Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 11:54 AM EDT

PDB ID	:	3Q8U
Title	:	Crystal structure of Staphylococcus aureus nucleoside diphosphate kinase complexed with ADP
Authors	:	Srivastava, S.K.; Rajasree, K.; Gopal, B.
Deposited on	:	2011-01-07
Resolution	:	2.22 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 (i) 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 (i)) were used in the production of this report:

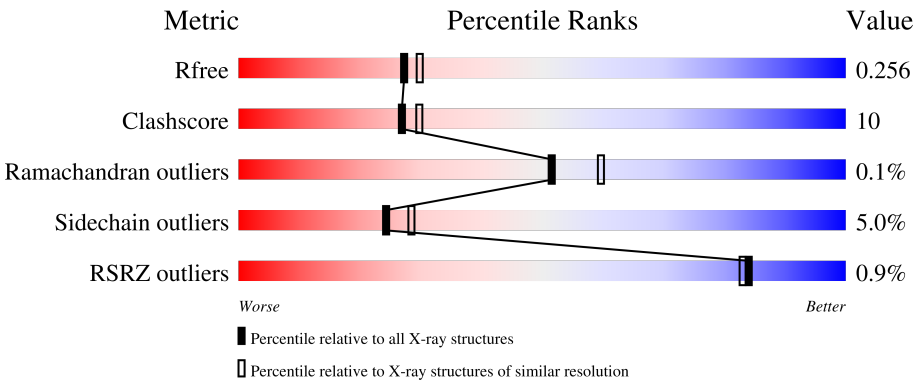
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	157	73% 17% • • 5%
1	B	157	75% 17% • • 5%
1	C	157	82% 10% • • 5%
1	D	157	.% 83% 10% • • 5%
1	E	157	.% 69% 24% • 5%

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Mol	Chain	Length	Quality of chain
1	F	157	3% 77% 14% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7566 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	1165	733	202	225	5	0	0	0
1	B	149	1158	730	202	221	5	0	0	0
1	C	149	1158	730	202	221	5	0	0	0
1	D	149	1161	731	202	223	5	0	0	0
1	E	149	1158	730	202	221	5	0	0	0
1	F	149	1158	730	202	221	5	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4
A	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
A	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
A	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
A	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
A	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
A	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
A	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4
B	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4
B	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
B	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
B	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
B	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
B	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
B	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
B	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4
C	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4

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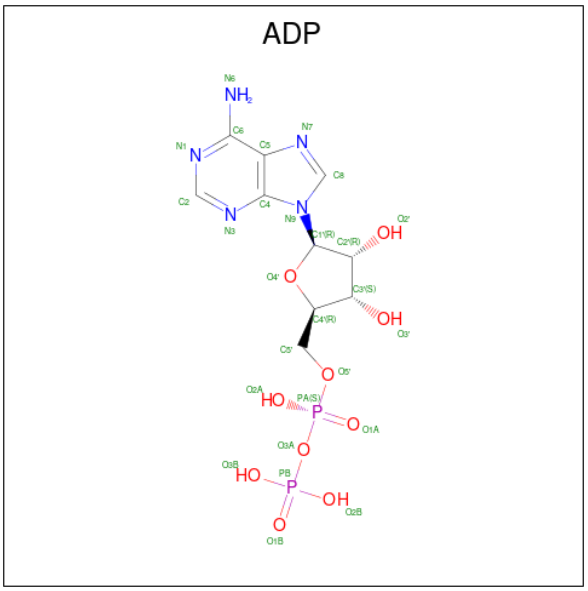
Chain	Residue	Modelled	Actual	Comment	Reference
C	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
C	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
C	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
C	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
C	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
C	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
C	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4
D	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4
D	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
D	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
D	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
D	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
D	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
D	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
D	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4
E	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4
E	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
E	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
E	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
E	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
E	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
E	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
E	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4
F	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4
F	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
F	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
F	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
F	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
F	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
F	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
F	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	85	85	85	0	0
			Total	O		
4	B	81	81	81	0	0
			Total	O		
4	C	76	76	76	0	0
			Total	O		
4	D	53	53	53	0	0
			Total	O		
4	E	95	95	95	0	0
			Total	O		
4	F	51	51	51	0	0

