



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:25 AM UTC

PDB ID : 5LVP / pdb_00005lvp
Title : Human PDK1 Kinase Domain in Complex with an HM-Peptide Bound to the PIF-Pocket
Authors : Schulze, J.O.; Saladino, G.; Busschots, K.; Neimanis, S.; Suess, E.; Odadzic, D.; Zeuzem, S.; Hindie, V.; Herbrand, A.K.; Lisa, M.N.; Alzari, P.M.; Gervasio, F.L.; Biondi, R.M.
Deposited on : 2016-09-14
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

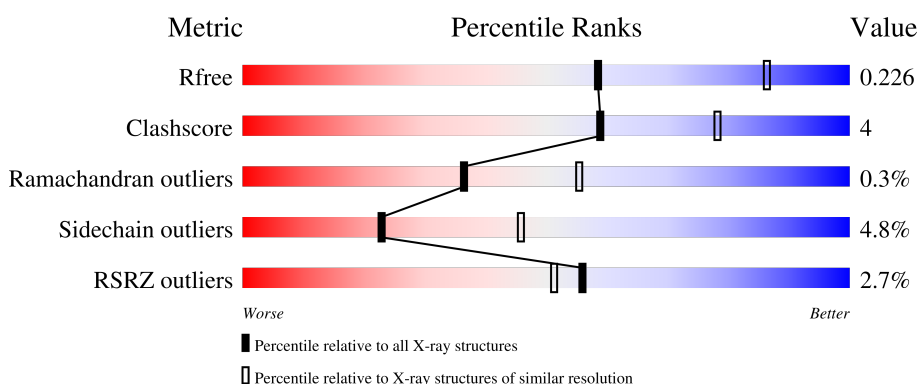
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	311	77% 11% 11%
1	B	311	78% 10% 11%
1	C	311	78% 10% 11%
1	D	311	73% 14% 11%
2	E	15	27% 20% 53%

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Mol	Chain	Length	Quality of chain
2	F	15	13%33%13%7%47%
2	G	15	13%40%13%47%
2	H	15	7%27%20%53%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9538 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 3-phosphoinositide-dependent protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	P	S	0	0	0
			2209	1435	362	404	1	7			
1	B	277	Total	C	N	O	P	S	0	0	0
			2222	1443	363	408	1	7			
1	C	276	Total	C	N	O	P	S	0	0	0
			2213	1437	364	404	1	7			
1	D	277	Total	C	N	O	P	S	0	0	0
			2235	1453	367	407	1	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	expression tag	UNP O15530
A	288	GLY	TYR	engineered mutation	UNP O15530
A	292	ALA	GLN	engineered mutation	UNP O15530
B	49	GLY	-	expression tag	UNP O15530
B	288	GLY	TYR	engineered mutation	UNP O15530
B	292	ALA	GLN	engineered mutation	UNP O15530
C	49	GLY	-	expression tag	UNP O15530
C	288	GLY	TYR	engineered mutation	UNP O15530
C	292	ALA	GLN	engineered mutation	UNP O15530
D	49	GLY	-	expression tag	UNP O15530
D	288	GLY	TYR	engineered mutation	UNP O15530
D	292	ALA	GLN	engineered mutation	UNP O15530

- Molecule 2 is a protein called hydrophobic-motif peptide of PKB/Akt.

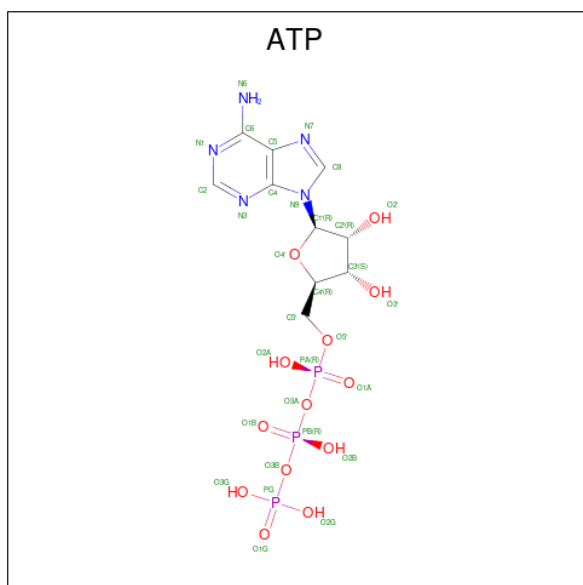
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	1
			57	38	7	11	1			
2	F	8	Total	C	N	O	P	0	0	1
			64	42	8	13	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	1
			64	42	8	13	1			
2	H	7	Total	C	N	O	P	0	0	0
			62	41	7	13	1			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl	0	0
			1 1		
4	C	1	Total Cl	0	0
			1 1		

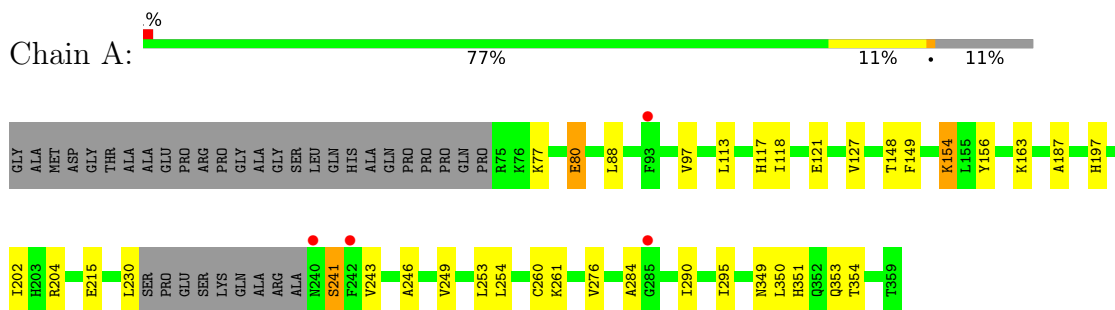
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total 75	O 75	0	0
5	B	71	Total 71	O 71	0	0
5	C	75	Total 75	O 75	0	0
5	D	65	Total 65	O 65	0	0

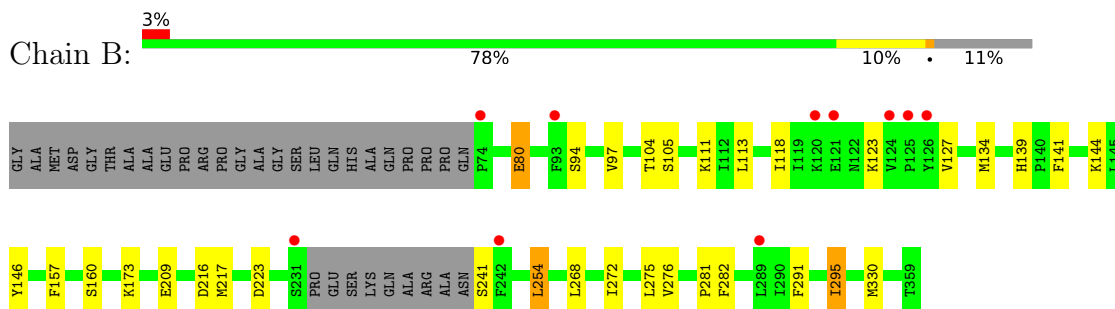
3 Residue-property plots [i](#)

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.

