



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:58 AM EDT

PDB ID : 2J9L / pdb_00002j9l
Title : Cytoplasmic Domain of the Human Chloride Transporter ClC-5 in complex with ATP
Authors : Meyer, S.; Savaresi, S.; Forster, I.C.; Dutzler, R.
Deposited on : 2006-11-13
Resolution : 2.30 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:

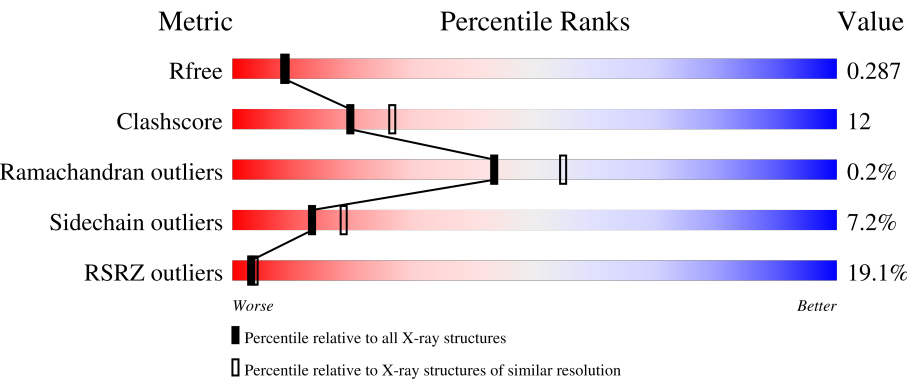
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	185	11% 71% 16% • 10%
1	B	185	7% 68% 22% • 8%
1	C	185	9% 68% 18% 5% • 7%
1	D	185	8% 69% 21% • 8%
1	E	185	12% 68% 19% • 10%

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Mol	Chain	Length	Quality of chain
1	F	185	57% 75% 10% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8466 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 CHLORIDE CHANNEL PROTEIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1326	849	226	245	6			
1	B	171	Total	C	N	O	S	0	0	0
			1362	875	231	250	6			
1	C	172	Total	C	N	O	S	0	0	0
			1371	880	233	252	6			
1	D	171	Total	C	N	O	S	0	0	0
			1353	866	231	250	6			
1	E	167	Total	C	N	O	S	0	0	0
			1326	849	226	245	6			
1	F	162	Total	C	N	O	S	0	0	0
			1265	811	217	231	6			

There are 54 discrepancies between the modelled and reference sequences:

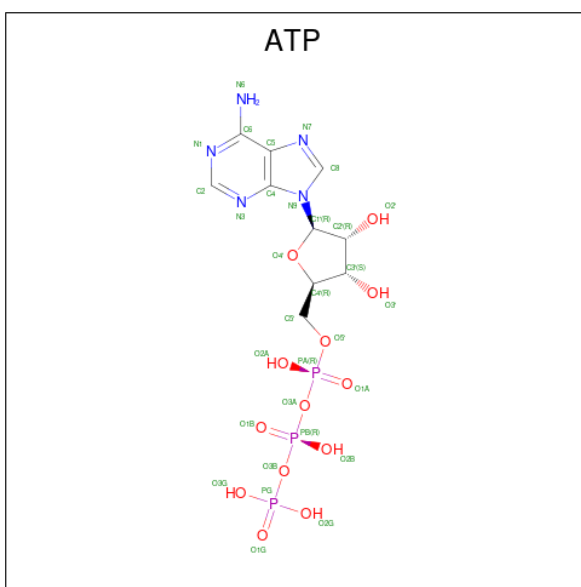
Chain	Residue	Modelled	Actual	Comment	Reference
A	570	MET	-	expression tag	UNP P51795
A	747	GLU	-	expression tag	UNP P51795
A	748	PHE	-	expression tag	UNP P51795
A	749	LEU	-	expression tag	UNP P51795
A	750	GLU	-	expression tag	UNP P51795
A	751	VAL	-	expression tag	UNP P51795
A	752	LEU	-	expression tag	UNP P51795
A	753	PHE	-	expression tag	UNP P51795
A	754	GLN	-	expression tag	UNP P51795
B	570	MET	-	expression tag	UNP P51795
B	747	GLU	-	expression tag	UNP P51795
B	748	PHE	-	expression tag	UNP P51795
B	749	LEU	-	expression tag	UNP P51795
B	750	GLU	-	expression tag	UNP P51795
B	751	VAL	-	expression tag	UNP P51795
B	752	LEU	-	expression tag	UNP P51795
B	753	PHE	-	expression tag	UNP P51795

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	GLN	-	expression tag	UNP P51795
C	570	MET	-	expression tag	UNP P51795
C	747	GLU	-	expression tag	UNP P51795
C	748	PHE	-	expression tag	UNP P51795
C	749	LEU	-	expression tag	UNP P51795
C	750	GLU	-	expression tag	UNP P51795
C	751	VAL	-	expression tag	UNP P51795
C	752	LEU	-	expression tag	UNP P51795
C	753	PHE	-	expression tag	UNP P51795
C	754	GLN	-	expression tag	UNP P51795
D	570	MET	-	expression tag	UNP P51795
D	747	GLU	-	expression tag	UNP P51795
D	748	PHE	-	expression tag	UNP P51795
D	749	LEU	-	expression tag	UNP P51795
D	750	GLU	-	expression tag	UNP P51795
D	751	VAL	-	expression tag	UNP P51795
D	752	LEU	-	expression tag	UNP P51795
D	753	PHE	-	expression tag	UNP P51795
D	754	GLN	-	expression tag	UNP P51795
E	570	MET	-	expression tag	UNP P51795
E	747	GLU	-	expression tag	UNP P51795
E	748	PHE	-	expression tag	UNP P51795
E	749	LEU	-	expression tag	UNP P51795
E	750	GLU	-	expression tag	UNP P51795
E	751	VAL	-	expression tag	UNP P51795
E	752	LEU	-	expression tag	UNP P51795
E	753	PHE	-	expression tag	UNP P51795
E	754	GLN	-	expression tag	UNP P51795
F	570	MET	-	expression tag	UNP P51795
F	747	GLU	-	expression tag	UNP P51795
F	748	PHE	-	expression tag	UNP P51795
F	749	LEU	-	expression tag	UNP P51795
F	750	GLU	-	expression tag	UNP P51795
F	751	VAL	-	expression tag	UNP P51795
F	752	LEU	-	expression tag	UNP P51795
F	753	PHE	-	expression tag	UNP P51795
F	754	GLN	-	expression tag	UNP P51795

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	D	3	Total	Cl	0	0
			3	3		
3	E	1	Total	Cl	0	0
			1	1		
3	F	2	Total	Cl	0	0
			2	2		

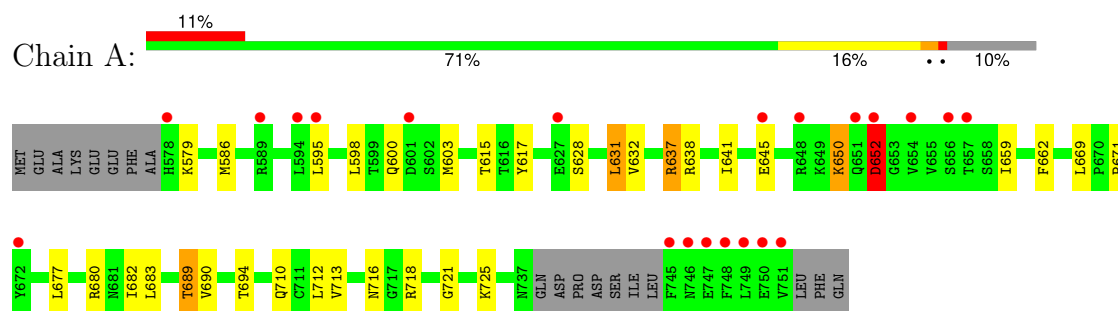
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	45	Total 45	O 45	0	0
4	C	67	Total 67	O 67	0	0
4	D	58	Total 58	O 58	0	0
4	E	33	Total 33	O 33	0	0
4	F	21	Total 21	O 21	0	0

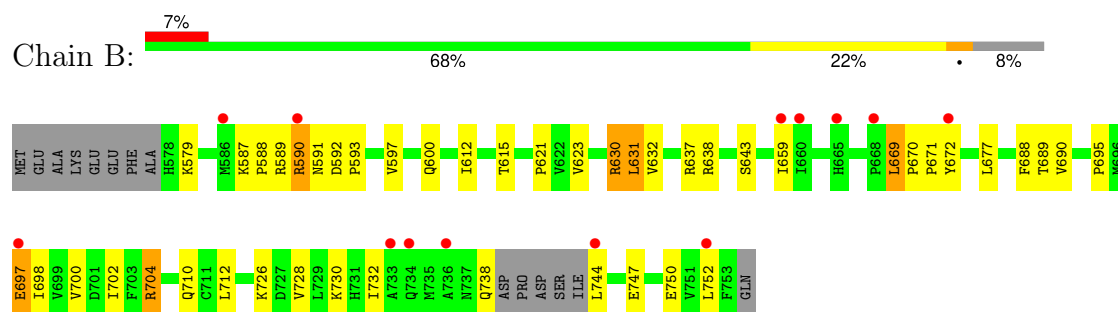
3 Residue-property plots

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

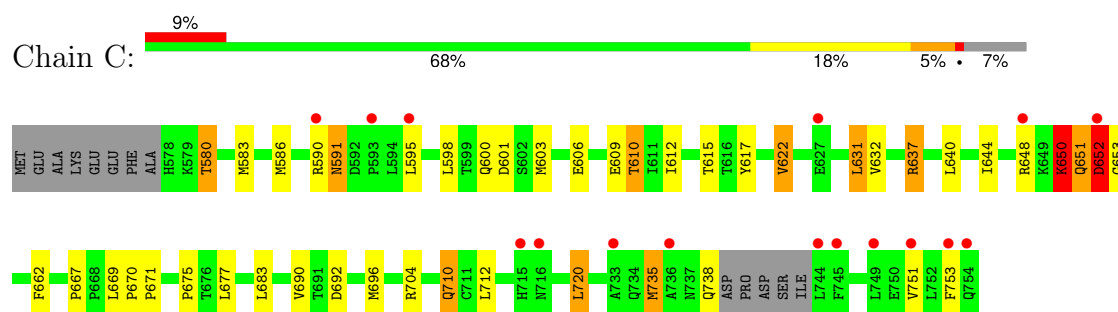
• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



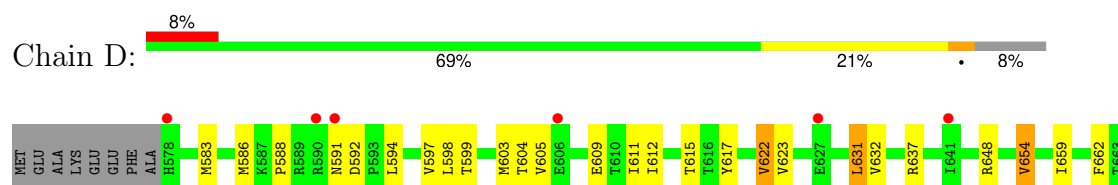
• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

