



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:15 PM UTC

PDB ID : 1XMI / pdb_00001xmi
Title : Crystal structure of human F508A NBD1 domain with ATP
Authors : Lewis, H.A.; Zhao, X.; Wang, C.; Sauder, J.M.; Rooney, I.; Noland, B.W.; Lorimer, D.; Kearins, M.C.; Conners, K.; Condon, B.; Maloney, P.C.; Guggino, W.B.; Hunt, J.F.; Emtage, S.; Structural GenomiX
Deposited on : 2004-10-02
Resolution : 2.25 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:

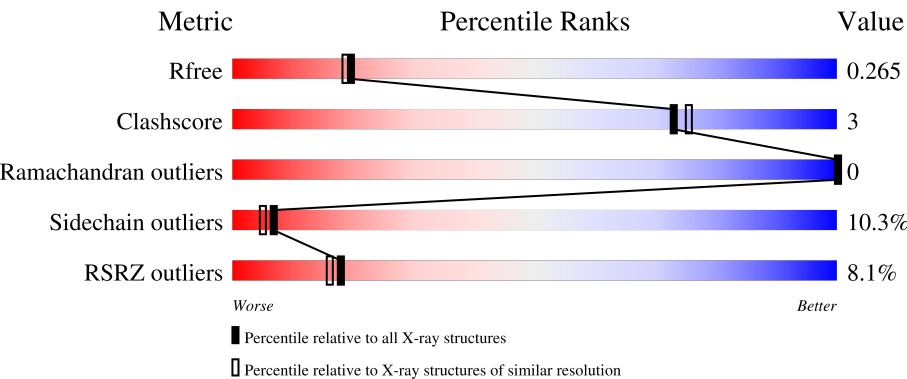
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	10% 76%15%8%
1	B	291	4% 73%14%11%
1	C	291	5% 80%12%7%
1	D	291	10% 80%11%8%

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Mol	Chain	Length	Quality of chain
1	E	291	7% 75% 15% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11228 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2056	1308	342	394	12			
1	B	258	Total	C	N	O	S	0	0	0
			2027	1294	334	386	13			
1	C	270	Total	C	N	O	S	0	0	0
			2117	1347	349	408	13			
1	D	268	Total	C	N	O	S	0	0	0
			2085	1325	344	403	13			
1	E	266	Total	C	N	O	S	0	0	0
			2079	1325	343	398	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	THR	cloning artifact	UNP P13569
A	429	SER	PHE	engineered mutation	UNP P13569
A	508	ALA	PHE	engineered mutation	UNP P13569
A	667	ARG	HIS	engineered mutation	UNP P13569
B	388	SER	THR	cloning artifact	UNP P13569
B	429	SER	PHE	engineered mutation	UNP P13569
B	508	ALA	PHE	engineered mutation	UNP P13569
B	667	ARG	HIS	engineered mutation	UNP P13569
C	388	SER	THR	cloning artifact	UNP P13569
C	429	SER	PHE	engineered mutation	UNP P13569
C	508	ALA	PHE	engineered mutation	UNP P13569
C	667	ARG	HIS	engineered mutation	UNP P13569
D	388	SER	THR	cloning artifact	UNP P13569
D	429	SER	PHE	engineered mutation	UNP P13569
D	508	ALA	PHE	engineered mutation	UNP P13569
D	667	ARG	HIS	engineered mutation	UNP P13569
E	388	SER	THR	cloning artifact	UNP P13569
E	429	SER	PHE	engineered mutation	UNP P13569
E	508	ALA	PHE	engineered mutation	UNP P13569

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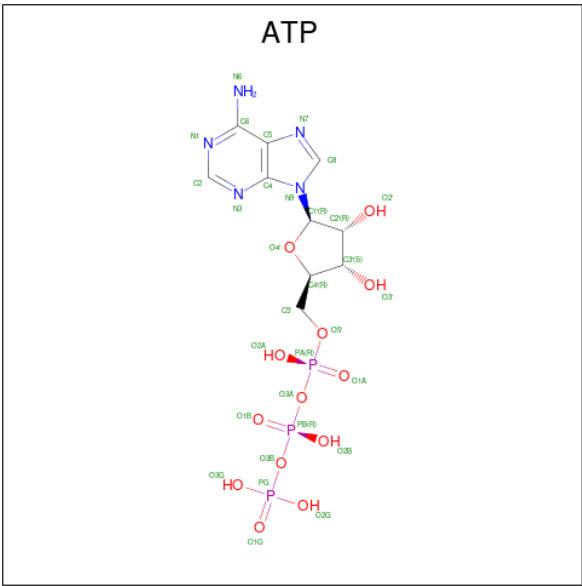
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Chain	Residue	Modelled	Actual	Comment	Reference
E	667	ARG	HIS	engineered mutation	UNP P13569

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

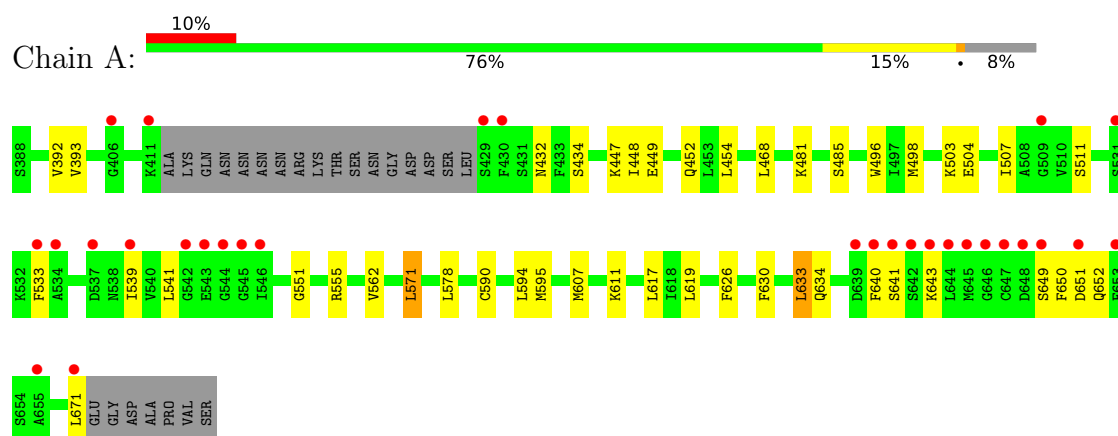
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	163	Total	O	0	0
			163	163		
4	C	146	Total	O	0	0
			146	146		
4	D	132	Total	O	0	0
			132	132		
4	E	108	Total	O	0	0
			108	108		

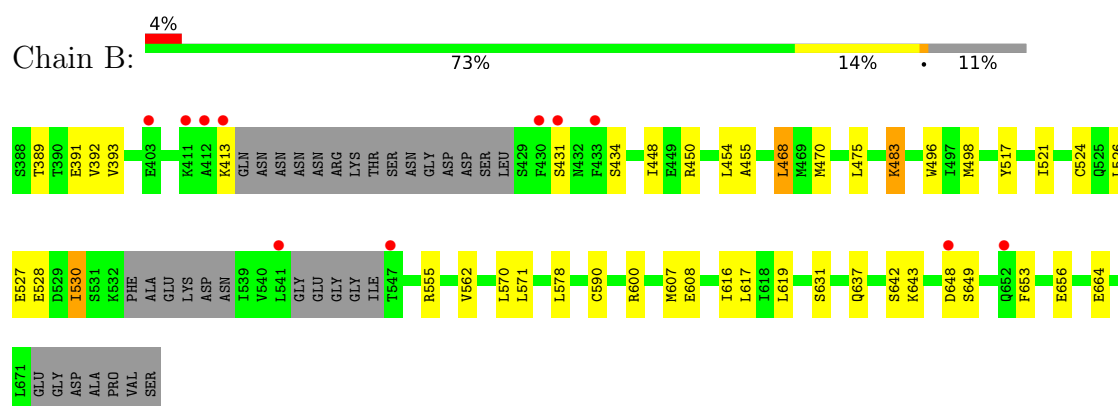
3 Residue-property plots [i](#)

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.

