



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 PM UTC

PDB ID : 2V7Q / pdb_00002v7q
Title : The structure of F1-ATPase inhibited by I1-60HIS, a monomeric form of the inhibitor protein, IF1.
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2007-07-31
Resolution : 2.10 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:

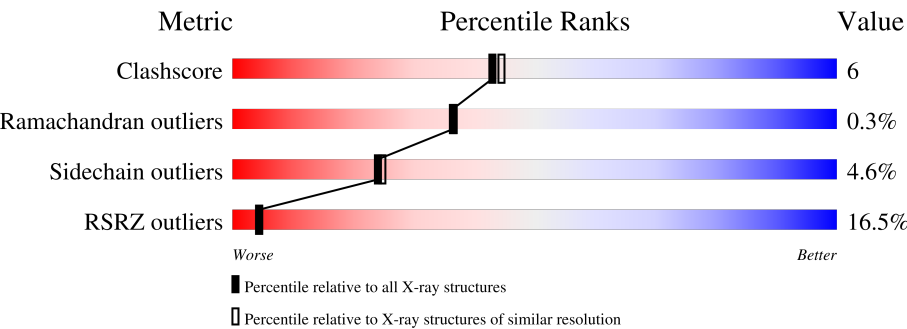
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	510	9% 82% 14% 5%
1	B	510	17% 81% 12% 6%
1	C	510	13% 76% 15% 7%
2	D	482	2% 85% 11% • •
2	E	482	20% 86% 9% • •
2	F	482	16% 85% 10% • •
3	G	272	35% 78% 17% • •

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Mol	Chain	Length	Quality of chain
4	H	146	26% 75% 13% 10%
5	I	50	64% 78% 14% 6%
6	J	66	5% 52% 12% 35%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27418 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	473	Total	C	N	O	S	0	0	0
			3607	2279	637	679	12			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	E	465	Total	C	N	O	S	0	0	0
			3523	2234	599	679	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2054	1293	357	396	8			

- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

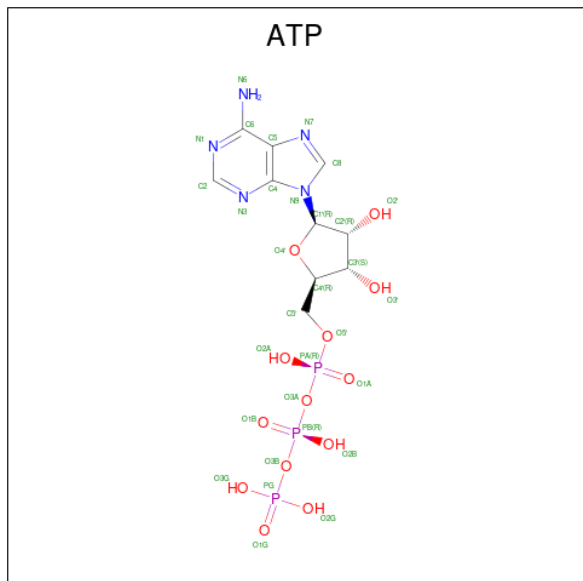
- Molecule 6 is a protein called ATPASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	43	Total	C	N	O		0	0	0
			339	206	71	62				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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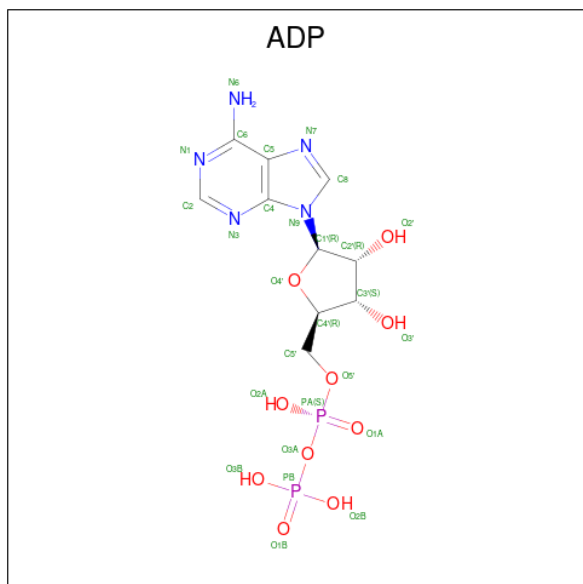
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

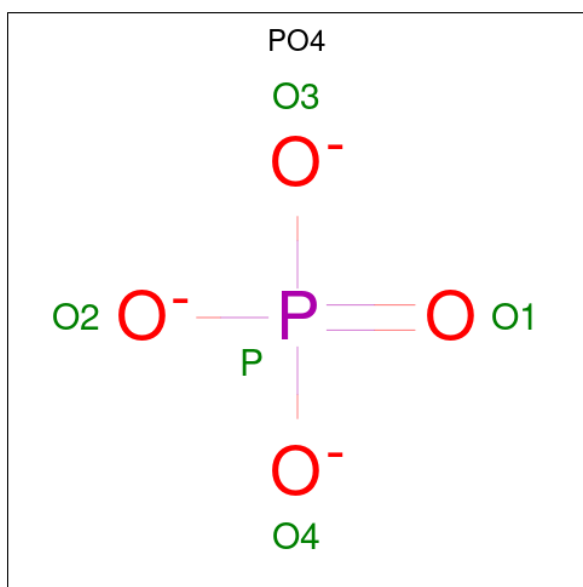
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	O	P	0	0
			5	4	1		

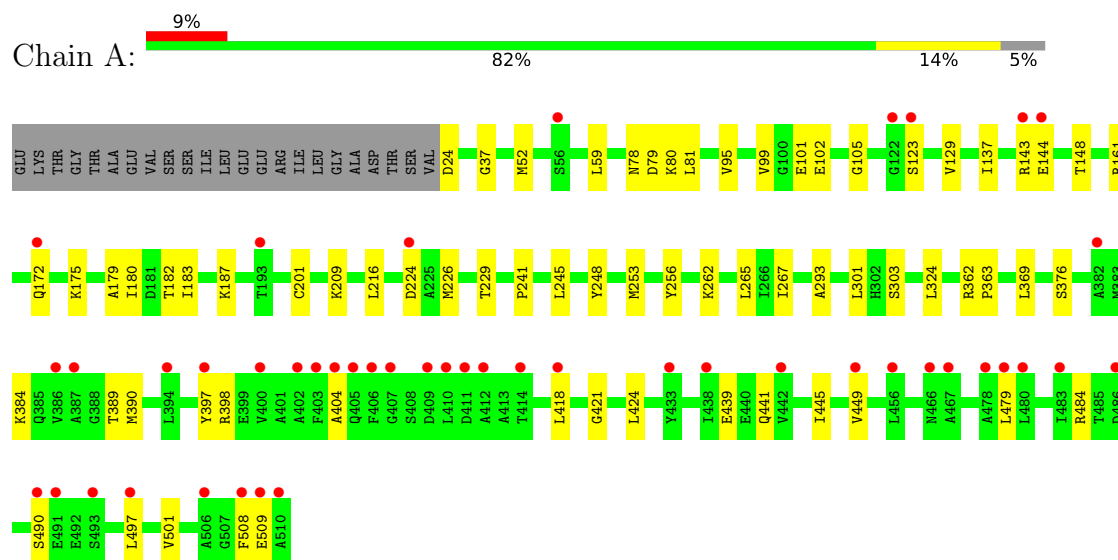
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	286	Total	O	0	0
			286	286		
11	B	294	Total	O	0	0
			294	294		
11	C	296	Total	O	0	0
			296	296		
11	D	367	Total	O	0	0
			367	367		
11	E	216	Total	O	0	0
			216	216		
11	F	316	Total	O	0	0
			316	316		
11	G	112	Total	O	0	0
			112	112		
11	H	27	Total	O	0	0
			27	27		
11	I	6	Total	O	0	0
			6	6		
11	J	20	Total	O	0	0
			20	20		

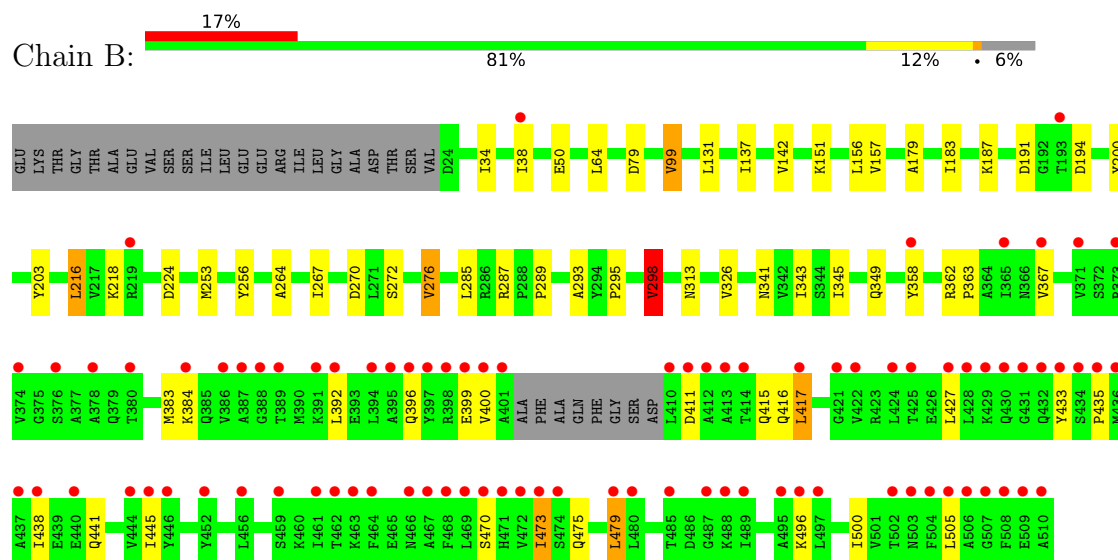
3 Residue-property plots [i](#)

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.

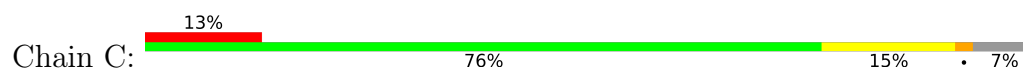
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

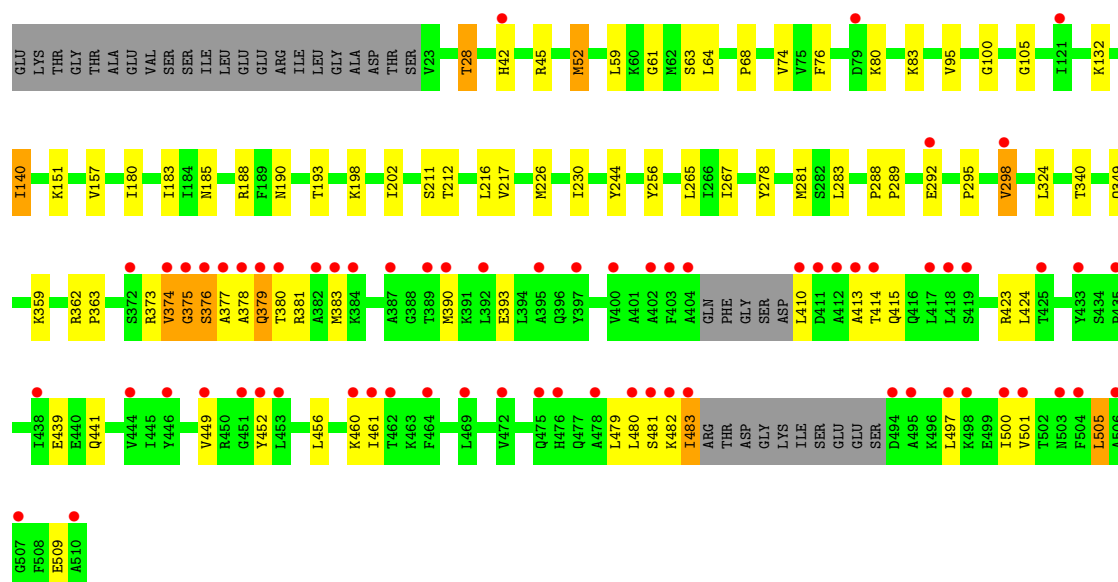


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

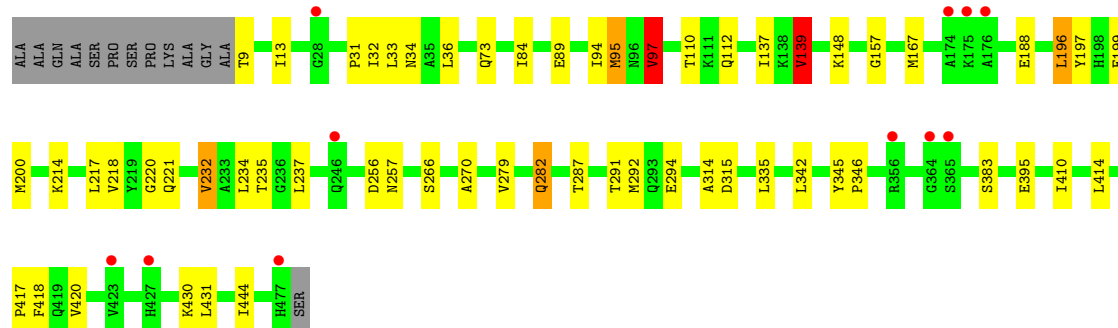
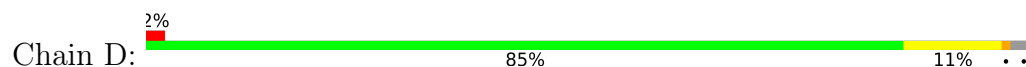