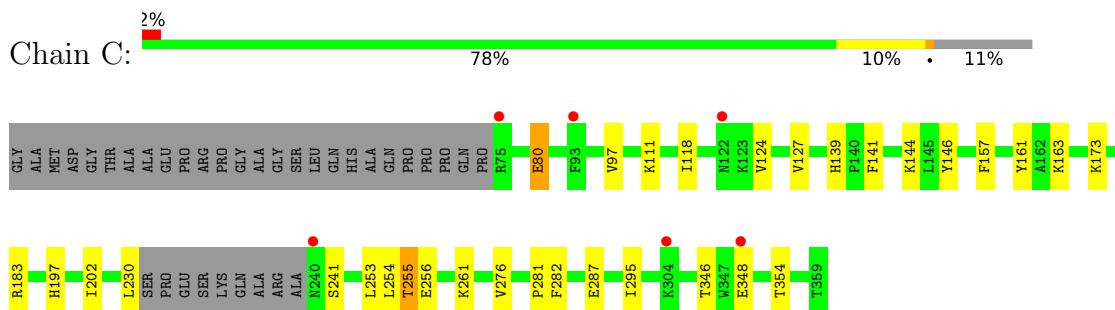
- Molecule 1: 3-phosphoinositide-dependent protein kinase 1



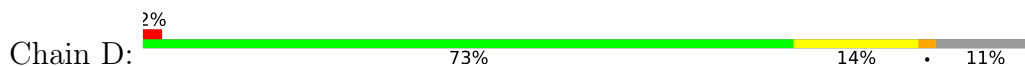
- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

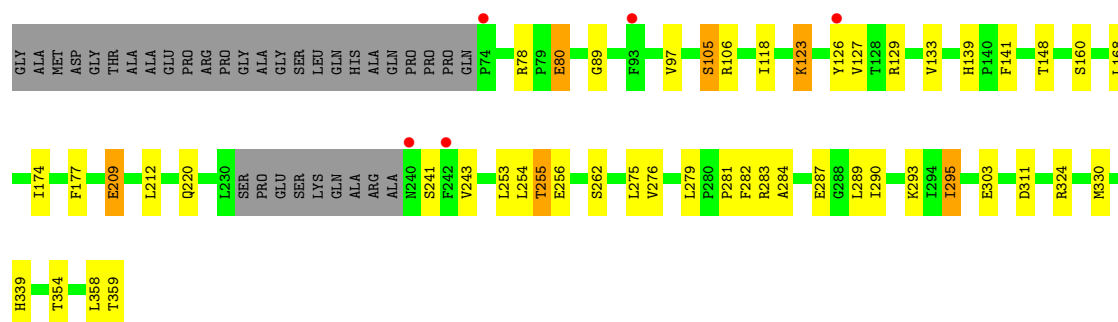


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

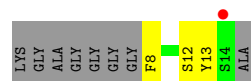
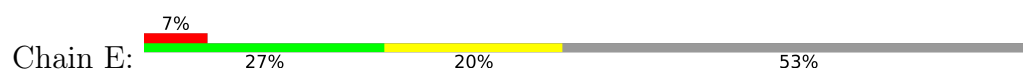


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

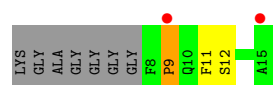
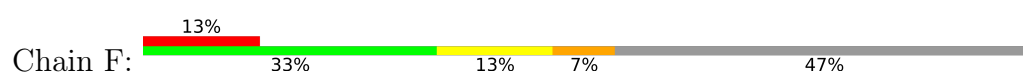




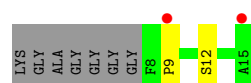
- Molecule 2: hydrophobic-motif peptide of PKB/Akt



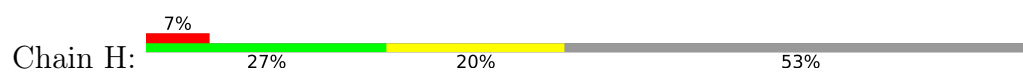
- Molecule 2: hydrophobic-motif peptide of PKB/Akt



- Molecule 2: hydrophobic-motif peptide of PKB/Akt



- Molecule 2: hydrophobic-motif peptide of PKB/Akt



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.83Å 168.51Å 94.88Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	94.75 – 2.50 94.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (94.75-2.50) 99.7 (94.75-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.174 , 0.226 0.175 , 0.226	Depositor DCC
R_{free} test set	2580 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9538	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 64.78 % 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 7.8499e-06. 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: ATP, SEP, CL

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	0.33	0/2250	0.52	0/3036
1	B	0.33	0/2265	0.52	0/3058
1	C	0.33	0/2254	0.52	1/3041 (0.0%)
1	D	0.33	0/2278	0.52	0/3071
2	E	0.27	0/49	0.51	0/65
2	F	0.36	0/56	0.78	0/74
2	G	0.26	0/56	0.50	0/74
2	H	0.35	0/54	0.59	0/71
All	All	0.33	0/9262	0.52	1/12490 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	THR	N-CA-C	-6.50	107.21	114.62