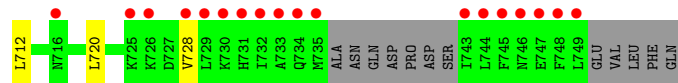
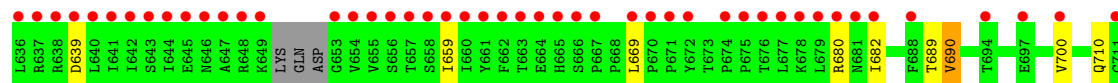




• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.33Å 148.10Å 79.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.30) 97.3 (20.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.263 , 0.295 0.260 , 0.287	Depositor DCC
R_{free} test set	3191 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.42	0/1348	0.76	1/1830 (0.1%)
1	B	0.38	0/1385	0.71	2/1880 (0.1%)
1	C	0.43	0/1394	0.79	0/1892
1	D	0.40	0/1375	0.70	0/1867
1	E	0.35	0/1348	0.78	1/1830 (0.1%)
1	F	0.30	0/1285	0.70	0/1745
All	All	0.38	0/8135	0.74	4/11044 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	652	ASP	N-CA-C	-6.99	104.37	113.17
1	A	652	ASP	N-CA-C	-6.27	105.20	112.92
1	B	669	LEU	CA-C-N	5.09	125.63	120.38
1	B	669	LEU	C-N-CA	5.09	125.63	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	650	LYS	Peptide
1	C	651	GLN	Peptide
1	C	652	ASP	Peptide

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	1326	0	1384	23	0
1	B	1362	0	1423	44	0
1	C	1371	0	1431	41	0
1	D	1353	0	1407	38	0
1	E	1326	0	1384	35	0
1	F	1265	0	1312	13	0
2	A	31	0	12	1	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	3	0	0	0	1
3	E	1	0	0	0	0
3	F	2	0	0	0	0
4	A	43	0	0	3	0
4	B	45	0	0	3	0
4	C	67	0	0	0	0
4	D	58	0	0	1	0
4	E	33	0	0	1	0
4	F	21	0	0	0	0
All	All	8466	0	8413	192	1

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 12.

All (192) 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:704:ARG:HH11	1:B:704:ARG:HG2	1.21	1.04
1:C:651:GLN:HB2	1:C:653:GLY:H	1.21	1.03
1:D:586:MET:CE	1:D:713:VAL:HB	1.88	1.02
1:B:630:ARG:HG2	1:B:630:ARG:HH11	1.26	1.01
1:D:598:LEU:HD22	1:D:603:MET:HE2	1.45	0.99
1:C:651:GLN:HB2	1:C:653:GLY:N	1.80	0.95
1:D:612:ILE:O	1:D:637:ARG:NH2	2.03	0.92
1:E:617:TYR:O	1:E:637:ARG:NH1	2.03	0.91
1:B:704:ARG:HH11	1:B:704:ARG:CG	1.85	0.89
1:D:586:MET:HE2	1:D:721:GLY:HA3	1.55	0.87
1:A:586:MET:HE2	1:A:721:GLY:HA3	1.59	0.85
1:B:587:LYS:HD3	1:B:589:ARG:HD3	1.58	0.83
1:A:586:MET:CE	1:A:713:VAL:HB	2.09	0.82
1:E:598:LEU:HD13	1:E:603:MET:HE2	1.61	0.82
1:B:590:ARG:H	1:B:590:ARG:HD3	1.46	0.79
2:A:1752:ATP:O3G	4:A:2041:HOH:O	1.99	0.79
1:E:622:VAL:CG1	1:E:683:LEU:HD11	2.12	0.79
1:E:622:VAL:HG11	1:E:683:LEU:HD11	1.65	0.79
1:D:586:MET:HE1	1:D:713:VAL:HB	1.66	0.77
1:E:622:VAL:HG11	1:E:683:LEU:CD1	2.14	0.77
1:C:644:ILE:O	1:C:648:ARG:HG3	1.84	0.77
1:D:662:PHE:O	1:D:680:ARG:HG2	1.85	0.76
1:D:586:MET:HE3	1:D:713:VAL:HB	1.67	0.76
1:A:586:MET:HE3	1:A:713:VAL:HB	1.66	0.76
1:C:609:GLU:OE1	1:C:648:ARG:NH1	2.19	0.76
1:C:606:GLU:O	1:C:610:THR:HG22	1.87	0.75
1:D:586:MET:HE2	1:D:721:GLY:CA	2.16	0.75
1:A:586:MET:HE2	1:A:721:GLY:CA	2.18	0.73
1:D:586:MET:HE3	1:D:713:VAL:CB	2.19	0.73
1:E:600:GLN:HE21	1:E:632:VAL:HG21	1.54	0.72
1:C:609:GLU:OE2	1:C:648:ARG:NH1	2.22	0.72
1:C:609:GLU:CD	1:C:648:ARG:NH1	2.48	0.72
1:B:597:VAL:HG23	1:B:621:PRO:HB2	1.72	0.71
1:D:586:MET:CE	1:D:713:VAL:CB	2.67	0.70
1:A:641:ILE:O	1:A:645:GLU:HB2	1.92	0.69
1:B:591:ASN:OD1	4:B:2004:HOH:O	2.09	0.69
1:B:697:GLU:H	1:B:697:GLU:CD	2.00	0.69
1:B:704:ARG:HG2	1:B:704:ARG:NH1	2.00	0.68
1:A:617:TYR:O	1:A:637:ARG:NH1	2.27	0.68
1:C:650:LYS:HB3	1:C:652:ASP:OD1	1.93	0.68
1:C:735:MET:HE3	1:C:735:MET:HA	1.76	0.67
1:C:583:MET:HB3	1:C:692:ASP:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:VAL:HG21	1:D:654:VAL:HG11	1.75	0.67
1:D:609:GLU:OE1	1:D:648:ARG:NH1	2.28	0.66
1:D:631:LEU:HD11	1:D:712:LEU:HD12	1.76	0.65
1:C:651:GLN:HB2	1:C:652:ASP:C	2.22	0.65
1:C:651:GLN:CB	1:C:653:GLY:H	2.06	0.65
1:B:630:ARG:HH11	1:B:630:ARG:CG	2.06	0.65
1:A:682:ILE:O	4:A:2027:HOH:O	2.14	0.65
1:D:598:LEU:CD2	1:D:603:MET:HE2	2.23	0.64
1:A:662:PHE:O	1:A:680:ARG:HG2	1.97	0.64
1:B:643:SER:OG	4:B:2024:HOH:O	2.15	0.64
1:D:605:VAL:HG21	1:D:654:VAL:CG1	2.27	0.63
1:B:697:GLU:CD	1:B:697:GLU:N	2.57	0.62
1:A:615:THR:O	1:A:637:ARG:NH2	2.32	0.62
1:E:746:ASN:HB3	1:E:749:LEU:HD12	1.82	0.61
1:A:652:ASP:N	1:A:652:ASP:OD1	2.33	0.61
1:C:586:MET:HE1	1:C:720:LEU:HD13	1.81	0.61
1:C:631:LEU:HD11	1:C:712:LEU:HD12	1.83	0.61
1:A:631:LEU:HD11	1:A:712:LEU:HD12	1.81	0.61
1:D:598:LEU:HD22	1:D:603:MET:CE	2.27	0.61
1:F:622:VAL:HG23	1:F:632:VAL:HB	1.83	0.60
1:C:591:ASN:C	1:C:591:ASN:HD22	2.08	0.60
1:C:704:ARG:NH2	1:C:751:VAL:O	2.34	0.60
1:F:598:LEU:HB2	1:F:622:VAL:HG12	1.83	0.60
1:B:630:ARG:HG2	1:B:630:ARG:NH1	2.04	0.59
1:A:598:LEU:HD22	1:A:603:MET:HE2	1.84	0.59
1:A:716:ASN:O	1:B:630:ARG:HG2	2.03	0.59
1:C:612:ILE:HD11	1:C:640:LEU:HB3	1.83	0.59
1:E:748:PHE:O	1:E:751:VAL:HG22	2.03	0.57
1:A:586:MET:HE3	1:A:713:VAL:CB	2.33	0.57
1:C:651:GLN:CB	1:C:653:GLY:N	2.63	0.57
1:E:735:MET:HB3	1:E:748:PHE:HB2	1.87	0.57
1:F:599:THR:OG1	1:F:603:MET:HG2	2.05	0.57
1:E:603:MET:HE1	1:E:611:ILE:HD12	1.87	0.56
1:E:600:GLN:NE2	1:E:632:VAL:HG21	2.21	0.56
1:B:752:LEU:HD21	1:D:752:LEU:HD23	1.87	0.56
1:B:704:ARG:CG	1:B:704:ARG:NH1	2.56	0.56
1:B:631:LEU:HD11	1:B:712:LEU:CD1	2.37	0.55
1:F:587:LYS:HE2	1:F:589:ARG:HG2	1.87	0.54
1:F:590:ARG:O	1:F:591:ASN:HB2	2.06	0.54
1:A:725:LYS:HE3	1:C:753:PHE:CE2	2.43	0.54
1:C:617:TYR:HA	2:C:1755:ATP:O1A	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:VAL:HG21	1:B:623:VAL:HG13	1.91	0.53
1:D:689:THR:HG22	4:D:2047:HOH:O	2.08	0.53
1:D:664:GLU:HG3	1:D:680:ARG:NH2	2.24	0.52
1:E:637:ARG:HB2	1:E:637:ARG:HH11	1.74	0.52
1:A:631:LEU:HD11	1:A:712:LEU:CD1	2.38	0.52
1:D:631:LEU:HD11	1:D:712:LEU:CD1	2.38	0.52
1:B:697:GLU:N	1:B:697:GLU:OE2	2.43	0.52
1:B:738:GLN:HG2	1:B:744:LEU:HD23	1.90	0.52
1:E:617:TYR:HA	2:E:1752:ATP:O1A	2.11	0.51
1:C:662:PHE:HB3	1:C:683:LEU:HD22	1.93	0.51
1:E:583:MET:HG2	1:E:692:ASP:O	2.11	0.51
1:A:650:LYS:HB3	1:A:652:ASP:OD1	2.10	0.51
1:E:583:MET:HB3	1:E:692:ASP:HB2	1.92	0.51
1:B:587:LYS:CD	1:B:589:ARG:HD3	2.37	0.50
1:D:667:PRO:O	1:D:669:LEU:HD22	2.11	0.50
1:B:659:ILE:HG13	1:B:669:LEU:HD21	1.93	0.50
1:D:615:THR:O	1:D:637:ARG:NH2	2.44	0.50
1:B:612:ILE:O	1:B:637:ARG:NH2	2.45	0.50
1:C:651:GLN:CB	1:C:652:ASP:C	2.84	0.50
1:E:622:VAL:HG11	1:E:683:LEU:HD13	1.90	0.49
1:B:726:LYS:HG2	1:B:730:LYS:HE3	1.93	0.49
1:C:598:LEU:O	1:C:622:VAL:HA	2.12	0.49
1:D:622:VAL:HG23	1:D:632:VAL:HB	1.93	0.49
1:F:700:VAL:HG22	1:F:728:VAL:HG13	1.94	0.49
1:B:630:ARG:CG	1:B:630:ARG:NH1	2.70	0.48
1:C:704:ARG:HH22	1:C:751:VAL:HA	1.79	0.48
1:B:638:ARG:HD2	4:B:2021:HOH:O	2.14	0.48
1:B:700:VAL:HG22	1:B:728:VAL:HG13	1.94	0.48
1:B:728:VAL:O	1:B:732:ILE:HG13	2.14	0.48
1:D:603:MET:HE1	1:D:611:ILE:HD12	1.95	0.48
1:D:617:TYR:HA	2:D:1753:ATP:O1A	2.13	0.48
1:B:698:ILE:O	1:B:702:ILE:HG13	2.13	0.48
1:A:689:THR:HG22	4:A:2036:HOH:O	2.15	0.47
1:B:704:ARG:NH1	1:B:704:ARG:HB3	2.29	0.47
1:C:600:GLN:HG3	1:C:601:ASP:HB2	1.96	0.47
1:D:586:MET:HE3	1:D:713:VAL:CG2	2.43	0.47
1:E:735:MET:HA	1:E:735:MET:HE2	1.95	0.47
1:C:652:ASP:OD1	1:C:652:ASP:N	2.44	0.47
1:E:588:PRO:HD3	1:E:595:LEU:HG	1.96	0.47
1:E:662:PHE:HB3	1:E:683:LEU:HD22	1.96	0.47
1:F:631:LEU:HD11	1:F:712:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ARG:H	1:B:590:ARG:CD	2.12	0.47
1:B:704:ARG:HH11	1:B:704:ARG:CB	2.28	0.47
1:E:622:VAL:HG22	1:E:632:VAL:HB	1.97	0.46
1:C:650:LYS:CB	1:C:652:ASP:OD1	2.63	0.46
1:C:590:ARG:O	1:C:591:ASN:ND2	2.49	0.46
1:D:609:GLU:CD	1:D:648:ARG:NH1	2.74	0.46
1:E:690:VAL:O	1:E:713:VAL:HA	2.15	0.46
1:D:583:MET:HB3	1:D:692:ASP:HB2	1.97	0.46
1:E:608:VAL:O	1:E:612:ILE:HG13	2.15	0.46
1:F:631:LEU:HD11	1:F:712:LEU:HD13	1.98	0.46
1:D:594:LEU:HD22	1:D:594:LEU:H	1.81	0.46
1:D:704:ARG:NH2	1:D:751:VAL:HG13	2.31	0.46
1:C:615:THR:O	1:C:637:ARG:NH2	2.49	0.46
1:D:604:THR:HA	1:D:659:ILE:HA	1.98	0.46
1:C:735:MET:HA	1:C:735:MET:CE	2.46	0.45
1:C:653:GLY:HA3	1:C:675:PRO:HG3	1.98	0.45
1:F:659:ILE:HD12	1:F:669:LEU:HD21	1.97	0.45
1:C:600:GLN:HE21	1:C:632:VAL:HG21	1.82	0.45
1:C:601:ASP:OD2	1:C:667:PRO:HB3	2.16	0.45
1:E:594:LEU:HD22	1:E:594:LEU:H	1.82	0.45
1:A:690:VAL:HG22	1:A:694:THR:OG1	2.17	0.45
1:D:588:PRO:HB2	1:D:592:ASP:HB2	1.99	0.45
1:A:586:MET:HE1	1:A:713:VAL:HB	1.96	0.45
1:E:670:PRO:HG2	1:E:673:THR:OG1	2.17	0.44
1:B:631:LEU:HD11	1:B:712:LEU:HD13	2.00	0.44
1:D:599:THR:OG1	1:D:603:MET:HG2	2.18	0.44
1:E:598:LEU:HD11	1:E:608:VAL:HG22	2.00	0.44
1:E:637:ARG:NH1	1:E:637:ARG:HB2	2.34	0.43
1:E:648:ARG:NH2	4:E:2014:HOH:O	2.51	0.43
1:B:615:THR:O	1:B:637:ARG:NH2	2.46	0.43
1:D:662:PHE:HB3	1:D:683:LEU:HD22	2.01	0.43
1:F:590:ARG:O	1:F:590:ARG:HD2	2.18	0.43
1:B:592:ASP:HB3	1:B:593:PRO:HD2	2.01	0.43
1:B:631:LEU:HD11	1:B:712:LEU:HD12	2.00	0.43
1:C:612:ILE:O	1:C:637:ARG:NH2	2.51	0.43
1:E:586:MET:O	1:E:589:ARG:HD2	2.19	0.43
1:C:710:GLN:HE21	1:C:710:GLN:HB3	1.72	0.43
1:F:639:ASP:HB3	1:F:682:ILE:HG12	2.01	0.42
1:E:622:VAL:CG1	1:E:683:LEU:CD1	2.85	0.42
1:B:669:LEU:HA	1:B:670:PRO:HD3	1.87	0.42
1:B:671:PRO:O	1:B:672:TYR:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:GLY:HA3	1:C:675:PRO:CG	2.49	0.42
1:D:597:VAL:HG11	1:D:623:VAL:HG22	2.01	0.42
1:D:622:VAL:CG2	1:D:632:VAL:HB	2.49	0.42
1:E:715:HIS:O	1:E:718:ARG:HB3	2.20	0.42
1:C:598:LEU:HD22	1:C:603:MET:HE1	2.02	0.42
1:D:586:MET:HE3	1:D:713:VAL:HG21	2.00	0.42
1:B:688:PHE:CE2	1:B:702:ILE:HG21	2.54	0.42
1:C:670:PRO:HA	1:C:671:PRO:HD3	1.92	0.42
1:D:604:THR:HG22	1:D:659:ILE:HG12	2.02	0.41
1:B:587:LYS:HA	1:B:588:PRO:C	2.45	0.41
1:C:644:ILE:O	1:C:648:ARG:CG	2.63	0.41
1:E:631:LEU:HD23	1:E:719:LEU:HD22	2.02	0.41
1:B:747:GLU:O	1:B:750:GLU:HB2	2.21	0.41
1:E:598:LEU:CD1	1:E:608:VAL:HG22	2.51	0.41
1:A:632:VAL:HG12	1:A:683:LEU:HD21	2.02	0.41
1:F:589:ARG:NE	1:F:589:ARG:HA	2.35	0.41
1:A:600:GLN:HE21	1:A:632:VAL:HG21	1.86	0.41
1:C:704:ARG:NH2	1:C:751:VAL:HG13	2.35	0.41
1:E:615:THR:C	1:E:637:ARG:NH2	2.79	0.40
1:B:579:LYS:HD3	1:B:695:PRO:HB3	2.03	0.40
1:C:580:THR:HG23	1:C:696:MET:HB2	2.04	0.40
1:F:689:THR:CG2	1:F:690:VAL:N	2.84	0.40
1:B:590:ARG:HD3	1:B:590:ARG:N	2.25	0.40
1:E:652:ASP:OD1	1:E:652:ASP:N	2.54	0.40
1:A:628:SER:HA	1:A:718:ARG:HH11	1.85	0.40
1:B:600:GLN:NE2	1:B:632:VAL:HG21	2.36	0.40
1:E:615:THR:O	1:E:637:ARG:NH2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1755:CL:CL	3:D:1755:CL:CL[2_665]	0.94	1.26