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

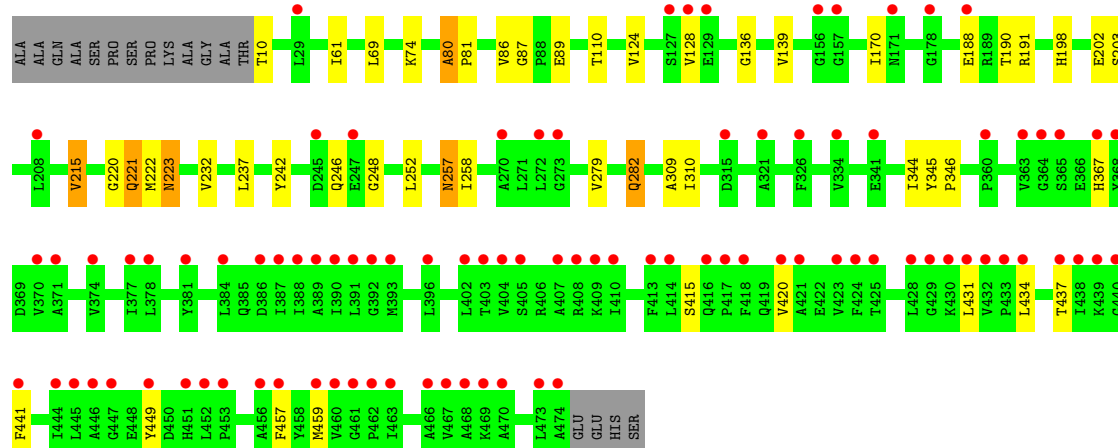
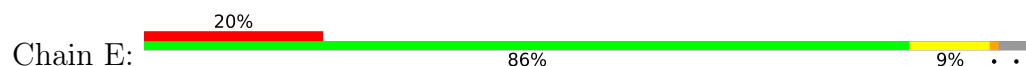




• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• Molecule 2: ATP SYNTHASE SUBUNIT BETA

WORLDWIDE
PDB
PROTEIN DATA BANK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	262.53Å 103.27Å 135.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 2.10 37.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.19-2.10) 98.9 (37.19-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.245 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27418	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: PO4, MG, ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	2/3766 (0.1%)	0.86	0/5080
1	B	0.60	0/3704	0.88	2/4995 (0.0%)
1	C	0.66	2/3655 (0.1%)	0.88	4/4930 (0.1%)
2	D	0.63	0/3616	0.87	3/4906 (0.1%)
2	E	0.55	0/3580	0.82	1/4857 (0.0%)
2	F	0.62	0/3587	0.84	2/4867 (0.0%)
3	G	0.51	0/2077	0.85	0/2787
4	H	0.49	0/982	0.83	0/1337
5	I	0.49	0/374	0.82	1/501 (0.2%)
6	J	0.57	1/343 (0.3%)	1.01	3/453 (0.7%)
All	All	0.60	5/25684 (0.0%)	0.86	16/34713 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	482	LYS	C-N	12.27	1.50	1.33
1	C	373	ARG	C-N	8.16	1.44	1.33
1	A	490	SER	CB-OG	6.37	1.54	1.42
1	A	137	ILE	CA-CB	6.12	1.57	1.54
6	J	23	GLY	C-N	-5.75	1.26	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-10.77	97.94	112.04
2	F	97	VAL	CB-CA-C	-8.92	100.35	112.04
6	J	18	ALA	O-C-N	-7.84	111.64	122.46
2	D	139	VAL	CB-CA-C	-7.74	102.06	111.97
1	C	379	GLN	N-CA-C	-7.63	102.78	112.93
1	B	298	VAL	CB-CA-C	-6.65	103.17	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	249	GLN	N-CA-C	6.31	119.47	109.81
1	C	482	LYS	O-C-N	5.40	129.77	122.59
1	C	482	LYS	CA-C-N	-5.36	112.05	121.70
1	C	482	LYS	C-N-CA	-5.36	112.05	121.70
6	J	18	ALA	CA-C-N	5.26	131.72	121.41
6	J	18	ALA	C-N-CA	5.26	131.72	121.41
2	D	232	VAL	N-CA-C	5.21	115.93	110.62
1	B	298	VAL	N-CA-C	5.18	115.90	110.62
5	I	36	LYS	N-CA-C	-5.17	106.24	112.54
2	E	80	ALA	N-CA-C	5.16	112.66	108.07

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	3715	0	3812	45	0
1	B	3656	0	3763	37	0
1	C	3607	0	3717	59	0
2	D	3558	0	3605	46	0
2	E	3523	0	3580	34	0
2	F	3530	0	3586	57	0
3	G	2054	0	2122	44	0
4	H	970	0	972	10	0
5	I	369	0	395	7	0
6	J	339	0	333	5	0
7	A	31	0	12	2	0
7	B	31	0	12	0	0
7	C	31	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	D	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	27	0	12	0	0
10	E	5	0	0	0	0
11	A	286	0	0	4	0
11	B	294	0	0	4	0
11	C	296	0	0	7	0
11	D	367	0	0	3	0
11	E	216	0	0	1	0
11	F	316	0	0	10	0
11	G	112	0	0	3	0
11	H	27	0	0	0	0
11	I	6	0	0	0	0
11	J	20	0	0	0	0
All	All	27418	0	25945	318	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 6.

