



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:05 PM EST

PDB ID : 1R0X  
Title : Cystic fibrosis transmembrane conductance regulator (CFTR) nucleotide-binding domain one (NBD1) with ATP  
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Deposited on : 2003-09-23  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16

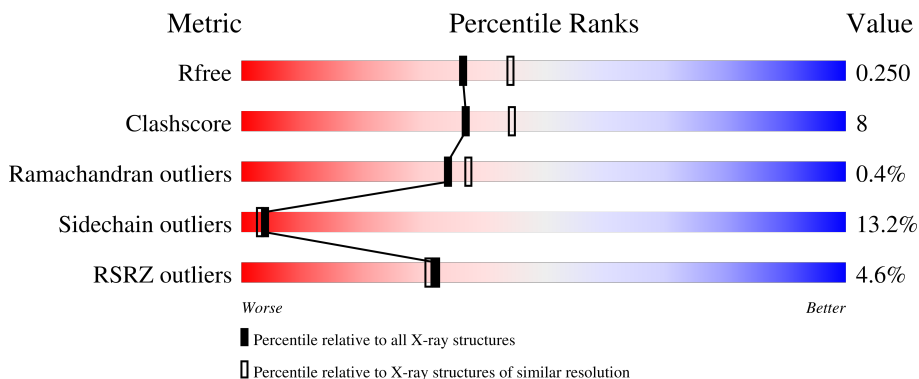
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	286	
1	B	286	
1	C	286	
1	D	286	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8852 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
			Total	C	N	O	S			
1	A	264	2082	1326	344	400	12	0	0	0
1	B	265	2089	1330	345	402	12	0	0	0
1	C	265	2089	1330	345	402	12	0	0	0
1	D	263	2076	1323	343	398	12	0	0	0

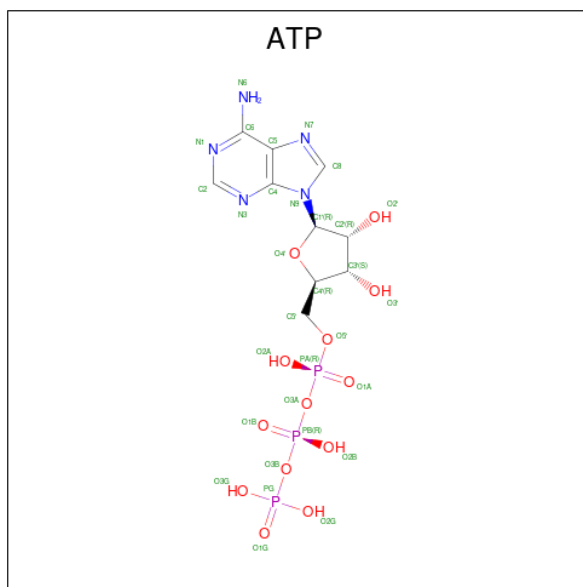
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	-	cloning artifact	UNP P26361
B	388	SER	-	cloning artifact	UNP P26361
C	388	SER	-	cloning artifact	UNP P26361
D	388	SER	-	cloning artifact	UNP P26361

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

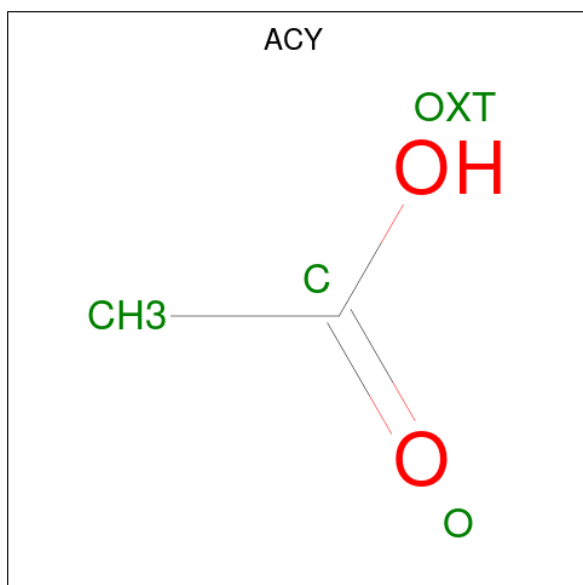
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

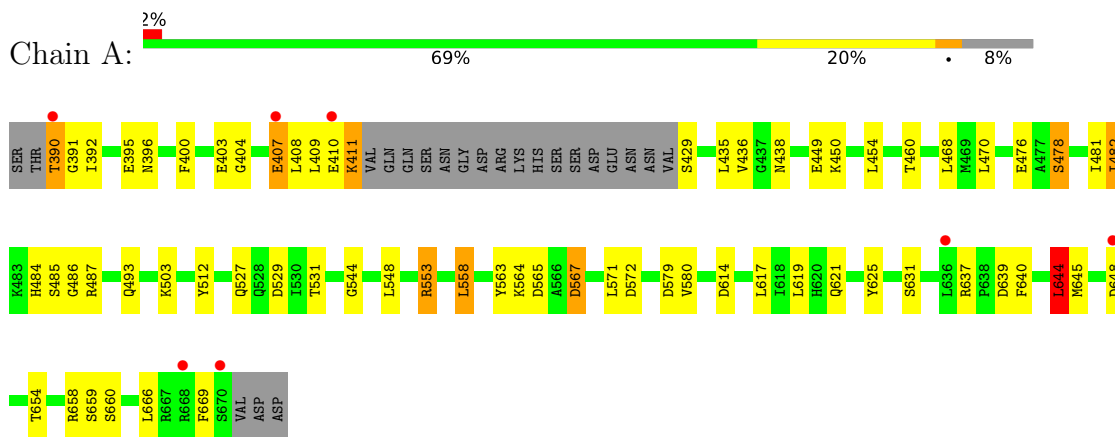
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	95	Total O 95 95	0	0
5	B	96	Total O 96 96	0	0
5	C	105	Total O 105 105	0	0
5	D	68	Total O 68 68	0	0

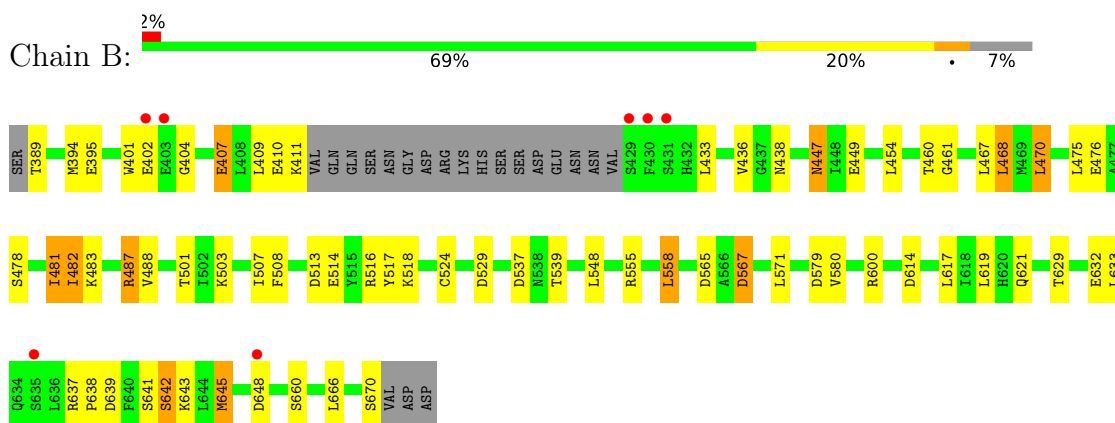
### 3 Residue-property plots [i](#)

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.