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/185 (88%)	154 (94%)	8 (5%)	1 (1%)	21	27
1	B	167/185 (90%)	163 (98%)	4 (2%)	0	100	100
1	C	168/185 (91%)	162 (96%)	5 (3%)	1 (1%)	21	27
1	D	167/185 (90%)	164 (98%)	3 (2%)	0	100	100
1	E	163/185 (88%)	159 (98%)	4 (2%)	0	100	100
1	F	156/185 (84%)	148 (95%)	8 (5%)	0	100	100
All	All	984/1110 (89%)	950 (96%)	32 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	652	ASP
1	A	671	PRO

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	156/173 (90%)	144 (92%)	12 (8%)	12	16
1	B	160/173 (92%)	151 (94%)	9 (6%)	19	28
1	C	161/173 (93%)	145 (90%)	16 (10%)	7	9
1	D	158/173 (91%)	147 (93%)	11 (7%)	14	19
1	E	156/173 (90%)	145 (93%)	11 (7%)	13	19
1	F	146/173 (84%)	138 (94%)	8 (6%)	19	28
All	All	937/1038 (90%)	870 (93%)	67 (7%)	13	18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	579	LYS
1	A	595	LEU
1	A	631	LEU
1	A	637	ARG
1	A	638	ARG
1	A	650	LYS
1	A	652	ASP
1	A	659	ILE
1	A	669	LEU
1	A	677	LEU
1	A	689	THR
1	A	710	GLN
1	B	590	ARG
1	B	630	ARG
1	B	631	LEU
1	B	677	LEU
1	B	689	THR
1	B	690	VAL
1	B	697	GLU
1	B	704	ARG
1	B	710	GLN
1	C	580	THR
1	C	591	ASN
1	C	595	LEU
1	C	610	THR
1	C	622	VAL
1	C	631	LEU
1	C	637	ARG
1	C	650	LYS
1	C	652	ASP
1	C	669	LEU
1	C	677	LEU
1	C	690	VAL
1	C	710	GLN
1	C	720	LEU
1	C	735	MET
1	C	738	GLN
1	D	591	ASN
1	D	622	VAL
1	D	631	LEU
1	D	654	VAL
1	D	669	LEU
1	D	677	LEU

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Mol	Chain	Res	Type
1	D	680	ARG
1	D	690	VAL
1	D	710	GLN
1	D	718	ARG
1	D	720	LEU
1	E	590	ARG
1	E	622	VAL
1	E	650	LYS
1	E	656	SER
1	E	669	LEU
1	E	677	LEU
1	E	690	VAL
1	E	710	GLN
1	E	718	ARG
1	E	746	ASN
1	E	751	VAL
1	F	580	THR
1	F	587	LYS
1	F	590	ARG
1	F	631	LEU
1	F	680	ARG
1	F	690	VAL
1	F	710	GLN
1	F	720	LEU