All (318) 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)
2:F:166:ILE:HG23	2:F:167:MET:HE2	1.24	1.14
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.29	1.08
2:D:167:MET:HE1	2:D:196:LEU:HD13	1.35	1.08
1:C:211:SER:HB3	2:F:126:MET:HE2	1.37	1.02
2:F:126:MET:HE3	11:F:2122:HOH:O	1.60	1.02
1:C:52:MET:HE1	1:C:76:PHE:HE1	1.20	1.00
3:G:140:ASP:OD1	5:I:42:ILE:HG12	1.61	0.99
2:F:282:GLN:H	2:F:282:GLN:HE21	1.03	0.99
2:E:282:GLN:H	2:E:282:GLN:HE21	1.06	0.99
2:D:282:GLN:H	2:D:282:GLN:HE21	0.99	0.97
1:C:52:MET:HE1	1:C:76:PHE:CE1	2.02	0.95
3:G:89:MET:HE1	3:G:112:ILE:HG23	1.55	0.86
2:F:166:ILE:HG23	2:F:167:MET:CE	2.05	0.86
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.05	0.86
2:F:292:MET:SD	11:F:2222:HOH:O	2.37	0.81
1:C:211:SER:HB3	2:F:126:MET:CE	2.10	0.81
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.64	0.80
1:C:132:LYS:HD3	11:C:2106:HOH:O	1.81	0.79
1:C:52:MET:CE	1:C:76:PHE:HE1	1.96	0.76
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.68	0.76
2:F:292:MET:CE	2:F:296:ILE:HD11	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:209:LYS:HE2	2:F:209:LYS:HA	1.69	0.75
2:F:292:MET:HE1	2:F:296:ILE:HD11	1.69	0.74
1:B:187:LYS:HE2	1:B:224:ASP:HB3	1.70	0.73
1:C:211:SER:CB	2:F:126:MET:HE2	2.17	0.73
2:D:167:MET:CE	2:D:196:LEU:HD13	2.17	0.71
1:A:52:MET:HG2	1:A:95:VAL:HG22	1.72	0.71
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.72	0.71
1:C:340:THR:HG22	11:C:2231:HOH:O	1.91	0.71
1:A:99:VAL:HG23	1:A:253:MET:HA	1.73	0.71
2:F:166:ILE:CG2	2:F:167:MET:HE2	2.14	0.70
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.74	0.70
2:D:282:GLN:HE21	2:D:282:GLN:N	1.82	0.70
2:F:223:ASN:HD22	2:F:223:ASN:H	1.39	0.70
2:D:200:MET:HE1	2:D:217:LEU:HD11	1.74	0.69
2:F:282:GLN:H	2:F:282:GLN:NE2	1.85	0.68
1:B:156:LEU:HD13	1:B:367:VAL:HG13	1.73	0.68
2:D:287:THR:O	2:D:291:THR:HG23	1.93	0.68
3:G:78:CYS:HB3	11:G:2032:HOH:O	1.91	0.68
2:D:282:GLN:H	2:D:282:GLN:NE2	1.82	0.68
1:C:28:THR:HG22	11:C:2006:HOH:O	1.94	0.67
2:F:291:THR:HG21	11:F:2221:HOH:O	1.93	0.67
3:G:86:ALA:HA	3:G:89:MET:HE3	1.77	0.67
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.78	0.66
1:C:52:MET:CE	1:C:95:VAL:HG22	2.16	0.65
3:G:85:VAL:HG12	3:G:89:MET:HE2	1.79	0.64
1:C:374:VAL:HG13	1:C:375:GLY:H	1.63	0.64
2:F:209:LYS:HA	2:F:209:LYS:CE	2.28	0.64
1:C:52:MET:HE3	1:C:95:VAL:CG2	2.18	0.63
2:E:223:ASN:HD22	2:E:223:ASN:H	1.45	0.63
1:A:389:THR:HB	1:A:449:VAL:HG21	1.79	0.63
2:F:282:GLN:HE21	2:F:282:GLN:N	1.87	0.63
1:B:295:PRO:O	1:B:298:VAL:HG22	1.99	0.63
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.81	0.63
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.82	0.62
2:E:257:ASN:HB2	2:E:309:ALA:O	2.00	0.62
2:F:12:ARG:HG2	2:F:74:LYS:HE2	1.82	0.61
2:F:96:ASN:C	2:F:96:ASN:HD22	2.08	0.61
2:E:203:SER:HB2	2:E:420:VAL:HG13	1.82	0.60
2:F:266:SER:HB3	2:F:282:GLN:HE22	1.65	0.60
2:F:249:GLN:HA	2:F:249:GLN:HE21	1.66	0.60
2:E:282:GLN:H	2:E:282:GLN:NE2	1.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ALA:HB2	1:A:418:LEU:HD22	1.85	0.59
2:D:137:ILE:HD12	2:D:418:PHE:CE1	2.37	0.59
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.83	0.59
1:C:340:THR:HG21	2:D:314:ALA:HB2	1.85	0.59
2:E:449:TYR:HB3	2:E:457:PHE:HZ	1.68	0.58
2:F:188:GLU:O	2:F:221:GLN:HB3	2.02	0.58
1:A:78:ASN:HD21	1:A:80:LYS:HD3	1.69	0.58
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.34	0.58
1:A:376:SER:HB3	1:A:384:LYS:HE3	1.84	0.58
2:D:395:GLU:CD	3:G:75:ARG:HD3	2.29	0.58
2:D:200:MET:CE	2:D:217:LEU:HD11	2.33	0.58
3:G:117:HIS:O	3:G:121:SER:HB2	2.03	0.58
5:I:37:THR:HG22	5:I:38:SER:H	1.69	0.58
2:E:257:ASN:C	2:E:257:ASN:HD22	2.10	0.58
1:A:303:SER:HB2	2:E:222:MET:HG2	1.86	0.57
1:C:244:TYR:CB	1:C:281:MET:HE1	2.34	0.57
2:E:198:HIS:O	2:E:202:GLU:HG2	2.04	0.57
1:A:497:LEU:O	1:A:501:VAL:HG23	2.04	0.57
1:C:376:SER:C	1:C:378:ALA:H	2.13	0.57
1:B:289:PRO:HB2	1:B:293:ALA:HA	1.88	0.56
6:J:8:VAL:HG23	6:J:9:ARG:H	1.71	0.56
2:F:345:TYR:HB2	2:F:459:MET:HE1	1.86	0.56
2:D:234:LEU:HD21	2:D:292:MET:HG3	1.87	0.56
1:A:187:LYS:HE3	1:A:224:ASP:HB3	1.87	0.56
1:B:183:ILE:HD11	1:B:267:ILE:HD13	1.88	0.55
1:B:218:LYS:HD2	2:E:128:VAL:HB	1.88	0.55
1:C:359:LYS:NZ	2:F:383:SER:OG	2.39	0.55
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.87	0.55
2:F:166:ILE:CG2	2:F:167:MET:CE	2.81	0.55
4:H:127:THR:O	4:H:131:ILE:HG12	2.07	0.55
2:D:221:GLN:HE21	2:D:221:GLN:HA	1.72	0.54
3:G:25:MET:HE2	3:G:25:MET:HA	1.88	0.54
1:C:439:GLU:HG3	1:C:480:LEU:HB3	1.89	0.54
2:D:97:VAL:HG22	11:D:2176:HOH:O	2.07	0.54
2:E:345:TYR:HB2	2:E:459:MET:HE1	1.88	0.54
1:C:379:GLN:HG2	1:C:380:THR:H	1.73	0.54
1:C:380:THR:HG22	1:C:381:ARG:H	1.72	0.54
3:G:2:THR:HG23	3:G:5:ASP:H	1.73	0.54
4:H:104:ASP:HB2	5:I:27:LYS:HB3	1.89	0.54
2:F:249:GLN:HA	2:F:249:GLN:NE2	2.22	0.54
1:A:24:ASP:N	11:A:2002:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:HD12	1:C:216:LEU:HD21	1.86	0.53
2:F:9:THR:N	11:F:2001:HOH:O	2.41	0.53
1:C:52:MET:HE2	1:C:61:GLY:O	2.08	0.53
1:C:265:LEU:HD11	1:C:324:LEU:HG	1.90	0.53
2:F:97:VAL:HG22	11:F:2173:HOH:O	2.08	0.53
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.90	0.53
2:F:167:MET:HE1	2:F:183:PHE:CE1	2.43	0.52
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.91	0.52
2:D:157:GLY:HA3	2:D:315:ASP:OD1	2.09	0.52
2:E:345:TYR:HA	2:E:346:PRO:C	2.35	0.52
2:D:89:GLU:HB2	2:D:110:THR:CG2	2.39	0.52
1:B:496:LYS:O	1:B:500:ILE:HG12	2.09	0.52
1:C:390:MET:HG3	1:C:424:LEU:HD13	1.90	0.52
4:H:22:SER:HA	4:H:94:ALA:O	2.10	0.52
1:B:287:ARG:HD3	11:B:2219:HOH:O	2.08	0.52
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.91	0.52
3:G:2:THR:HG22	3:G:5:ASP:CG	2.35	0.51
1:A:37:GLY:HA2	1:A:79:ASP:CG	2.35	0.51
2:F:126:MET:CE	11:F:2122:HOH:O	2.35	0.51
2:F:292:MET:HE2	2:F:296:ILE:HD11	1.92	0.51
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.93	0.51
1:C:151:LYS:HG2	1:C:441:GLN:HG2	1.92	0.51
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.92	0.51
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.93	0.51
2:D:188:GLU:O	2:D:221:GLN:HB3	2.11	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.22	0.51
2:F:252:LEU:HD23	2:F:305:THR:HB	1.93	0.51
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.93	0.51
1:B:358:TYR:HB3	11:B:2258:HOH:O	2.11	0.51
2:D:279:VAL:HG12	2:D:279:VAL:O	2.10	0.50
1:A:390:MET:HE2	1:A:424:LEU:HB3	1.93	0.50
1:B:479:LEU:HG	1:B:496:LYS:HD3	1.93	0.50
3:G:78:CYS:HB3	3:G:228:ARG:HG3	1.91	0.50
1:A:99:VAL:CG2	1:A:256:TYR:HB2	2.41	0.50
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.92	0.50
2:E:257:ASN:C	2:E:257:ASN:ND2	2.70	0.50
2:E:258:ILE:HG21	2:E:310:ILE:HG12	1.93	0.50
2:F:223:ASN:HD22	2:F:223:ASN:N	2.05	0.50
5:I:44:ILE:HD13	5:I:44:ILE:H	1.75	0.50
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.93	0.50
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LEU:HA	1:C:500:ILE:HG22	1.93	0.49
2:E:223:ASN:HD22	2:E:223:ASN:N	2.10	0.49
11:C:2234:HOH:O	3:G:2:THR:HG21	2.11	0.49
2:D:395:GLU:OE1	3:G:75:ARG:NH1	2.40	0.49
2:F:391:LEU:HD22	3:G:77:LEU:HD21	1.93	0.49
2:E:242:TYR:CD1	2:E:246:GLN:HG3	2.47	0.49
1:C:380:THR:HB	1:C:383:MET:HB3	1.95	0.49
2:E:86:VAL:O	2:E:110:THR:OG1	2.30	0.49
3:G:131:VAL:HG22	5:I:42:ILE:HD12	1.94	0.49
2:D:291:THR:HG21	11:D:2116:HOH:O	2.13	0.49
2:F:139:VAL:HG23	11:F:2296:HOH:O	2.13	0.49
1:A:183:ILE:HD11	1:A:267:ILE:HD13	1.94	0.49
1:B:343:ILE:HG12	1:B:349:GLN:HG2	1.95	0.49
2:D:89:GLU:HB2	2:D:110:THR:HG22	1.95	0.49
1:A:102:GLU:HG3	1:A:123:SER:HA	1.94	0.49
1:A:175:LYS:HE3	7:A:1511:ATP:O1B	2.13	0.49
1:A:172:GLN:NE2	7:A:1511:ATP:O1G	2.41	0.48
1:B:392:LEU:HB2	11:B:2262:HOH:O	2.12	0.48
2:E:203:SER:CB	2:E:420:VAL:HG13	2.43	0.48
2:F:266:SER:HB3	2:F:282:GLN:NE2	2.27	0.48
1:B:411:ASP:HB3	1:B:415:GLN:HB2	1.94	0.48
1:B:272:SER:O	1:B:276:VAL:HG13	2.14	0.48
3:G:75:ARG:O	3:G:82:HIS:HE1	1.97	0.48
1:A:248:TYR:OH	1:A:301:LEU:HD12	2.13	0.48
1:B:362:ARG:HA	1:B:363:PRO:C	2.38	0.48
1:C:481:SER:C	1:C:483:ILE:H	2.21	0.48
1:A:143:ARG:HB2	11:A:2118:HOH:O	2.14	0.48
2:D:97:VAL:HG13	2:D:232:VAL:HG13	1.95	0.48
1:B:441:GLN:O	1:B:445:ILE:HG12	2.14	0.48
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.49	0.47
1:C:376:SER:C	1:C:378:ALA:N	2.72	0.47
3:G:140:ASP:HB3	5:I:42:ILE:HG13	1.96	0.47
2:D:395:GLU:OE2	3:G:75:ARG:HD3	2.15	0.47
1:C:379:GLN:HG2	1:C:380:THR:N	2.29	0.47
3:G:87:LYS:HA	3:G:90:LYS:HE2	1.97	0.47
1:A:201:CYS:O	1:A:229:THR:HA	2.14	0.47
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.97	0.47
3:G:75:ARG:NH2	3:G:228:ARG:HG2	2.29	0.47
1:C:452:TYR:HB3	1:C:505:LEU:HD12	1.97	0.47
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.50	0.47
1:A:369:LEU:HD21	6:J:8:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:TYR:CG	1:C:281:MET:HE1	2.49	0.47
1:C:185:ASN:O	1:C:188:ARG:HG2	2.14	0.47
3:G:2:THR:CG2	3:G:5:ASP:H	2.27	0.47
1:A:105:GLY:HA2	1:A:226:MET:O	2.15	0.46
3:G:10:LEU:HD22	3:G:14:LYS:HE3	1.97	0.46
3:G:81:ILE:HD13	3:G:227:ALA:CB	2.45	0.46
3:G:262:LEU:O	3:G:266:ILE:HG12	2.15	0.46
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.50	0.46
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.30	0.46
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.96	0.46
2:D:188:GLU:H	2:D:221:GLN:NE2	2.13	0.46
2:F:167:MET:HE1	2:F:183:PHE:HE1	1.77	0.46
1:B:38:ILE:HD11	1:B:64:LEU:HD23	1.97	0.46
1:C:295:PRO:HD2	1:C:298:VAL:HG13	1.97	0.46
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.81	0.46
3:G:140:ASP:CG	5:I:42:ILE:HG12	2.34	0.46
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.51	0.46
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.98	0.46
2:F:163:THR:O	2:F:167:MET:HG2	2.17	0.45
2:E:188:GLU:O	2:E:221:GLN:HG3	2.17	0.45
1:A:441:GLN:O	1:A:445:ILE:HG12	2.16	0.45
2:E:437:THR:O	2:E:441:PHE:HD1	1.99	0.45
1:C:80:LYS:HG2	2:F:32:ILE:HG21	1.99	0.45
2:F:139:VAL:HG22	2:F:414:LEU:HB3	1.98	0.45
1:B:99:VAL:HG22	1:B:253:MET:HA	1.99	0.45
1:C:413:ALA:C	1:C:415:GLN:H	2.25	0.45
1:C:456:LEU:HD11	1:C:460:LYS:HD2	1.97	0.45
2:D:410:ILE:HG13	2:D:444:ILE:HG21	1.97	0.45
1:C:100:GLY:HA2	1:C:256:TYR:CZ	2.52	0.45
1:C:212:THR:HA	2:F:356:ARG:HH22	1.81	0.45
1:A:99:VAL:HG21	1:A:256:TYR:HB2	1.99	0.45
1:A:479:LEU:HD11	1:A:497:LEU:HG	1.98	0.45
1:B:187:LYS:NZ	1:B:191:ASP:OD2	2.49	0.45
1:C:140:ILE:HD12	11:C:2110:HOH:O	2.16	0.45
2:D:167:MET:HE1	2:D:196:LEU:CD1	2.24	0.45
3:G:72:SER:HB2	3:G:82:HIS:HD2	1.82	0.45
3:G:72:SER:CB	3:G:82:HIS:HD2	2.29	0.45
3:G:214:TYR:CE2	4:H:23:PRO:HB3	2.52	0.45
4:H:41:GLN:HA	4:H:59:ARG:HG3	1.98	0.45
1:A:101:GLU:OE1	1:A:262:LYS:NZ	2.38	0.44
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.53	0.44
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.53	0.44
3:G:133:ARG:HG3	11:G:2055:HOH:O	2.17	0.44
3:G:209:LEU:O	3:G:213:ILE:HG22	2.16	0.44
1:B:38:ILE:HD12	1:B:285:LEU:HD21	1.99	0.44
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.18	0.44
2:F:274:ARG:NH2	11:F:2203:HOH:O	2.51	0.44
1:B:156:LEU:HD13	1:B:367:VAL:CG1	2.46	0.44
2:D:214:LYS:HE3	11:D:2193:HOH:O	2.17	0.44
3:G:75:ARG:HG3	11:G:2032:HOH:O	2.18	0.44
2:E:190:THR:OG1	2:E:221:GLN:HG2	2.18	0.44
6:J:20:GLY:O	6:J:23:GLY:N	2.51	0.44
4:H:83:THR:HB	4:H:91:GLN:HG2	2.00	0.43
1:A:99:VAL:HG22	1:A:256:TYR:CB	2.48	0.43
1:A:508:PHE:CD2	1:A:509:GLU:HG2	2.53	0.43
1:C:42:HIS:HD2	11:C:2010:HOH:O	2.00	0.43
1:B:270:ASP:HB2	1:B:326:VAL:O	2.19	0.43
2:D:345:TYR:HA	2:D:346:PRO:C	2.43	0.43
3:G:89:MET:HE1	3:G:112:ILE:HD12	1.99	0.43
1:A:144:GLU:HB3	1:A:161:ARG:HD2	2.01	0.43
2:E:282:GLN:HE21	2:E:282:GLN:N	1.91	0.43
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.53	0.43
11:A:2114:HOH:O	2:E:191:ARG:HG3	2.19	0.43
1:B:470:SER:O	1:B:473:ILE:HG22	2.19	0.43
1:C:52:MET:CE	1:C:76:PHE:CE1	2.83	0.43
2:D:95:MET:HG2	2:D:218:VAL:HG22	2.01	0.43
2:D:417:PRO:HG2	2:D:430:LYS:HG2	2.00	0.43
3:G:87:LYS:O	3:G:91:SER:HB2	2.19	0.43
4:H:40:THR:OG1	4:H:56:GLN:CG	2.67	0.43
1:B:50:GLU:OE2	2:F:67:GLU:HG3	2.19	0.43
1:A:148:THR:HA	1:A:182:THR:HG23	2.01	0.43
1:C:278:TYR:CD2	1:C:295:PRO:HG2	2.54	0.43
2:F:96:ASN:C	2:F:96:ASN:ND2	2.76	0.43
2:F:108:ILE:HG22	2:F:110:THR:HG23	2.00	0.43
1:B:435:PRO:HG2	11:B:2063:HOH:O	2.18	0.43
3:G:141:ALA:HB1	3:G:213:ILE:HG23	2.00	0.43
1:C:190:ASN:HA	1:C:198:LYS:HG2	2.01	0.42
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.42
1:B:383:MET:HG3	1:B:438:ILE:HD11	2.01	0.42
1:C:64:LEU:HD23	1:C:64:LEU:HA	1.86	0.42
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:178:ILE:CG2	3:G:180:SER:HB2	2.47	0.42
1:B:341:ASN:O	1:B:345:ILE:HG13	2.19	0.42
2:D:342:LEU:HD11	6:J:16:ARG:HH21	1.83	0.42
2:F:139:VAL:HG21	11:F:2258:HOH:O	2.19	0.42
3:G:261:GLU:HG2	3:G:262:LEU:N	2.34	0.42
1:A:59:LEU:HD11	1:A:81:LEU:HD12	2.02	0.42
2:F:422:GLU:HG2	2:F:427:HIS:O	2.19	0.42
1:A:265:LEU:HD11	1:A:324:LEU:HG	2.02	0.42
2:E:10:THR:HG21	2:E:74:LYS:HD2	2.01	0.42
2:E:248:GLY:HA3	11:E:2187:HOH:O	2.18	0.42
3:G:181:LEU:HD23	3:G:184:ILE:HB	2.01	0.42
1:B:179:ALA:HB1	1:B:267:ILE:HG12	2.02	0.42
1:B:203:TYR:CZ	1:B:216:LEU:HD21	2.55	0.42
2:E:258:ILE:CG2	2:E:310:ILE:HG12	2.50	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.17	0.42
6:J:37:ARG:HD3	6:J:37:ARG:HA	1.80	0.42
1:C:105:GLY:HA2	1:C:226:MET:O	2.20	0.41
1:A:129:VAL:HG21	1:A:245:LEU:HD21	2.02	0.41
2:E:80:ALA:HB1	2:E:81:PRO:HD2	2.02	0.41
2:F:32:ILE:O	2:F:33:LEU:HB2	2.20	0.41
3:G:117:HIS:CE1	3:G:118:ARG:HG3	2.56	0.41
1:A:180:ILE:CD1	1:A:216:LEU:HD21	2.50	0.41
1:B:433:TYR:C	1:B:435:PRO:HD3	2.45	0.41
2:F:97:VAL:HG13	2:F:232:VAL:HB	2.01	0.41
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.20	0.41
1:C:288:PRO:HB2	2:D:270:ALA:HB1	2.02	0.41
1:C:375:GLY:O	1:C:377:ALA:N	2.53	0.41
1:C:374:VAL:N	11:C:2256:HOH:O	2.50	0.41
2:F:177:HIS:HE1	2:F:250:ASP:HB3	1.85	0.41
2:F:435:LYS:HG2	11:F:2299:HOH:O	2.21	0.41
1:A:241:PRO:O	1:A:245:LEU:HB2	2.21	0.41
1:B:200:TYR:O	1:B:264:ALA:HA	2.21	0.41
1:C:497:LEU:O	1:C:501:VAL:HG23	2.21	0.41
3:G:13:ILE:HD13	3:G:242:MET:HE2	2.03	0.41
4:H:66:HIS:HA	4:H:72:THR:HG22	2.03	0.41
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.41
2:D:97:VAL:HG13	2:D:232:VAL:CG1	2.51	0.41
2:E:69:LEU:HD23	2:E:69:LEU:HA	1.88	0.41
3:G:260:LYS:HE3	3:G:264:GLU:OE2	2.21	0.41
1:A:398:ARG:HD3	11:A:2239:HOH:O	2.20	0.40
1:C:183:ILE:HD11	1:C:267:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:345:TYR:HA	2:F:346:PRO:C	2.45	0.40
1:B:151:LYS:HE3	1:B:151:LYS:HB2	1.96	0.40
1:C:362:ARG:HA	1:C:363:PRO:C	2.46	0.40
3:G:72:SER:HB2	3:G:82:HIS:CD2	2.55	0.40
1:A:362:ARG:HA	1:A:363:PRO:C	2.46	0.40
1:B:396:GLN:HB3	1:B:417:LEU:HD11	2.02	0.40
3:G:2:THR:HG22	3:G:5:ASP:OD2	2.22	0.40
1:B:313:ASN:C	1:B:313:ASN:OD1	2.64	0.40
2:D:256:ASP:HA	2:D:257:ASN:HA	1.94	0.40
4:H:40:THR:OG1	4:H:56:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