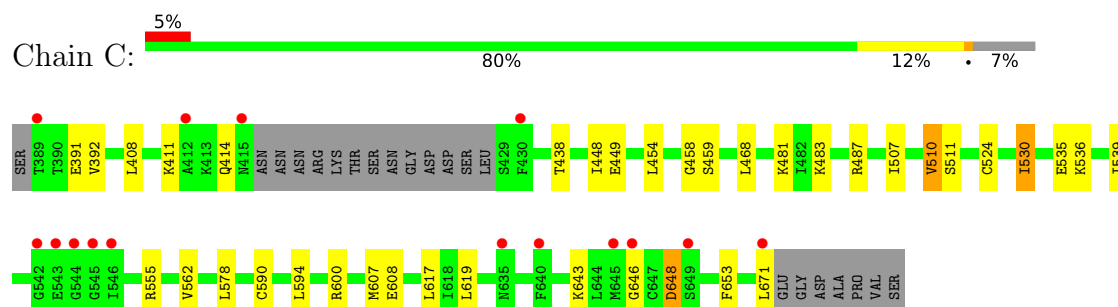
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



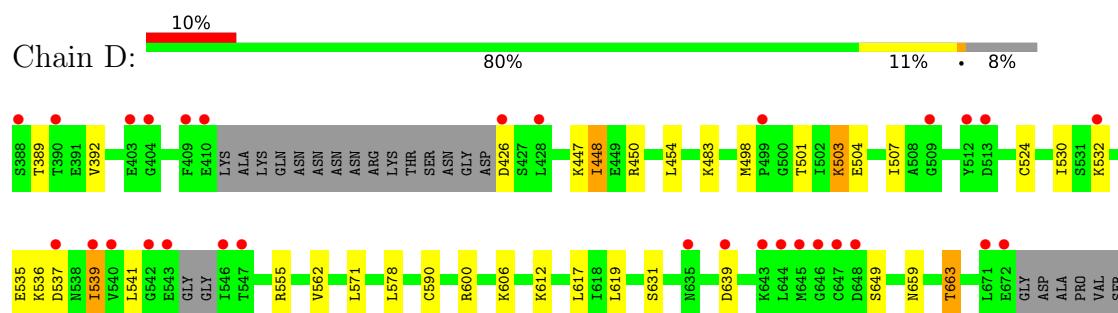
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



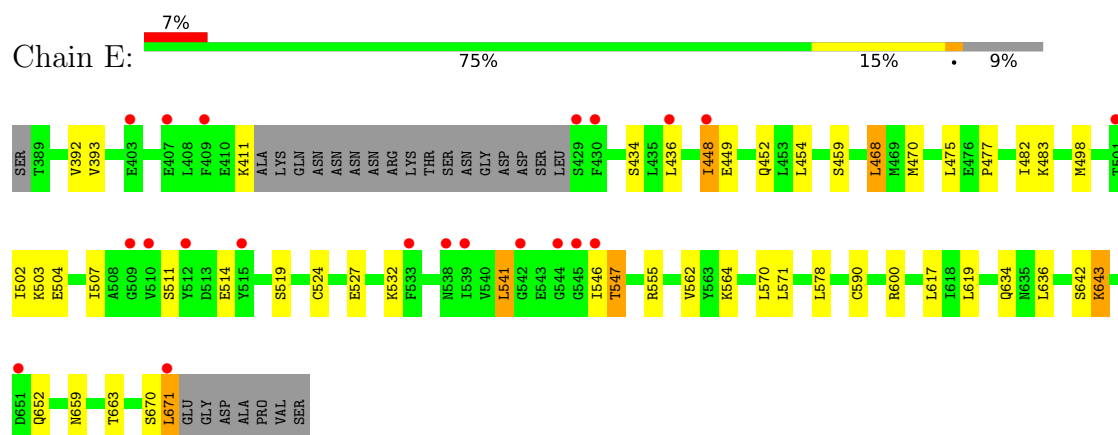
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



● Molecule 1: Cystic fibrosis transmembrane conductance regulator



● Molecule 1: Cystic fibrosis transmembrane conductance regulator



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	144.46Å 154.02Å 136.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.20 – 2.25 27.20 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.20-2.25) 99.8 (27.20-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.212 , 0.265 (Not available) , 0.265	Depositor DCC
R_{free} test set	3582 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11228	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: MG, ATP

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	0.39	0/2091	0.81	0/2813
1	B	0.40	0/2059	0.81	0/2762
1	C	0.41	0/2152	0.81	0/2890
1	D	0.41	0/2118	0.81	0/2845
1	E	0.40	0/2114	0.82	0/2839
All	All	0.40	0/10534	0.81	0/14149

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	2056	0	2014	14	0
1	B	2027	0	2033	15	0
1	C	2117	0	2106	12	0
1	D	2085	0	2056	12	0
1	E	2079	0	2068	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
4	A	155	0	0	0	0
4	B	163	0	0	0	0
4	C	146	0	0	0	0
4	D	132	0	0	1	0
4	E	108	0	0	0	0
All	All	11228	0	10337	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 3.