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

Mol	Chain	Res	Type
1	A	600	GLN
1	A	746	ASN
1	B	600	GLN
1	B	710	GLN
1	B	715	HIS
1	B	731	HIS
1	B	734	GLN
1	B	738	GLN
1	C	591	ASN
1	C	600	GLN
1	C	646	ASN
1	C	665	HIS
1	C	710	GLN
1	C	731	HIS

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Mol	Chain	Res	Type
1	C	734	GLN
1	C	738	GLN
1	D	591	ASN
1	D	710	GLN
1	D	738	GLN
1	E	591	ASN
1	E	600	GLN
1	E	737	ASN
1	F	600	GLN
1	F	731	HIS

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 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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
2	ATP	A	1752	-	32,33,33	1.44	5 (15%)	48,52,52	1.72	9 (18%)
2	ATP	B	1754	-	32,33,33	1.42	5 (15%)	48,52,52	1.76	9 (18%)
2	ATP	E	1752	-	32,33,33	1.50	7 (21%)	48,52,52	1.73	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	C	1755	-	32,33,33	1.41	4 (12%)	48,52,52	1.79	10 (20%)
2	ATP	F	1750	-	32,33,33	1.39	6 (18%)	48,52,52	1.75	10 (20%)
2	ATP	D	1753	-	32,33,33	1.50	5 (15%)	48,52,52	1.72	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	1752	-	-	8/22/38/38	0/3/3/3
2	ATP	B	1754	-	-	2/22/38/38	0/3/3/3
2	ATP	E	1752	-	-	3/22/38/38	0/3/3/3
2	ATP	C	1755	-	-	3/22/38/38	0/3/3/3
2	ATP	F	1750	-	-	7/22/38/38	0/3/3/3
2	ATP	D	1753	-	-	4/22/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1752	ATP	PG-O1G	4.33	1.63	1.50
2	D	1753	ATP	PG-O1G	4.24	1.63	1.50
2	E	1752	ATP	PG-O1G	4.22	1.63	1.50
2	F	1750	ATP	PG-O1G	4.01	1.63	1.50
2	C	1755	ATP	PG-O1G	3.96	1.62	1.50
2	B	1754	ATP	PG-O1G	3.68	1.61	1.50
2	D	1753	ATP	C5-N7	-3.32	1.33	1.39
2	B	1754	ATP	C5-N7	-3.22	1.33	1.39
2	A	1752	ATP	C5-N7	-3.22	1.33	1.39
2	E	1752	ATP	C5-N7	-3.20	1.33	1.39
2	C	1755	ATP	C5-N7	-3.17	1.33	1.39
2	F	1750	ATP	C5-N7	-3.12	1.33	1.39
2	E	1752	ATP	PB-O3A	2.79	1.62	1.59
2	D	1753	ATP	PG-O2G	2.68	1.64	1.54
2	E	1752	ATP	PA-O3A	2.58	1.62	1.59
2	D	1753	ATP	C4-N9	-2.50	1.32	1.37
2	C	1755	ATP	C8-N9	-2.46	1.33	1.37
2	A	1752	ATP	PG-O2G	2.38	1.63	1.54
2	D	1753	ATP	C8-N9	-2.33	1.33	1.37
2	E	1752	ATP	C8-N9	-2.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1754	ATP	PG-O2G	2.31	1.63	1.54
2	A	1752	ATP	C8-N9	-2.28	1.33	1.37
2	E	1752	ATP	PG-O2G	2.26	1.63	1.54
2	F	1750	ATP	C8-N9	-2.21	1.33	1.37
2	C	1755	ATP	C4-N9	-2.19	1.33	1.37
2	A	1752	ATP	C4-N9	-2.18	1.33	1.37
2	F	1750	ATP	C4-N9	-2.17	1.33	1.37
2	B	1754	ATP	C8-N9	-2.15	1.33	1.37
2	F	1750	ATP	PG-O2G	2.12	1.62	1.54
2	B	1754	ATP	PA-O3A	2.09	1.61	1.59
2	E	1752	ATP	C4-N9	-2.08	1.33	1.37
2	F	1750	ATP	PB-O3A	2.08	1.61	1.59

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1754	ATP	C5-C4-N3	-5.58	119.03	126.72
2	C	1755	ATP	C5-C4-N3	-5.43	119.24	126.72
2	A	1752	ATP	C5-C4-N3	-5.28	119.44	126.72
2	E	1752	ATP	C5-C4-N3	-5.26	119.48	126.72
2	F	1750	ATP	C5-C4-N3	-5.18	119.58	126.72
2	D	1753	ATP	C5-C4-N3	-4.95	119.90	126.72
2	D	1753	ATP	N3-C2-N1	-4.81	121.31	128.58
2	A	1752	ATP	N3-C2-N1	-4.70	121.47	128.58
2	B	1754	ATP	N3-C2-N1	-4.68	121.50	128.58
2	E	1752	ATP	N3-C2-N1	-4.64	121.56	128.58
2	F	1750	ATP	N3-C2-N1	-4.56	121.68	128.58
2	C	1755	ATP	N3-C2-N1	-4.36	121.98	128.58
2	B	1754	ATP	N3-C4-N9	3.89	133.79	127.17
2	E	1752	ATP	N3-C4-N9	3.65	133.37	127.17
2	A	1752	ATP	N3-C4-N9	3.64	133.35	127.17
2	B	1754	ATP	C2-N3-C4	3.63	120.71	111.83
2	F	1750	ATP	N3-C4-N9	3.59	133.27	127.17
2	C	1755	ATP	N9-C8-N7	-3.54	108.91	113.94
2	A	1752	ATP	C2-N3-C4	3.53	120.46	111.83
2	E	1752	ATP	C2-N3-C4	3.53	120.46	111.83
2	C	1755	ATP	C2-N3-C4	3.53	120.45	111.83
2	F	1750	ATP	C2-N3-C4	3.48	120.34	111.83
2	D	1753	ATP	C2-N3-C4	3.46	120.28	111.83
2	D	1753	ATP	N9-C8-N7	-3.42	109.08	113.94
2	A	1752	ATP	N9-C8-N7	-3.40	109.11	113.94
2	C	1755	ATP	C4-C5-N7	-3.40	106.70	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1755	ATP	O3G-PG-O3B	3.35	115.86	104.64
2	E	1752	ATP	N9-C8-N7	-3.33	109.21	113.94
2	D	1753	ATP	N3-C4-N9	3.29	132.76	127.17
2	C	1755	ATP	N3-C4-N9	3.24	132.68	127.17
2	F	1750	ATP	N9-C8-N7	-3.24	109.34	113.94
2	B	1754	ATP	N9-C8-N7	-3.17	109.44	113.94
2	C	1755	ATP	C5-N7-C8	3.15	108.40	103.45
2	E	1752	ATP	C5-N7-C8	2.84	107.91	103.45
2	A	1752	ATP	C5-N7-C8	2.82	107.88	103.45
2	B	1754	ATP	C5-N7-C8	2.79	107.83	103.45
2	F	1750	ATP	C5-N7-C8	2.74	107.76	103.45
2	F	1750	ATP	O3G-PG-O3B	2.73	113.78	104.64
2	D	1753	ATP	C5-N7-C8	2.67	107.64	103.45
2	E	1752	ATP	C4-C5-N7	-2.65	107.55	110.58
2	A	1752	ATP	O3G-PG-O3B	2.63	113.46	104.64
2	F	1750	ATP	C4-C5-N7	-2.60	107.61	110.58
2	A	1752	ATP	C4-C5-N7	-2.58	107.63	110.58
2	D	1753	ATP	C4-C5-N7	-2.58	107.64	110.58
2	E	1752	ATP	O3G-PG-O3B	2.52	113.08	104.64
2	B	1754	ATP	C4-C5-N7	-2.48	107.75	110.58
2	F	1750	ATP	C5'-C4'-C3'	-2.48	106.30	115.21
2	D	1753	ATP	C4-N9-C8	2.43	108.29	105.74
2	B	1754	ATP	O3G-PG-O3B	2.40	112.67	104.64
2	E	1752	ATP	C4-N9-C8	2.32	108.18	105.74
2	A	1752	ATP	C4-N9-C8	2.32	108.17	105.74
2	D	1753	ATP	O3G-PG-O3B	2.29	112.31	104.64
2	F	1750	ATP	C4-N9-C8	2.28	108.14	105.74
2	B	1754	ATP	C5'-C4'-C3'	-2.21	107.27	115.21
2	C	1755	ATP	C5-C4-N9	2.08	108.08	105.81
2	C	1755	ATP	C4-N9-C8	2.07	107.91	105.74

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1752	ATP	C5'-O5'-PA-O1A
2	F	1750	ATP	PB-O3B-PG-O2G
2	F	1750	ATP	C5'-O5'-PA-O1A
2	F	1750	ATP	C5'-O5'-PA-O2A
2	F	1750	ATP	C5'-O5'-PA-O3A
2	A	1752	ATP	O4'-C4'-C5'-O5'
2	A	1752	ATP	PB-O3A-PA-O1A