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	485/510 (95%)	472 (97%)	13 (3%)	0	100	100
1	B	475/510 (93%)	459 (97%)	15 (3%)	1 (0%)	43	44
1	C	467/510 (92%)	447 (96%)	16 (3%)	4 (1%)	14	10
2	D	467/482 (97%)	451 (97%)	16 (3%)	0	100	100
2	E	463/482 (96%)	448 (97%)	14 (3%)	1 (0%)	43	44
2	F	464/482 (96%)	452 (97%)	10 (2%)	2 (0%)	30	28
3	G	257/272 (94%)	244 (95%)	11 (4%)	2 (1%)	16	12
4	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
5	I	45/50 (90%)	42 (93%)	2 (4%)	1 (2%)	5	2
6	J	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
All	All	3293/3510 (94%)	3177 (96%)	105 (3%)	11 (0%)	36	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	VAL
1	B	194	ASP
2	F	247	GLU
5	I	29	GLU
3	G	148	LEU
1	C	376	SER
1	C	509	GLU
2	F	28	GLY
3	G	195	ASP
1	C	375	GLY
2	E	279	VAL

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	B	328/413 (79%)	311 (95%)	17 (5%)	21	20
1	C	381/413 (92%)	361 (95%)	20 (5%)	21	20
2	D	379/386 (98%)	364 (96%)	15 (4%)	28	29
2	E	375/386 (97%)	364 (97%)	11 (3%)	37	42
2	F	376/386 (97%)	362 (96%)	14 (4%)	30	33
3	G	225/230 (98%)	211 (94%)	14 (6%)	16	14
4	H	104/109 (95%)	97 (93%)	7 (7%)	15	12
5	I	38/41 (93%)	36 (95%)	2 (5%)	20	19
6	J	30/50 (60%)	28 (93%)	2 (7%)	15	12
All	All	2236/2414 (93%)	2134 (95%)	102 (5%)	24	25

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	99	VAL
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	142	VAL
1	B	157	VAL
1	B	216	LEU
1	B	276	VAL
1	B	298	VAL
1	B	384	LYS
1	B	399	GLU
1	B	400	VAL
1	B	416	GLN
1	B	417	LEU
1	B	427	LEU
1	B	473	ILE
1	B	475	GLN
1	B	479	LEU
1	B	505	LEU
1	C	28	THR
1	C	52	MET
1	C	59	LEU
1	C	63	SER
1	C	74	VAL
1	C	83	LYS
1	C	140	ILE
1	C	157	VAL
1	C	193	THR
1	C	217	VAL
1	C	292	GLU
1	C	298	VAL
1	C	349	GLN
1	C	393	GLU
1	C	410	LEU
1	C	414	THR
1	C	449	VAL
1	C	479	LEU
1	C	483	ILE
1	C	505	LEU
2	D	9	THR
2	D	36	LEU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	139	VAL
2	D	148	LYS

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Mol	Chain	Res	Type
2	D	196	LEU
2	D	199	GLU
2	D	237	LEU
2	D	282	GLN
2	D	335	LEU
2	D	383	SER
2	D	420	VAL
2	D	431	LEU
2	E	61	ILE
2	E	89	GLU
2	E	124	VAL
2	E	139	VAL
2	E	215	VAL
2	E	221	GLN
2	E	223	ASN
2	E	237	LEU
2	E	252	LEU
2	E	257	ASN
2	E	282	GLN
2	F	10	THR
2	F	67	GLU
2	F	96	ASN
2	F	97	VAL
2	F	173	VAL
2	F	223	ASN
2	F	274	ARG
2	F	279	VAL
2	F	282	GLN
2	F	356	ARG
2	F	386	ASP
2	F	419	GLN
2	F	423	VAL
2	F	455	GLN
3	G	10	LEU
3	G	67	LEU
3	G	81	ILE
3	G	108	VAL
3	G	119	THR
3	G	125	LEU
3	G	126	VAL
3	G	133	ARG
3	G	169	ILE

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Mol	Chain	Res	Type
3	G	184	ILE
3	G	199	ASP
3	G	200	VAL
3	G	261	GLU
3	G	262	LEU
4	H	40	THR
4	H	42	THR
4	H	54	THR
4	H	91	GLN
4	H	105	LEU
4	H	112	LEU
4	H	118	GLU
5	I	44	ILE
5	I	46	LYS
6	J	26	GLU
6	J	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	186	GLN
1	B	330	GLN
1	B	349	GLN
1	B	475	GLN
1	C	263	HIS
1	C	349	GLN
1	C	396	GLN
2	D	24	GLN
2	D	112	GLN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	D	379	GLN
2	D	385	GLN
2	D	442	GLN
2	E	24	GLN
2	E	112	GLN
2	E	194	ASN
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	442	GLN

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Mol	Chain	Res	Type
2	E	443	GLN
2	F	96	ASN
2	F	177	HIS
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	249	GLN
2	F	282	GLN
2	F	361	ASN
2	F	367	HIS
2	F	379	GLN
2	F	455	GLN
3	G	82	HIS
3	G	120	HIS
3	G	234	ASN
4	H	85	ASN
4	H	91	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 11 ligands modelled in this entry, 5 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
7	ATP	C	1511	8	32,33,33	1.44	5 (15%)	48,52,52	1.85	10 (20%)
9	ADP	F	1475	8	28,29,29	1.39	3 (10%)	43,45,45	1.83	9 (20%)
7	ATP	A	1511	8	32,33,33	1.41	5 (15%)	48,52,52	1.92	10 (20%)
10	PO4	E	1475	-	4,4,4	0.95	0	6,6,6	0.48	0
9	ADP	D	1478	8	28,29,29	1.51	5 (17%)	43,45,45	1.93	7 (16%)
7	ATP	B	1511	8	32,33,33	1.62	6 (18%)	48,52,52	1.79	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
7	ATP	C	1511	8	-	3/22/38/38	0/3/3/3
9	ADP	F	1475	8	-	2/16/32/32	0/3/3/3
7	ATP	A	1511	8	-	4/22/38/38	0/3/3/3
9	ADP	D	1478	8	-	2/16/32/32	0/3/3/3
7	ATP	B	1511	8	-	0/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1511	ATP	C5-C4	4.95	1.47	1.39
9	D	1478	ADP	C5-C4	4.95	1.47	1.39
7	A	1511	ATP	C5-C4	4.89	1.47	1.39
9	F	1475	ADP	C5-C4	4.71	1.47	1.39
7	C	1511	ATP	C5-C4	4.61	1.47	1.39
7	B	1511	ATP	PA-O3A	3.89	1.63	1.59
9	D	1478	ADP	C5-C6	3.00	1.49	1.41
7	A	1511	ATP	C5-C6	2.95	1.49	1.41
7	B	1511	ATP	PB-O3B	2.90	1.62	1.59
9	F	1475	ADP	C5-C6	2.84	1.48	1.41
7	B	1511	ATP	C5-C6	2.72	1.48	1.41
7	C	1511	ATP	C5-C6	2.69	1.48	1.41
7	C	1511	ATP	PA-O3A	2.52	1.62	1.59
7	C	1511	ATP	C8-N7	2.44	1.36	1.31
7	A	1511	ATP	C5-N7	-2.43	1.34	1.39
9	D	1478	ADP	C5-N7	-2.36	1.34	1.39
7	B	1511	ATP	C5-N7	-2.31	1.34	1.39
7	A	1511	ATP	PA-O3A	2.30	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1511	ATP	C5-N7	-2.30	1.34	1.39
9	D	1478	ADP	PA-O3A	2.28	1.62	1.59
9	F	1475	ADP	C8-N7	2.18	1.35	1.31
7	B	1511	ATP	C8-N7	2.16	1.35	1.31
7	A	1511	ATP	C8-N7	2.11	1.35	1.31
9	D	1478	ADP	C8-N7	2.06	1.35	1.31