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	2209	0	2199	19	0
1	B	2222	0	2212	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2213	0	2203	14	0
1	D	2235	0	2238	27	0
2	E	57	0	39	1	0
2	F	64	0	45	1	0
2	G	64	0	45	0	0
2	H	62	0	44	2	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	75	0	0	3	0
5	B	71	0	0	1	0
5	C	75	0	0	1	0
5	D	65	0	0	1	0
All	All	9538	0	9073	80	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 (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:HIS:HD2	1:B:141:PHE:H	1.30	0.80
1:D:139:HIS:HD2	1:D:141:PHE:H	1.30	0.77
1:D:255:THR:HG22	1:D:256:GLU:HG3	1.68	0.75
1:C:139:HIS:HD2	1:C:141:PHE:H	1.34	0.73
1:A:118:ILE:HD13	1:A:127:VAL:HG21	1.74	0.69
1:B:118:ILE:HD13	1:B:127:VAL:HG21	1.78	0.66
1:D:118:ILE:HD13	1:D:127:VAL:HG21	1.78	0.66
1:D:123:LYS:HG3	1:D:126:TYR:HB3	1.80	0.63
1:B:139:HIS:CD2	1:B:141:PHE:H	2.14	0.63
1:C:255:THR:HG22	1:C:256:GLU:HG3	1.81	0.62
1:C:139:HIS:CD2	1:C:141:PHE:H	2.18	0.61
1:D:139:HIS:CD2	1:D:141:PHE:H	2.18	0.59
1:C:118:ILE:HD13	1:C:127:VAL:HG21	1.85	0.58
1:B:118:ILE:HG23	1:B:123:LYS:HB2	1.85	0.57
1:B:173:LYS:HG3	5:C:518:HOH:O	2.05	0.56
1:B:254:LEU:HD13	1:B:295:ILE:HD13	1.88	0.56
1:D:284:ALA:HB3	1:D:290:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HD11	1:A:230:LEU:HD21	1.88	0.54
1:D:148:THR:OG1	2:H:13:TYR:HB3	2.08	0.53
1:A:197:HIS:HB3	1:A:261:LYS:HD3	1.89	0.53
1:A:350:LEU:N	5:A:603:HOH:O	2.41	0.53
1:D:262:SER:OG	1:D:324:ARG:HD2	2.10	0.52
1:C:348:GLU:O	1:D:105:SER:OG	2.26	0.51
1:A:113:LEU:HD13	1:A:118:ILE:HD11	1.92	0.50
1:D:139:HIS:HE1	5:D:642:HOH:O	1.95	0.50
1:C:144:LYS:HD3	1:C:146:TYR:CE2	2.47	0.50
1:A:246:ALA:O	1:A:249:VAL:HG12	2.12	0.49
1:A:163:LYS:HD3	1:A:215:GLU:HG3	1.93	0.49
1:D:174:ILE:HD11	1:D:177:PHE:CD1	2.47	0.49
1:B:295:ILE:H	1:B:295:ILE:HG12	1.40	0.48
1:D:148:THR:HB	2:H:11:PHE:CE2	2.49	0.48
1:A:260:CYS:HB2	5:A:623:HOH:O	2.13	0.48
1:D:289:LEU:O	1:D:293:LYS:HG3	2.14	0.47
1:B:113:LEU:HD13	1:B:118:ILE:HD11	1.96	0.47
1:A:80:GLU:H	1:A:80:GLU:CD	2.20	0.47
1:A:284:ALA:HB3	1:A:290:ILE:HG13	1.97	0.47
1:D:295:ILE:H	1:D:295:ILE:HG12	1.54	0.47
1:B:144:LYS:HD3	1:B:146:TYR:CE2	2.50	0.47
1:C:197:HIS:HB3	1:C:261:LYS:HD3	1.95	0.47
3:D:500:ATP:O1B	3:D:500:ATP:H5'2	2.14	0.47
1:A:349:ASN:O	1:A:353:GLN:HG3	2.15	0.47
1:D:78:ARG:NH2	1:D:80:GLU:HG3	2.30	0.47
1:A:154:LYS:HD3	1:A:156:TYR:OH	2.15	0.46
1:B:80:GLU:CD	1:B:80:GLU:H	2.22	0.46
1:A:148:THR:HB	2:F:11:PHE:CE2	2.51	0.46
1:D:89:GLY:HA3	3:D:500:ATP:H4'	1.96	0.46
1:D:168:LEU:HD22	1:D:209:GLU:HG2	1.96	0.46
1:D:281:PRO:HG2	1:D:282:PHE:CD2	2.51	0.46
1:D:358:LEU:HD23	1:D:358:LEU:HA	1.77	0.46
1:A:204:ARG:NH1	1:A:241:SEP:O2P	2.44	0.45
1:A:351:HIS:HD2	5:A:603:HOH:O	2.00	0.45
1:B:281:PRO:HG2	1:B:282:PHE:CD2	2.51	0.45
1:D:118:ILE:HG23	1:D:123:LYS:HB3	1.98	0.45
1:B:111:LYS:HB3	1:B:157:PHE:HB2	1.98	0.45
1:C:80:GLU:H	1:C:80:GLU:CD	2.25	0.44
1:D:311:ASP:OD2	1:D:339:HIS:NE2	2.42	0.43
1:D:359:THR:OXT	1:D:359:THR:OG1	2.30	0.43
1:D:330:MET:HB3	1:D:330:MET:HE3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LYS:HB3	1:C:157:PHE:HB2	2.00	0.43
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.86	0.43
1:B:94:SER:OG	3:B:401:ATP:O1A	2.33	0.43
1:B:146:TYR:HE1	1:B:160:SER:HB3	1.84	0.42
1:B:104:THR:O	1:B:105:SER:HB2	2.19	0.42
1:B:216:ASP:O	1:B:217:MET:HB2	2.19	0.42
1:A:117:HIS:HD1	1:A:117:HIS:C	2.27	0.42
5:B:540:HOH:O	1:C:173:LYS:HG3	2.20	0.42
1:D:212:LEU:O	1:D:220:GLN:N	2.48	0.42
1:A:77:LYS:HB2	1:A:149:PHE:CD2	2.55	0.42
1:D:129:ARG:O	1:D:133:VAL:HG23	2.20	0.41
1:B:144:LYS:HD3	1:B:146:TYR:CZ	2.54	0.41
1:D:177:PHE:CD2	1:D:275:LEU:HD22	2.56	0.41
1:B:268:LEU:O	1:B:272:ILE:HG13	2.20	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.88	0.41
1:A:187:ALA:HB1	1:A:350:LEU:HD11	2.02	0.41
1:B:291:PHE:O	1:B:295:ILE:HG12	2.21	0.41
1:C:124:VAL:HG22	2:E:8:PHE:CE2	2.56	0.40
1:C:161:TYR:CZ	1:C:163:LYS:HA	2.56	0.40
1:C:202:ILE:HD11	1:C:230:LEU:HD21	2.03	0.40
1:D:279:LEU:HB3	1:D:283:ARG:HD3	2.03	0.40
1:C:281:PRO:HG2	1:C:282:PHE:CD2	2.57	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	271/311 (87%)	262 (97%)	9 (3%)	0	100	100
1	B	273/311 (88%)	260 (95%)	12 (4%)	1 (0%)	30	49
1	C	271/311 (87%)	260 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	272/311 (88%)	258 (95%)	14 (5%)	0	100	100
2	E	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
2	F	5/15 (33%)	4 (80%)	0	1 (20%)	0	0
2	G	5/15 (33%)	3 (60%)	1 (20%)	1 (20%)	0	0
2	H	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
All	All	1105/1304 (85%)	1053 (95%)	49 (4%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	9	PRO
2	G	9	PRO
1	B	223	ASP

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	233/266 (88%)	223 (96%)	10 (4%)	26	51
1	B	235/266 (88%)	227 (97%)	8 (3%)	32	60
1	C	233/266 (88%)	223 (96%)	10 (4%)	26	51
1	D	238/266 (90%)	222 (93%)	16 (7%)	15	31
2	E	4/7 (57%)	3 (75%)	1 (25%)	0	1
2	F	5/7 (71%)	4 (80%)	1 (20%)	1	2
2	G	5/7 (71%)	5 (100%)	0	100	100
2	H	5/7 (71%)	5 (100%)	0	100	100
All	All	958/1092 (88%)	912 (95%)	46 (5%)	23	46

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	97	VAL
1	A	121	GLU
1	A	154	LYS
1	A	243	VAL
1	A	253	LEU
1	A	254	LEU
1	A	276	VAL
1	A	295	ILE
1	A	354	THR
1	B	80	GLU
1	B	97	VAL
1	B	134	MET
1	B	209	GLU
1	B	254	LEU
1	B	276	VAL
1	B	295	ILE
1	B	330	MET
1	C	80	GLU
1	C	97	VAL
1	C	183	ARG
1	C	253	LEU
1	C	254	LEU
1	C	276	VAL
1	C	287	GLU
1	C	295	ILE
1	C	346	THR
1	C	354	THR
1	D	80	GLU
1	D	97	VAL
1	D	105	SER
1	D	106	ARG
1	D	123	LYS
1	D	160	SER
1	D	209	GLU
1	D	243	VAL
1	D	253	LEU
1	D	254	LEU
1	D	255	THR
1	D	276	VAL
1	D	287	GLU
1	D	295	ILE
1	D	303	GLU

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Mol	Chain	Res	Type
1	D	354	THR
2	E	13	TYR
2	F	9	PRO

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	351	HIS
1	B	139	HIS
1	B	352	GLN
1	B	353	GLN
1	C	139	HIS
1	C	353	GLN
1	D	139	HIS
1	D	351	HIS
1	D	353	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	B	241	1	8,9,10	1.70	1 (12%)	7,12,14	1.48	1 (14%)
2	SEP	H	12	2	8,9,10	1.71	1 (12%)	7,12,14	1.80	2 (28%)
1	SEP	A	241	1	8,9,10	1.64	1 (12%)	7,12,14	1.80	1 (14%)
1	SEP	D	241	1	8,9,10	1.63	1 (12%)	7,12,14	1.41	1 (14%)
2	SEP	E	12	2	8,9,10	1.66	1 (12%)	7,12,14	1.59	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	F	12	2	8,9,10	1.67	1 (12%)	7,12,14	1.65	1 (14%)
2	SEP	G	12	2	8,9,10	1.65	1 (12%)	7,12,14	1.49	1 (14%)
1	SEP	C	241	1	8,9,10	1.66	1 (12%)	7,12,14	1.73	1 (14%)