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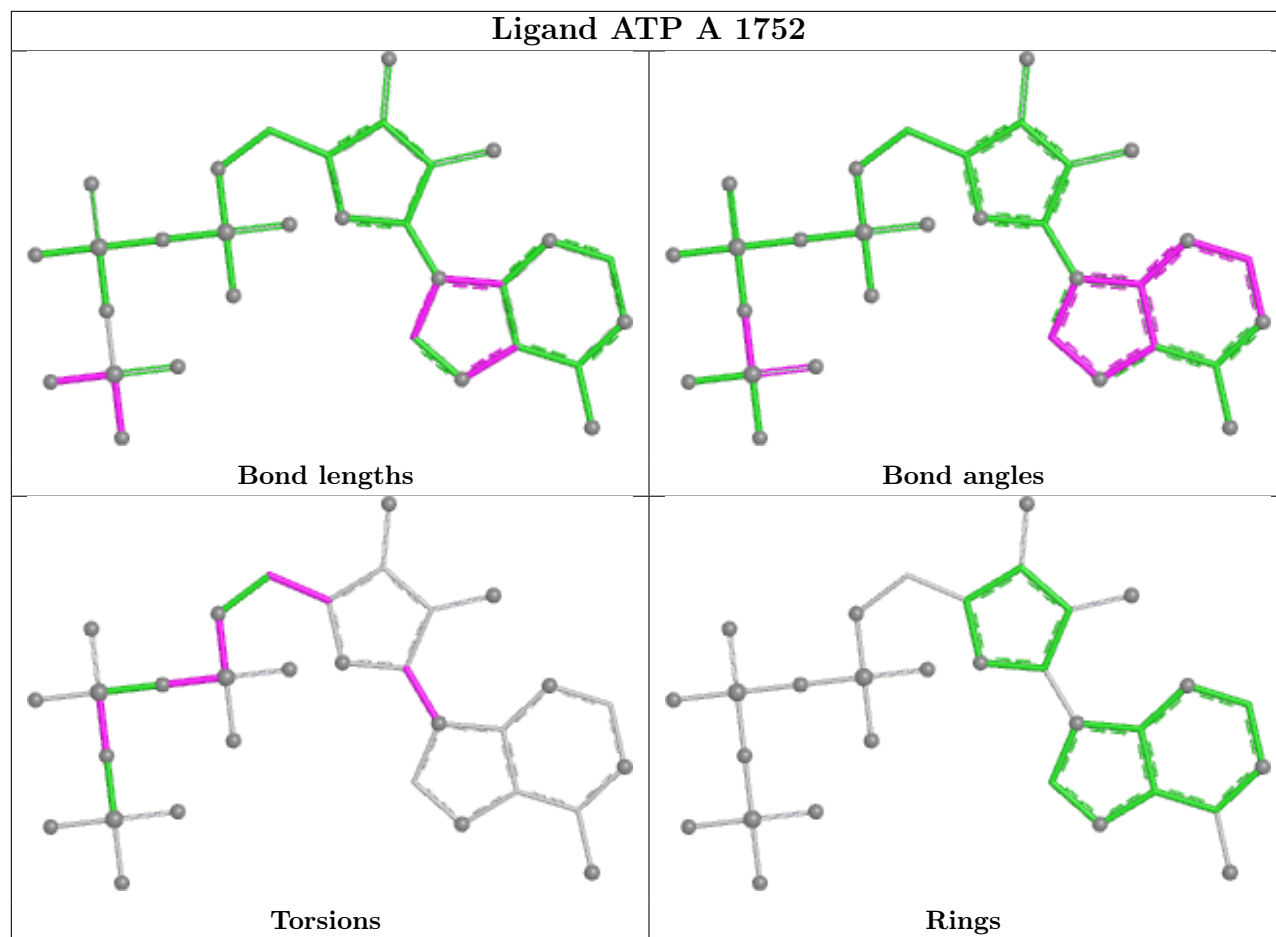
Mol	Chain	Res	Type	Atoms
2	E	1752	ATP	PB-O3A-PA-O1A
2	A	1752	ATP	C3'-C4'-C5'-O5'
2	A	1752	ATP	PB-O3A-PA-O5'
2	D	1753	ATP	PB-O3A-PA-O5'
2	E	1752	ATP	PB-O3A-PA-O5'
2	F	1750	ATP	PB-O3A-PA-O5'
2	D	1753	ATP	PB-O3B-PG-O1G
2	B	1754	ATP	C2'-C1'-N9-C8
2	C	1755	ATP	C2'-C1'-N9-C8
2	D	1753	ATP	C2'-C1'-N9-C8
2	C	1755	ATP	PA-O3A-PB-O2B
2	A	1752	ATP	C2'-C1'-N9-C8
2	B	1754	ATP	PG-O3B-PB-O2B
2	D	1753	ATP	O4'-C1'-N9-C8
2	E	1752	ATP	C2'-C1'-N9-C8
2	F	1750	ATP	C2'-C1'-N9-C8
2	A	1752	ATP	O4'-C1'-N9-C8
2	A	1752	ATP	PG-O3B-PB-O2B
2	C	1755	ATP	PA-O3A-PB-O1B
2	F	1750	ATP	PB-O3A-PA-O2A

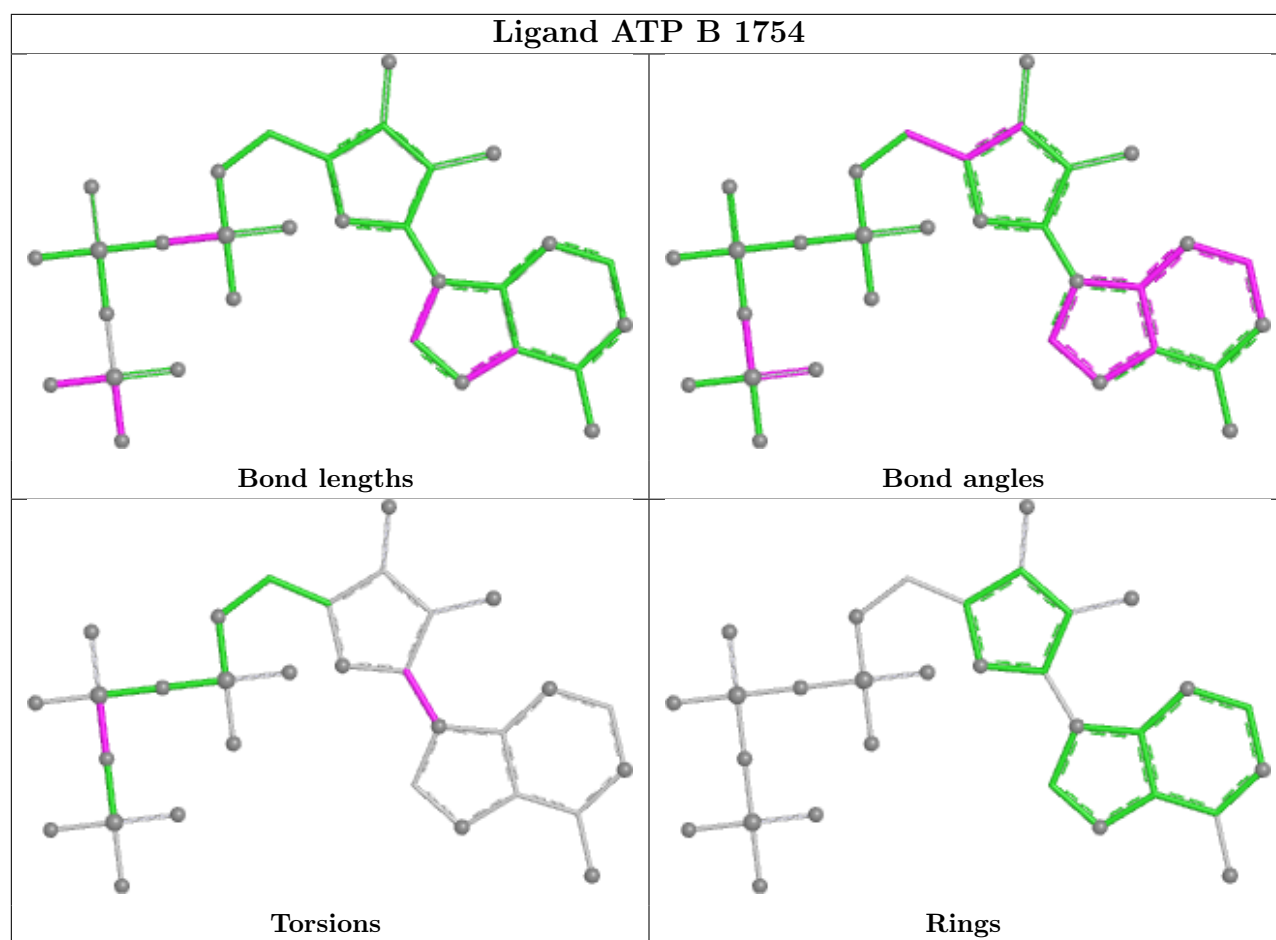
There are no ring outliers.

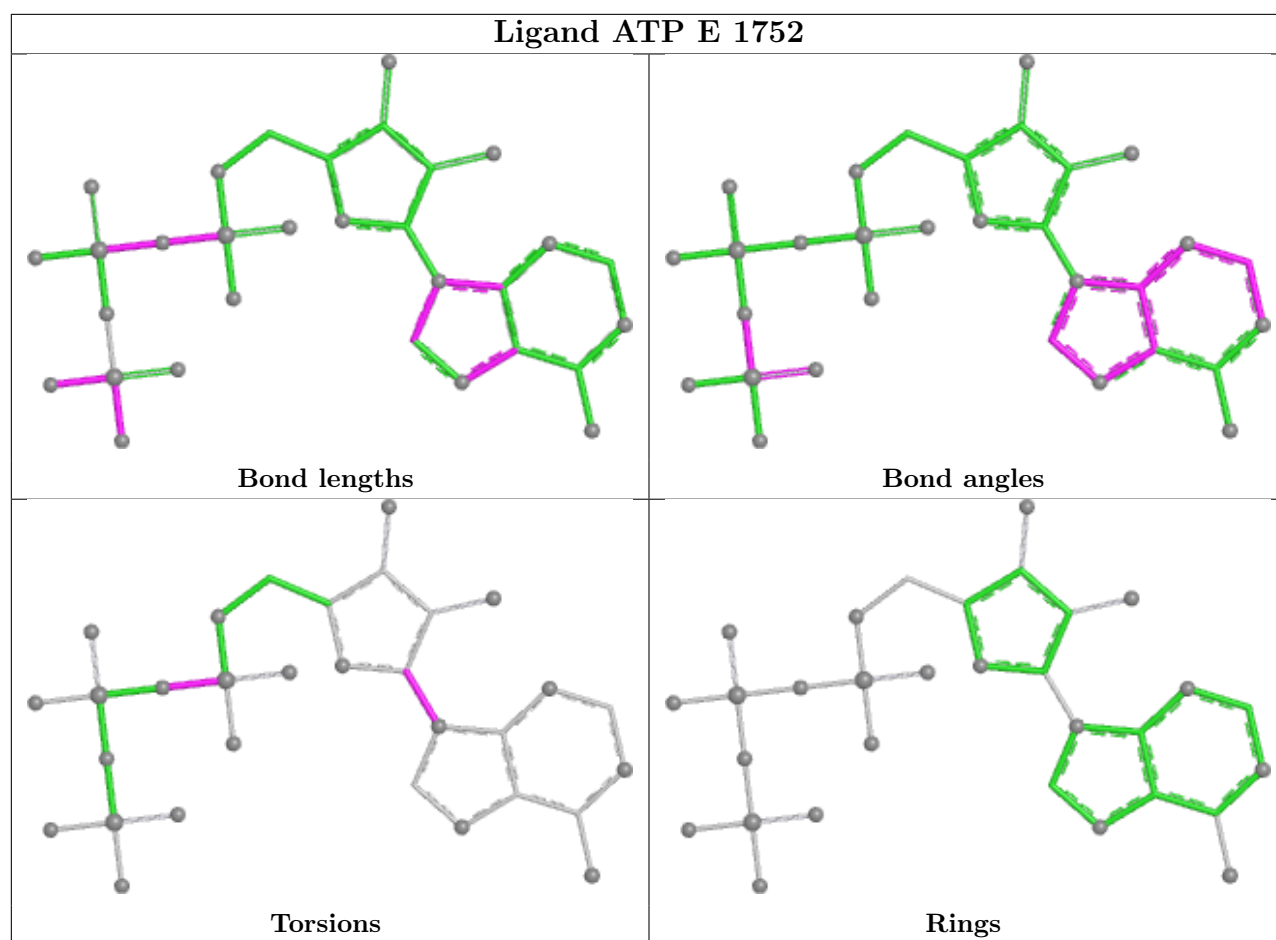
4 monomers are involved in 4 short contacts:

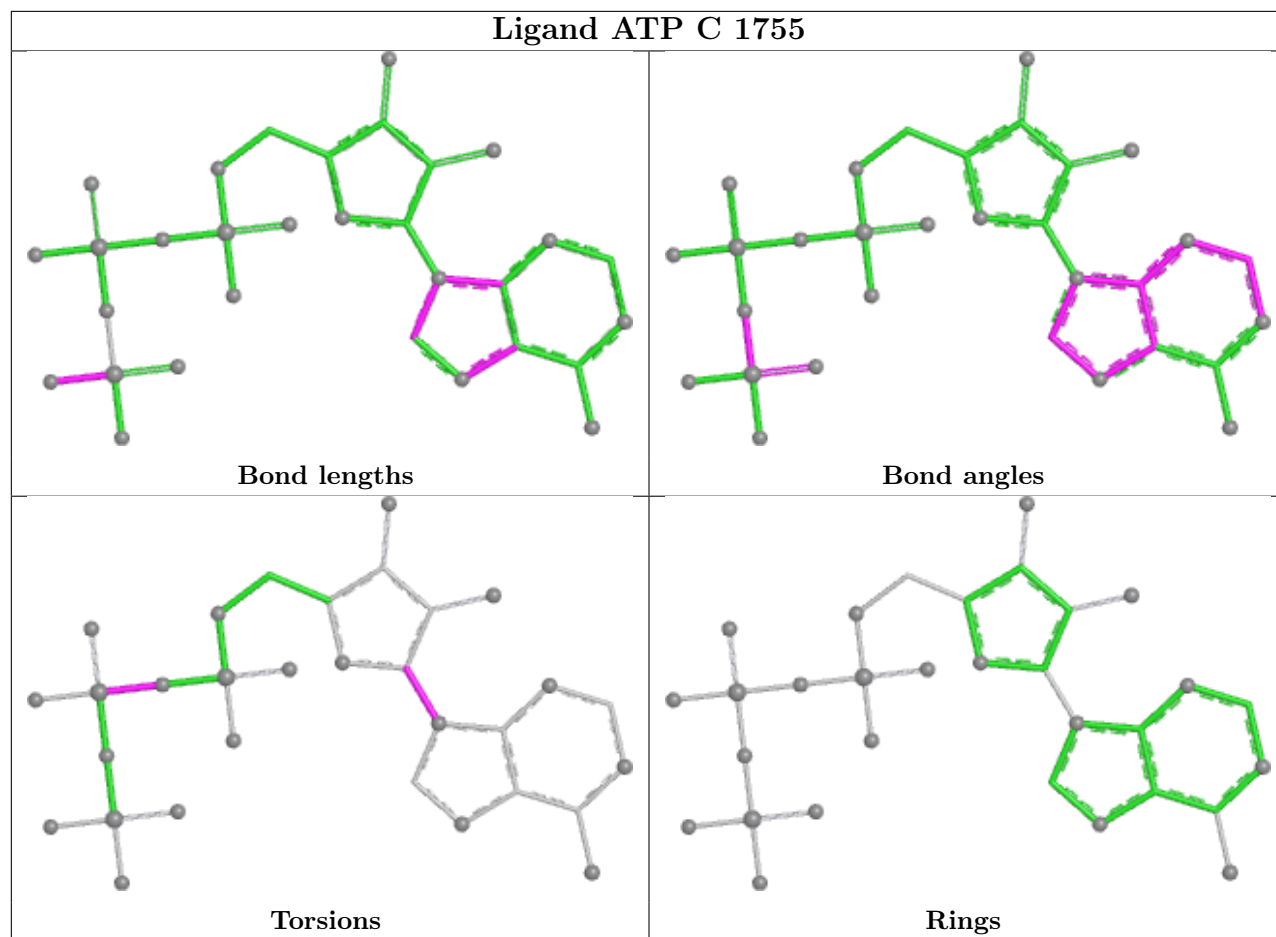
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1752	ATP	1	0
2	E	1752	ATP	1	0
2	C	1755	ATP	1	0
2	D	1753	ATP	1	0

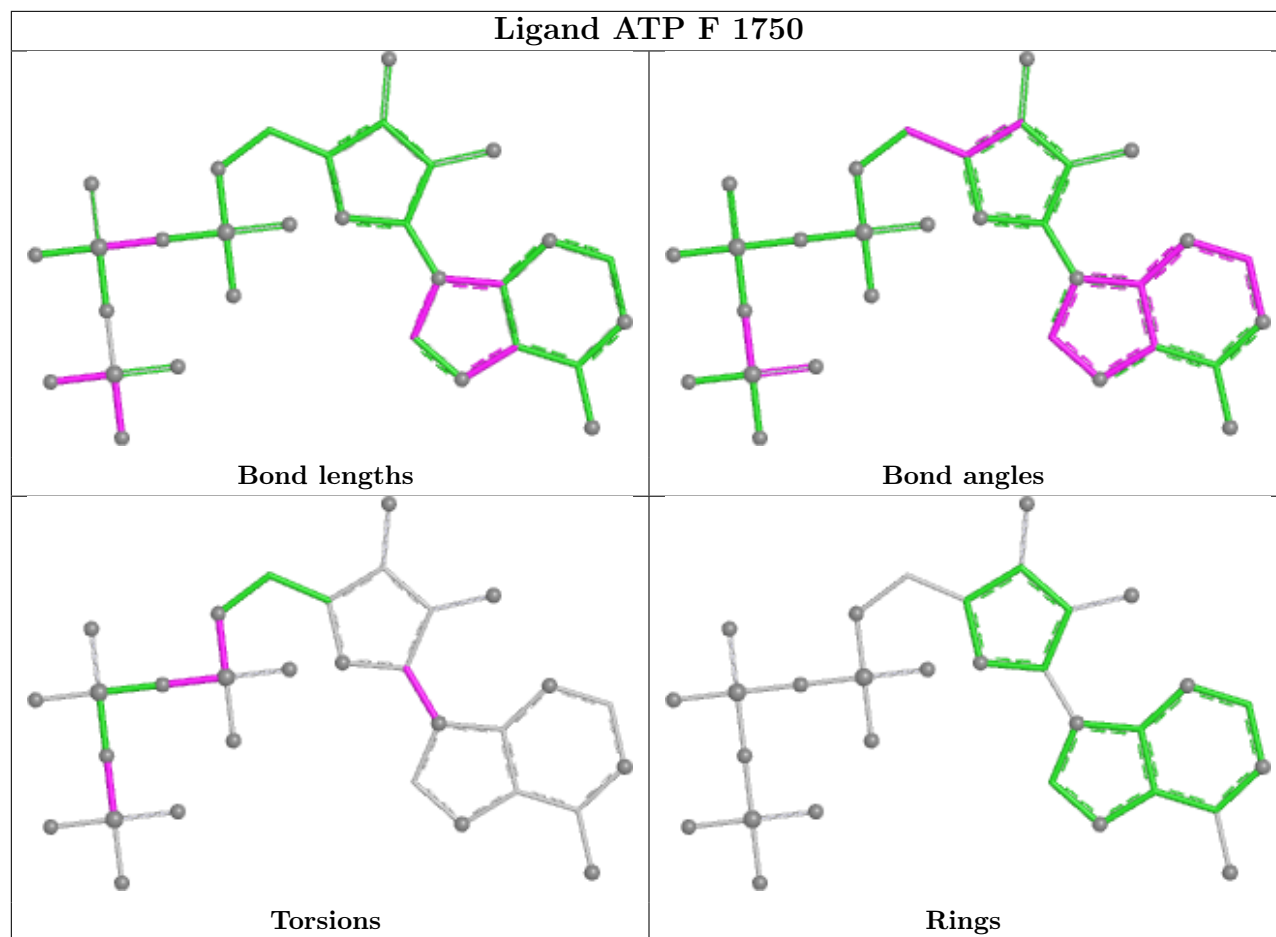
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