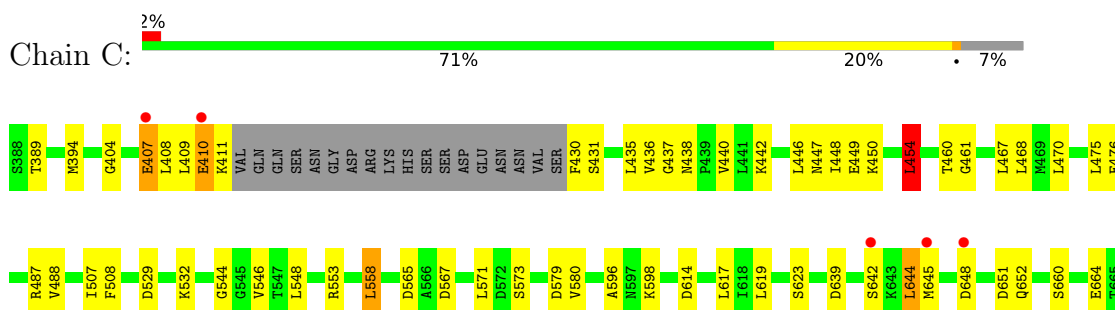
- Molecule 1: Cystic fibrosis transmembrane conductance regulator

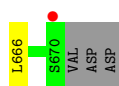


- Molecule 1: Cystic fibrosis transmembrane conductance regulator

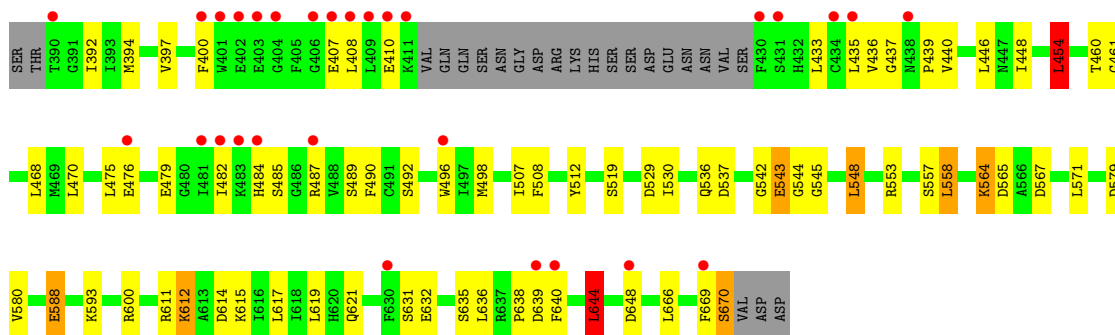


- Molecule 1: Cystic fibrosis transmembrane conductance regulator





- Molecule 1: Cystic fibrosis transmembrane conductance regulator



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.29Å 173.29Å 110.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.20 – 2.20 39.28 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.20-2.20) 98.5 (39.28-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.20Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.211 , 0.266 0.209 , 0.250	Depositor DCC
$R_{free}$ test set	4273 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ACY, 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	0.82	1/2117 (0.0%)	0.93	10/2846 (0.4%)
1	B	0.81	0/2124	0.95	12/2856 (0.4%)
1	C	0.84	0/2124	0.97	13/2856 (0.5%)
1	D	0.71	0/2111	0.89	10/2838 (0.4%)
All	All	0.80	1/8476 (0.0%)	0.93	45/11396 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	563	TYR	CE2-CZ	5.29	1.45	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	ASP	CB-CG-OD2	7.87	125.39	118.30
1	B	513	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	614	ASP	CB-CG-OD2	7.10	124.69	118.30
1	C	579	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	651	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	579	ASP	CB-CG-OD2	6.77	124.40	118.30
1	C	639	ASP	CB-CG-OD2	6.76	124.38	118.30
1	D	579	ASP	CB-CG-OD2	6.75	124.38	118.30
1	B	614	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	614	ASP	CB-CG-OD2	6.61	124.25	118.30
1	D	558	LEU	CB-CG-CD2	6.57	122.17	111.00
1	C	567	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	558	LEU	CB-CG-CD2	6.50	122.04	111.00
1	D	644	LEU	CA-CB-CG	-6.50	100.36	115.30
1	D	529	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	537	ASP	CB-CG-OD2	6.38	124.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	644	LEU	CA-CB-CG	-6.31	100.79	115.30
1	C	644	LEU	CA-CB-CG	-6.18	101.09	115.30
1	B	567	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	565	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	470	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	572	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	565	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	648	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	648	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	470	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	558	LEU	CB-CG-CD2	5.72	120.73	111.00
1	C	529	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	470	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	567	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	614	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	558	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	648	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	553	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	600	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	639	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	567	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	454	LEU	CA-CB-CG	5.22	127.32	115.30
1	C	454	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	558	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	579	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	529	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	558	LEU	CA-CB-CG	5.07	126.95	115.30
1	B	468	LEU	CB-CG-CD1	5.06	119.60	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2082	0	2078	26	0
1	B	2089	0	2085	41	0
1	C	2089	0	2086	33	0
1	D	2076	0	2074	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	2	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	8	0	6	2	0
5	A	95	0	0	2	0
5	B	96	0	0	2	0
5	C	105	0	0	7	0
5	D	68	0	0	3	0
All	All	8852	0	8389	132	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 8.