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
1	SEP	B	241	1	-	0/6/8/10	-
2	SEP	H	12	2	-	0/6/8/10	-
1	SEP	A	241	1	-	1/6/8/10	-
1	SEP	D	241	1	-	2/6/8/10	-
2	SEP	E	12	2	-	4/6/8/10	-
2	SEP	F	12	2	-	1/6/8/10	-
2	SEP	G	12	2	-	2/6/8/10	-
1	SEP	C	241	1	-	2/6/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	SEP	P-O1P	3.69	1.61	1.50
2	F	12	SEP	P-O1P	3.62	1.61	1.50
2	G	12	SEP	P-O1P	3.58	1.61	1.50
1	A	241	SEP	P-O1P	3.56	1.61	1.50
2	H	12	SEP	P-O1P	3.55	1.61	1.50
1	C	241	SEP	P-O1P	3.52	1.61	1.50
1	D	241	SEP	P-O1P	3.50	1.61	1.50
2	E	12	SEP	P-O1P	3.49	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	SEP	OG-CB-CA	4.12	112.15	108.14
1	C	241	SEP	OG-CB-CA	3.99	112.02	108.14
1	B	241	SEP	OG-CB-CA	3.42	111.47	108.14
2	H	12	SEP	OG-CB-CA	3.39	111.44	108.14
2	F	12	SEP	OG-CB-CA	3.18	111.24	108.14
1	D	241	SEP	OG-CB-CA	3.12	111.19	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	12	SEP	OG-CB-CA	3.06	111.12	108.14
2	E	12	SEP	OG-CB-CA	3.04	111.10	108.14
2	E	12	SEP	O3P-P-OG	2.24	112.52	106.67
2	H	12	SEP	O3P-P-OG	2.16	112.30	106.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	12	SEP	CA-CB-OG-P
2	E	12	SEP	CB-OG-P-O1P
2	E	12	SEP	CB-OG-P-O2P
2	G	12	SEP	CA-CB-OG-P
2	G	12	SEP	CB-OG-P-O1P
1	C	241	SEP	CB-OG-P-O3P
1	D	241	SEP	CB-OG-P-O3P
1	A	241	SEP	CA-CB-OG-P
1	C	241	SEP	CA-CB-OG-P
1	D	241	SEP	CA-CB-OG-P
2	F	12	SEP	CA-CB-OG-P
2	E	12	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	241	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ATP	B	401	-	32,33,33	1.44	6 (18%)	48,52,52	1.95	11 (22%)
3	ATP	A	500	-	32,33,33	1.38	6 (18%)	48,52,52	1.83	9 (18%)
3	ATP	D	500	-	32,33,33	1.50	7 (21%)	48,52,52	1.85	9 (18%)
3	ATP	C	401	-	32,33,33	1.32	4 (12%)	48,52,52	1.87	13 (27%)

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
3	ATP	B	401	-	-	1/22/38/38	0/3/3/3
3	ATP	A	500	-	-	1/22/38/38	0/3/3/3
3	ATP	D	500	-	-	7/22/38/38	0/3/3/3
3	ATP	C	401	-	-	4/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	ATP	C5-C4	4.59	1.47	1.39
3	C	401	ATP	C5-C4	4.53	1.47	1.39
3	A	500	ATP	C5-C4	4.51	1.47	1.39
3	B	401	ATP	C5-C4	4.40	1.46	1.39
3	B	401	ATP	PA-O3A	3.09	1.62	1.59
3	D	500	ATP	PA-O3A	2.89	1.62	1.59
3	D	500	ATP	C5-N7	-2.72	1.34	1.39
3	C	401	ATP	C5-C6	2.71	1.48	1.41
3	D	500	ATP	PB-O3A	2.62	1.62	1.59
3	B	401	ATP	PB-O3A	2.53	1.62	1.59
3	D	500	ATP	C8-N7	2.46	1.36	1.31
3	A	500	ATP	C5-C6	2.45	1.47	1.41
3	A	500	ATP	C8-N7	2.41	1.36	1.31
3	C	401	ATP	C8-N7	2.39	1.36	1.31
3	D	500	ATP	PB-O3B	2.38	1.62	1.59
3	B	401	ATP	C8-N7	2.31	1.36	1.31
3	C	401	ATP	C5-N7	-2.26	1.35	1.39
3	B	401	ATP	C5-N7	-2.22	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ATP	C5-C6	2.19	1.47	1.41
3	A	500	ATP	PB-O3B	2.18	1.61	1.59
3	A	500	ATP	C5-N7	-2.09	1.35	1.39
3	D	500	ATP	C4-N9	-2.04	1.33	1.37
3	A	500	ATP	PB-O3A	2.02	1.61	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ATP	C5-C4-N3	-6.39	117.92	126.72
3	C	401	ATP	C5-C4-N3	-6.13	118.28	126.72
3	A	500	ATP	C5-C4-N3	-5.70	118.86	126.72
3	B	401	ATP	N3-C4-N9	5.47	136.47	127.17
3	D	500	ATP	C5-C4-N3	-5.44	119.23	126.72
3	D	500	ATP	N3-C4-N9	5.22	136.05	127.17
3	C	401	ATP	N3-C4-N9	4.77	135.28	127.17
3	A	500	ATP	N3-C4-N9	4.70	135.15	127.17
3	B	401	ATP	C2-N3-C4	4.25	122.21	111.83
3	C	401	ATP	C2-N3-C4	3.98	121.56	111.83
3	D	500	ATP	N3-C2-N1	-3.83	122.79	128.58
3	A	500	ATP	C2-N3-C4	3.83	121.18	111.83
3	B	401	ATP	N3-C2-N1	-3.81	122.82	128.58
3	C	401	ATP	N3-C2-N1	-3.69	123.00	128.58
3	D	500	ATP	C2-N3-C4	3.58	120.58	111.83
3	C	401	ATP	C4-C5-N7	-3.58	106.48	110.58
3	A	500	ATP	N3-C2-N1	-3.58	123.17	128.58
3	A	500	ATP	C2'-C1'-N9	-3.38	104.92	113.30
3	D	500	ATP	C4-N9-C8	3.32	109.22	105.74
3	A	500	ATP	C4-C5-N7	-3.04	107.11	110.58
3	A	500	ATP	C4-N9-C8	3.00	108.88	105.74
3	D	500	ATP	O3'-C3'-C2'	-2.96	102.32	111.82
3	D	500	ATP	N6-C6-N1	2.84	124.70	118.38
3	C	401	ATP	C5-N7-C8	2.83	107.90	103.45
3	C	401	ATP	C2'-C1'-N9	-2.68	106.63	113.30
3	B	401	ATP	C2'-C1'-N9	-2.68	106.66	113.30
3	D	500	ATP	C5-C6-N6	-2.58	116.90	123.29
3	B	401	ATP	C4-N9-C8	2.42	108.28	105.74
3	D	500	ATP	C2'-C1'-N9	-2.40	107.35	113.30
3	B	401	ATP	C3'-C2'-C1'	2.38	105.97	101.46
3	C	401	ATP	C4-N9-C8	2.37	108.23	105.74
3	B	401	ATP	C4-C5-N7	-2.33	107.92	110.58
3	B	401	ATP	C5-C6-N6	-2.29	117.61	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ATP	O2B-PB-O1B	2.27	123.01	112.44
3	A	500	ATP	C5-N7-C8	2.21	106.92	103.45
3	C	401	ATP	C2-N1-C6	2.19	122.33	118.73
3	B	401	ATP	O3G-PG-O2G	2.14	115.84	107.80
3	C	401	ATP	C6-C5-N7	2.13	136.19	132.09
3	C	401	ATP	N9-C8-N7	-2.10	110.95	113.94
3	B	401	ATP	O4'-C1'-N9	2.03	111.98	108.09
3	C	401	ATP	O4'-C1'-N9	2.02	111.96	108.09
3	A	500	ATP	N9-C8-N7	-2.00	111.09	113.94