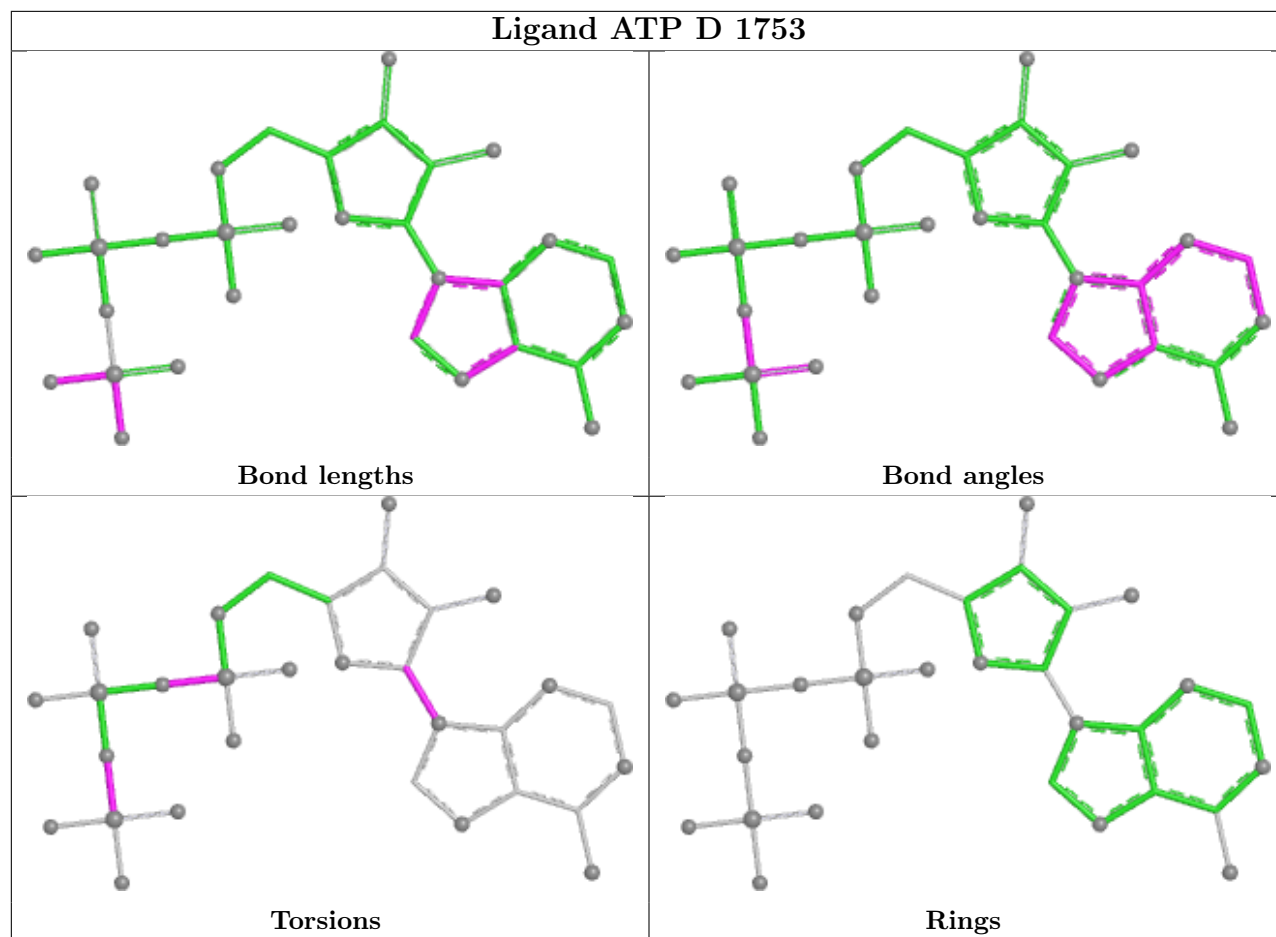












5.7 Other polymers [i](#)

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, 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	167/185 (90%)	0.75	21 (12%) 8 9	18, 25, 39, 93	0
1	B	171/185 (92%)	0.49	13 (7%) 20 21	16, 23, 39, 42	0
1	C	172/185 (92%)	0.38	16 (9%) 14 16	18, 23, 34, 40	0
1	D	171/185 (92%)	0.47	15 (8%) 15 17	18, 23, 37, 81	0
1	E	167/185 (90%)	0.72	22 (13%) 7 8	21, 27, 47, 51	0
1	F	162/185 (87%)	3.09	106 (65%) 0 0	29, 72, 132, 139	0
All	All	1010/1110 (90%)	0.97	193 (19%) 3 4	16, 26, 97, 139	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	659	ILE	8.8
1	F	641	ILE	8.7
1	F	665	HIS	8.3
1	A	751	VAL	7.8
1	F	749	LEU	7.4
1	F	664	GLU	7.3
1	F	658	SER	7.3
1	F	662	PHE	7.2
1	F	653	GLY	7.0
1	F	663	THR	6.9
1	F	666	SER	6.9
1	D	744	LEU	6.9
1	F	642	ILE	6.8
1	F	597	VAL	6.6
1	F	596	THR	6.6
1	F	746	ASN	6.4
1	D	748	PHE	6.4
1	F	655	VAL	6.3
1	F	747	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	F	598	LEU	5.9
1	F	660	ILE	5.8
1	F	679	LEU	5.7
1	F	661	TYR	5.7
1	F	745	PHE	5.6
1	D	752	LEU	5.6
1	F	595	LEU	5.6
1	A	750	GLU	5.6
1	F	602	SER	5.6
1	F	601	ASP	5.4
1	F	617	TYR	5.4
1	A	748	PHE	5.3
1	F	748	PHE	5.3
1	F	643	SER	5.3
1	F	728	VAL	5.3
1	A	749	LEU	5.3
1	F	578	HIS	5.2
1	F	654	VAL	5.2
1	F	657	THR	5.1
1	A	746	ASN	5.1
1	F	743	ILE	5.0
1	A	745	PHE	5.0
1	F	644	ILE	5.0
1	F	599	THR	4.9
1	D	751	VAL	4.9
1	F	672	TYR	4.7
1	F	610	THR	4.5
1	F	669	LEU	4.4
1	F	639	ASP	4.4
1	F	671	PRO	4.3
1	F	729	LEU	4.3
1	F	656	SER	4.3
1	F	677	LEU	4.3
1	F	600	GLN	4.3
1	F	730	LYS	4.3
1	A	747	GLU	4.2
1	E	642	ILE	4.2
1	F	603	MET	4.2
1	F	618	SER	4.1
1	F	620	PHE	4.1
1	F	608	VAL	4.1
1	C	744	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	587	LYS	4.0
1	F	688	PHE	4.0
1	F	588	PRO	3.9
1	F	646	ASN	3.9
1	F	604	THR	3.8
1	F	607	ASP	3.8
1	F	594	LEU	3.8
1	E	651	GLN	3.8
1	F	680	ARG	3.8
1	F	744	LEU	3.8
1	F	725	LYS	3.7
1	F	605	VAL	3.7
1	C	749	LEU	3.7
1	F	581	LEU	3.6
1	F	733	ALA	3.6
1	F	678	LYS	3.5
1	F	731	HIS	3.5
1	F	645	GLU	3.5
1	D	749	LEU	3.5
1	D	739	ASP	3.5
1	F	638	ARG	3.4
1	B	672	TYR	3.4
1	A	672	TYR	3.3
1	C	751	VAL	3.3
1	E	595	LEU	3.3
1	C	716	ASN	3.3
1	F	732	ILE	3.3
1	E	650	LYS	3.2
1	E	657	THR	3.2
1	F	670	PRO	3.2
1	E	610	THR	3.2
1	F	649	LYS	3.2
1	F	615	THR	3.2
1	F	636	LEU	3.1
1	F	667	PRO	3.1
1	F	735	MET	3.1
1	D	745	PHE	3.1
1	F	586	MET	3.1
1	E	654	VAL	3.0
1	E	746	ASN	3.0
1	F	616	THR	3.0
1	B	733	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	754	GLN	2.9
1	F	613	SER	2.9
1	F	711	CYS	2.9
1	B	736	ALA	2.9
1	A	657	THR	2.9
1	F	611	ILE	2.9
1	C	648	ARG	2.8
1	F	694	THR	2.8
1	F	648	ARG	2.8
1	A	651	GLN	2.8
1	F	734	GLN	2.8
1	F	700	VAL	2.8
1	F	585	VAL	2.7
1	F	592	ASP	2.7
1	F	627	GLU	2.7
1	F	624	VAL	2.7
1	A	645	GLU	2.7
1	D	641	ILE	2.7
1	E	652	ASP	2.6
1	E	594	LEU	2.6
1	A	595	LEU	2.6
1	A	578	HIS	2.6
1	F	640	LEU	2.6
1	C	733	ALA	2.6
1	C	736	ALA	2.6
1	F	619	GLY	2.6
1	F	676	THR	2.6
1	E	601	ASP	2.5
1	C	590	ARG	2.5
1	D	590	ARG	2.5
1	F	637	ARG	2.5
1	C	595	LEU	2.5
1	E	647	ALA	2.5
1	F	716	ASN	2.5
1	D	750	GLU	2.5
1	F	606	GLU	2.5
1	A	648	ARG	2.5
1	E	656	SER	2.5
1	F	589	ARG	2.5
1	F	674	PRO	2.5
1	F	726	LYS	2.4
1	A	601	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	652	ASP	2.4
1	C	745	PHE	2.4
1	B	744	LEU	2.4
1	D	606	GLU	2.4
1	D	578	HIS	2.3
1	B	665	HIS	2.3
1	C	652	ASP	2.3
1	D	701	ASP	2.3
1	A	627	GLU	2.3
1	D	627	GLU	2.3
1	F	675	PRO	2.3
1	B	586	MET	2.3
1	B	697	GLU	2.3
1	C	715	HIS	2.3
1	B	734	GLN	2.3
1	A	656	SER	2.2
1	C	753	PHE	2.2
1	E	745	PHE	2.2
1	F	623	VAL	2.2
1	D	591	ASN	2.2
1	B	668	PRO	2.2
1	F	593	PRO	2.2
1	E	733	ALA	2.2
1	B	752	LEU	2.2
1	E	749	LEU	2.2
1	B	590	ARG	2.2
1	F	681	ASN	2.2
1	F	609	GLU	2.2
1	F	682	ILE	2.2
1	A	589	ARG	2.2
1	C	627	GLU	2.2
1	F	580	THR	2.2
1	E	648	ARG	2.1
1	E	591	ASN	2.1
1	F	632	VAL	2.1
1	F	697	GLU	2.1
1	F	635	VAL	2.1
1	B	659	ILE	2.1
1	E	592	ASP	2.1
1	E	653	GLY	2.1
1	E	649	LYS	2.1
1	A	594	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	612	ILE	2.1
1	A	654	VAL	2.1
1	F	647	ALA	2.0
1	E	655	VAL	2.0
1	B	660	ILE	2.0
1	C	593	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

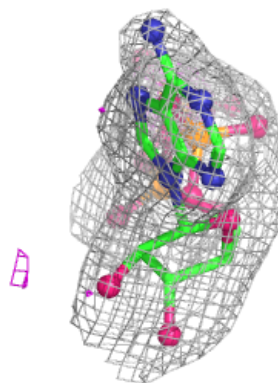
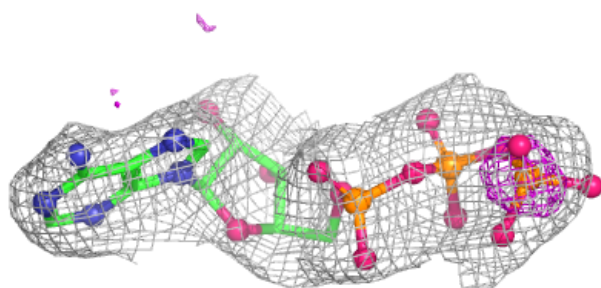
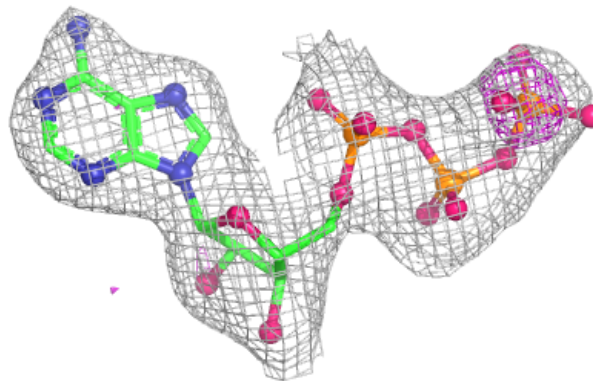
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	C	1756	1/1	0.73	0.22	124,124,124,124	0
3	CL	A	1753	1/1	0.76	0.19	87,87,87,87	0
3	CL	D	1754	1/1	0.76	0.24	83,83,83,83	0
3	CL	F	3001	1/1	0.76	0.16	80,80,80,80	0
2	ATP	F	1750	31/31	0.84	0.11	95,95,98,98	0
3	CL	F	1751	1/1	0.85	0.32	108,108,108,108	0
2	ATP	E	1752	31/31	0.88	0.11	65,66,71,71	0
2	ATP	B	1754	31/31	0.90	0.10	44,48,61,62	0
3	CL	E	1753	1/1	0.91	0.13	99,99,99,99	0
2	ATP	D	1753	31/31	0.91	0.10	42,44,58,58	0
2	ATP	C	1755	31/31	0.91	0.11	41,45,58,58	0
3	CL	D	3001	1/1	0.92	0.16	70,70,70,70	0
2	ATP	A	1752	31/31	0.92	0.10	49,51,61,62	0
3	CL	B	3002	1/1	0.93	0.12	64,64,64,64	0
3	CL	B	3001	1/1	0.94	0.13	68,68,68,68	0
3	CL	D	1755	1/1	0.97	0.14	51,51,51,51	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.