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:E:670:SER:O	1:E:671:LEU:HB2	1.85	0.77
1:D:530:ILE:HG12	1:D:537:ASP:HB3	1.77	0.66
1:E:524:CYS:O	1:E:555:ARG:HD2	2.03	0.59
1:B:392:VAL:HB	1:B:448:ILE:HG22	1.83	0.59
1:D:524:CYS:O	1:D:555:ARG:HD2	2.03	0.58
1:E:659:ASN:O	1:E:663:THR:HG23	2.04	0.57
1:D:392:VAL:HB	1:D:448:ILE:HG23	1.87	0.56
1:C:459:SER:HB3	1:C:643:LYS:O	2.05	0.56
1:D:659:ASN:O	1:D:663:THR:CG2	2.55	0.55
1:C:524:CYS:O	1:C:555:ARG:HD2	2.07	0.55
1:E:546:ILE:O	1:E:547:THR:HG22	2.06	0.55
1:E:393:VAL:HB	1:E:483:LYS:HB2	1.89	0.55
1:A:393:VAL:HG22	1:A:447:LYS:HG3	1.90	0.54
1:D:501:THR:HG23	1:D:504:GLU:H	1.71	0.54
1:B:524:CYS:O	1:B:555:ARG:HD2	2.08	0.53
1:D:659:ASN:O	1:D:663:THR:HG22	2.08	0.53
1:A:607:MET:HE2	1:A:630:PHE:HZ	1.73	0.53
1:D:503:LYS:O	1:D:507:ILE:HG12	2.09	0.53
1:A:448:ILE:HG13	1:A:452:GLN:HB2	1.91	0.52
1:E:470:MET:HB2	1:E:475:LEU:HD23	1.90	0.52
1:B:526:LEU:HB3	1:B:530:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:VAL:HG21	1:B:590:CYS:SG	2.51	0.51
1:A:485:SER:HB2	1:B:527:GLU:HG2	1.93	0.50
1:A:562:VAL:HG11	1:A:594:LEU:HD23	1.92	0.50
1:D:389:THR:HG23	1:D:450:ARG:HB3	1.93	0.50
1:B:455:ALA:HB3	1:B:616:ILE:HG22	1.94	0.48
1:E:477:PRO:HG3	1:E:482:ILE:HD12	1.94	0.48
1:C:562:VAL:HG11	1:C:594:LEU:HD23	1.94	0.48
1:D:562:VAL:HG21	1:D:590:CYS:SG	2.53	0.48
1:C:562:VAL:HG21	1:C:590:CYS:SG	2.54	0.48
1:B:517:TYR:O	1:B:521:ILE:HG12	2.13	0.48
1:A:633:LEU:HD21	1:A:640:PHE:CD2	2.49	0.47
1:A:392:VAL:HB	1:A:448:ILE:HG22	1.95	0.47
1:E:459:SER:HB3	1:E:643:LYS:O	2.15	0.47
1:E:468:LEU:HG	1:E:570:LEU:HB3	1.96	0.47
1:E:562:VAL:HG21	1:E:590:CYS:SG	2.55	0.46
1:A:650:PHE:C	1:A:652:GLN:H	2.24	0.46
1:B:393:VAL:HB	1:B:483:LYS:HB2	1.98	0.45
1:B:468:LEU:HG	1:B:570:LEU:HB3	1.97	0.45
1:C:392:VAL:HB	1:C:448:ILE:HG22	1.99	0.45
1:C:507:ILE:HG23	1:C:510:VAL:O	2.16	0.45
1:E:502:ILE:HG13	1:E:541:LEU:HD11	1.98	0.45
1:A:626:PHE:CE2	1:A:633:LEU:HB2	2.52	0.45
1:C:530:ILE:O	1:C:536:LYS:HA	2.17	0.45
1:C:648:ASP:HB3	1:C:653:PHE:CE1	2.52	0.44
1:B:555:ARG:NH1	1:B:664:GLU:OE2	2.49	0.44
1:A:562:VAL:HG21	1:A:590:CYS:SG	2.58	0.44
1:A:571:LEU:HD21	1:A:595:MET:HE1	1.98	0.44
1:C:458:GLY:O	1:C:646:GLY:HA3	2.18	0.43
1:E:503:LYS:O	1:E:507:ILE:HG12	2.18	0.43
1:D:447:LYS:HB3	4:D:777:HOH:O	2.19	0.43
1:C:648:ASP:HB3	1:C:653:PHE:HE1	1.85	0.42
1:B:470:MET:HB2	1:B:475:LEU:HD23	2.00	0.42
1:B:496:TRP:CZ2	1:B:498:MET:HG3	2.55	0.41
1:A:551:GLY:O	1:A:555:ARG:HG3	2.20	0.41
1:B:648:ASP:HB3	1:B:653:PHE:CZ	2.56	0.41
1:D:392:VAL:HB	1:D:448:ILE:CG2	2.50	0.41
1:E:392:VAL:HB	1:E:448:ILE:HG22	2.02	0.41
1:C:391:GLU:HG3	1:C:449:GLU:HA	2.02	0.41
1:A:503:LYS:O	1:A:507:ILE:HG12	2.21	0.41
1:D:535:GLU:HB2	1:D:539:ILE:HB	2.03	0.41
1:C:459:SER:HA	1:C:646:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:THR:HG23	1:B:450:ARG:HB3	2.02	0.40
1:B:521:ILE:HD12	1:B:530:ILE:CD1	2.52	0.40
1:A:496:TRP:CZ2	1:A:498:MET:HG3	2.57	0.40
1:E:448:ILE:HG13	1:E:452:GLN:HB2	2.04	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	263/291 (90%)	252 (96%)	11 (4%)	0	100	100
1	B	250/291 (86%)	246 (98%)	4 (2%)	0	100	100
1	C	266/291 (91%)	258 (97%)	8 (3%)	0	100	100
1	D	262/291 (90%)	253 (97%)	9 (3%)	0	100	100
1	E	262/291 (90%)	256 (98%)	6 (2%)	0	100	100
All	All	1303/1455 (90%)	1265 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	220/252 (87%)	197 (90%)	23 (10%)	6	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	224/252 (89%)	202 (90%)	22 (10%)	7	5
1	C	232/252 (92%)	210 (90%)	22 (10%)	8	6
1	D	227/252 (90%)	206 (91%)	21 (9%)	8	6
1	E	227/252 (90%)	199 (88%)	28 (12%)	4	3
All	All	1130/1260 (90%)	1014 (90%)	116 (10%)	7	5

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	A	434	SER
1	A	449	GLU
1	A	454	LEU
1	A	468	LEU
1	A	481	LYS
1	A	504	GLU
1	A	511	SER
1	A	533	PHE
1	A	539	ILE
1	A	541	LEU
1	A	571	LEU
1	A	578	LEU
1	A	611	LYS
1	A	617	LEU
1	A	619	LEU
1	A	633	LEU
1	A	634	GLN
1	A	641	SER
1	A	643	LYS
1	A	649	SER
1	A	651	ASP
1	A	671	LEU
1	B	391	GLU
1	B	413	LYS
1	B	431	SER
1	B	434	SER
1	B	454	LEU
1	B	468	LEU
1	B	483	LYS
1	B	528	GLU
1	B	530	ILE

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Mol	Chain	Res	Type
1	B	571	LEU
1	B	578	LEU
1	B	600	ARG
1	B	607	MET
1	B	608	GLU
1	B	617	LEU
1	B	619	LEU
1	B	631	SER
1	B	637	GLN
1	B	642	SER
1	B	643	LYS
1	B	649	SER
1	B	656	GLU
1	C	408	LEU
1	C	411	LYS
1	C	414	GLN
1	C	438	THR
1	C	454	LEU
1	C	468	LEU
1	C	481	LYS
1	C	483	LYS
1	C	487	ARG
1	C	510	VAL
1	C	511	SER
1	C	530	ILE
1	C	535	GLU
1	C	539	ILE
1	C	578	LEU
1	C	600	ARG
1	C	607	MET
1	C	608	GLU
1	C	617	LEU
1	C	619	LEU
1	C	648	ASP
1	C	671	LEU
1	D	426	ASP
1	D	448	ILE
1	D	454	LEU
1	D	483	LYS
1	D	498	MET
1	D	503	LYS
1	D	532	LYS

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Mol	Chain	Res	Type
1	D	536	LYS
1	D	539	ILE
1	D	541	LEU
1	D	571	LEU
1	D	578	LEU
1	D	600	ARG
1	D	606	LYS
1	D	612	LYS
1	D	617	LEU
1	D	619	LEU
1	D	631	SER
1	D	639	ASP
1	D	649	SER
1	D	663	THR
1	E	411	LYS
1	E	434	SER
1	E	436	LEU
1	E	448	ILE
1	E	449	GLU
1	E	454	LEU
1	E	468	LEU
1	E	498	MET
1	E	504	GLU
1	E	511	SER
1	E	514	GLU
1	E	519	SER
1	E	527	GLU
1	E	532	LYS
1	E	541	LEU
1	E	547	THR
1	E	564	LYS
1	E	571	LEU
1	E	578	LEU
1	E	600	ARG
1	E	617	LEU
1	E	619	LEU
1	E	634	GLN
1	E	636	LEU
1	E	642	SER
1	E	643	LYS
1	E	652	GLN
1	E	671	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	A	484	HIS
1	A	493	GLN
1	A	637	GLN
1	B	432	ASN
1	B	452	GLN
1	B	637	GLN
1	C	432	ASN
1	C	484	HIS
1	C	637	GLN
1	D	432	ASN
1	D	538	ASN
1	D	637	GLN
1	E	452	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	1	2	32,33,33	1.15	5 (15%)	48,52,52	1.72	8 (16%)
3	ATP	D	4	2	32,33,33	1.13	3 (9%)	48,52,52	1.77	9 (18%)
3	ATP	A	2	2	32,33,33	1.14	4 (12%)	48,52,52	1.76	9 (18%)
3	ATP	E	5	2	32,33,33	1.09	3 (9%)	48,52,52	1.75	9 (18%)
3	ATP	C	3	2	32,33,33	1.07	3 (9%)	48,52,52	1.74	10 (20%)