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O3A
3	D	500	ATP	C5'-O5'-PA-O2A
3	D	500	ATP	O4'-C4'-C5'-O5'
3	D	500	ATP	C3'-C4'-C5'-O5'
3	D	500	ATP	PG-O3B-PB-O2B
3	A	500	ATP	C5'-O5'-PA-O1A
3	B	401	ATP	C5'-O5'-PA-O1A
3	D	500	ATP	C5'-O5'-PA-O1A
3	D	500	ATP	C5'-O5'-PA-O3A
3	D	500	ATP	PG-O3B-PB-O1B
3	C	401	ATP	PB-O3A-PA-O2A

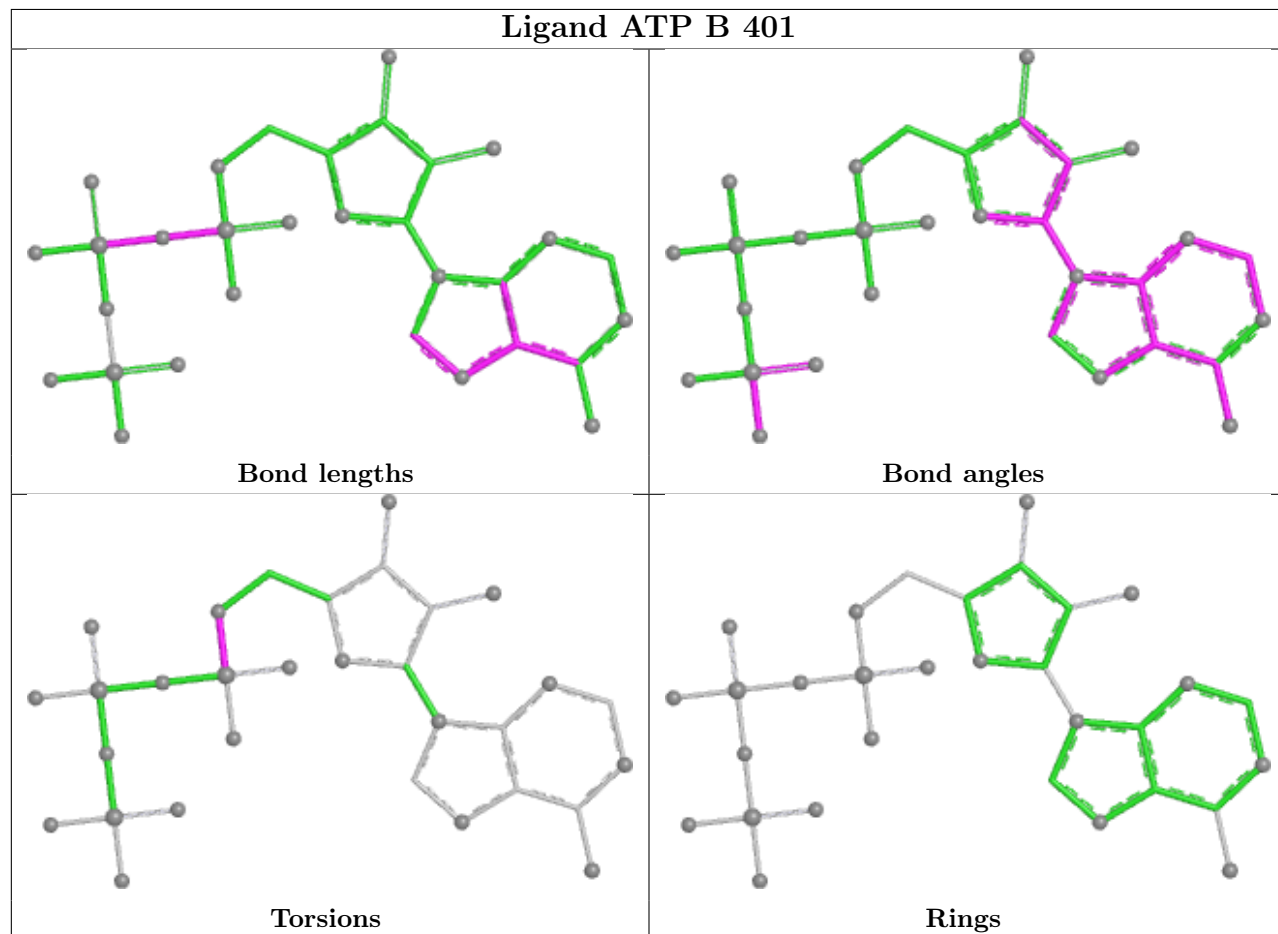
There are no ring outliers.

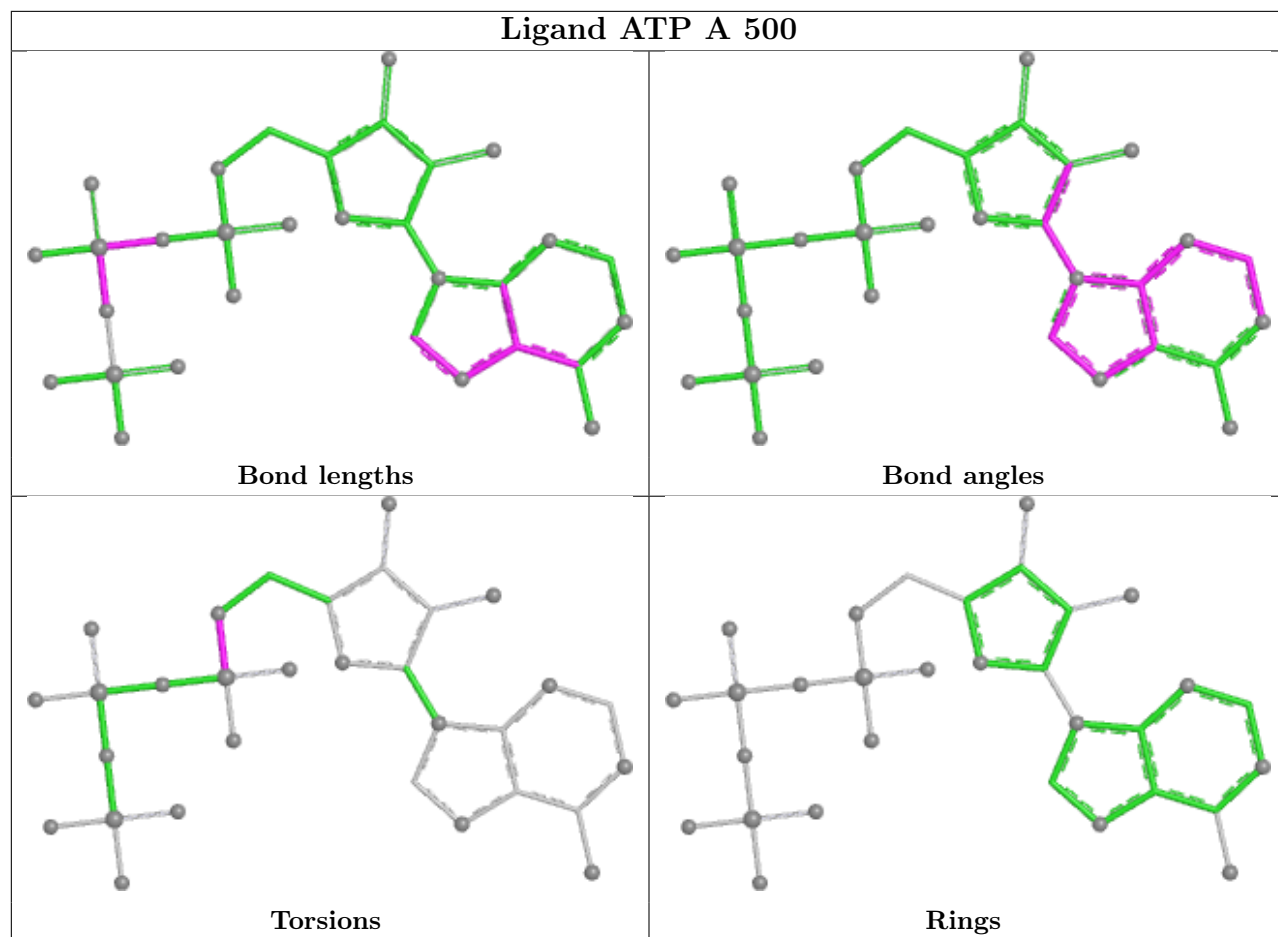
2 monomers are involved in 3 short contacts:

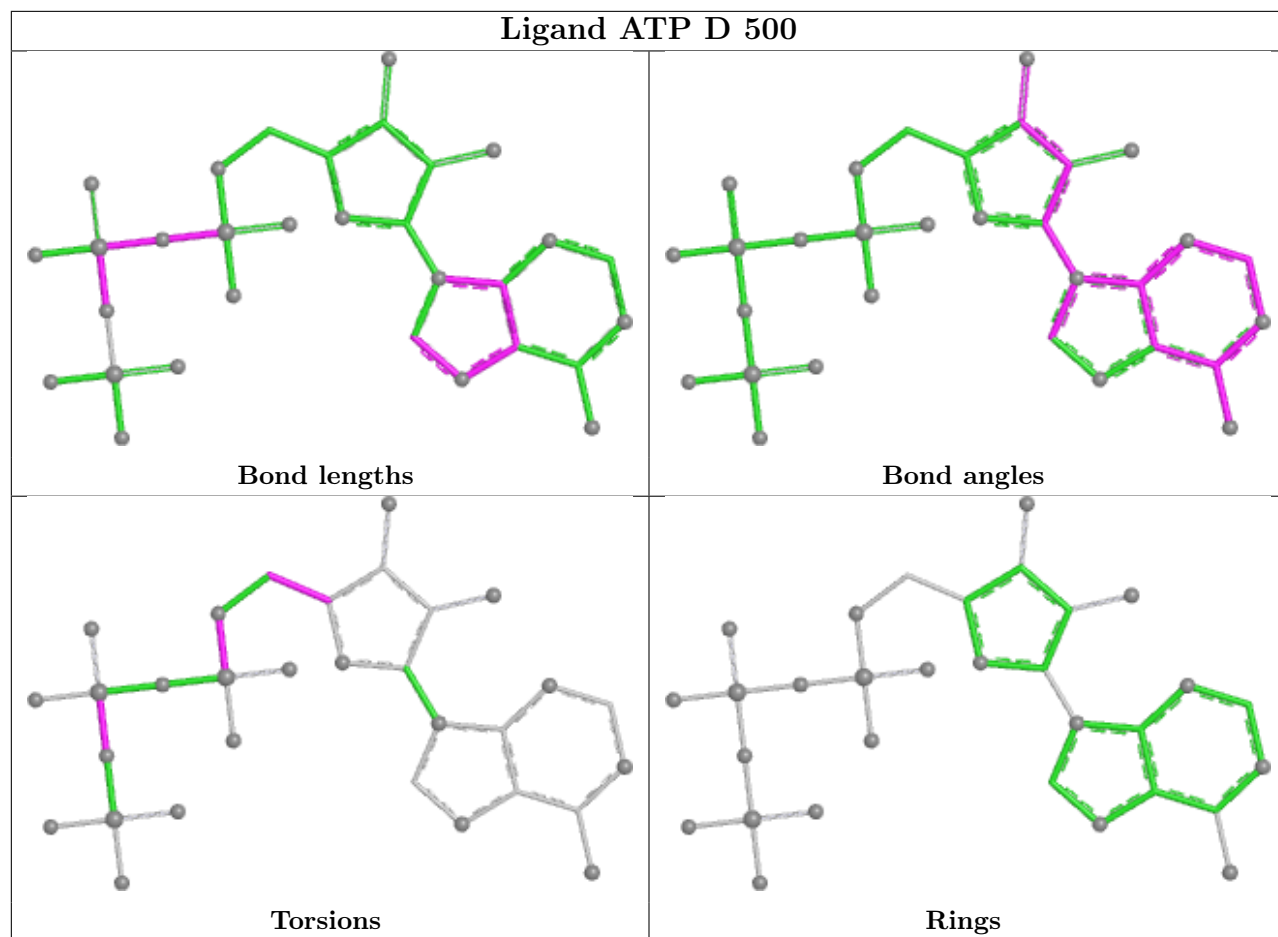
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ATP	1	0
3	D	500	ATP	2	0