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1511	ATP	C5-C4-N3	-6.30	118.04	126.72
9	D	1478	ADP	C5-C4-N3	-6.30	118.04	126.72
7	B	1511	ATP	C5-C4-N3	-5.90	118.60	126.72
7	C	1511	ATP	C5-C4-N3	-5.71	118.85	126.72
9	F	1475	ADP	C5-C4-N3	-5.66	118.92	126.72
7	A	1511	ATP	N3-C4-N9	5.03	135.72	127.17
9	D	1478	ADP	N3-C4-N9	5.00	135.66	127.17
7	B	1511	ATP	N3-C4-N9	4.93	135.55	127.17
9	F	1475	ADP	N3-C4-N9	4.52	134.86	127.17
7	C	1511	ATP	N3-C4-N9	4.35	134.57	127.17
7	A	1511	ATP	C2-N3-C4	4.16	121.99	111.83
9	D	1478	ADP	C4-C5-N7	-3.97	106.05	110.58
9	F	1475	ADP	C2-N3-C4	3.92	121.40	111.83
9	F	1475	ADP	N3-C2-N1	-3.87	122.72	128.58
7	C	1511	ATP	C4-C5-N7	-3.83	106.21	110.58
7	B	1511	ATP	C2-N3-C4	3.82	121.17	111.83
9	D	1478	ADP	C2-N3-C4	3.81	121.12	111.83
7	C	1511	ATP	C2-N3-C4	3.72	120.91	111.83
7	A	1511	ATP	N3-C2-N1	-3.67	123.02	128.58
7	A	1511	ATP	C4-C5-N7	-3.60	106.47	110.58
7	B	1511	ATP	N3-C2-N1	-3.59	123.15	128.58
9	F	1475	ADP	C4-C5-N7	-3.43	106.66	110.58
7	C	1511	ATP	N3-C2-N1	-3.37	123.49	128.58
9	D	1478	ADP	N3-C2-N1	-3.14	123.83	128.58
7	B	1511	ATP	C4-C5-N7	-3.04	107.11	110.58
9	D	1478	ADP	C5-N7-C8	2.97	108.12	103.45
7	A	1511	ATP	O2B-PB-O3B	2.94	115.21	107.27
7	C	1511	ATP	C5-N7-C8	2.73	107.74	103.45
7	A	1511	ATP	C5-N7-C8	2.70	107.70	103.45
7	B	1511	ATP	C4-N9-C8	2.65	108.52	105.74
7	C	1511	ATP	C4-N9-C8	2.62	108.49	105.74
9	D	1478	ADP	C4-N9-C8	2.57	108.43	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	1475	ADP	C4-N9-C8	2.55	108.42	105.74
7	A	1511	ATP	C4-N9-C8	2.46	108.32	105.74
9	F	1475	ADP	C5-N7-C8	2.42	107.25	103.45
7	C	1511	ATP	C6-C5-N7	2.41	136.73	132.09
9	F	1475	ADP	C6-C5-N7	2.32	136.56	132.09
7	B	1511	ATP	C5-N7-C8	2.22	106.94	103.45
9	F	1475	ADP	C2-N1-C6	2.17	122.30	118.73
7	A	1511	ATP	O2A-PA-O1A	2.17	122.53	112.44
7	A	1511	ATP	C6-C5-N7	2.15	136.24	132.09
7	C	1511	ATP	O4'-C1'-N9	2.11	112.15	108.09
7	C	1511	ATP	N9-C8-N7	-2.08	110.98	113.94
7	B	1511	ATP	C2-N1-C6	2.02	122.05	118.73
7	B	1511	ATP	O3B-PG-O1G	-2.01	100.44	111.04

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1511	ATP	PB-O3B-PG-O2G
7	C	1511	ATP	PB-O3B-PG-O2G
9	D	1478	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O1B
7	A	1511	ATP	PB-O3B-PG-O1G
7	A	1511	ATP	PB-O3B-PG-O3G
7	C	1511	ATP	PB-O3B-PG-O3G
9	D	1478	ADP	PA-O3A-PB-O3B
7	A	1511	ATP	PG-O3B-PB-O1B
7	C	1511	ATP	PG-O3B-PB-O1B

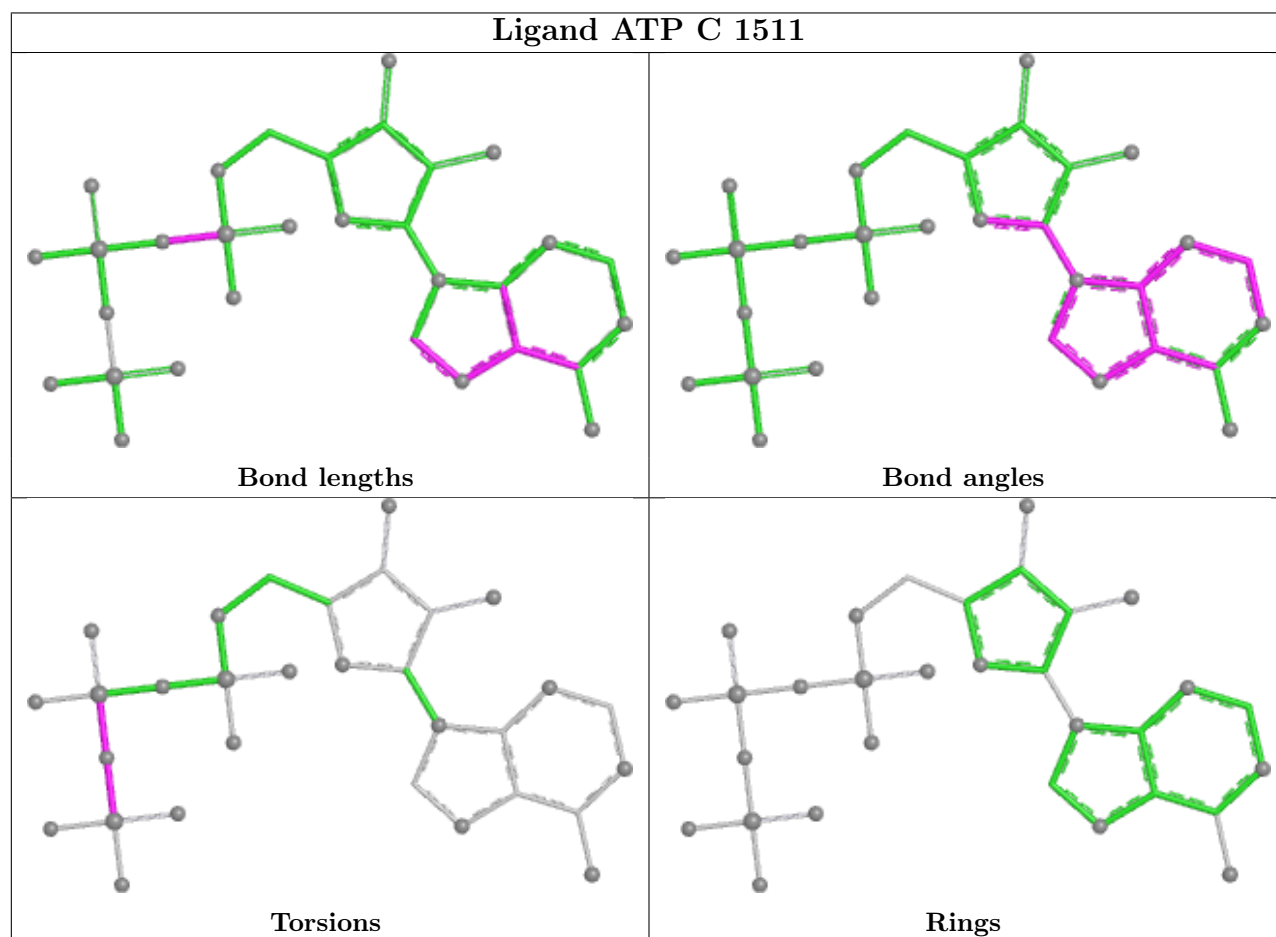
There are no ring outliers.

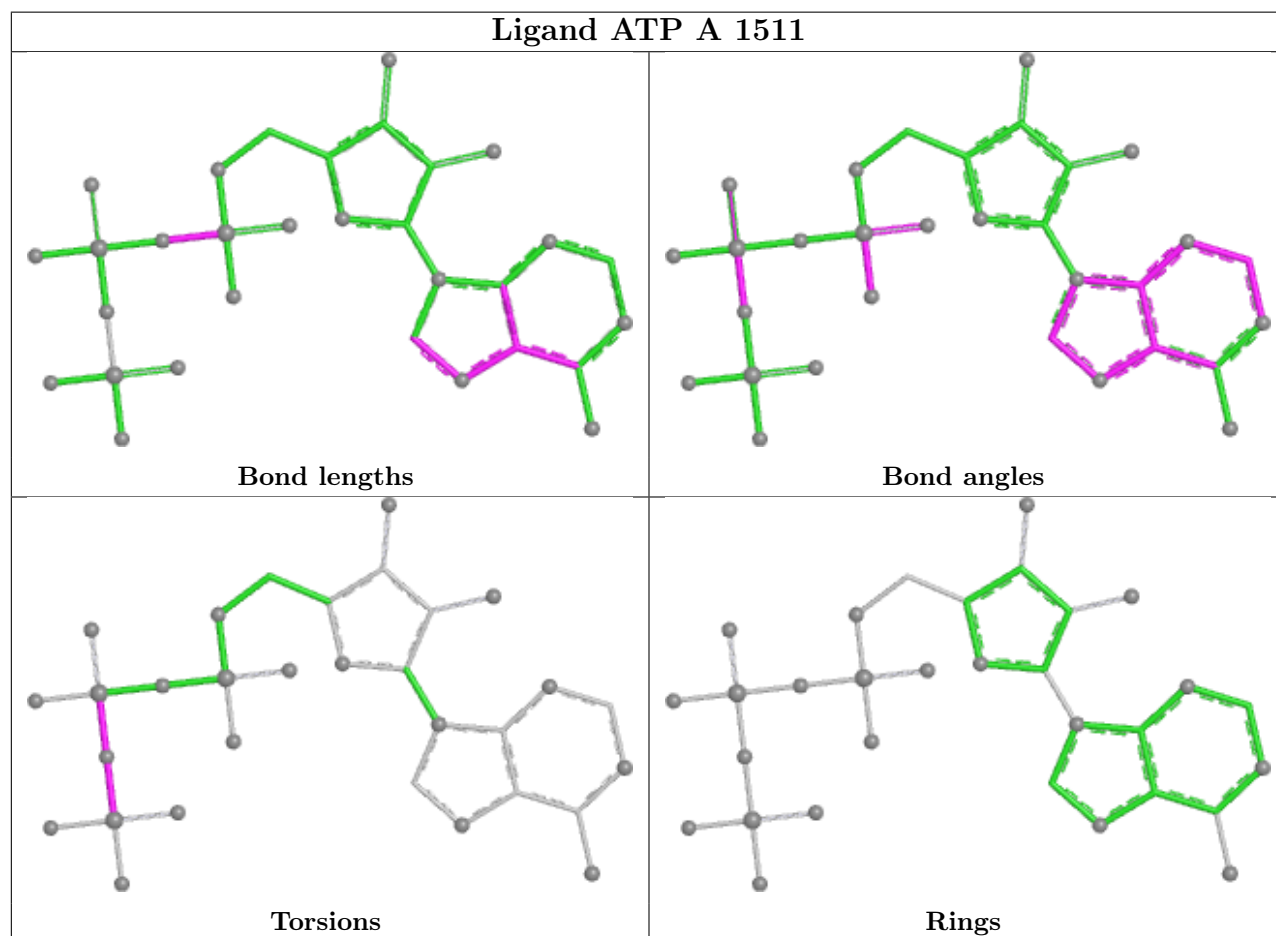
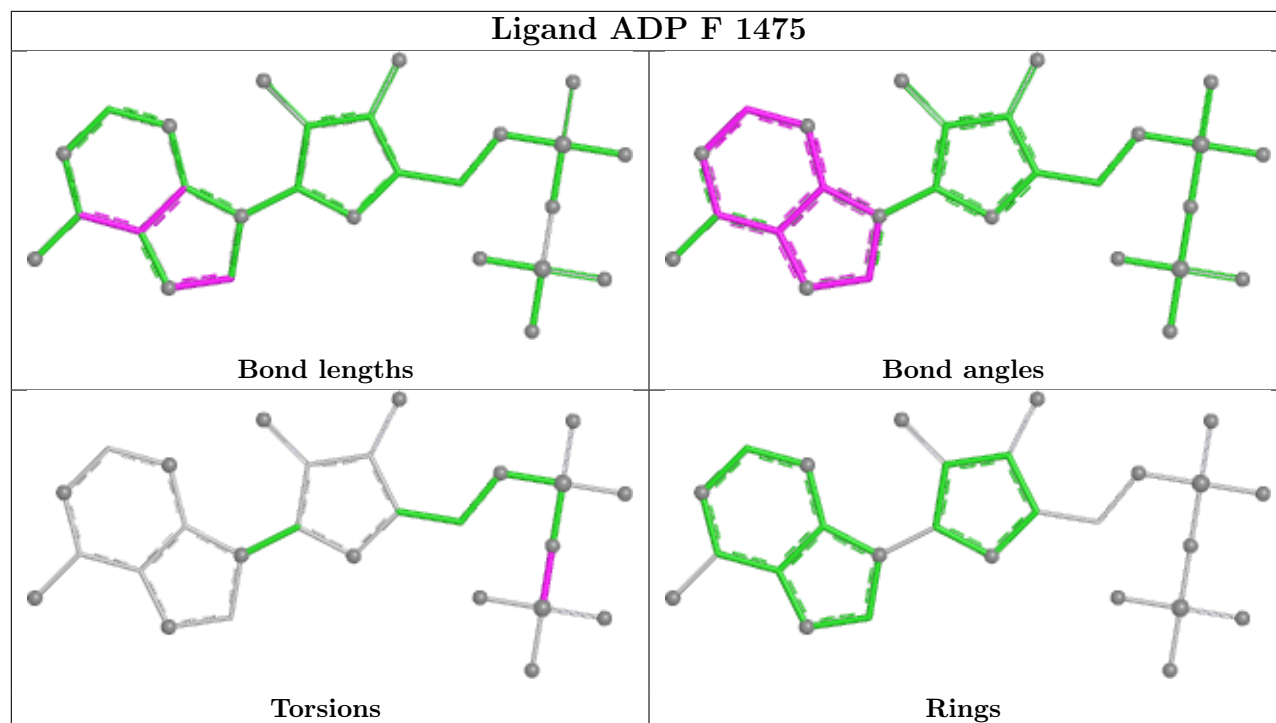
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1511	ATP	2	0