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	1	2	-	2/22/38/38	0/3/3/3
3	ATP	D	4	2	-	2/22/38/38	0/3/3/3
3	ATP	A	2	2	-	2/22/38/38	0/3/3/3
3	ATP	E	5	2	-	2/22/38/38	0/3/3/3
3	ATP	C	3	2	-	2/22/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	ATP	C2-N3	2.93	1.39	1.33
3	D	4	ATP	C2-N1	2.89	1.39	1.33
3	C	3	ATP	C2-N3	2.75	1.38	1.33
3	E	5	ATP	C2-N3	2.74	1.38	1.33
3	A	2	ATP	C2-N3	2.73	1.38	1.33
3	B	1	ATP	C2-N1	2.72	1.38	1.33
3	C	3	ATP	C2-N1	2.72	1.38	1.33
3	B	1	ATP	C2-N3	2.69	1.38	1.33
3	E	5	ATP	C2-N1	2.69	1.38	1.33
3	A	2	ATP	C2-N1	2.56	1.38	1.33
3	A	2	ATP	PB-O3B	2.23	1.61	1.59
3	A	2	ATP	C8-N7	2.21	1.35	1.31
3	D	4	ATP	C8-N7	2.17	1.35	1.31
3	E	5	ATP	C8-N7	2.16	1.35	1.31
3	B	1	ATP	C8-N7	2.09	1.35	1.31
3	B	1	ATP	PB-O3B	2.09	1.61	1.59
3	C	3	ATP	C8-N7	2.02	1.35	1.31
3	B	1	ATP	C5-N7	-2.02	1.35	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	ATP	N3-C2-N1	-6.10	119.35	128.58
3	C	3	ATP	N3-C2-N1	-6.05	119.42	128.58
3	D	4	ATP	N3-C2-N1	-5.91	119.64	128.58
3	B	1	ATP	N3-C2-N1	-5.84	119.75	128.58
3	A	2	ATP	N3-C2-N1	-5.79	119.81	128.58
3	D	4	ATP	C5-C4-N3	-4.56	120.43	126.72
3	A	2	ATP	C5-C4-N3	-4.52	120.49	126.72
3	B	1	ATP	C5-C4-N3	-4.50	120.52	126.72
3	C	3	ATP	C5-C4-N3	-4.34	120.74	126.72
3	E	5	ATP	C5-C4-N3	-4.25	120.87	126.72
3	E	5	ATP	N9-C8-N7	-4.06	108.17	113.94
3	A	2	ATP	N9-C8-N7	-4.02	108.23	113.94
3	D	4	ATP	N9-C8-N7	-3.87	108.44	113.94
3	C	3	ATP	N9-C8-N7	-3.84	108.49	113.94
3	B	1	ATP	N9-C8-N7	-3.75	108.61	113.94
3	A	2	ATP	C5-N7-C8	3.62	109.14	103.45
3	D	4	ATP	C2-N3-C4	3.54	120.48	111.83
3	E	5	ATP	C2-N3-C4	3.53	120.45	111.83
3	D	4	ATP	C5-N7-C8	3.51	108.97	103.45
3	C	3	ATP	C2-N3-C4	3.49	120.35	111.83
3	A	2	ATP	C2-N3-C4	3.48	120.33	111.83
3	B	1	ATP	C2-N3-C4	3.48	120.32	111.83
3	E	5	ATP	C5-N7-C8	3.44	108.85	103.45
3	B	1	ATP	C5-N7-C8	3.33	108.68	103.45
3	C	3	ATP	C5-N7-C8	3.30	108.64	103.45
3	B	1	ATP	N3-C4-N9	3.11	132.45	127.17
3	C	3	ATP	N3-C4-N9	3.04	132.34	127.17
3	D	4	ATP	N3-C4-N9	3.01	132.29	127.17
3	A	2	ATP	N3-C4-N9	2.97	132.22	127.17
3	E	5	ATP	N3-C4-N9	2.89	132.08	127.17
3	A	2	ATP	C4-C5-N7	-2.59	107.62	110.58
3	D	4	ATP	O2B-PB-O3A	2.55	114.17	107.27
3	D	4	ATP	C4-C5-N7	-2.51	107.71	110.58
3	A	2	ATP	O2B-PB-O3A	2.51	114.05	107.27
3	B	1	ATP	O2B-PB-O3A	2.36	113.64	107.27
3	E	5	ATP	O2B-PB-O3A	2.28	113.44	107.27
3	E	5	ATP	C4-C5-N7	-2.28	107.98	110.58
3	B	1	ATP	C4-C5-N7	-2.18	108.09	110.58
3	C	3	ATP	C4-C5-N7	-2.17	108.11	110.58
3	C	3	ATP	O2B-PB-O3B	2.12	113.00	107.27
3	E	5	ATP	C4-N9-C8	2.10	107.95	105.74
3	D	4	ATP	O2G-PG-O3B	2.09	111.63	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	ATP	O2G-PG-O3B	2.01	111.37	104.64
3	A	2	ATP	O2G-PG-O3B	2.01	111.37	104.64
3	C	3	ATP	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

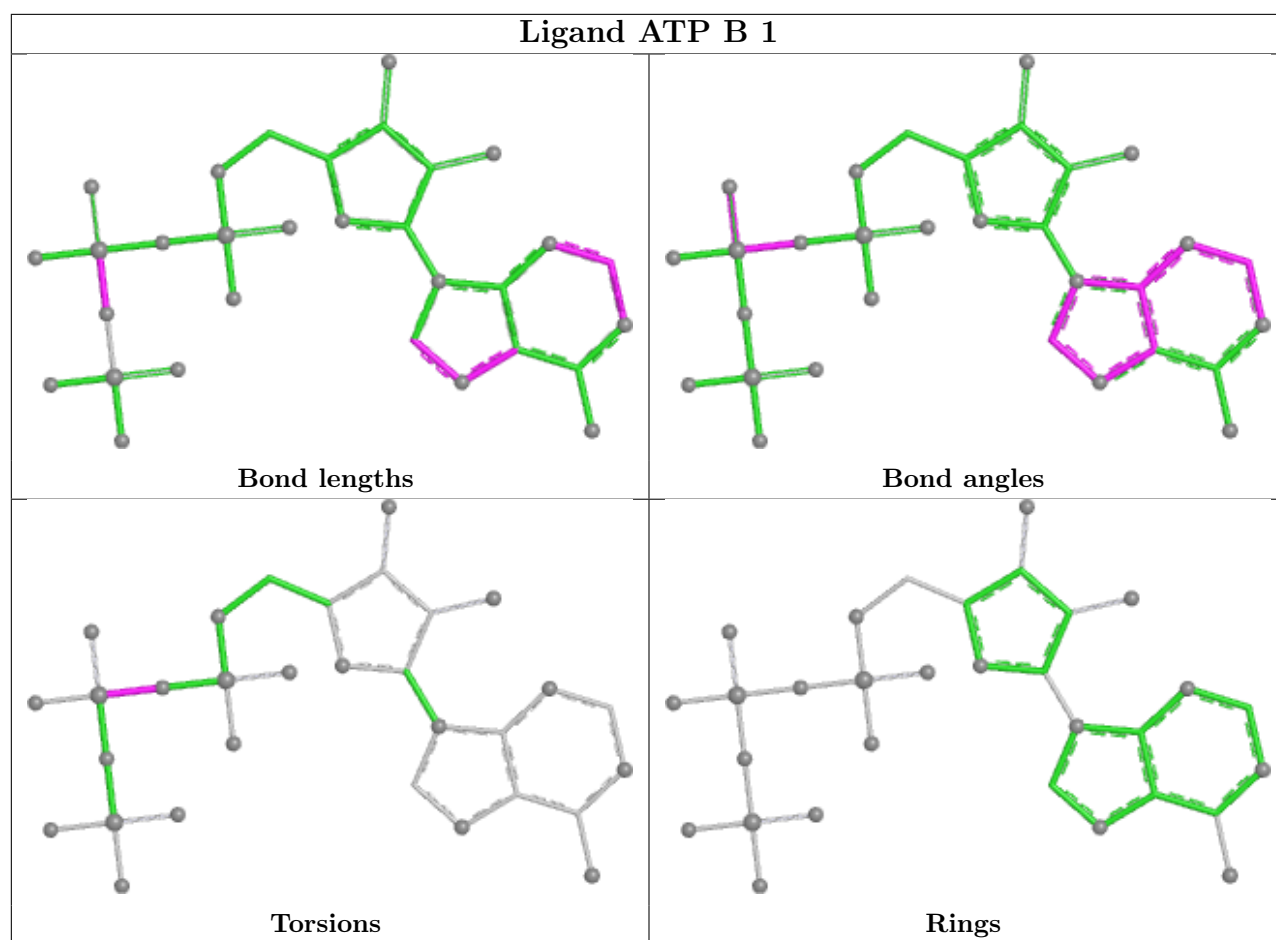
All (10) torsion outliers are listed below:

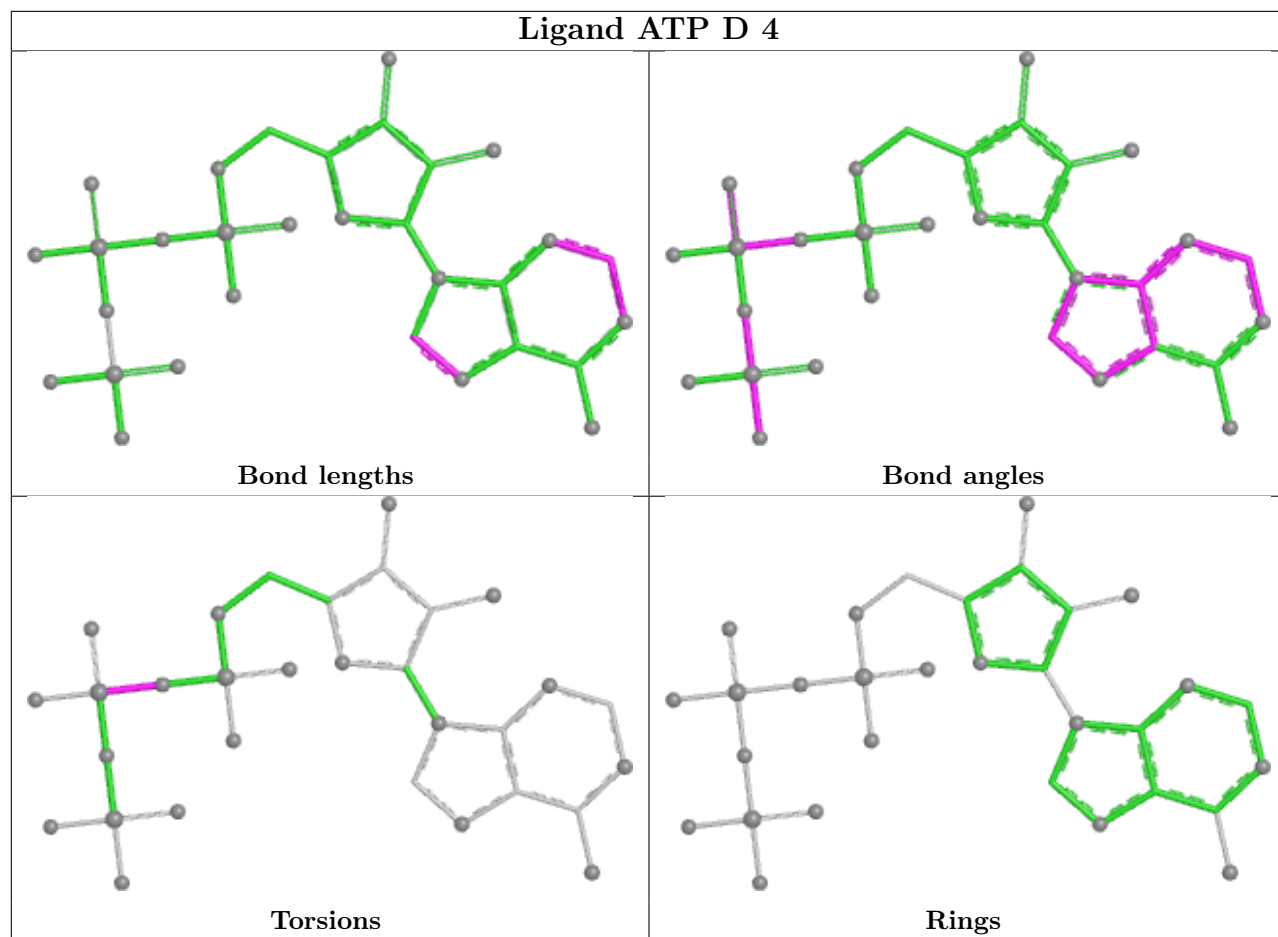
Mol	Chain	Res	Type	Atoms
3	A	2	ATP	PA-O3A-PB-O2B
3	E	5	ATP	PA-O3A-PB-O2B
3	B	1	ATP	PA-O3A-PB-O2B
3	C	3	ATP	PA-O3A-PB-O2B
3	D	4	ATP	PA-O3A-PB-O2B
3	C	3	ATP	PA-O3A-PB-O1B
3	A	2	ATP	PA-O3A-PB-O1B
3	D	4	ATP	PA-O3A-PB-O1B
3	E	5	ATP	PA-O3A-PB-O1B
3	B	1	ATP	PA-O3A-PB-O1B

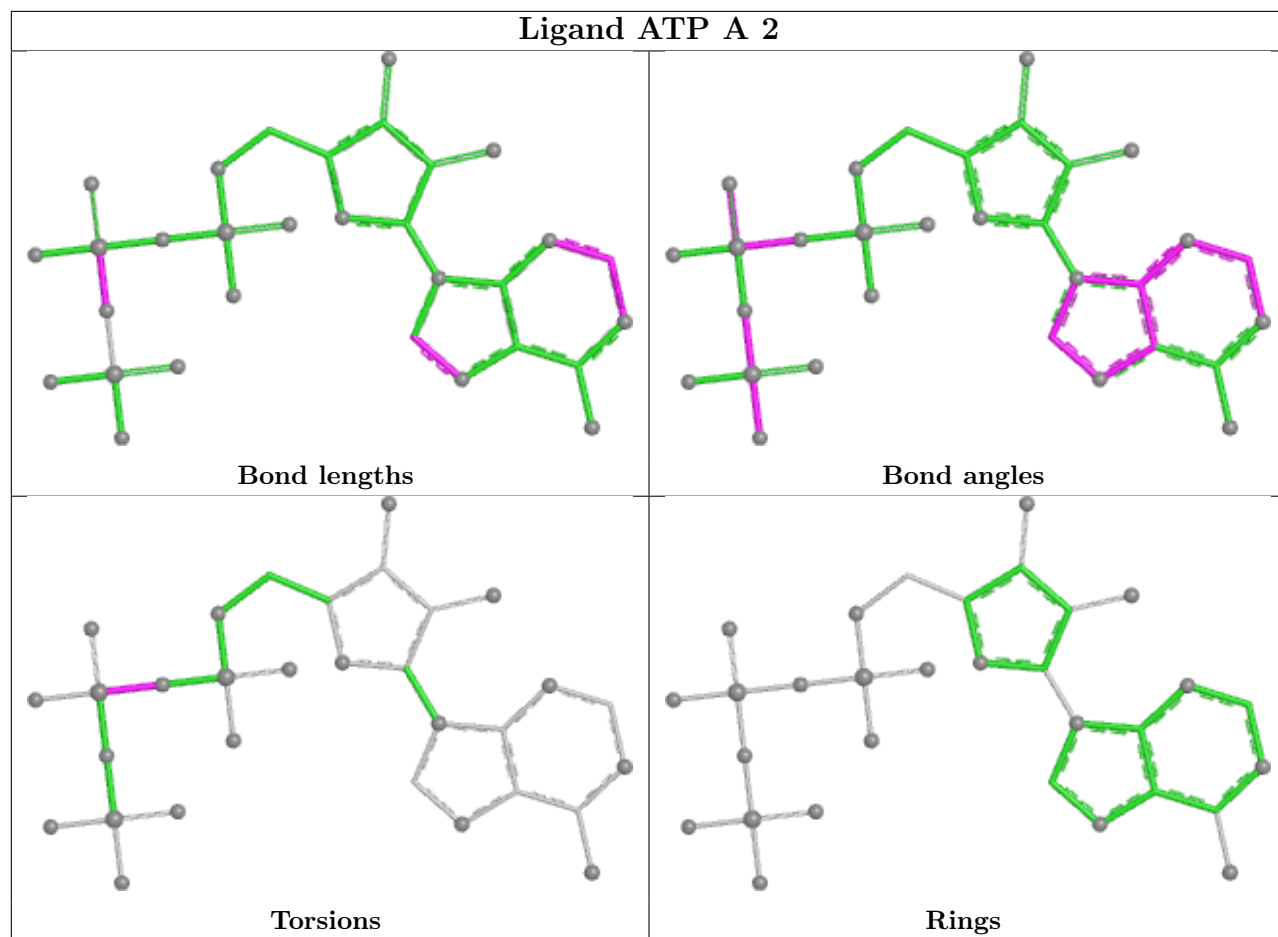
There are no ring outliers.