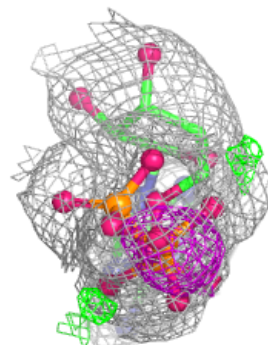
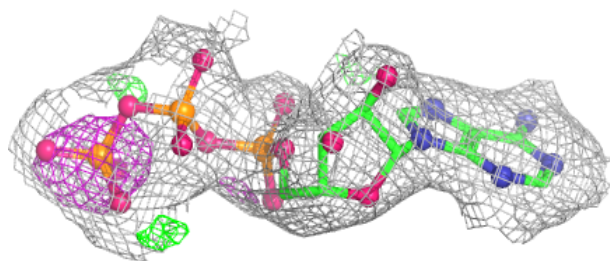
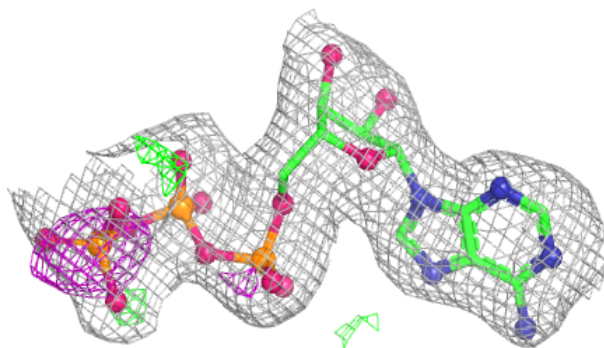
Electron density around ATP F 1750:

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

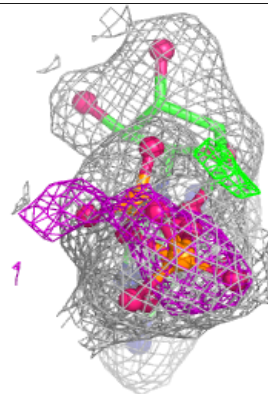
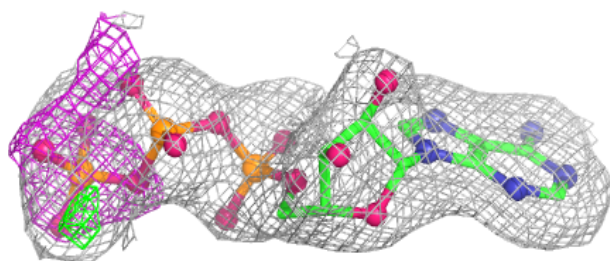
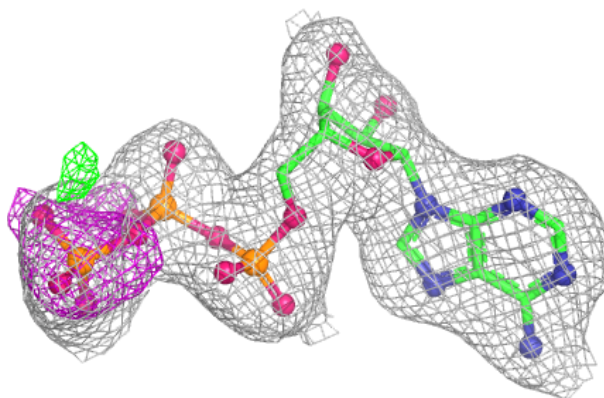


Electron density around ATP E 1752:

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

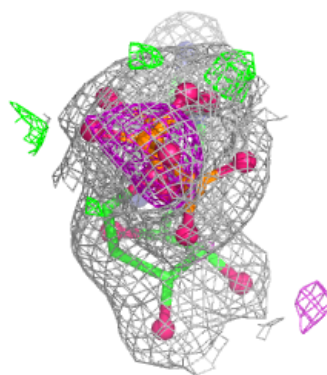
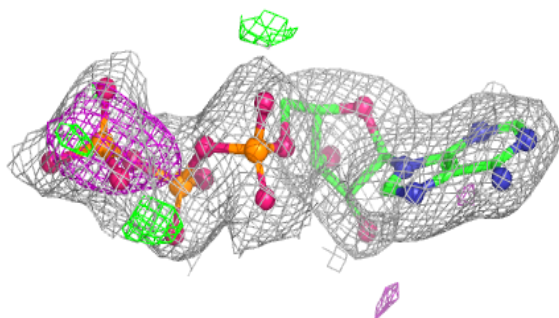
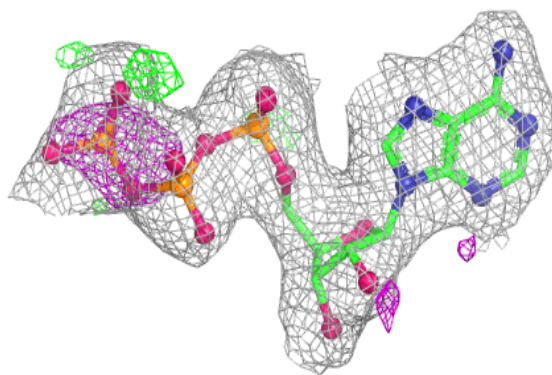
**Electron density around ATP B 1754:**

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

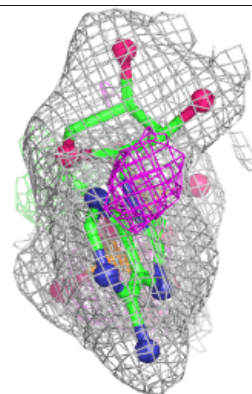
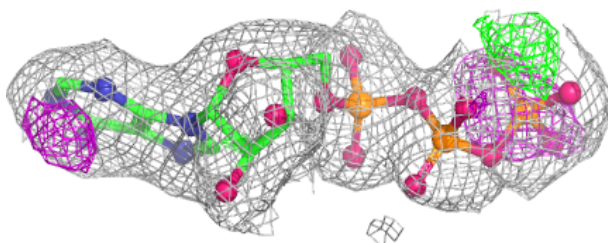
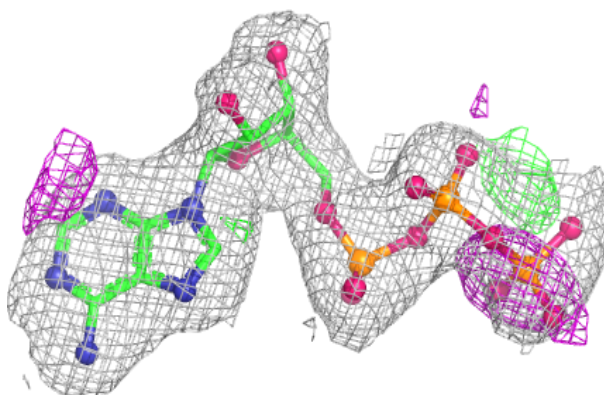


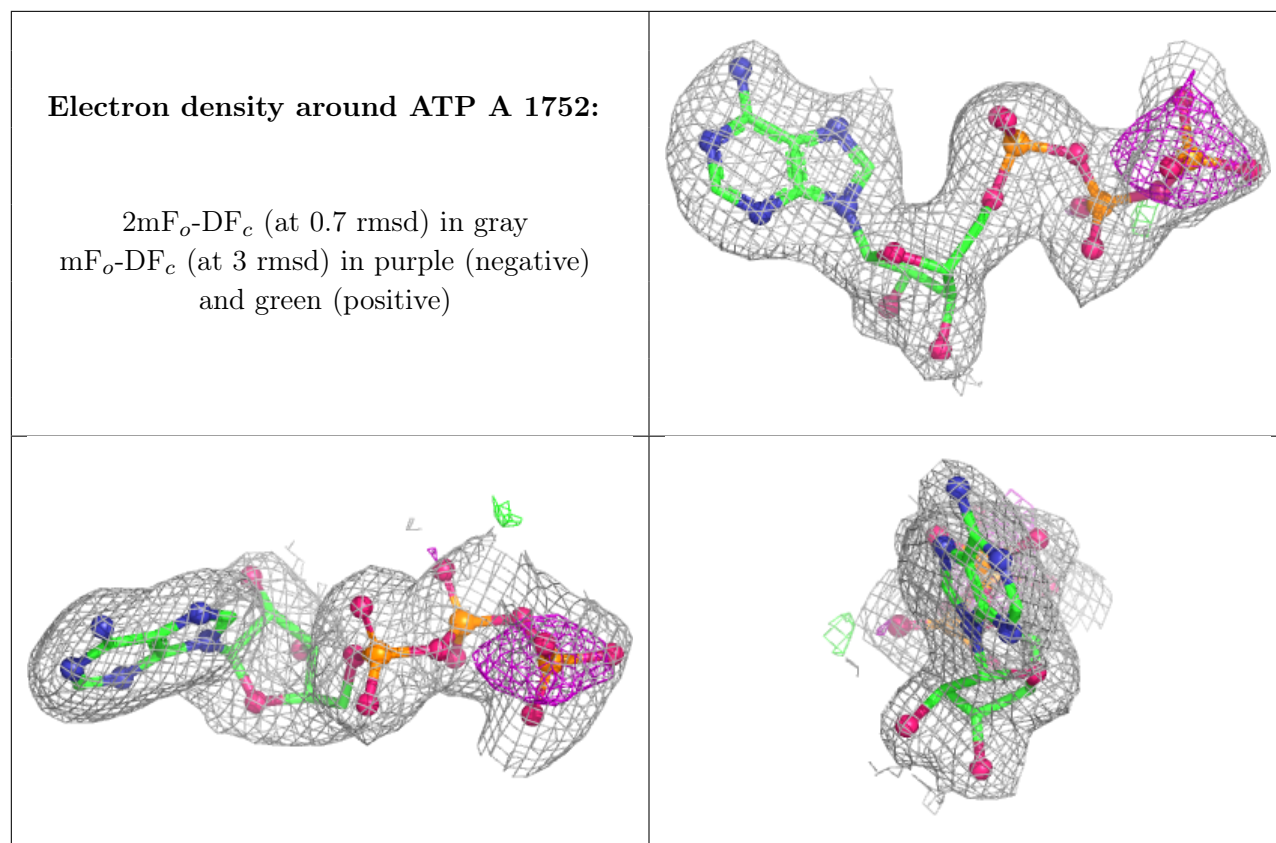
Electron density around ATP D 1753:

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

**Electron density around ATP C 1755:**

$2mF_o-DF_c$ (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.