3 Residue-property plots (i)

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

• Molecule 1: Nucleoside diphosphate kinase

Chain A: 73% 17% • • 5%

M1 E2 R3 L6 R15 E20 V33 G34 G35 Q39 V40 P41 M42 E43 T47 D60 L61 I62 V75 E76 G77 E78 N82 R85 T91 N92 P93 S94 R102 L107 R111 N112 D118 E124 R125 E133 N134 E135 I136 P142 A145

E149 LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Nucleoside diphosphate kinase

Chain B: 75% 17% • • 5%

M1 L6 M7 I8 R15 R27 L30 V33 G34 G35 Q39 M42 E43 T47 E51 D60 L61 A72 M73 V74 V75 R85 I88 T91 R102 L107 T108 V109 G110 R111 N112 H115 N128 N134 E135 I136 E149 LEU GLU HIS

HIS HIS HIS HIS HIS

• Molecule 1: Nucleoside diphosphate kinase

Chain C: 82% 10% • • 5%

M1 E2 R3 R15 E20 R27 V33 K36 E46 Q53 D60 L61 N82 N92 E95 R102 L107 N112 N134 E135 I136 R143 E149 LEU GLU HIS HIS HIS HIS HIS HIS

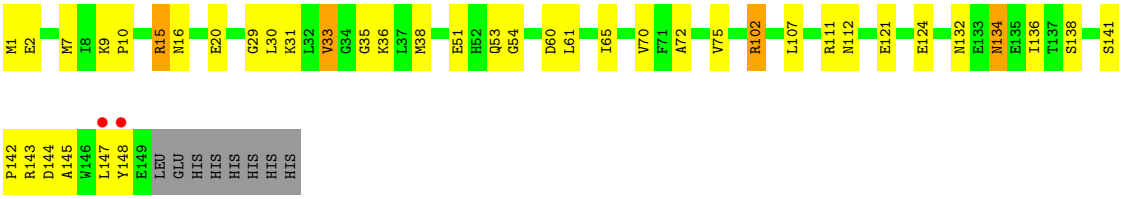
• Molecule 1: Nucleoside diphosphate kinase

Chain D: % 83% 10% • • 5%

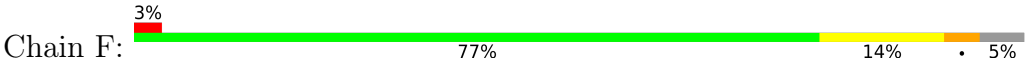
M1 R15 V33 V40 T47 G54 K55 P56 L61 T66 V74 H86 S94 R102 L107 N112 N134 E135 I136 P142 E149 LEU GLU HIS HIS HIS HIS HIS HIS

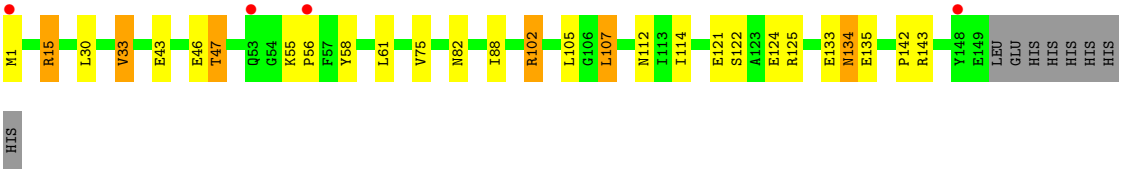
• Molecule 1: Nucleoside diphosphate kinase

Chain E: % 69% 24% • 5%



- Molecule 1: Nucleoside diphosphate kinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.27Å 103.06Å 127.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.52 – 2.22 34.52 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.52-2.22) 97.8 (34.52-2.22)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.258 0.180 , 0.256	Depositor DCC
R_{free} test set	2230 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7566	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.01	3/1188 (0.3%)	1.07	7/1607 (0.4%)
1	B	0.98	0/1181	0.99	5/1598 (0.3%)
1	C	1.00	1/1181 (0.1%)	0.98	5/1598 (0.3%)
1	D	0.97	0/1184	1.02	5/1602 (0.3%)
1	E	1.00	1/1181 (0.1%)	0.98	3/1598 (0.2%)
1	F	0.95	1/1181 (0.1%)	0.97	4/1598 (0.3%)
All	All	0.98	6/7096 (0.1%)	1.00	29/9601 (0.3%)