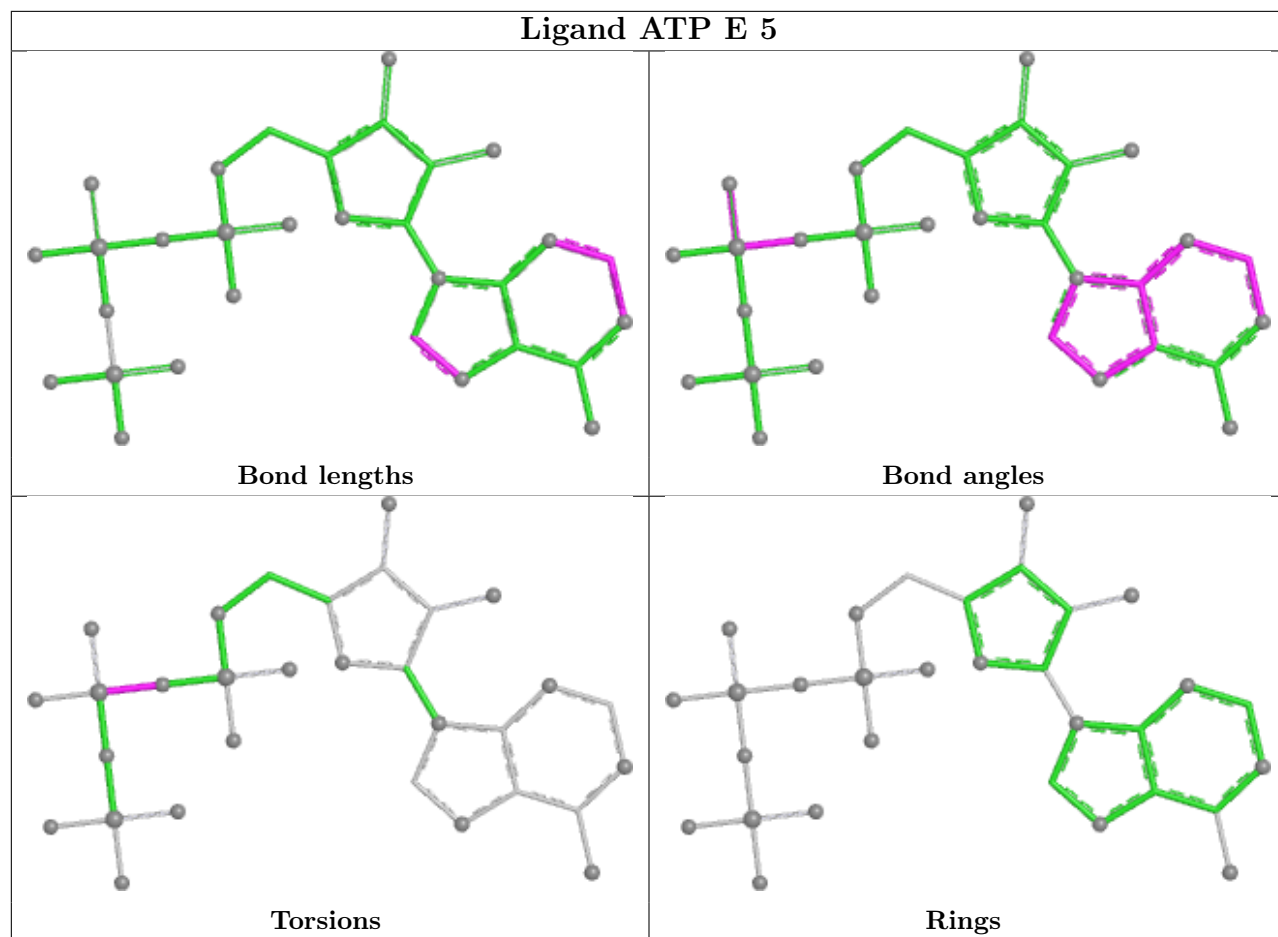
No monomer is involved in short contacts.

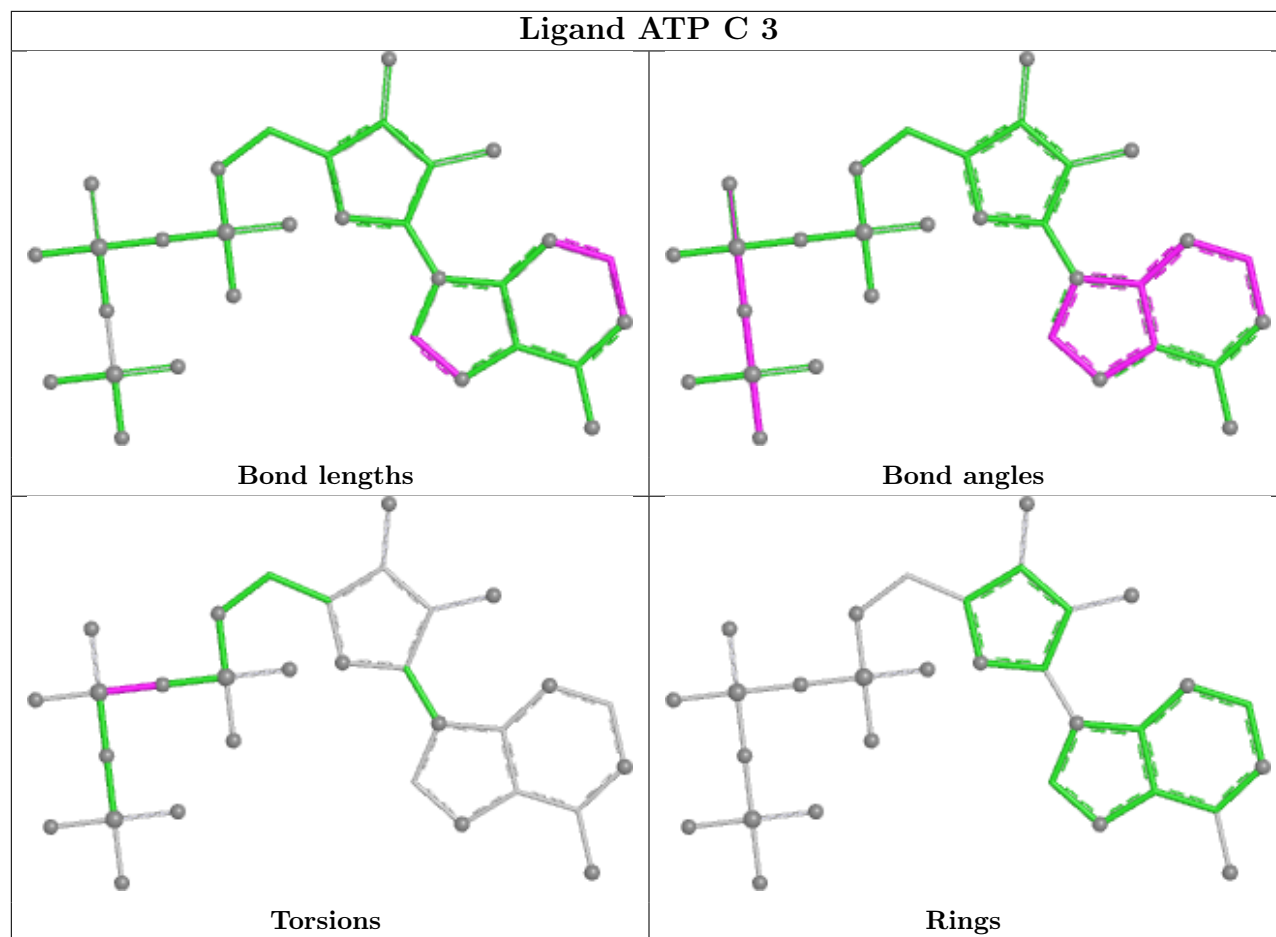
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	267/291 (91%)	0.38	30 (11%) 10 9	10, 28, 62, 73	0
1	B	258/291 (88%)	0.18	11 (4%) 40 39	12, 27, 47, 76	0
1	C	270/291 (92%)	0.24	15 (5%) 30 28	9, 26, 56, 72	0
1	D	268/291 (92%)	0.49	30 (11%) 10 9	11, 33, 59, 69	0
1	E	266/291 (91%)	0.51	21 (7%) 18 17	14, 32, 58, 68	0
All	All	1329/1455 (91%)	0.36	107 (8%) 18 16	9, 29, 59, 76	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	545	GLY	7.4
1	A	544	GLY	6.3
1	A	646	GLY	6.0
1	A	411	LYS	5.2
1	D	426	ASP	5.1
1	E	546	ILE	4.9
1	D	646	GLY	4.8
1	D	647	CYS	4.4
1	C	671	LEU	4.4
1	A	546	ILE	4.1
1	D	645	MET	4.0
1	A	543	GLU	3.9
1	E	671	LEU	3.9
1	A	533	PHE	3.9
1	E	533	PHE	3.8
1	E	542	GLY	3.8
1	C	544	GLY	3.7
1	A	643	LYS	3.7
1	D	546	ILE	3.7
1	C	412	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	546	ILE	3.6
1	A	647	CYS	3.6
1	A	542	GLY	3.5
1	B	412	ALA	3.5
1	C	543	GLU	3.5
1	A	641	SER	3.4
1	C	430	PHE	3.4
1	A	649	SER	3.3
1	D	543	GLU	3.3
1	E	545	GLY	3.2
1	B	547	THR	3.2
1	D	671	LEU	3.2
1	E	448	ILE	3.1
1	A	539	ILE	3.1
1	A	642	SER	3.1
1	B	430	PHE	3.0
1	D	542	GLY	3.0
1	A	645	MET	3.0
1	D	509	GLY	3.0
1	D	403	GLU	3.0
1	D	428	LEU	2.9
1	A	534	ALA	2.9
1	B	648	ASP	2.9
1	A	639	ASP	2.9
1	C	415	ASN	2.9
1	B	411	LYS	2.9
1	D	643	LYS	2.9
1	D	388	SER	2.8
1	C	646	GLY	2.7
1	A	671	LEU	2.7
1	D	644	LEU	2.7
1	A	545	GLY	2.7
1	E	429	SER	2.7
1	D	639	ASP	2.6
1	C	640	PHE	2.6
1	A	651	ASP	2.5
1	A	640	PHE	2.5
1	E	651	ASP	2.5
1	A	644	LEU	2.5
1	A	537	ASP	2.5
1	A	648	ASP	2.5
1	D	547	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	531	SER	2.4
1	C	542	GLY	2.4
1	C	389	THR	2.4
1	E	436	LEU	2.4
1	E	403	GLU	2.4
1	C	649	SER	2.4
1	D	540	VAL	2.3
1	D	537	ASP	2.3
1	E	510	VAL	2.3
1	B	431	SER	2.3
1	E	515	TYR	2.3
1	B	413	LYS	2.3
1	D	539	ILE	2.3
1	A	653	PHE	2.2
1	A	406	GLY	2.2
1	E	407	GLU	2.2
1	A	655	ALA	2.2
1	D	512	TYR	2.2
1	E	430	PHE	2.2
1	A	429	SER	2.2
1	E	501	THR	2.2
1	B	433	PHE	2.2
1	D	648	ASP	2.2
1	B	403	GLU	2.2
1	E	512	TYR	2.1
1	D	672	GLU	2.1
1	E	509	GLY	2.1
1	B	652	GLN	2.1
1	E	409	PHE	2.1
1	A	430	PHE	2.1
1	A	509	GLY	2.1
1	D	404	GLY	2.1
1	D	532	LYS	2.1
1	D	410	GLU	2.1
1	D	513	ASP	2.1
1	D	499	PRO	2.1
1	E	544	GLY	2.0
1	D	409	PHE	2.0
1	C	645	MET	2.0
1	D	390	THR	2.0
1	B	541	LEU	2.0
1	C	635	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	635	ASN	2.0
1	E	538	ASN	2.0
1	E	539	ILE	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](#)