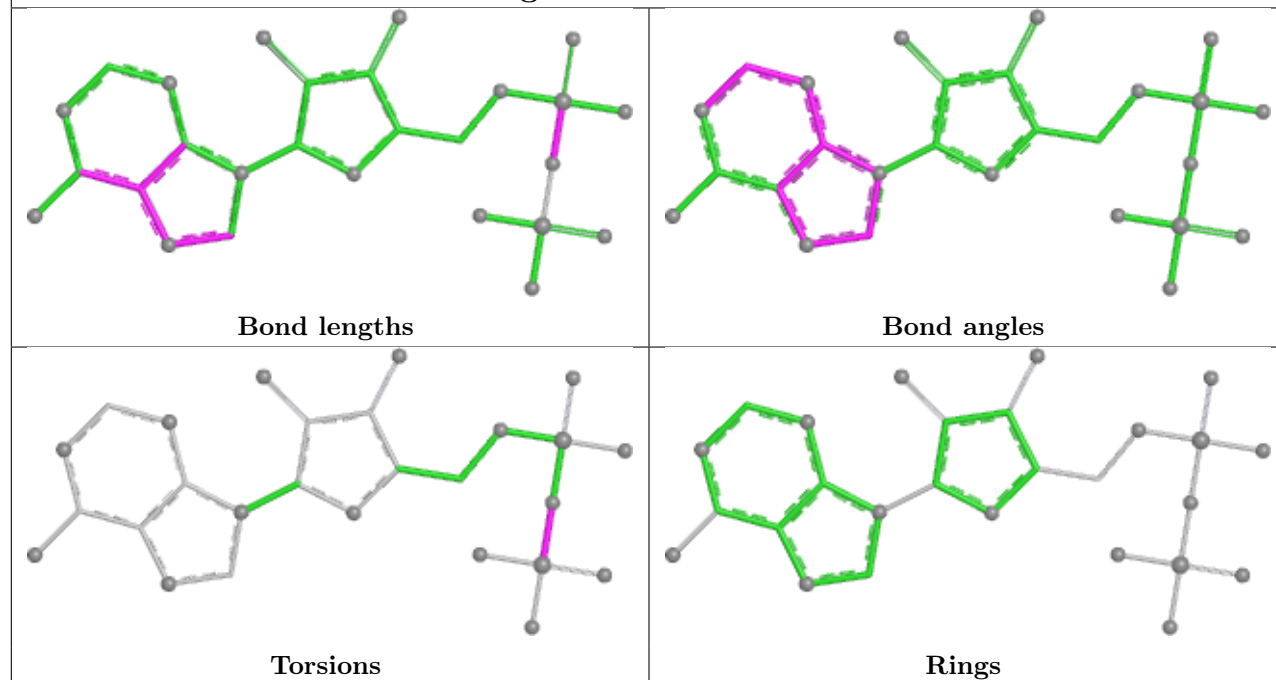
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

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

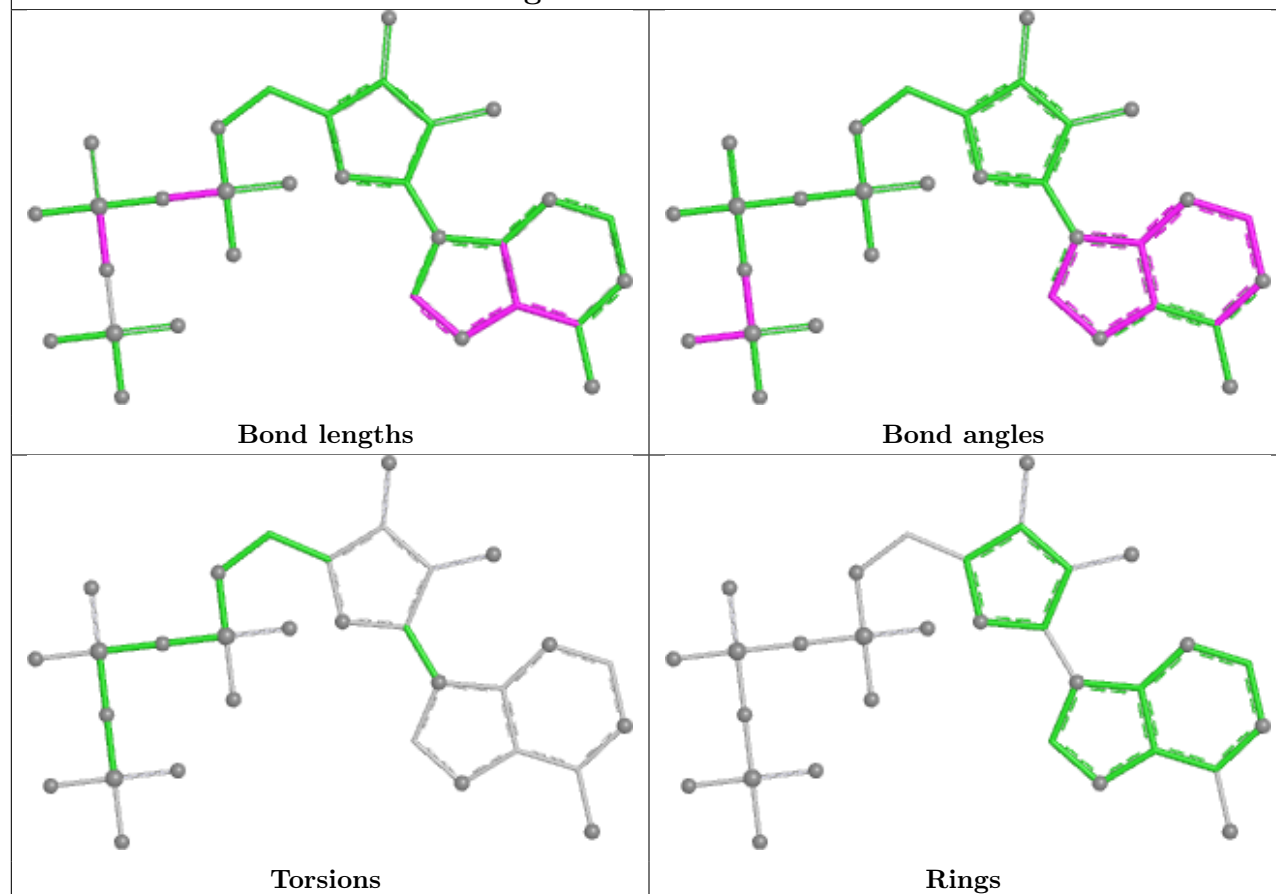




Ligand ADP D 1478



Ligand ATP B 1511



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	487/510 (95%)	0.70	46 (9%)	14 14	22, 34, 60, 86	0
1	B	479/510 (93%)	0.92	87 (18%)	3 3	21, 33, 70, 82	0
1	C	473/510 (92%)	0.85	68 (14%)	6 6	22, 32, 65, 87	0
2	D	469/482 (97%)	0.36	11 (2%)	61 64	21, 30, 47, 65	0
2	E	465/482 (96%)	1.13	94 (20%)	3 3	23, 40, 84, 89	0
2	F	466/482 (96%)	0.87	75 (16%)	4 5	22, 32, 58, 77	0
3	G	263/272 (96%)	1.67	94 (35%)	1 1	26, 53, 83, 93	0
4	H	131/146 (89%)	1.64	38 (29%)	1 1	36, 54, 75, 76	0
5	I	47/50 (94%)	2.79	32 (68%)	0 0	46, 60, 105, 108	0
6	J	43/66 (65%)	0.54	3 (6%)	22 24	12, 24, 56, 65	0
All	All	3323/3510 (94%)	0.93	548 (16%)	4 4	12, 35, 74, 108	0