All (132) 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:467:LEU:HG	5:C:282:HOH:O	1.26	1.35
4:D:9:ACY:H1	5:D:318:HOH:O	1.69	0.93
1:C:436:VAL:HB	1:C:438:ASN:HD21	1.32	0.92
1:A:527:GLN:HB2	5:A:189:HOH:O	1.77	0.85
1:C:389:THR:HG21	1:C:598:LYS:HA	1.60	0.81
1:C:580:VAL:CG2	5:C:245:HOH:O	2.31	0.78
1:B:487:ARG:NH2	1:B:567:ASP:OD1	2.17	0.77
1:D:496:TRP:HH2	1:D:508:PHE:CZ	2.03	0.76
1:C:436:VAL:HB	1:C:438:ASN:ND2	2.05	0.72
1:C:440:VAL:HG11	1:C:475:LEU:HD21	1.69	0.72
1:D:397:VAL:HG11	1:D:470:LEU:HD21	1.71	0.70
1:B:436:VAL:HB	1:B:438:ASN:HD21	1.55	0.70
1:D:400:PHE:HA	1:D:439:PRO:HA	1.73	0.70
1:D:496:TRP:CH2	1:D:508:PHE:CZ	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ARG:NH2	1:B:567:ASP:CG	2.45	0.70
1:A:395:GLU:HB2	1:A:481:ILE:HB	1.74	0.68
1:D:437:GLY:HA2	5:D:374:HOH:O	1.94	0.67
1:B:516:ARG:HH11	1:B:516:ARG:HG3	1.61	0.66
1:B:629:THR:OG1	1:B:632:GLU:HG3	1.95	0.65
1:A:482:ILE:HD11	1:A:484:HIS:HD2	1.61	0.63
1:C:580:VAL:HG23	5:C:245:HOH:O	1.96	0.63
1:C:404:GLY:HA2	1:C:407:GLU:HG2	1.81	0.62
1:D:487:ARG:HG3	1:D:487:ARG:HH21	1.64	0.62
1:A:390:THR:HA	1:A:450:LYS:NZ	2.15	0.61
1:C:430:PHE:N	5:C:258:HOH:O	2.33	0.61
1:B:476:GLU:HG2	5:B:93:HOH:O	2.00	0.61
1:A:544:GLY:O	1:A:553:ARG:HD3	2.00	0.61
1:D:588:GLU:HG2	5:D:355:HOH:O	2.00	0.61
1:C:389:THR:O	1:C:450:LYS:HE3	2.01	0.60
5:A:62:HOH:O	1:B:621:GLN:HG2	2.01	0.60
1:B:476:GLU:H	1:B:476:GLU:CD	2.02	0.59
1:B:404:GLY:O	1:B:407:GLU:HG2	2.04	0.58
1:A:482:ILE:HD11	1:A:484:HIS:CD2	2.38	0.57
1:A:436:VAL:CG1	1:A:438:ASN:HD21	2.18	0.57
1:A:390:THR:HG21	1:A:485:SER:H	1.68	0.57
1:D:448:ILE:HD13	1:D:615:LYS:HD2	1.87	0.57
1:C:409:LEU:C	1:C:411:LYS:H	2.07	0.56
1:A:409:LEU:HD13	3:A:1:ATP:C8	2.41	0.56
1:A:390:THR:HG23	1:A:391:GLY:O	2.06	0.55
1:B:404:GLY:HA2	1:B:407:GLU:HG2	1.88	0.55
1:B:461:GLY:O	3:B:2:ATP:H3'	2.08	0.54
1:D:436:VAL:O	1:D:436:VAL:HG12	2.08	0.53
1:B:395:GLU:HB2	1:B:481:ILE:HG23	1.90	0.53
1:B:516:ARG:NH1	1:B:516:ARG:HG3	2.20	0.53
1:B:487:ARG:HG3	1:B:487:ARG:NH2	2.24	0.53
1:D:635:SER:O	1:D:638:PRO:HD3	2.09	0.53
1:A:436:VAL:HG12	1:A:438:ASN:HD21	1.73	0.52
1:C:394:MET:HB2	1:C:446:LEU:HG	1.90	0.52
1:D:543:GLU:HG3	1:D:544:GLY:N	2.24	0.52
1:D:640:PHE:CE2	1:D:644:LEU:HD13	2.45	0.52
1:B:436:VAL:HB	1:B:438:ASN:ND2	2.25	0.52
1:C:436:VAL:O	1:C:436:VAL:HG12	2.10	0.52
1:C:448:ILE:HD11	1:C:454:LEU:HG	1.92	0.51
1:B:409:LEU:C	1:B:411:LYS:H	2.13	0.51
1:C:461:GLY:O	3:C:3:ATP:H3'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:GLY:HA2	1:C:407:GLU:CG	2.40	0.51
1:D:507:ILE:CD1	1:D:512:TYR:HD1	2.24	0.51
1:A:436:VAL:HG12	1:A:438:ASN:ND2	2.25	0.51
1:A:409:LEU:C	1:A:411:LYS:H	2.14	0.50
1:B:487:ARG:HG3	1:B:487:ARG:HH21	1.76	0.50
1:B:638:PRO:O	1:B:642:SER:HB3	2.11	0.50
1:A:503:LYS:NZ	1:A:512:TYR:CE1	2.80	0.50
1:D:542:GLY:N	4:D:8:ACY:OXT	2.39	0.50
1:B:633:LEU:HD12	1:B:637:ARG:HB2	1.93	0.50
1:C:404:GLY:O	1:C:407:GLU:HG2	2.12	0.50
1:B:394:MET:CE	1:B:467:LEU:HD11	2.42	0.50
1:C:596:ALA:O	5:C:295:HOH:O	2.19	0.50
1:B:487:ARG:HH11	1:B:565:ASP:CG	2.14	0.50
1:D:394:MET:HB2	1:D:446:LEU:HG	1.93	0.50
1:B:447:ASN:HD22	1:B:447:ASN:C	2.15	0.50
1:C:404:GLY:CA	1:C:407:GLU:HG2	2.42	0.50
1:C:448:ILE:CD1	1:C:454:LEU:HG	2.42	0.49
1:A:639:ASP:HB3	1:A:669:PHE:CE1	2.47	0.49
1:C:440:VAL:HG11	1:C:475:LEU:CD2	2.38	0.49
1:C:440:VAL:CG1	1:C:475:LEU:HD21	2.39	0.49
1:D:507:ILE:HD13	1:D:512:TYR:HD1	1.78	0.49
1:A:476:GLU:CD	1:A:476:GLU:H	2.15	0.49
1:A:654:THR:O	1:A:658:ARG:HG3	2.13	0.49
1:B:507:ILE:HD11	1:B:517:TYR:CD1	2.48	0.48
1:C:409:LEU:O	1:C:411:LYS:N	2.46	0.48
1:B:487:ARG:CG	1:B:567:ASP:OD2	2.62	0.48
1:D:490:PHE:CE2	1:D:492:SER:HB3	2.48	0.48
1:D:639:ASP:HB3	1:D:669:PHE:CD1	2.48	0.48
1:A:436:VAL:HB	1:A:438:ASN:HD21	1.79	0.48
1:B:470:LEU:HD12	1:B:475:LEU:O	2.14	0.47
1:B:482:ILE:HD11	5:B:198:HOH:O	2.13	0.47
1:B:389:THR:N	1:B:567:ASP:OD1	2.48	0.47
1:D:448:ILE:CD1	1:D:615:LYS:HD2	2.43	0.47
1:D:545:GLY:O	1:D:548:LEU:HB2	2.14	0.47
1:B:487:ARG:HG3	1:B:567:ASP:OD2	2.15	0.46
1:A:486:GLY:HA3	1:A:567:ASP:OD2	2.16	0.46
1:C:409:LEU:C	1:C:411:LYS:N	2.68	0.46
1:A:487:ARG:HG3	1:A:487:ARG:HH21	1.80	0.46
1:B:487:ARG:CG	1:B:487:ARG:HH21	2.29	0.46
1:D:507:ILE:CD1	1:D:512:TYR:CD1	2.98	0.46
1:A:400:PHE:HD2	1:A:478:SER:HG	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLY:HA2	5:C:262:HOH:O	2.16	0.45
1:D:440:VAL:HG11	1:D:475:LEU:HD21	1.99	0.45
1:A:390:THR:HA	1:A:450:LYS:HZ3	1.79	0.45
1:C:430:PHE:CA	5:C:258:HOH:O	2.65	0.45
1:B:501:THR:HA	1:B:539:THR:O	2.17	0.45
1:D:489:SER:HB2	1:D:564:LYS:HD2	1.99	0.45
1:B:503:LYS:HD2	1:B:517:TYR:CZ	2.52	0.44
1:C:404:GLY:C	1:C:407:GLU:HG2	2.37	0.44
1:C:580:VAL:HG21	1:C:652:GLN:HG2	2.00	0.44
1:C:475:LEU:HD12	1:C:476:GLU:OE1	2.17	0.44
1:D:496:TRP:HH2	1:D:508:PHE:CE2	2.35	0.44
1:D:530:ILE:O	1:D:536:GLN:HA	2.17	0.44
1:A:640:PHE:CZ	1:A:644:LEU:HD13	2.52	0.44
1:B:514:GLU:O	1:B:518:LYS:HG3	2.18	0.43
1:B:401:TRP:CE2	1:B:433:LEU:HD13	2.54	0.43
1:C:436:VAL:CB	1:C:438:ASN:HD21	2.15	0.43
1:D:588:GLU:OE2	1:D:593:LYS:NZ	2.48	0.43
1:D:448:ILE:HD11	1:D:454:LEU:HG	2.01	0.43
1:D:612:LYS:HD2	1:D:612:LYS:HA	1.72	0.43
1:B:436:VAL:CB	1:B:438:ASN:HD21	2.29	0.42
1:A:404:GLY:HA2	1:A:407:GLU:HG2	2.00	0.42
1:D:461:GLY:O	3:D:4:ATP:H2'	2.20	0.42
1:D:487:ARG:HG3	1:D:487:ARG:NH2	2.32	0.42
1:D:544:GLY:O	1:D:553:ARG:HD3	2.20	0.42
1:B:507:ILE:O	1:B:508:PHE:C	2.58	0.42
1:A:625:TYR:CE1	1:A:637:ARG:HD2	2.55	0.42
1:B:524:CYS:O	1:B:555:ARG:HD2	2.20	0.41
1:B:641:SER:O	1:B:645:MET:HB2	2.21	0.41
1:B:404:GLY:HA2	1:B:407:GLU:CG	2.49	0.41
1:C:544:GLY:O	1:C:553:ARG:HD3	2.19	0.41
1:B:389:THR:HG22	1:C:449:GLU:HG3	2.03	0.41
1:A:409:LEU:HD13	3:A:1:ATP:H8	1.83	0.41
1:B:487:ARG:HH21	1:B:567:ASP:CG	2.13	0.41
1:B:394:MET:HE3	1:B:467:LEU:HD11	2.03	0.40
1:D:669:PHE:O	1:D:670:SER:HB2	2.21	0.40
1:C:394:MET:CE	1:C:467:LEU:HD11	2.51	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	260/286 (91%)	251 (96%)	8 (3%)	1 (0%)	34	37
1	B	261/286 (91%)	252 (97%)	8 (3%)	1 (0%)	34	37
1	C	261/286 (91%)	249 (95%)	10 (4%)	2 (1%)	19	19
1	D	259/286 (91%)	245 (95%)	14 (5%)	0	100	100
All	All	1041/1144 (91%)	997 (96%)	40 (4%)	4 (0%)	34	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	410	GLU
1	C	508	PHE
1	A	410	GLU
1	B	410	GLU