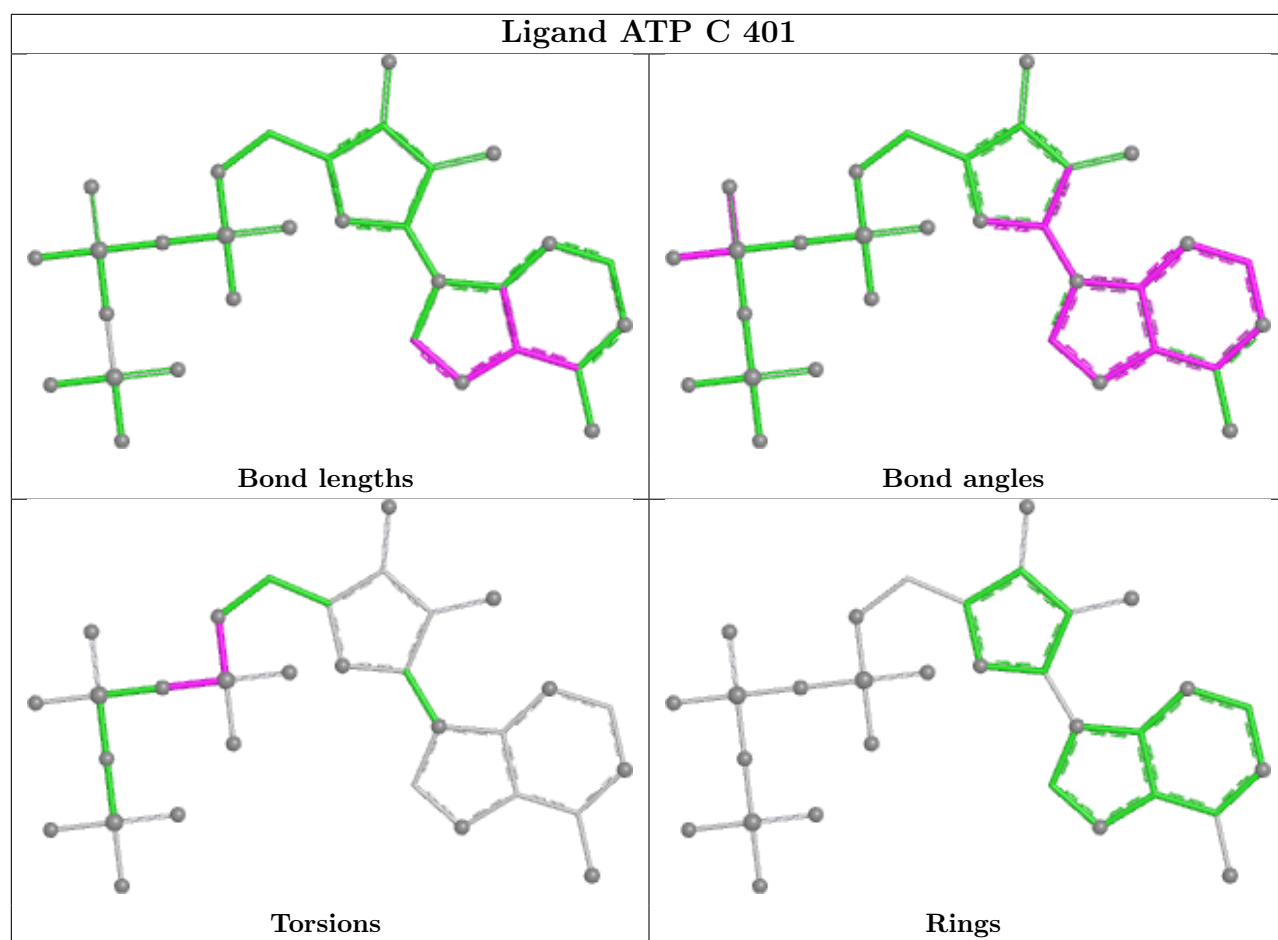
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	275/311 (88%)	-0.35	4 (1%) 72 68	23, 40, 89, 117	0
1	B	276/311 (88%)	-0.25	10 (3%) 46 41	22, 44, 89, 110	0
1	C	275/311 (88%)	-0.28	6 (2%) 62 58	22, 43, 84, 130	0
1	D	276/311 (88%)	-0.32	5 (1%) 67 64	23, 41, 87, 123	0
2	E	6/15 (40%)	1.31	1 (16%) 4 3	76, 83, 90, 93	0
2	F	7/15 (46%)	2.07	2 (28%) 1 1	67, 80, 91, 122	0
2	G	7/15 (46%)	1.99	2 (28%) 1 1	71, 86, 112, 133	0
2	H	6/15 (40%)	1.13	1 (16%) 4 3	70, 87, 91, 97	0
All	All	1128/1304 (86%)	-0.26	31 (2%) 56 51	22, 43, 90, 133	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	15	ALA	6.4
1	D	240	ASN	6.0
1	A	240	ASN	5.1
2	G	15	ALA	4.9
1	C	240	ASN	4.8
1	C	93	PHE	4.6
1	D	242	PHE	3.9
1	D	93	PHE	3.8
1	D	74	PRO	3.7
1	B	93	PHE	3.3
1	B	74	PRO	3.3
1	A	242	PHE	3.2
2	E	14	SER	3.0
2	F	9	PRO	2.7
1	B	126	TYR	2.7
1	B	242	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	PHE	2.6
1	C	75	ARG	2.5
1	B	231	SER	2.5
2	H	14	SER	2.5
2	G	9	PRO	2.4
1	B	289	LEU	2.4
1	C	348	GLU	2.4
1	B	125	PRO	2.3
1	D	126	TYR	2.3
1	C	122	ASN	2.2
1	C	304	LYS	2.2
1	B	120	LYS	2.2
1	B	121	GLU	2.2
1	A	285	GLY	2.1
1	B	124	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	SEP	F	12	10/11	0.77	0.13	82,95,124,125	0
1	SEP	B	241	10/11	0.79	0.13	91,100,110,112	0
1	SEP	D	241	10/11	0.81	0.13	104,115,121,124	0
2	SEP	G	12	10/11	0.81	0.12	88,101,123,124	0
2	SEP	H	12	10/11	0.84	0.13	76,94,121,123	0
1	SEP	A	241	10/11	0.86	0.12	93,99,106,107	0
2	SEP	E	12	10/11	0.87	0.12	81,99,117,118	0
1	SEP	C	241	10/11	0.87	0.11	84,100,108,112	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

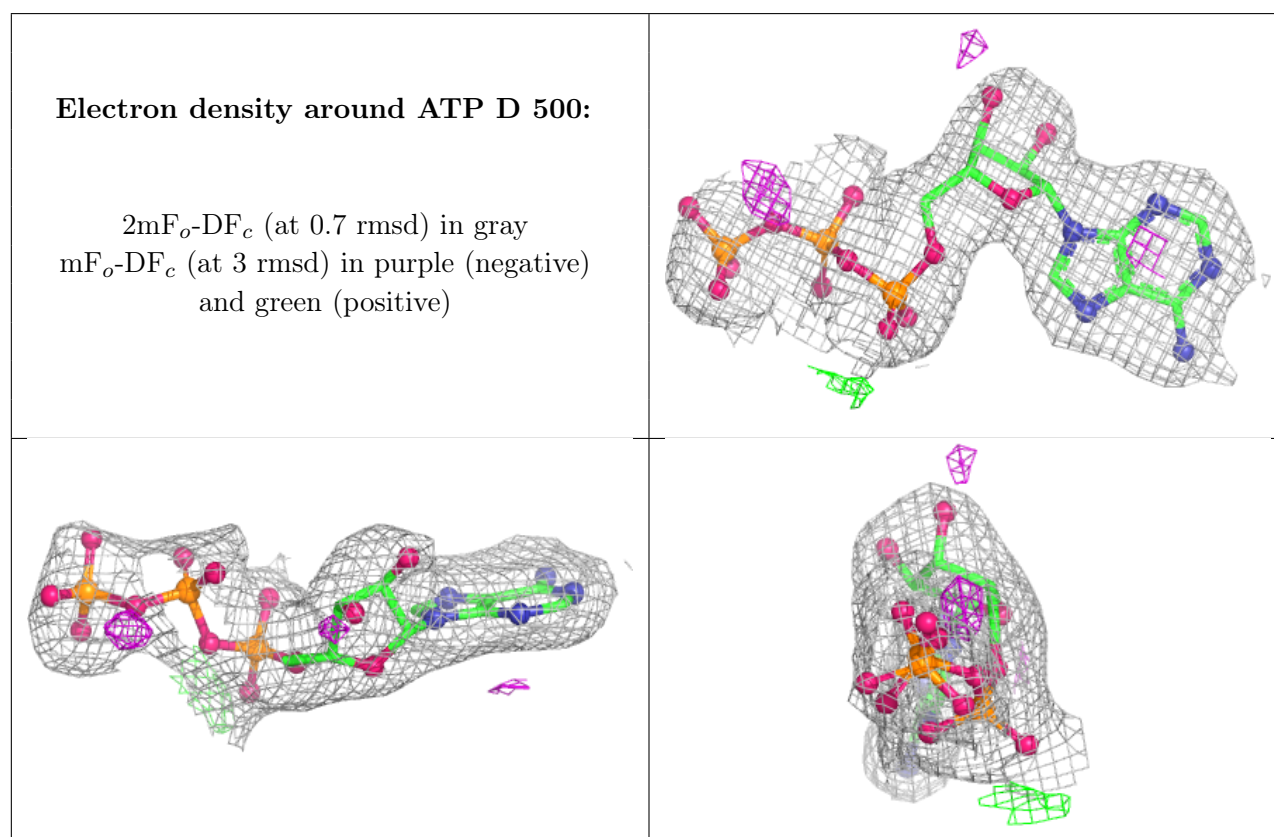
6.4 Ligands [i](#)

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.