All (548) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	ALA	6.9
1	C	374	VAL	6.3
5	I	45	VAL	6.2
1	A	406	PHE	5.9
2	E	388	ILE	5.9
2	E	457	PHE	5.9
1	B	401	ALA	5.8
1	B	434	SER	5.7
5	I	39	GLY	5.7
2	E	389	ALA	5.6
5	I	34	ALA	5.6
2	E	387	ILE	5.4
1	B	510	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	430	GLN	5.3
4	H	86	ALA	5.1
1	C	380	THR	5.1
1	C	483	ILE	5.0
5	I	41	THR	5.0
1	B	400	VAL	5.0
4	H	120	LEU	4.9
1	C	378	ALA	4.8
5	I	42	ILE	4.8
3	G	139	GLY	4.8
1	B	507	GLY	4.7
1	B	472	VAL	4.7
1	B	431	GLY	4.6
3	G	56	ASP	4.6
1	C	376	SER	4.6
2	F	176	ALA	4.6
1	B	508	PHE	4.5
5	I	47	VAL	4.5
2	E	432	VAL	4.5
5	I	25	ALA	4.5
3	G	187	ALA	4.5
4	H	45	PHE	4.4
1	B	410	LEU	4.4
2	F	392	GLY	4.3
5	I	44	ILE	4.3
2	E	474	ALA	4.3
3	G	192	ILE	4.3
1	A	479	LEU	4.3
3	G	193	TYR	4.3
1	C	375	GLY	4.2
1	C	414	THR	4.2
2	E	446	ALA	4.2
5	I	30	PHE	4.1
1	B	464	PHE	4.1
1	A	410	LEU	4.1
2	E	428	LEU	4.1
1	A	397	TYR	4.0
2	E	452	LEU	4.0
1	B	414	THR	4.0
1	B	437	ALA	4.0
2	E	396	LEU	4.0
1	B	438	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	407	GLY	4.0
5	I	37	THR	3.9
2	F	28	GLY	3.9
1	B	497	LEU	3.9
1	C	410	LEU	3.9
5	I	26	LEU	3.9
2	F	424	PHE	3.9
5	I	36	LYS	3.9
4	H	44	ALA	3.9
1	C	482	LYS	3.9
2	F	388	ILE	3.9
2	E	466	ALA	3.9
1	B	367	VAL	3.8
3	G	184	ILE	3.8
1	C	413	ALA	3.8
1	B	435	PRO	3.8
5	I	35	MET	3.8
3	G	59	THR	3.8
2	F	374	VAL	3.8
3	G	77	LEU	3.8
3	G	57	ILE	3.7
3	G	34	ALA	3.7
2	E	431	LEU	3.7
3	G	181	LEU	3.7
2	E	456	ALA	3.7
5	I	24	ASP	3.7
3	G	124	PHE	3.7
3	G	213	ILE	3.7
2	E	445	LEU	3.7
2	E	418	PHE	3.7
1	B	432	GLN	3.7
1	C	510	ALA	3.7
1	B	433	TYR	3.7
2	E	423	VAL	3.6
3	G	144	ILE	3.6
1	C	372	SER	3.6
1	C	379	GLN	3.6
1	B	495	ALA	3.5
3	G	127	THR	3.5
3	G	138	PHE	3.5
3	G	132	GLY	3.5
1	A	400	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	404	VAL	3.5
3	G	136	PRO	3.4
1	C	412	ALA	3.4
3	G	191	SER	3.4
4	H	135	ILE	3.4
1	B	506	ALA	3.4
3	G	179	PHE	3.4
1	C	480	LEU	3.4
2	F	246	GLN	3.4
3	G	40	PRO	3.4
2	F	438	ILE	3.4
1	B	384	LYS	3.4
1	C	400	VAL	3.4
3	G	112	ILE	3.4
3	G	153	TYR	3.3
2	E	390	ILE	3.3
2	F	407	ALA	3.3
1	B	444	VAL	3.3
5	I	22	VAL	3.3
3	G	180	SER	3.3
2	E	447	GLY	3.3
3	G	131	VAL	3.3
5	I	32	ALA	3.3
1	B	445	ILE	3.3
1	C	403	PHE	3.3
3	G	183	THR	3.2
2	E	467	VAL	3.2
1	B	378	ALA	3.2
1	C	392	LEU	3.2
2	F	402	LEU	3.2
2	E	326	PHE	3.2
1	B	411	ASP	3.2
2	F	386	ASP	3.2
4	H	99	THR	3.2
5	I	40	SER	3.2
1	C	501	VAL	3.2
1	B	473	ILE	3.2
1	B	480	LEU	3.2
3	G	186	SER	3.2
1	A	414	THR	3.2
1	B	509	GLU	3.2
1	C	404	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	394	LEU	3.2
1	B	428	LEU	3.2
1	A	508	PHE	3.2
2	E	424	PHE	3.2
1	A	506	ALA	3.1
2	F	378	LEU	3.1
1	B	395	ALA	3.1
1	C	411	ASP	3.1
2	E	460	VAL	3.1
2	F	400	ASP	3.1
2	F	423	VAL	3.1
3	G	140	ASP	3.1
1	B	459	SER	3.1
1	B	387	ALA	3.1
3	G	55	ALA	3.1
1	C	418	LEU	3.1
3	G	137	THR	3.1
3	G	135	PRO	3.1
1	B	505	LEU	3.1
1	B	388	GLY	3.0
1	B	462	THR	3.0
2	F	340	ALA	3.0
3	G	41	ALA	3.0
3	G	38	LEU	3.0
1	B	489	ILE	3.0
1	C	481	SER	3.0
1	B	193	THR	3.0
4	H	71	THR	3.0
3	G	214	TYR	3.0
1	B	429	LYS	3.0
1	A	405	GLN	3.0
3	G	141	ALA	3.0
5	I	7	ALA	3.0
2	E	364	GLY	3.0
1	B	358	TYR	3.0
2	E	386	ASP	3.0
5	I	4	TRP	3.0
4	H	102	MET	3.0
1	B	412	ALA	3.0
1	A	394	LEU	3.0
2	F	384	LEU	3.0
4	H	100	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	130	GLU	3.0
2	D	28	GLY	3.0
2	E	461	GLY	3.0
5	I	28	THR	3.0
3	G	33	ARG	2.9
3	G	134	ARG	2.9
1	B	413	ALA	2.9
1	B	469	LEU	2.9
2	F	452	LEU	2.9
1	A	386	VAL	2.9
1	B	487	GLY	2.9
2	E	429	GLY	2.9
3	G	31	TYR	2.9
1	B	470	SER	2.9
2	F	371	ALA	2.9
2	F	456	ALA	2.9
3	G	32	ALA	2.9
2	F	396	LEU	2.9
2	F	425	THR	2.9
3	G	215	TYR	2.9
1	C	382	ALA	2.9
2	E	470	ALA	2.9
1	B	392	LEU	2.9
1	C	451	GLY	2.9
2	E	404	VAL	2.9
2	F	420	VAL	2.9
1	B	391	LYS	2.9
1	B	397	TYR	2.9
1	C	504	PHE	2.9
2	F	381	TYR	2.9
2	F	458	TYR	2.9
3	G	270	ALA	2.9
1	C	497	LEU	2.8
1	B	219	ARG	2.8
1	B	398	ARG	2.8
2	E	367	HIS	2.8
1	B	467	ALA	2.8
3	G	37	GLU	2.8
1	A	442	VAL	2.8
1	B	386	VAL	2.8
3	G	143	VAL	2.8
1	B	461	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	444	ILE	2.8
2	E	441	PHE	2.8
1	A	122	GLY	2.8
2	F	368	TYR	2.8
1	A	478	ALA	2.8
3	G	269	ALA	2.8
3	G	51	LEU	2.8
3	G	146	LEU	2.8
4	H	62	LEU	2.8
2	E	363	VAL	2.8
2	E	462	PRO	2.8
3	G	200	VAL	2.8
1	C	121	ILE	2.8
2	D	365	SER	2.8
3	G	190	MET	2.8
1	A	404	ALA	2.8
2	E	381	TYR	2.8
2	E	468	ALA	2.8
3	G	80	ALA	2.8
1	B	424	LEU	2.8
1	C	453	LEU	2.8
3	G	148	LEU	2.8
3	G	168	VAL	2.8
6	J	8	VAL	2.8
2	F	379	GLN	2.7
2	F	383	SER	2.7
5	I	38	SER	2.7
2	F	177	HIS	2.7
4	H	43	GLY	2.7
1	B	496	LYS	2.7
2	E	439	LYS	2.7
4	H	123	ALA	2.7
2	F	445	LEU	2.7
1	B	380	THR	2.7
2	F	403	THR	2.7
2	E	453	PRO	2.7
1	B	365	ILE	2.7
3	G	161	ILE	2.7
1	B	488	LYS	2.7
1	A	382	ALA	2.7
1	B	373	ARG	2.7
4	H	145	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	433	TYR	2.7
2	E	420	VAL	2.7
1	C	494	ASP	2.7
2	F	418	PHE	2.7
2	E	272	LEU	2.7
2	E	473	LEU	2.7
2	E	417	PRO	2.7
2	E	127	SER	2.7
2	F	370	VAL	2.7
2	F	415	SER	2.7
4	H	98	VAL	2.7
2	E	430	LYS	2.7
3	G	75	ARG	2.7
1	C	506	ALA	2.6
2	E	171	ASN	2.6
2	F	391	LEU	2.6
3	G	207	TYR	2.6
2	F	429	GLY	2.6
1	A	491	GLU	2.6
2	E	371	ALA	2.6
4	H	50	ALA	2.6
2	F	9	THR	2.6
4	H	76	PHE	2.6
2	E	409	LYS	2.6
3	G	44	TYR	2.6
5	I	11	TYR	2.6
2	D	423	VAL	2.6
5	I	12	ILE	2.6
1	C	476	HIS	2.6
2	E	208	LEU	2.6
2	F	271	LEU	2.6
3	G	272	LEU	2.6
5	I	43	LYS	2.6
1	C	464	PHE	2.6
2	E	413	PHE	2.6
3	G	126	VAL	2.6
4	H	41	GLN	2.6
4	H	68	GLU	2.6
1	B	503	ASN	2.6
3	G	271	ALA	2.6
2	E	245	ASP	2.6
1	B	440	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	129	GLU	2.5
2	E	128	VAL	2.5
2	E	410	ILE	2.5
2	E	368	TYR	2.5
2	D	477	HIS	2.5
2	E	315	ASP	2.5
2	F	365	SER	2.5
2	E	416	GLN	2.5
1	C	472	VAL	2.5
2	E	178	GLY	2.5
2	F	463	ILE	2.5
3	G	108	VAL	2.5
3	G	66	HIS	2.5
1	A	449	VAL	2.5
2	E	438	ILE	2.5
2	E	463	ILE	2.5
1	B	446	TYR	2.5
1	C	433	TYR	2.5
3	G	199	ASP	2.5
1	A	172	GLN	2.5
3	G	261	GLU	2.5
4	H	117	SER	2.5
5	I	15	SER	2.5
1	A	402	ALA	2.5
1	A	510	ALA	2.5
1	C	478	ALA	2.5
1	B	456	LEU	2.5
4	H	103	LEU	2.5
1	B	436	MET	2.5
1	B	471	HIS	2.5
2	F	457	PHE	2.5
1	A	411	ASP	2.4
1	B	425	THR	2.4
3	G	83	SER	2.4
3	G	177	PRO	2.4
1	A	418	LEU	2.4
1	B	463	LYS	2.4
4	H	105	LEU	2.4
5	I	46	LYS	2.4
4	H	59	ARG	2.4
1	A	403	PHE	2.4
1	A	144	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	387	ILE	2.4
4	H	15	GLN	2.4
2	E	334	VAL	2.4
2	F	405	SER	2.4
6	J	10	SER	2.4
4	H	16	MET	2.4
1	A	387	ALA	2.4
1	A	412	ALA	2.4
1	C	402	ALA	2.4
1	C	417	LEU	2.4
2	E	378	LEU	2.4
2	F	473	LEU	2.4
1	B	421	GLY	2.4
1	B	468	PHE	2.4
2	E	188	GLU	2.4
3	G	165	PHE	2.4
1	B	371	VAL	2.4
2	F	377	ILE	2.4
1	B	376	SER	2.4
3	G	267	SER	2.4
2	E	403	THR	2.4
2	F	474	ALA	2.4
3	G	145	ALA	2.4
3	G	210	ALA	2.4
5	I	19	ALA	2.4
2	E	402	LEU	2.4
3	G	128	PHE	2.4
2	E	370	VAL	2.4
2	E	374	VAL	2.4
2	E	365	SER	2.4
3	G	94	ALA	2.3
4	H	140	ALA	2.3
1	A	456	LEU	2.3
1	B	427	LEU	2.3
2	F	373	GLY	2.3
3	G	79	GLY	2.3
1	C	79	ASP	2.3
2	E	393	MET	2.3
4	H	142	VAL	2.3
2	E	425	THR	2.3
1	C	292	GLU	2.3
1	C	475	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	246	GLN	2.3
2	F	174	ALA	2.3
4	H	108	ALA	2.3
2	E	157	GLY	2.3
2	E	434	LEU	2.3
2	F	248	GLY	2.3
2	E	459	MET	2.3
1	B	504	PHE	2.3
1	A	483	ILE	2.3
1	C	461	ILE	2.3
1	C	444	VAL	2.3
1	B	396	GLN	2.3
1	C	389	THR	2.3
2	F	417	PRO	2.3
1	C	495	ALA	2.3
2	E	421	ALA	2.3
2	F	421	ALA	2.3
2	E	449	TYR	2.3
3	G	142	SER	2.3
2	F	441	PHE	2.3
3	G	81	ILE	2.3
2	F	460	VAL	2.3
1	B	502	THR	2.3
2	E	433	PRO	2.3
1	B	466	ASN	2.3
1	C	387	ALA	2.3
4	H	67	ALA	2.3
2	F	199	GLU	2.2
2	F	247	GLU	2.2
2	F	385	GLN	2.2
4	H	133	ILE	2.2
3	G	218	LYS	2.2
1	C	383	MET	2.2
2	D	174	ALA	2.2
2	E	156	GLY	2.2
1	B	417	LEU	2.2
2	E	384	LEU	2.2
1	A	509	GLU	2.2
3	G	188	GLU	2.2
1	B	389	THR	2.2
1	C	460	LYS	2.2
1	C	462	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	364	GLY	2.2
2	E	440	GLY	2.2
2	E	270	ALA	2.2
6	J	18	ALA	2.2
2	E	391	LEU	2.2
3	G	149	LEU	2.2
3	G	151	SER	2.2
2	F	412	ARG	2.2
1	C	384	LYS	2.2
2	F	376	LYS	2.2
1	C	425	THR	2.2
1	C	435	PRO	2.2
2	E	360	PRO	2.2
2	F	453	PRO	2.2
3	G	182	ASP	2.2
1	C	449	VAL	2.2
3	G	85	VAL	2.2
5	I	1	VAL	2.2
4	H	97	ALA	2.2
4	H	115	ALA	2.2
2	D	427	HIS	2.2
2	F	272	LEU	2.2
1	B	452	TYR	2.2
1	C	446	TYR	2.2
1	C	452	TYR	2.2
1	A	193	THR	2.2
2	F	471	ASP	2.2
4	H	104	ASP	2.2
4	H	127	THR	2.2
1	B	399	GLU	2.1
2	E	247	GLU	2.1
2	F	390	ILE	2.1
2	F	398	GLU	2.1
4	H	131	ILE	2.1
1	C	507	GLY	2.1
2	F	419	GLN	2.1
5	I	23	ARG	2.1
1	A	123	SER	2.1
1	B	474	SER	2.1
2	D	175	LYS	2.1
5	I	31	LYS	2.1
1	C	503	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	409	ASP	2.1
1	A	486	ASP	2.1
4	H	113	GLU	2.1
2	E	437	THR	2.1
1	C	438	ILE	2.1
2	F	410	ILE	2.1
3	G	169	ILE	2.1
1	B	374	VAL	2.1
1	C	298	VAL	2.1
2	F	273	GLY	2.1
1	A	143	ARG	2.1
2	D	356	ARG	2.1
1	C	395	ALA	2.1
4	H	110	ALA	2.1
1	A	480	LEU	2.1
1	A	497	LEU	2.1
1	C	498	LYS	2.1
2	E	29	LEU	2.1
2	F	431	LEU	2.1
2	F	434	LEU	2.1
4	H	32	ASN	2.1
1	B	485	THR	2.1
1	A	438	ILE	2.1
1	C	500	ILE	2.1
2	F	426	GLY	2.1
2	F	472	LYS	2.1
2	E	321	ALA	2.1
1	B	479	LEU	2.1
3	G	125	LEU	2.1
3	G	185	SER	2.1
2	E	341	GLU	2.1
2	F	436	GLU	2.1
3	G	205	GLN	2.1
2	E	408	ARG	2.1
2	E	451	HIS	2.1
1	B	38	ILE	2.1
2	E	469	LYS	2.1
3	G	212	ILE	2.1
1	B	422	VAL	2.1
1	A	56	SER	2.1
1	A	493	SER	2.1
2	D	176	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	405	SER	2.1
2	E	407	ALA	2.1
2	F	27	GLU	2.0
2	F	397	SER	2.1
3	G	73	SER	2.1
3	G	198	ALA	2.1
2	E	414	LEU	2.0
3	G	217	LEU	2.0
5	I	33	ASN	2.0
1	A	224	ASP	2.0
2	F	455	GLN	2.0
3	G	74	ASP	2.0
3	G	78	CYS	2.0
3	G	42	ARG	2.0
1	C	42	HIS	2.0
2	E	392	GLY	2.0
2	E	377	ILE	2.0
2	E	129	GLU	2.0
1	A	490	SER	2.0
1	C	390	MET	2.0
1	C	419	SER	2.0
3	G	72	SER	2.0
1	A	467	ALA	2.0
5	I	21	ALA	2.0
1	A	466	ASN	2.0
1	C	469	LEU	2.0
3	G	201	LEU	2.0
3	G	228	ARG	2.0
4	H	42	THR	2.0
2	E	273	GLY	2.0
1	C	397	TYR	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](#)

