	3.1
1	B	123	ARG	3.1
1	C	240	LEU	3.1
1	A	291	ILE	3.1
1	A	102	TYR	3.0
1	B	12	THR	3.0
1	A	353	ASP	3.0
1	C	319	LEU	3.0
1	A	432	GLU	3.0
1	C	27	ASP	3.0
1	B	388	GLU	3.0
1	B	244	ASP	3.0
1	C	318	ALA	2.9
1	C	286	TYR	2.9
1	C	280	ASN	2.9
1	C	449	ASP	2.9
1	A	11	LYS	2.9
1	B	309	ILE	2.9
1	C	320	GLU	2.9
1	C	432	GLU	2.9
1	A	215	LEU	2.9
1	A	323	ILE	2.9
1	B	156	HIS	2.9
1	B	170	LEU	2.9
1	A	157	VAL	2.9
1	A	219	GLU	2.9
1	C	323	ILE	2.9
1	A	373	GLN	2.8
1	B	408	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	243	LEU	2.8
1	A	245	VAL	2.8
1	B	393	HIS	2.8
1	C	326	ILE	2.8
1	C	67	LEU	2.7
1	A	34	GLN	2.7
1	C	279	ILE	2.7
1	A	216	GLU	2.7
1	A	449	ASP	2.7
1	B	219	GLU	2.7
1	B	122	LEU	2.7
1	A	36	ALA	2.7
1	A	80	ALA	2.7
1	A	330	ALA	2.7
1	B	167	THR	2.7
1	B	214	ASP	2.7
1	A	114	GLU	2.7
1	A	292	ALA	2.6
1	A	233	GLU	2.6
1	A	420	ASN	2.6
1	C	393	HIS	2.6
1	C	128	LYS	2.6
1	A	357	ARG	2.6
1	A	405	TYR	2.6
1	B	235	ILE	2.6
1	B	294	LEU	2.6
1	A	427	LYS	2.6
1	B	426	GLU	2.6
1	A	377	ILE	2.6
1	A	404	ARG	2.5
1	C	421	GLY	2.5
1	A	126	GLU	2.5
1	B	128	LYS	2.5
1	B	350	ILE	2.5
1	C	416	LEU	2.5
1	A	396	GLU	2.5
1	B	105	GLU	2.5
1	A	375	ILE	2.5
1	A	13	GLN	2.5
1	A	140	PRO	2.5
1	A	213	PHE	2.4
1	A	315	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	415	LEU	2.4
1	A	328	ILE	2.4
1	C	122	LEU	2.4
1	A	105	GLU	2.4
1	B	168	LYS	2.4
1	C	90	LYS	2.4
1	A	327	VAL	2.4
1	C	124	ILE	2.4
1	A	68	LEU	2.4
1	B	31	LEU	2.4
1	B	243	LEU	2.4
1	A	435	GLU	2.4
1	C	104	THR	2.4
1	A	141	CYS	2.4
1	A	294	LEU	2.4
1	A	394	LEU	2.4
1	B	231	LYS	2.3
1	A	326	ILE	2.3
1	A	386	ILE	2.3
1	C	419	ILE	2.3
1	A	409	LEU	2.3
1	B	428	GLU	2.3
1	A	351	PRO	2.3
1	B	104	THR	2.3
1	B	126	GLU	2.3
1	B	320	GLU	2.3
1	A	79	LEU	2.3
1	B	314	TYR	2.3
1	B	103	SER	2.3
1	A	181	GLN	2.3
1	B	407	VAL	2.3
1	A	416	LEU	2.3
1	B	140	PRO	2.3
1	B	422	LYS	2.3
1	C	106	ILE	2.3
1	A	200	VAL	2.3
1	A	82	ALA	2.2
1	A	342	GLU	2.2
1	A	225	LYS	2.2
1	B	427	LYS	2.2
1	A	66	VAL	2.2
1	A	300	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	301	VAL	2.2
1	B	415	LEU	2.2
1	B	44	ASN	2.2
1	B	88	GLY	2.2
1	B	233	GLU	2.2
1	A	12	THR	2.2
1	A	180	LEU	2.2
1	C	385	ASN	2.2
1	A	168	LYS	2.2
1	A	393	HIS	2.2
1	B	293	GLU	2.2
1	C	389	GLU	2.2
1	A	69	ALA	2.2
1	A	352	LEU	2.2
1	A	355	LEU	2.2
1	B	328	ILE	2.2
1	C	328	ILE	2.2
1	A	156	HIS	2.2
1	B	448	ALA	2.2
1	C	239	THR	2.2
1	C	357	ARG	2.1
1	A	403	LEU	2.1
1	B	27	ASP	2.1
1	A	45	ALA	2.1
1	A	65	ALA	2.1
1	A	172	LEU	2.1
1	A	235	ILE	2.1
1	A	441	LYS	2.1
1	B	315	LEU	2.1
1	B	319	LEU	2.1
1	A	285	LYS	2.1
1	B	361	ILE	2.1
1	C	420	ASN	2.1
1	C	98	GLY	2.1
1	A	14	ARG	2.1
1	A	165	LYS	2.1
1	A	199	ALA	2.1
1	A	426	GLU	2.1
1	A	410	LEU	2.1
1	A	214	ASP	2.1
1	A	227	ASP	2.1
1	A	237	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	286	TYR	2.1
1	A	322	SER	2.0
1	A	43	GLU	2.0
1	A	86	GLU	2.0
1	C	30	GLY	2.0
1	A	401	THR	2.0
1	C	110	GLU	2.0
1	C	31	LEU	2.0
1	A	184	ARG	2.0
1	A	384	ILE	2.0
1	C	309	ILE	2.0
1	B	418	LYS	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](#)