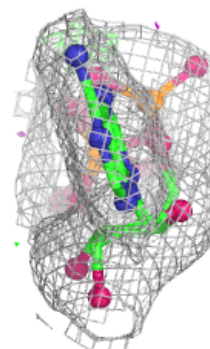
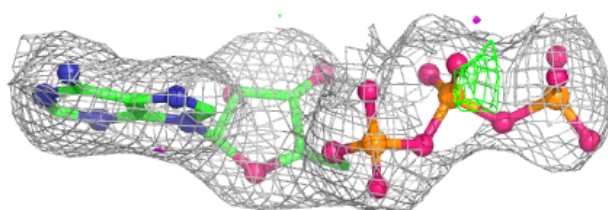
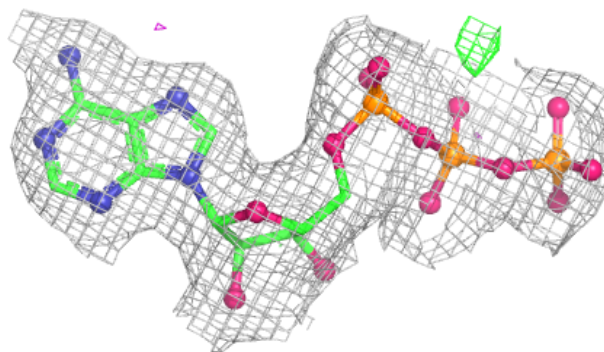
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATP	D	500	31/31	0.92	0.09	23,58,96,98	3
4	CL	B	402	1/1	0.92	0.18	76,76,76,76	0
3	ATP	C	401	31/31	0.93	0.08	25,50,79,87	3
3	ATP	B	401	31/31	0.94	0.07	25,50,77,87	2
3	ATP	A	500	31/31	0.94	0.08	24,52,93,99	2
4	CL	C	402	1/1	0.98	0.11	64,64,64,64	0

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.

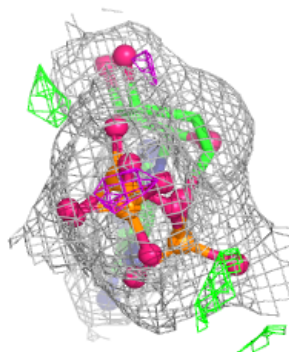
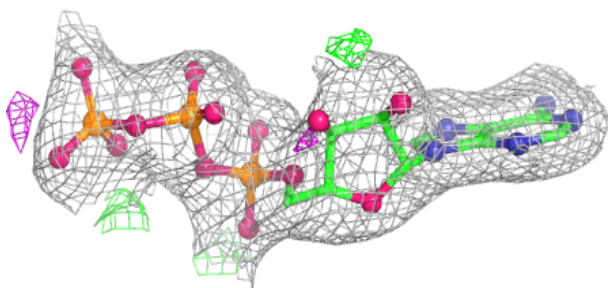
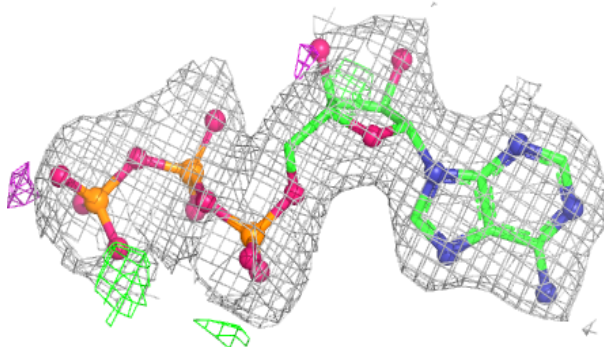


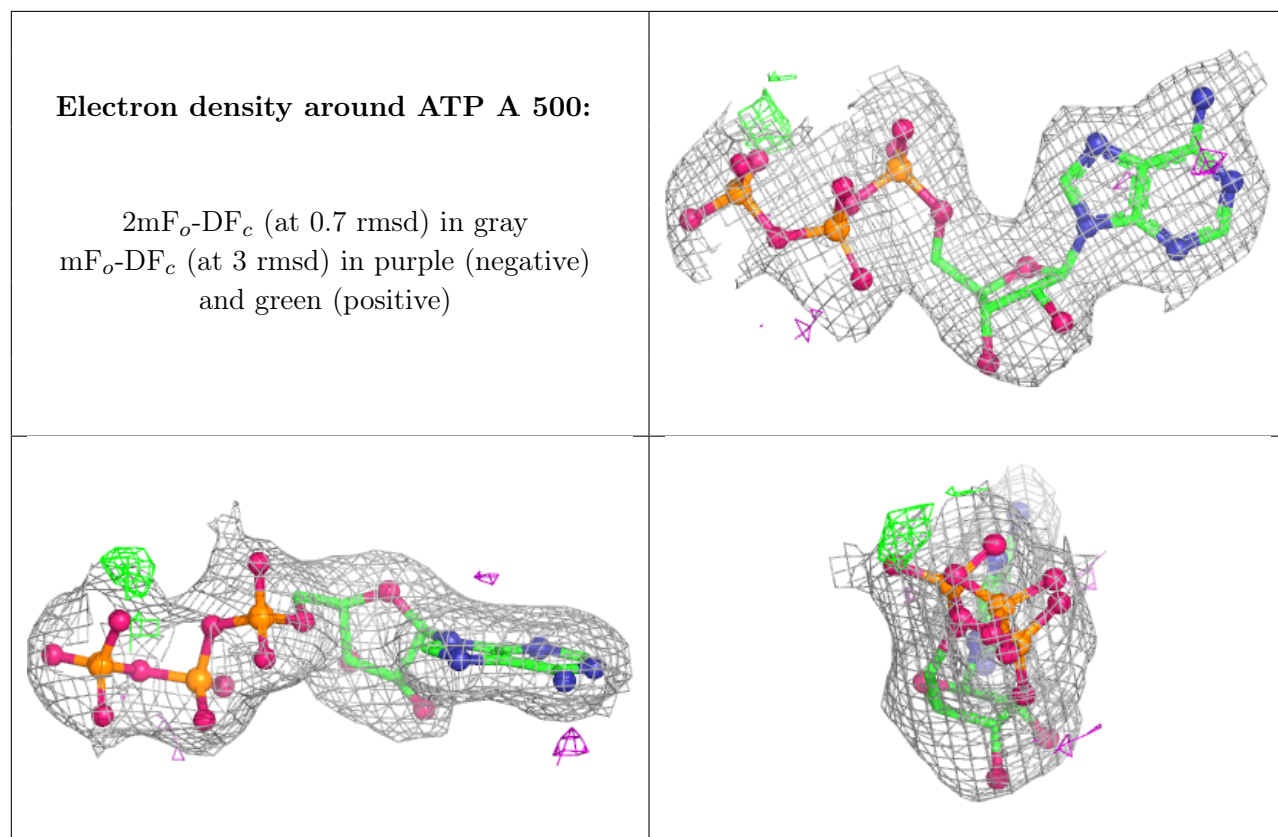
Electron density around ATP C 401:

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

**Electron density around ATP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.