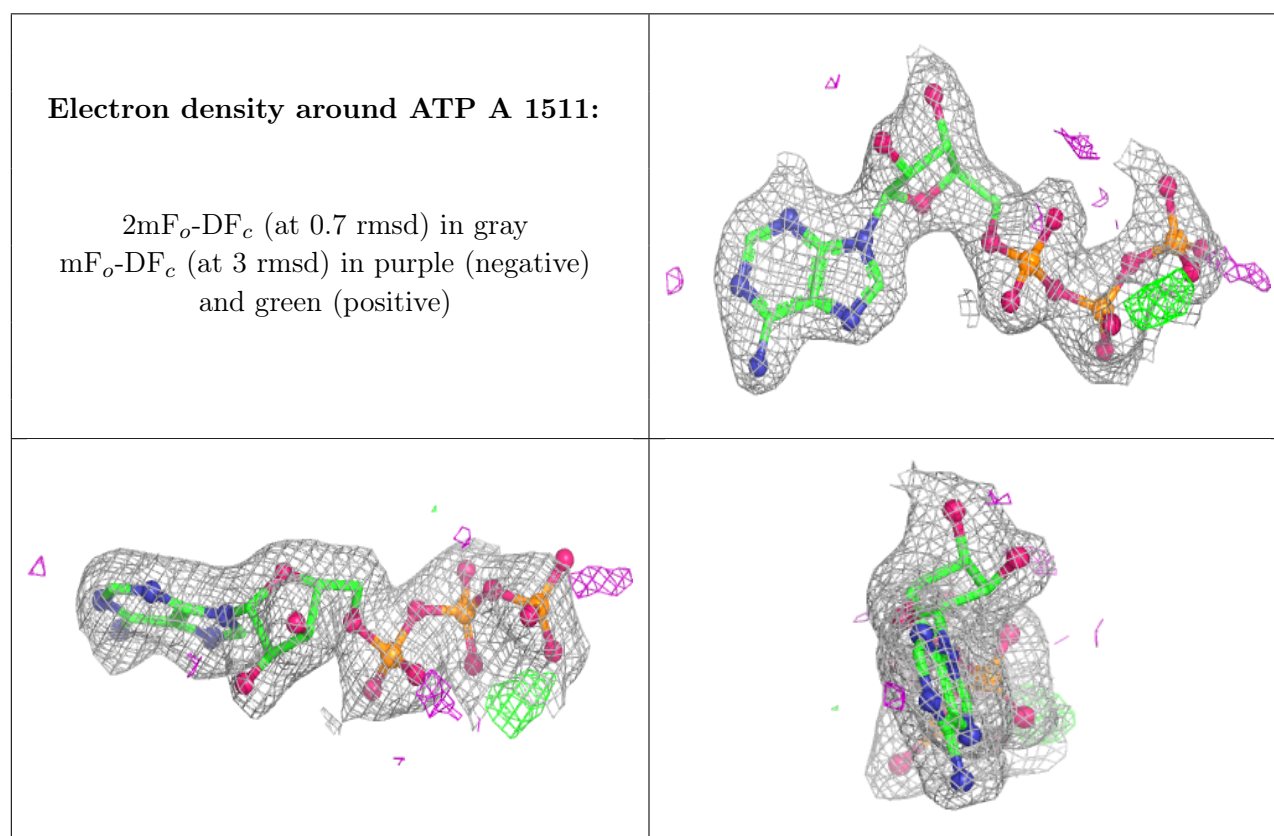
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

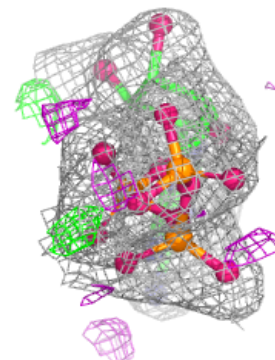
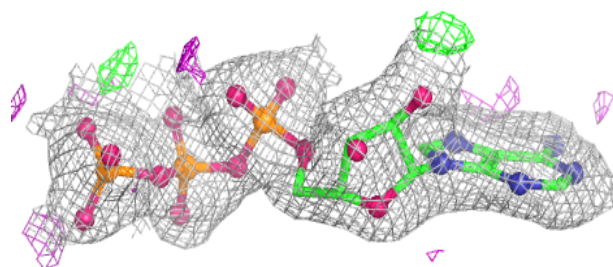
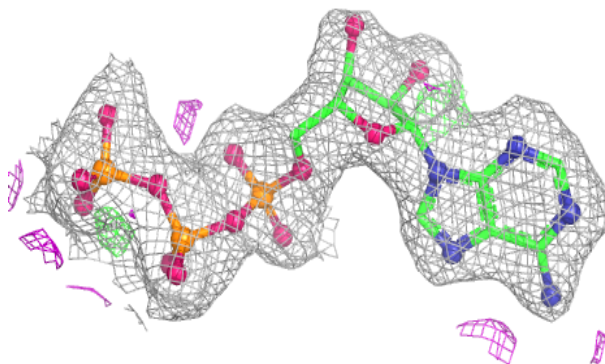
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PO4	E	1475	5/5	0.72	0.11	88,90,90,90	0
8	MG	F	1476	1/1	0.77	0.12	27,27,27,27	0
8	MG	A	1512	1/1	0.85	0.13	27,27,27,27	0
8	MG	C	1512	1/1	0.89	0.07	29,29,29,29	0
8	MG	B	1512	1/1	0.91	0.12	27,27,27,27	0
8	MG	D	1479	1/1	0.93	0.07	24,24,24,24	0
7	ATP	A	1511	31/31	0.95	0.08	23,28,38,40	4
7	ATP	B	1511	31/31	0.96	0.07	23,34,37,44	0
9	ADP	F	1475	27/27	0.96	0.07	27,32,37,41	0
7	ATP	C	1511	31/31	0.96	0.07	25,30,37,39	4
9	ADP	D	1478	27/27	0.98	0.06	22,29,33,36	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.

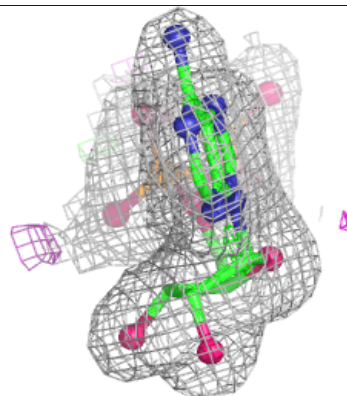
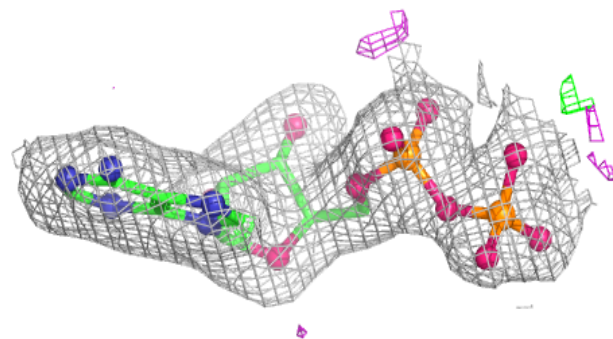
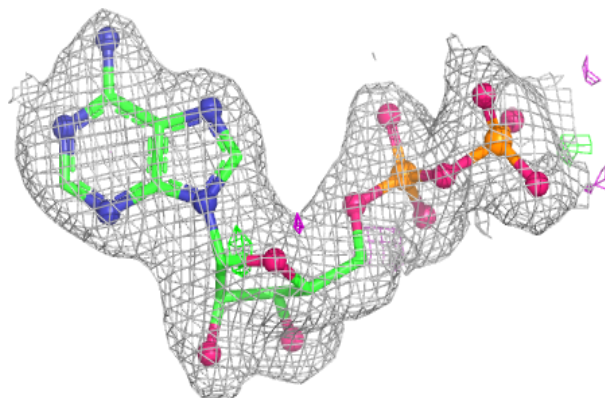


Electron density around ATP B 1511:

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

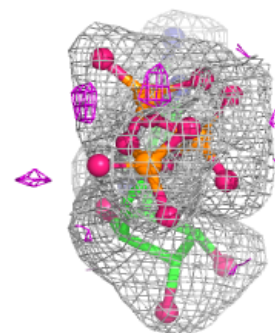
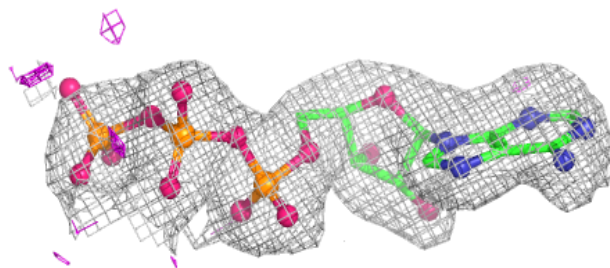
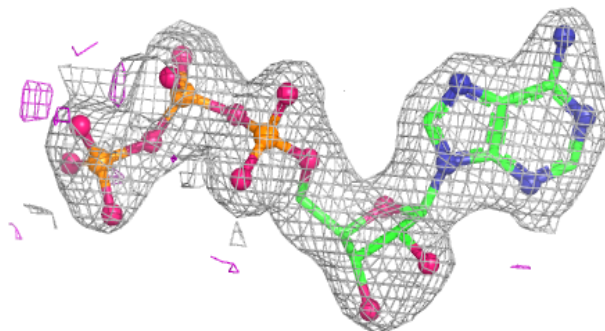
**Electron density around ADP F 1475:**

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

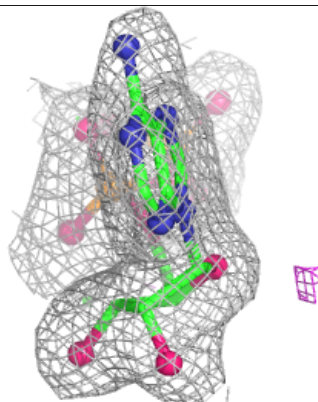
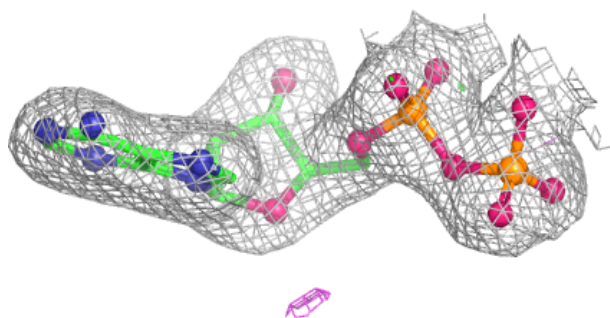
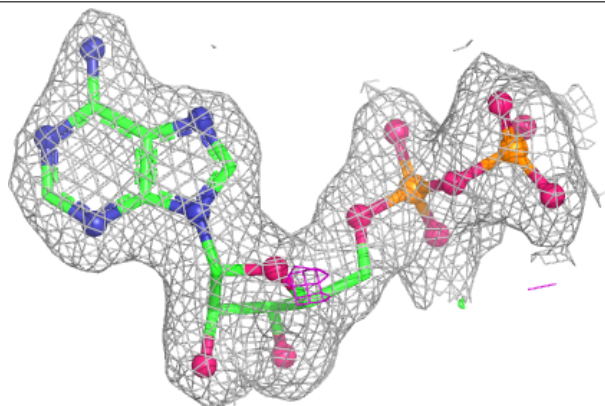


Electron density around ATP C 1511:

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

**Electron density around ADP D 1478:**

$2mF_o-DF_c$ (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.