### 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	231/252 (92%)	199 (86%)	32 (14%)	3	3
1	B	232/252 (92%)	207 (89%)	25 (11%)	6	6
1	C	232/252 (92%)	204 (88%)	28 (12%)	5	4
1	D	230/252 (91%)	193 (84%)	37 (16%)	2	2
All	All	925/1008 (92%)	803 (87%)	122 (13%)	4	3

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	THR
1	A	392	ILE
1	A	396	ASN
1	A	403	GLU
1	A	407	GLU
1	A	408	LEU
1	A	411	LYS
1	A	429	SER
1	A	435	LEU
1	A	449	GLU
1	A	454	LEU
1	A	460	THR
1	A	468	LEU
1	A	478	SER
1	A	482	ILE
1	A	493	GLN
1	A	531	THR
1	A	548	LEU
1	A	558	LEU
1	A	564	LYS
1	A	571	LEU
1	A	580	VAL
1	A	617	LEU
1	A	619	LEU
1	A	621	GLN
1	A	631	SER
1	A	644	LEU
1	A	645	MET
1	A	648	ASP
1	A	659	SER
1	A	660	SER
1	A	666	LEU
1	B	402	GLU
1	B	407	GLU
1	B	447	ASN
1	B	449	GLU
1	B	454	LEU
1	B	460	THR
1	B	468	LEU
1	B	478	SER
1	B	481	ILE
1	B	482	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	483	LYS
1	B	487	ARG
1	B	488	VAL
1	B	548	LEU
1	B	558	LEU
1	B	571	LEU
1	B	580	VAL
1	B	617	LEU
1	B	619	LEU
1	B	642	SER
1	B	643	LYS
1	B	645	MET
1	B	660	SER
1	B	666	LEU
1	B	670	SER
1	C	407	GLU
1	C	408	LEU
1	C	410	GLU
1	C	431	SER
1	C	435	LEU
1	C	442	LYS
1	C	447	ASN
1	C	454	LEU
1	C	460	THR
1	C	468	LEU
1	C	487	ARG
1	C	488	VAL
1	C	507	ILE
1	C	532	LYS
1	C	546	VAL
1	C	548	LEU
1	C	558	LEU
1	C	571	LEU
1	C	573	SER
1	C	617	LEU
1	C	619	LEU
1	C	623	SER
1	C	642	SER
1	C	644	LEU
1	C	645	MET
1	C	660	SER
1	C	664	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	666	LEU
1	D	392	ILE
1	D	407	GLU
1	D	408	LEU
1	D	410	GLU
1	D	433	LEU
1	D	435	LEU
1	D	454	LEU
1	D	460	THR
1	D	468	LEU
1	D	476	GLU
1	D	479	GLU
1	D	482	ILE
1	D	484	HIS
1	D	485	SER
1	D	498	MET
1	D	519	SER
1	D	537	ASP
1	D	543	GLU
1	D	548	LEU
1	D	557	SER
1	D	558	LEU
1	D	564	LYS
1	D	571	LEU
1	D	580	VAL
1	D	588	GLU
1	D	600	ARG
1	D	611	ARG
1	D	612	LYS
1	D	617	LEU
1	D	619	LEU
1	D	621	GLN
1	D	631	SER
1	D	632	GLU
1	D	636	LEU
1	D	644	LEU
1	D	666	LEU
1	D	670	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	ASN
1	A	484	HIS
1	A	538	ASN
1	B	438	ASN
1	B	447	ASN
1	B	538	ASN
1	C	438	ASN
1	C	447	ASN
1	C	538	ASN
1	D	438	ASN
1	D	538	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	A	1	2	26,33,33	1.24	2 (7%)	31,52,52	1.55	7 (22%)
4	ACY	D	8	-	1,3,3	1.92	0	0,3,3	0.00	-
3	ATP	B	2	2	26,33,33	1.11	2 (7%)	31,52,52	1.41	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACY	C	7	-	1,3,3	1.98	0	0,3,3	0.00	-
4	ACY	D	9	-	1,3,3	0.28	0	0,3,3	0.00	-
3	ATP	C	3	2	26,33,33	1.19	2 (7%)	31,52,52	1.45	2 (6%)
4	ACY	A	5	-	1,3,3	1.55	0	0,3,3	0.00	-
3	ATP	D	4	2	26,33,33	1.27	2 (7%)	31,52,52	1.59	5 (16%)
4	ACY	A	10	-	1,3,3	0.30	0	0,3,3	0.00	-
4	ACY	B	6	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-

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	2	2	-	2/18/38/38	0/3/3/3
3	ATP	A	1	2	-	1/18/38/38	0/3/3/3
3	ATP	D	4	2	-	3/18/38/38	0/3/3/3
3	ATP	C	3	2	-	0/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	ATP	C2-N3	4.63	1.39	1.32
3	A	1	ATP	C2-N3	4.24	1.38	1.32
3	C	3	ATP	C2-N3	3.82	1.38	1.32
3	B	2	ATP	C2-N3	3.71	1.38	1.32
3	D	4	ATP	C2-N1	3.00	1.39	1.33
3	C	3	ATP	C2-N1	2.85	1.39	1.33
3	A	1	ATP	C2-N1	2.75	1.39	1.33
3	B	2	ATP	C2-N1	2.38	1.38	1.33
4	B	6	ACY	CH3-C	2.28	1.51	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	ATP	N3-C2-N1	-5.90	119.45	128.68
3	B	2	ATP	N3-C2-N1	-5.54	120.02	128.68
3	D	4	ATP	N3-C2-N1	-5.34	120.34	128.68
3	A	1	ATP	N3-C2-N1	-4.86	121.09	128.68
3	D	4	ATP	PB-O3B-PG	-3.49	120.86	132.83
3	C	3	ATP	PA-O3A-PB	-3.33	121.39	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	ATP	C3'-C2'-C1'	2.94	105.40	100.98
3	A	1	ATP	C3'-C2'-C1'	2.91	105.36	100.98
3	A	1	ATP	PA-O3A-PB	-2.44	124.44	132.83
3	A	1	ATP	O2'-C2'-C1'	-2.43	101.88	110.85
3	B	2	ATP	O2G-PG-O3B	2.43	112.78	104.64
3	D	4	ATP	PA-O3A-PB	-2.42	124.51	132.83
3	A	1	ATP	O3G-PG-O3B	2.29	112.31	104.64
3	B	2	ATP	PA-O3A-PB	-2.18	125.35	132.83
3	B	2	ATP	PB-O3B-PG	-2.10	125.60	132.83
3	D	4	ATP	O3G-PG-O3B	2.10	111.67	104.64
3	A	1	ATP	O2G-PG-O3B	2.10	111.66	104.64
3	A	1	ATP	PB-O3B-PG	-2.09	125.66	132.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	ATP	C5'-O5'-PA-O1A
3	D	4	ATP	C5'-O5'-PA-O2A
3	B	2	ATP	PA-O3A-PB-O2B
3	A	1	ATP	O4'-C4'-C5'-O5'
3	D	4	ATP	C5'-O5'-PA-O3A
3	B	2	ATP	C5'-O5'-PA-O1A