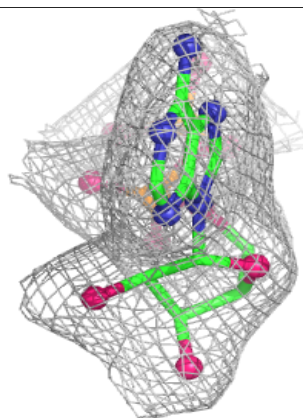
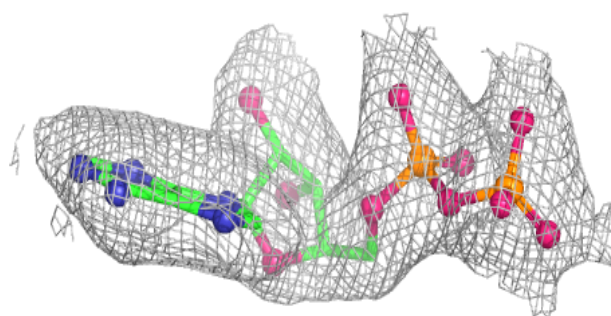
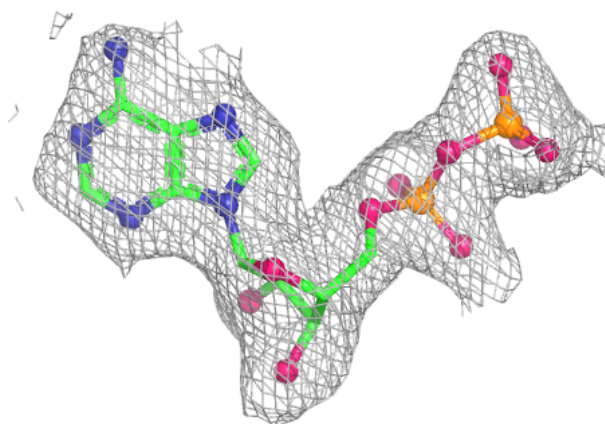
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	C	1450	27/27	0.96	0.08	33,44,51,52	0
2	ADP	B	1449	27/27	0.98	0.06	30,35,38,38	0
2	ADP	A	1450	27/27	0.99	0.04	18,27,29,33	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.