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	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	GLU	CD-OE1	-6.02	1.19	1.25
1	F	124	GLU	CG-CD	5.49	1.60	1.51
1	A	145	ALA	CA-CB	5.47	1.64	1.52
1	A	133	GLU	CD-OE2	-5.37	1.19	1.25
1	E	124	GLU	CG-CD	5.17	1.59	1.51
1	C	20	GLU	CB-CG	5.02	1.61	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	ARG	NE-CZ-NH1	-13.36	113.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	15	ARG	NE-CZ-NH1	-11.79	114.41	120.30
1	A	15	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	F	102	ARG	NE-CZ-NH2	10.45	125.53	120.30
1	F	102	ARG	NE-CZ-NH1	-10.45	115.08	120.30
1	E	15	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	C	15	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	D	15	ARG	NE-CZ-NH1	-8.85	115.87	120.30
1	C	15	ARG	NE-CZ-NH2	8.83	124.71	120.30
1	A	102	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	A	102	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	E	102	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	B	102	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	C	102	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	B	102	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	C	102	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	F	15	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	15	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	D	102	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	107	LEU	CB-CG-CD2	6.00	121.21	111.00
1	A	61	LEU	CA-CB-CG	5.80	128.65	115.30
1	D	33	VAL	CG1-CB-CG2	5.72	120.05	110.90
1	D	102	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	B	51	GLU	CB-CA-C	-5.52	99.35	110.40
1	D	15	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	33	VAL	CG1-CB-CG2	5.43	119.58	110.90
1	B	107	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	33	VAL	CB-CA-C	5.03	120.96	111.40
1	F	33	VAL	CB-CA-C	5.02	120.94	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	54	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1165	0	1149	32	1
1	B	1158	0	1143	28	0
1	C	1158	0	1143	17	0
1	D	1161	0	1145	12	1
1	E	1158	0	1143	43	0
1	F	1158	0	1142	20	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	85	0	0	19	0
4	B	81	0	0	16	2
4	C	76	0	0	9	0
4	D	53	0	0	1	0
4	E	95	0	0	14	2
4	F	51	0	0	5	0
All	All	7566	0	6937	144	3

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 10.