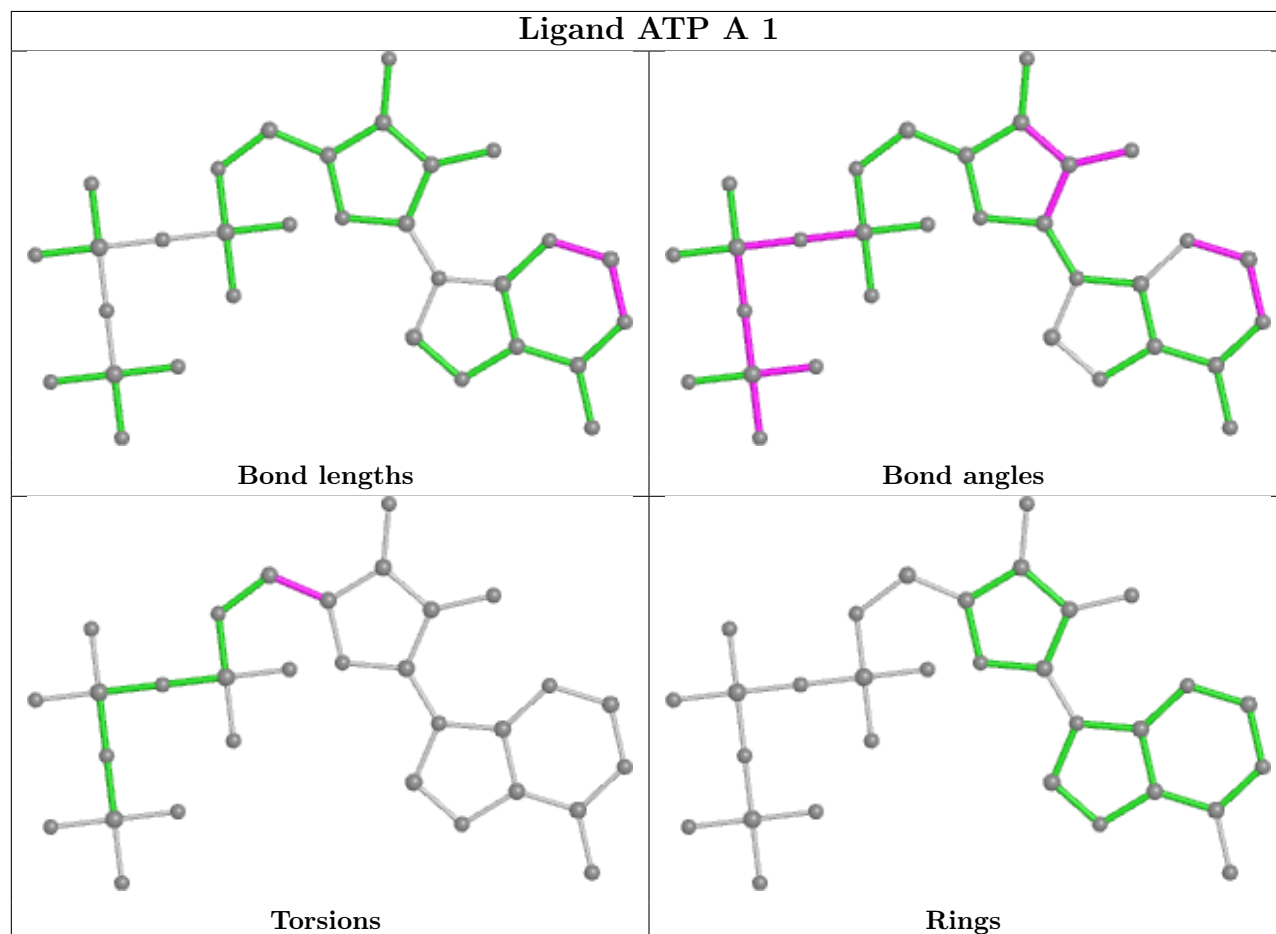
There are no ring outliers.

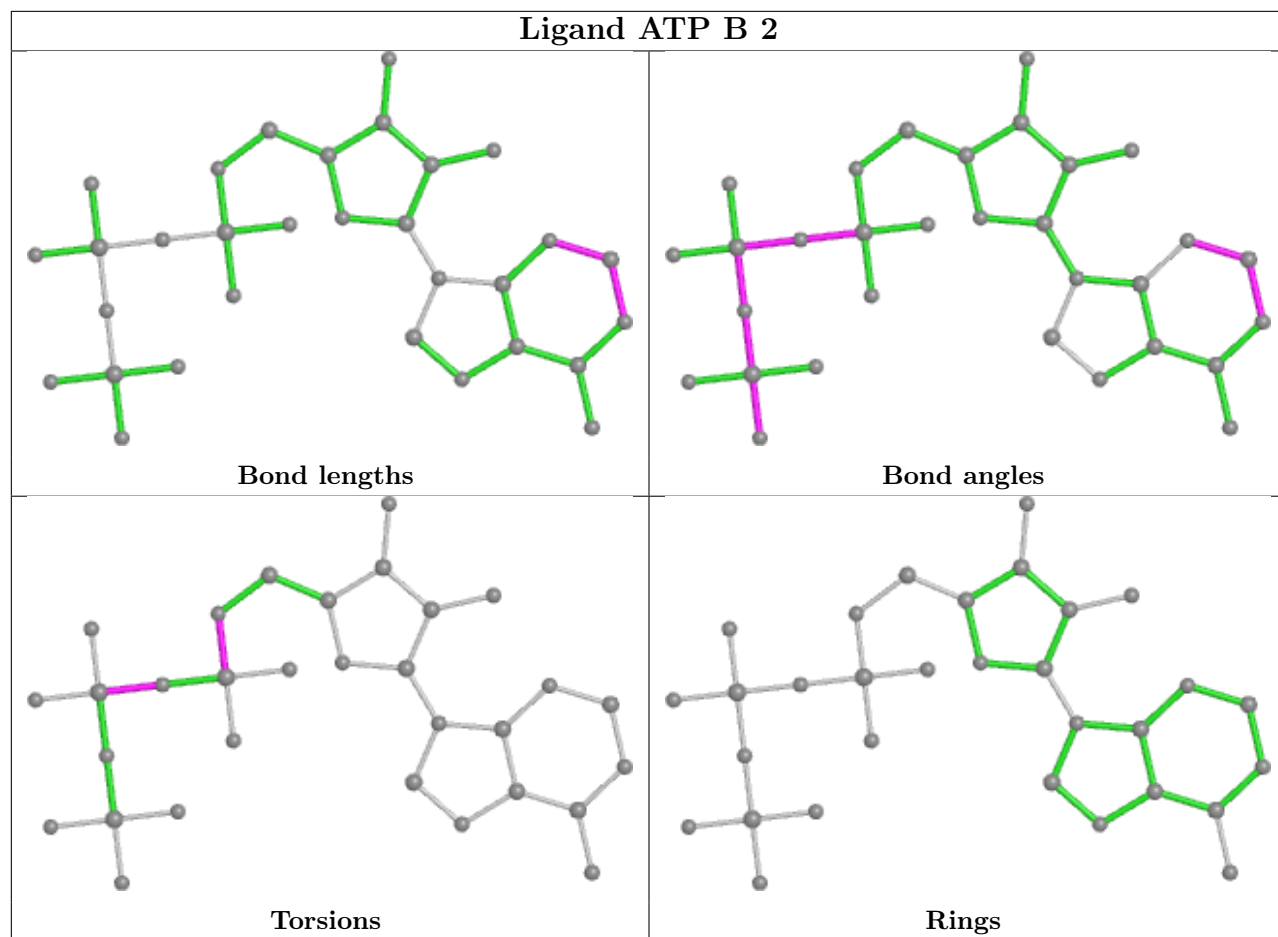
6 monomers are involved in 7 short contacts:

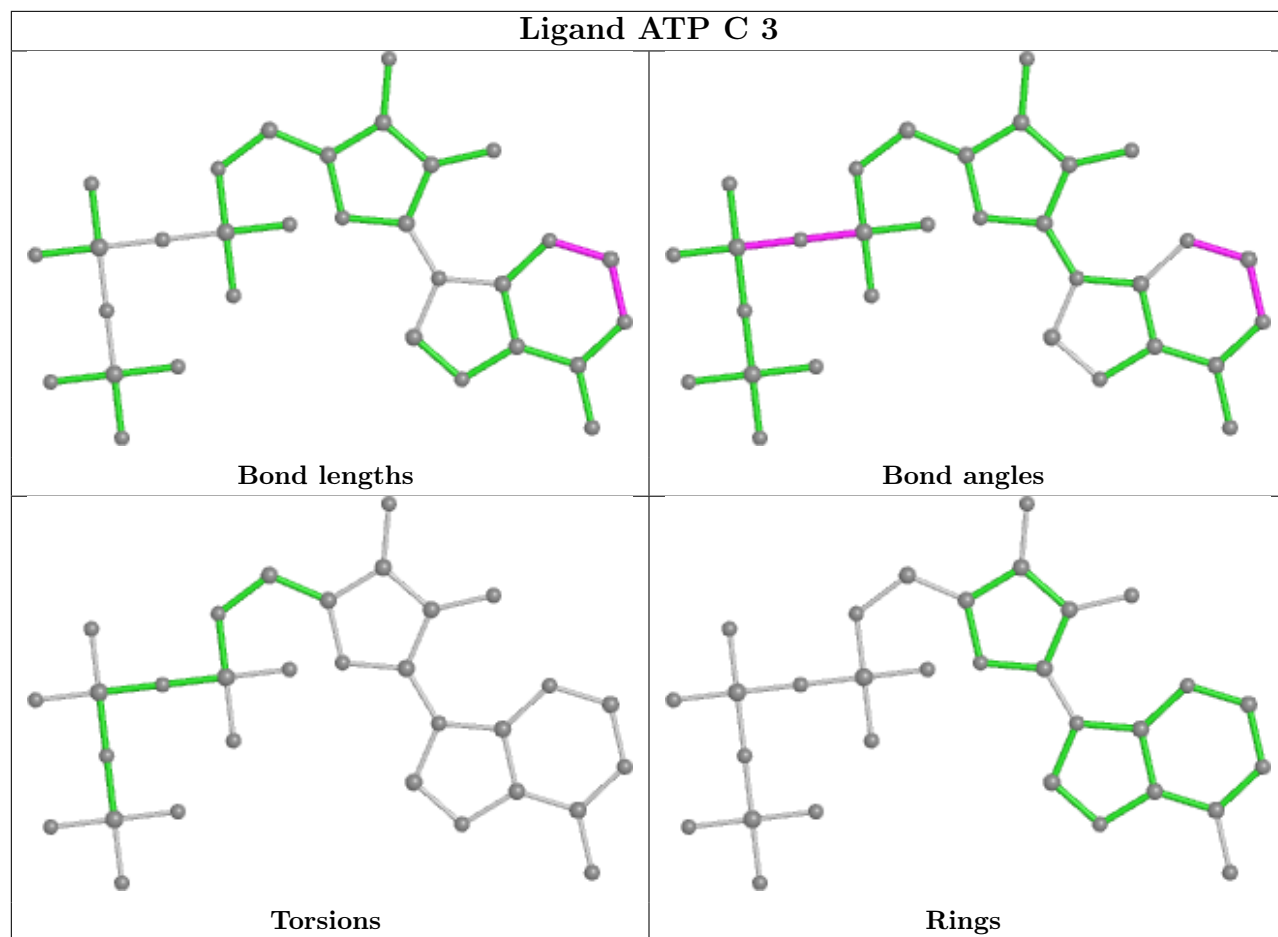
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	ATP	2	0
4	D	8	ACY	1	0
3	B	2	ATP	1	0
4	D	9	ACY	1	0
3	C	3	ATP	1	0
3	D	4	ATP	1	0