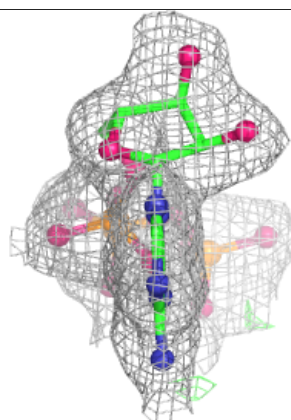
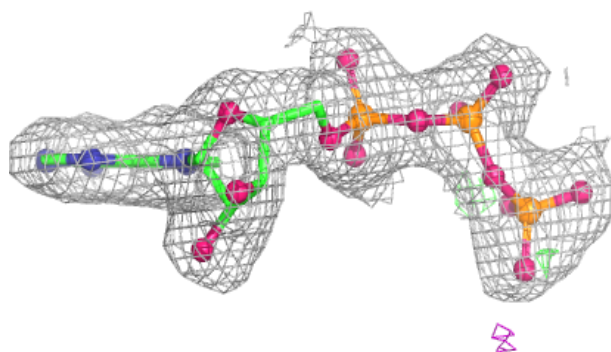
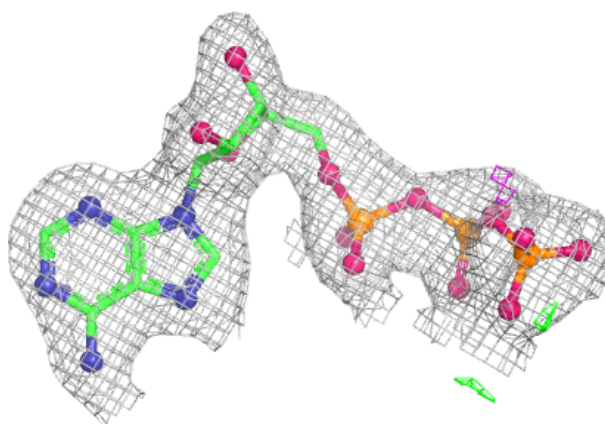
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	D	9	1/1	0.94	0.03	13,13,13,13	0
2	MG	E	10	1/1	0.95	0.04	20,20,20,20	0
2	MG	B	6	1/1	0.96	0.03	18,18,18,18	0
2	MG	C	8	1/1	0.97	0.04	16,16,16,16	0
3	ATP	E	5	31/31	0.97	0.06	17,23,30,32	0
3	ATP	A	2	31/31	0.98	0.05	12,17,25,26	0
3	ATP	B	1	31/31	0.98	0.06	13,20,26,33	0
3	ATP	C	3	31/31	0.98	0.06	9,21,25,29	0
3	ATP	D	4	31/31	0.98	0.05	8,17,24,29	0
2	MG	A	7	1/1	0.98	0.03	18,18,18,18	0

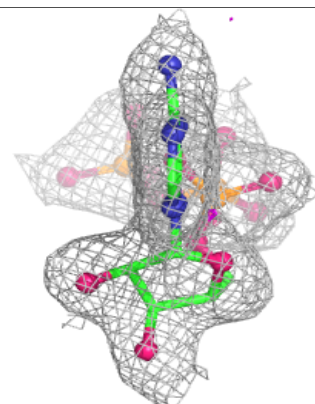
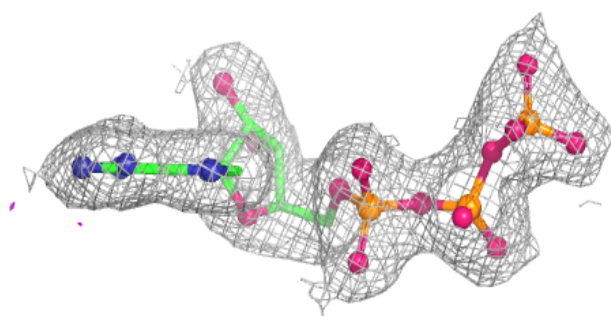
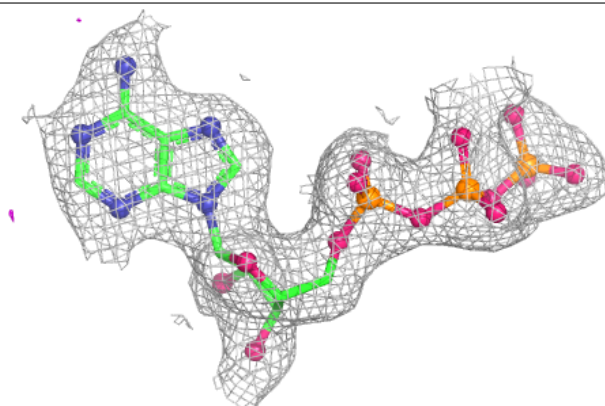
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP E 5:

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

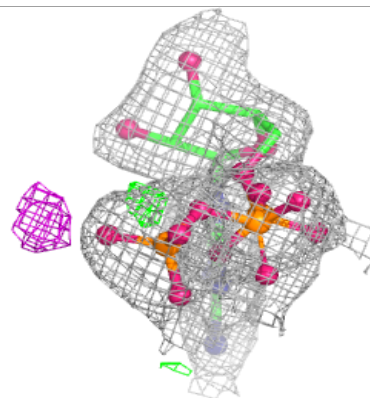
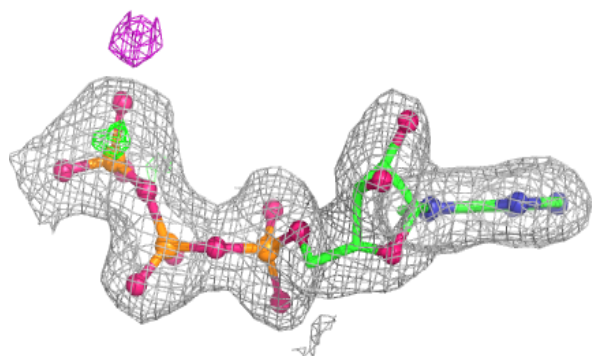
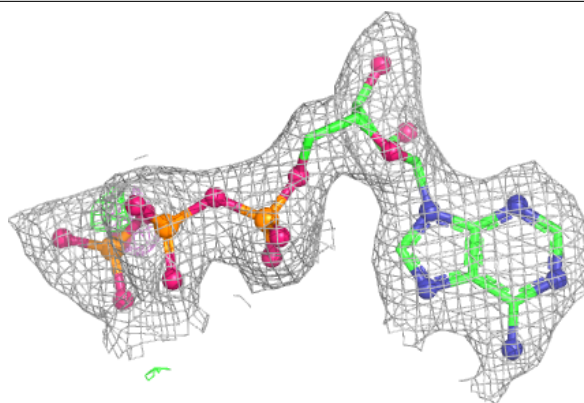
**Electron density around ATP A 2:**

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

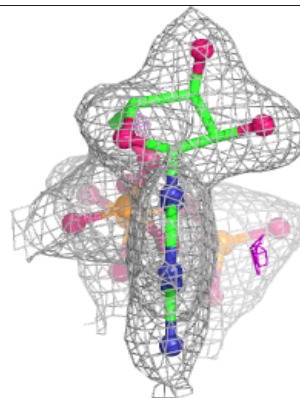
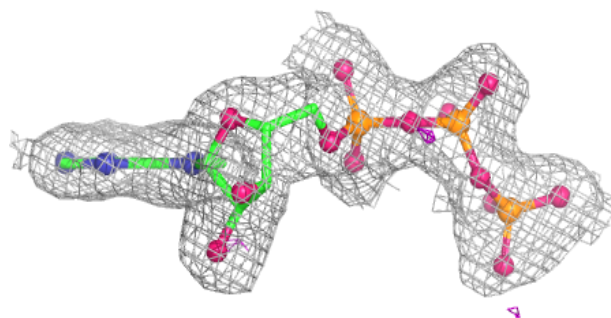
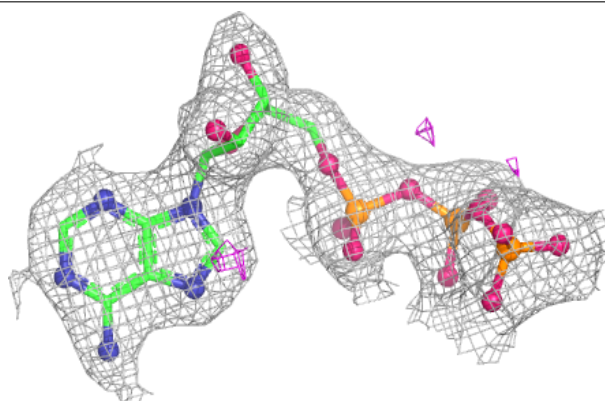


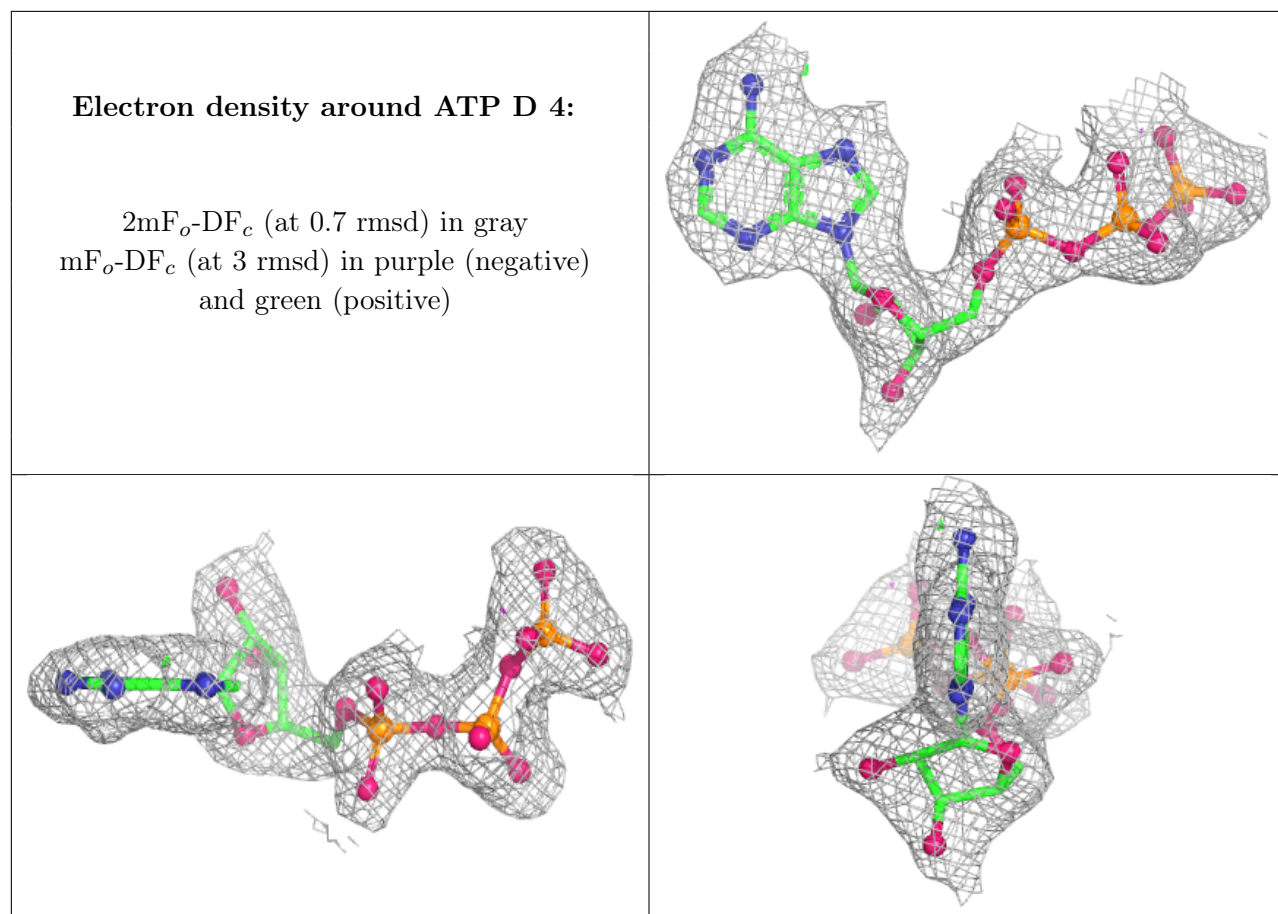
Electron density around ATP B 1:

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

**Electron density around ATP C 3:**

$2mF_o-DF_c$ (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.