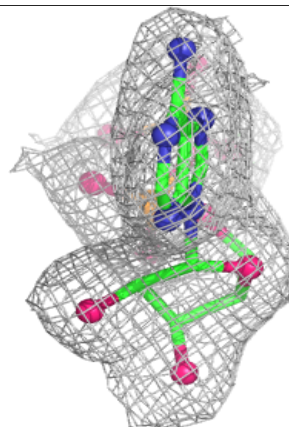
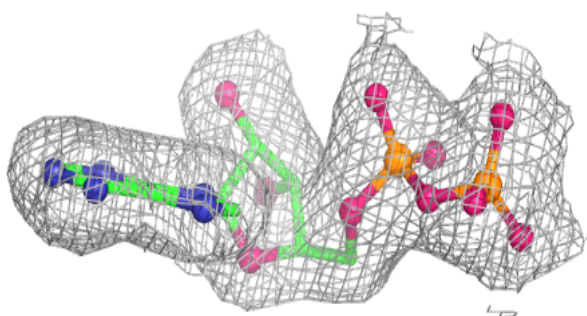
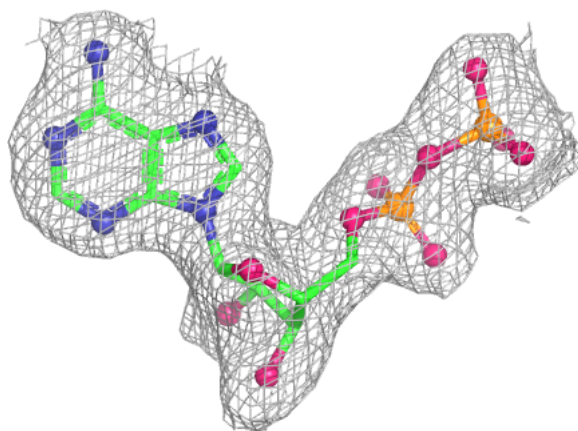
Electron density around ADP C 1450:

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



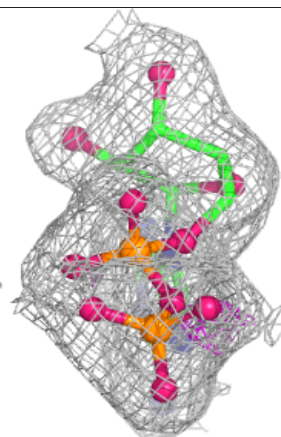
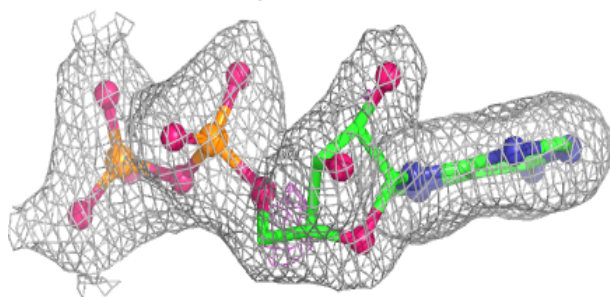
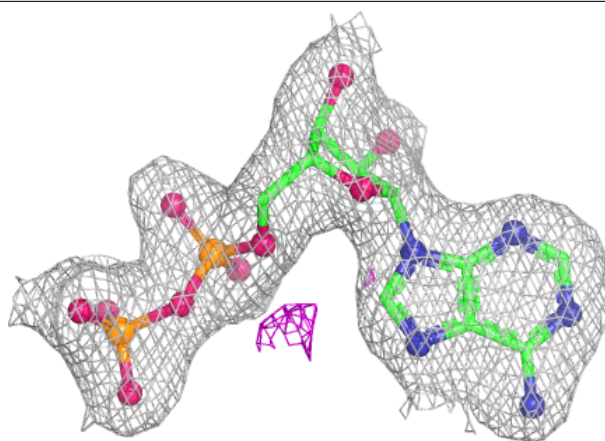
Electron density around ADP B 1449:

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



Electron density around ADP A 1450:

$2mF_o-DF_c$ (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.