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

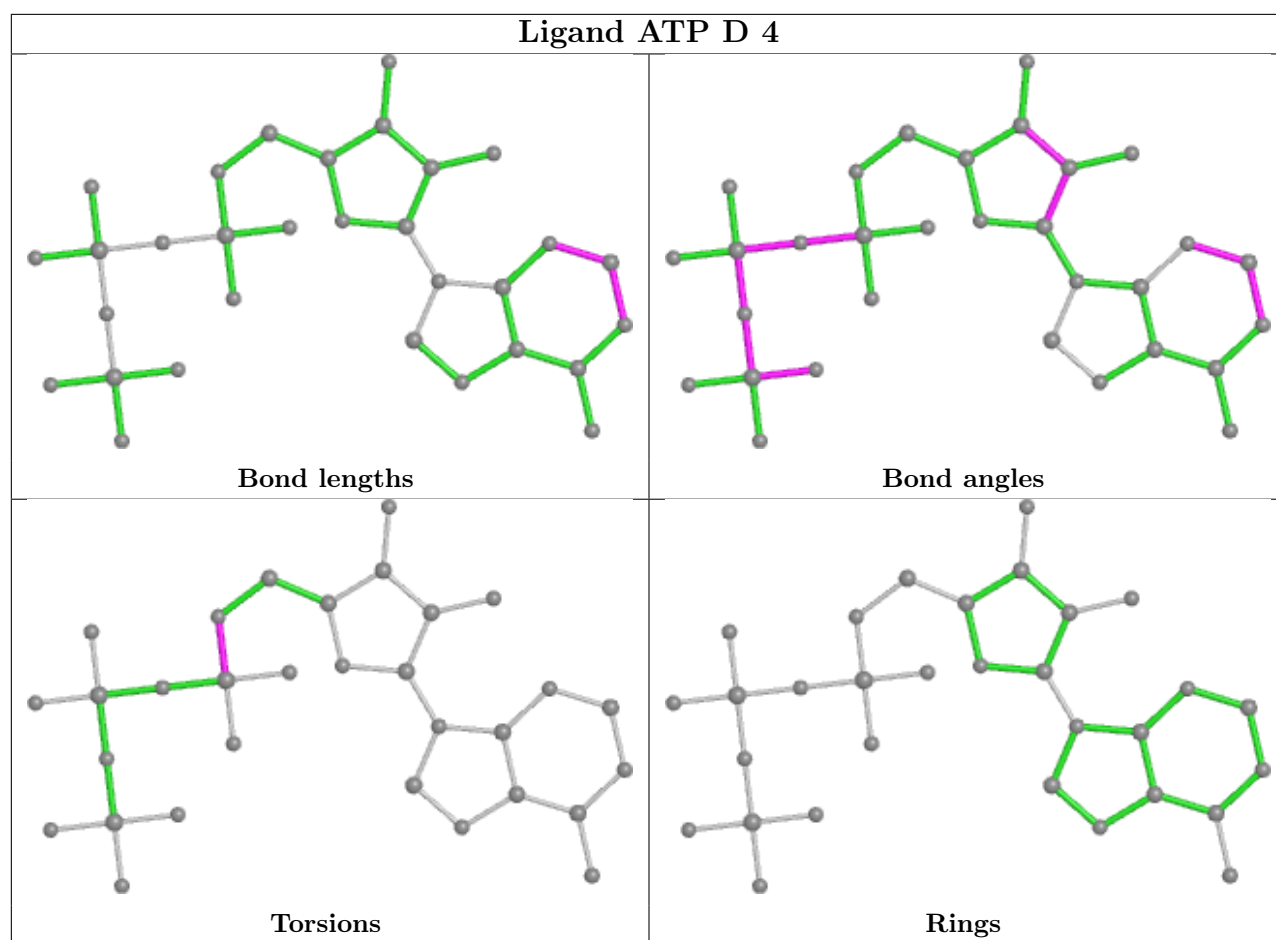
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/286 (92%)	-0.13	7 (2%) 54 52	19, 35, 55, 65	0
1	B	265/286 (92%)	-0.04	7 (2%) 56 53	20, 35, 56, 64	0
1	C	265/286 (92%)	-0.14	6 (2%) 60 58	19, 33, 53, 67	0
1	D	263/286 (91%)	0.30	29 (11%) 5 4	22, 44, 84, 91	0
All	All	1057/1144 (92%)	-0.00	49 (4%) 32 31	19, 35, 64, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	PHE	10.8
1	D	401	TRP	8.9
1	A	390	THR	5.7
1	D	403	GLU	5.0
1	D	407	GLU	4.9
1	D	406	GLY	4.7
1	B	648	ASP	4.7
1	D	434	CYS	4.5
1	B	403	GLU	4.5
1	D	404	GLY	4.5
1	B	430	PHE	4.2
1	D	408	LEU	4.1
1	D	431	SER	3.9
1	D	402	GLU	3.6
1	D	410	GLU	3.6
1	D	496	TRP	3.2
1	D	487	ARG	3.0
1	D	481	ILE	3.0
1	D	482	ILE	3.0
1	D	409	LEU	3.0
1	C	410	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	400	PHE	2.8
1	C	407	GLU	2.8
1	B	635	SER	2.7
1	B	429	SER	2.6
1	D	438	ASN	2.6
1	C	645	MET	2.6
1	C	670	SER	2.6
1	D	390	THR	2.5
1	B	402	GLU	2.5
1	D	640	PHE	2.5
1	D	476	GLU	2.5
1	D	669	PHE	2.5
1	D	648	ASP	2.5
1	A	407	GLU	2.5
1	C	642	SER	2.5
1	D	484	HIS	2.4
1	D	411	LYS	2.4
1	A	668	ARG	2.4
1	D	483	LYS	2.3
1	A	410	GLU	2.3
1	A	648	ASP	2.3
1	A	636	LEU	2.2
1	D	435	LEU	2.2
1	D	639	ASP	2.2
1	C	648	ASP	2.1
1	B	431	SER	2.1
1	A	670	SER	2.0
1	D	630	PHE	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 monosaccharides 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,

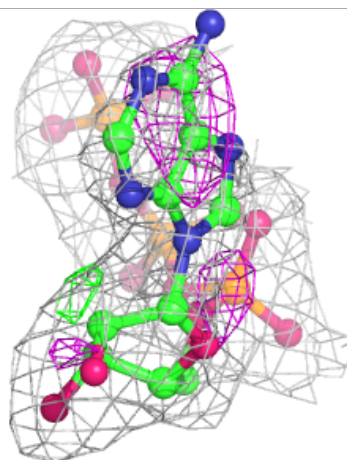
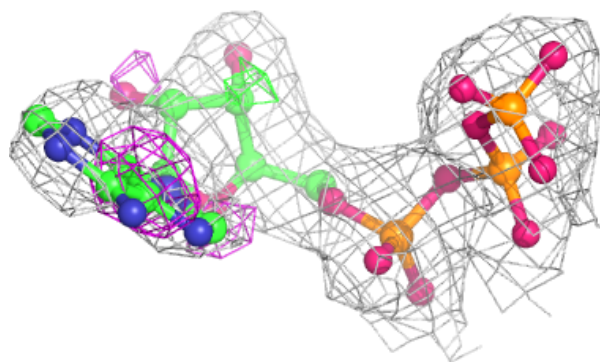
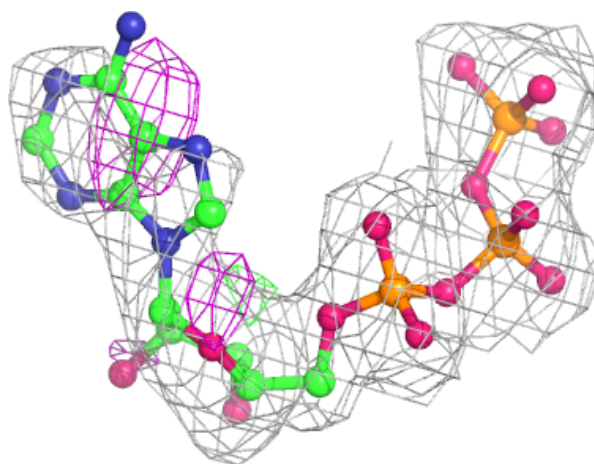
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	14	1/1	0.65	0.14	62,62,62,62	0
2	MG	C	12	1/1	0.86	0.06	37,37,37,37	0
4	ACY	D	9	4/4	0.90	0.12	33,35,35,36	0
3	ATP	A	1	31/31	0.92	0.18	33,55,70,71	0
3	ATP	D	4	31/31	0.92	0.22	42,72,86,86	0
4	ACY	D	8	4/4	0.94	0.17	43,44,45,45	0
3	ATP	B	2	31/31	0.95	0.14	27,48,66,67	0
4	ACY	A	10	4/4	0.95	0.14	41,41,41,42	0
2	MG	A	13	1/1	0.96	0.03	35,35,35,35	0
2	MG	B	11	1/1	0.96	0.09	39,39,39,39	0
3	ATP	C	3	31/31	0.96	0.12	31,50,66,68	0
4	ACY	A	5	4/4	0.98	0.10	31,31,32,32	0
4	ACY	B	6	4/4	0.98	0.12	36,36,36,36	0
4	ACY	C	7	4/4	0.99	0.10	34,35,35,35	0

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

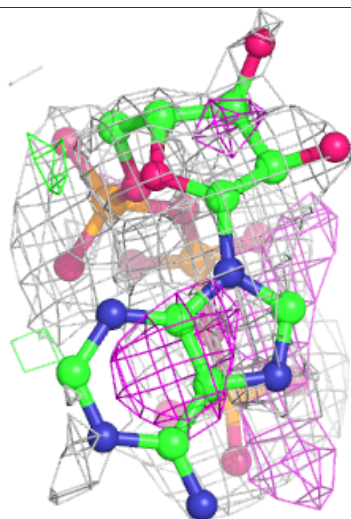
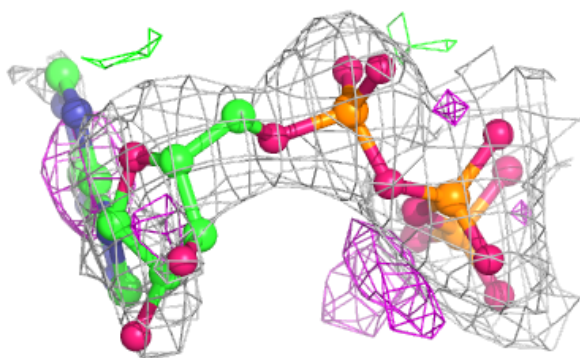
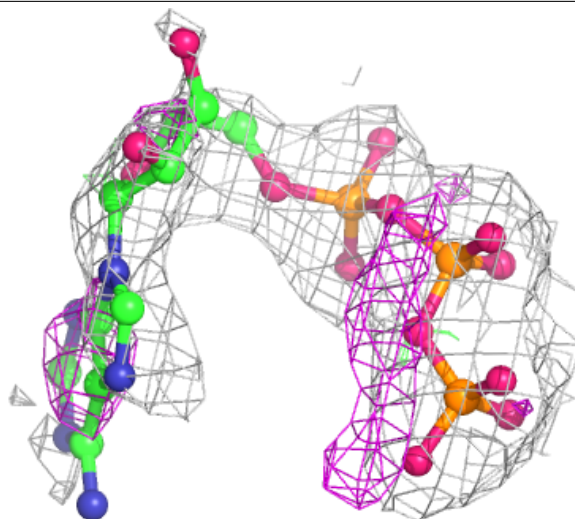
**Electron density around ATP A 1:**

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



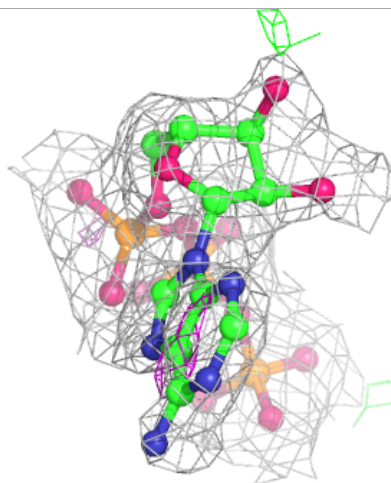
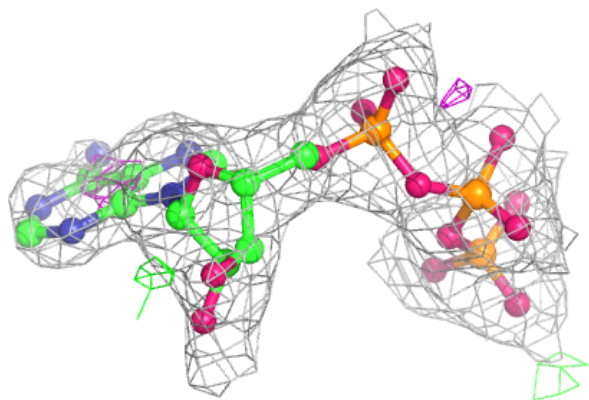
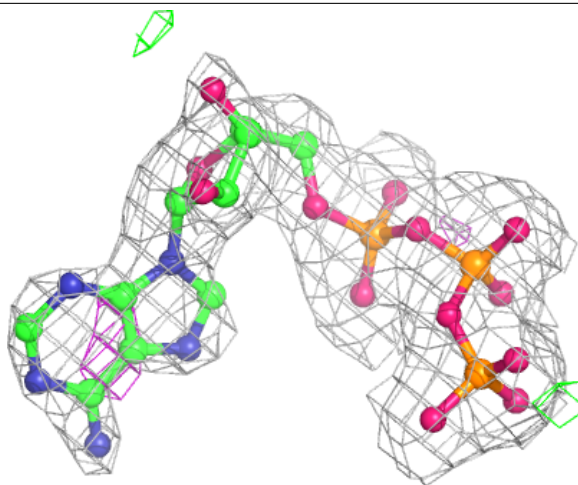
**Electron density around ATP D 4:**

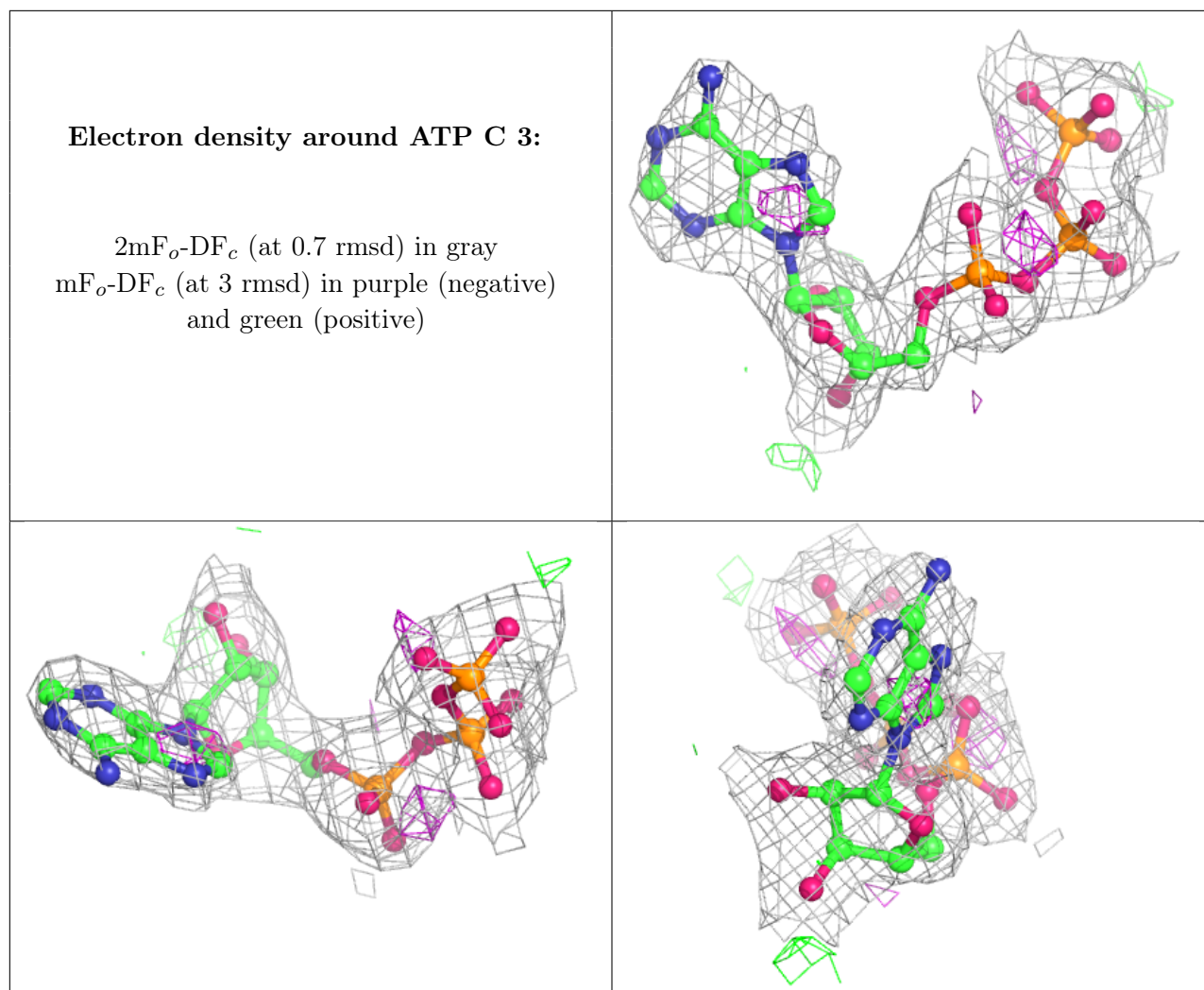
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP B 2:**

$2mF_o-DF_c$  (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.