All (144) 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:F:122:SER:HB3	4:F:430:HOH:O	1.15	1.32
4:A:168:HOH:O	1:E:60:ASP:HB3	1.29	1.31
1:C:82:ASN:HB3	4:C:401:HOH:O	1.28	1.27
1:A:82:ASN:HB3	4:A:414:HOH:O	1.22	1.27
1:E:145:ALA:HB2	4:E:368:HOH:O	1.32	1.25
1:E:145:ALA:HB3	4:E:388:HOH:O	1.22	1.25
1:F:133:GLU:CG	4:F:349:HOH:O	1.83	1.22
1:B:75:VAL:HB	4:B:392:HOH:O	1.05	1.21
1:B:60:ASP:HB3	4:B:176:HOH:O	1.45	1.14
1:A:1:MET:HG3	4:A:397:HOH:O	0.97	1.13
1:F:82:ASN:HB3	4:F:434:HOH:O	0.96	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:HB3	4:A:339:HOH:O	1.53	1.07
1:E:145:ALA:HB1	4:E:386:HOH:O	1.54	1.06
1:E:54:GLY:N	4:E:360:HOH:O	1.61	0.98
1:A:1:MET:CG	4:A:397:HOH:O	1.70	0.89
1:E:7:MET:CE	1:E:65:ILE:HD11	2.05	0.87
1:C:60:ASP:HB3	4:C:435:HOH:O	1.76	0.86
1:E:51:GLU:HG2	4:E:163:HOH:O	1.77	0.85
1:F:15:ARG:NH1	1:F:105:LEU:O	2.10	0.83
1:A:39:GLN:NE2	4:A:356:HOH:O	2.11	0.82
1:B:111:ARG:NE	4:B:366:HOH:O	2.00	0.80
1:E:7:MET:HE3	1:E:65:ILE:HD11	1.63	0.79
1:F:102:ARG:HD2	1:F:112:ASN:HB2	1.64	0.78
1:A:78:GLU:HG3	4:A:445:HOH:O	1.83	0.78
1:A:111:ARG:NH1	4:A:415:HOH:O	2.13	0.78
1:B:111:ARG:NH1	4:B:366:HOH:O	2.16	0.77
2:C:158:ADP:H8	2:C:158:ADP:H5'1	1.51	0.74
1:E:145:ALA:CB	4:E:388:HOH:O	1.96	0.74
1:B:75:VAL:CB	4:B:392:HOH:O	1.86	0.72
1:E:20:GLU:HG2	4:E:373:HOH:O	1.90	0.71
1:B:111:ARG:CZ	4:B:366:HOH:O	2.38	0.71
1:E:7:MET:HE1	1:E:65:ILE:HD11	1.74	0.69
1:E:102:ARG:HD2	1:E:112:ASN:HB2	1.75	0.69
1:B:30:LEU:HB3	1:B:75:VAL:CG1	2.22	0.69
1:B:39:GLN:NE2	4:B:326:HOH:O	2.27	0.68
1:E:20:GLU:CG	4:E:373:HOH:O	2.41	0.68
1:C:15:ARG:HD2	4:F:173:HOH:O	1.94	0.68
1:A:1:MET:SD	4:A:397:HOH:O	2.31	0.67
1:A:142:PRO:HB3	1:F:142:PRO:HB2	1.77	0.67
1:C:27:ARG:HD3	4:C:199:HOH:O	1.94	0.66
1:C:46:GLU:OE2	4:C:438:HOH:O	2.13	0.66
1:E:143:ARG:HG3	1:E:147:LEU:HD12	1.77	0.66
1:C:102:ARG:HD2	1:C:112:ASN:HB2	1.79	0.64
1:E:132:ASN:HB2	1:E:134:ASN:ND2	2.14	0.63
1:E:20:GLU:CD	4:E:373:HOH:O	2.37	0.62
1:B:107:LEU:HB2	1:E:147:LEU:HD22	1.81	0.61
1:D:149:GLU:OE2	1:D:149:GLU:HA	2.01	0.60
1:B:75:VAL:CG1	4:B:392:HOH:O	2.35	0.59
1:E:33:VAL:HG13	1:E:136:ILE:HG23	1.84	0.59
1:B:43:GLU:O	1:B:47:THR:HG23	2.02	0.59
1:E:31:LYS:HE2	1:E:141:SER:OG	2.04	0.58
1:A:43:GLU:O	1:A:47:THR:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:322:HOH:O	1:D:15:ARG:HD2	2.03	0.57
1:E:132:ASN:HB2	1:E:134:ASN:HD21	1.69	0.57
1:F:47:THR:O	1:F:125:ARG:NH2	2.37	0.57
1:A:102:ARG:HD3	1:A:112:ASN:O	2.05	0.57
4:D:382:HOH:O	1:F:15:ARG:HD2	2.04	0.57
1:A:102:ARG:HD2	1:A:112:ASN:HB2	1.86	0.56
1:A:133:GLU:HG3	4:A:334:HOH:O	2.04	0.56
1:E:7:MET:HE3	1:E:9:LYS:HG2	1.86	0.56
1:E:53:GLN:CA	4:E:360:HOH:O	2.51	0.56
1:B:35:GLY:HA2	1:B:72:ALA:O	2.06	0.56
1:B:51:GLU:HG3	4:B:288:HOH:O	2.06	0.56
1:A:20:GLU:HG2	4:A:442:HOH:O	2.06	0.55
1:A:33:VAL:HG13	1:A:136:ILE:HG23	1.89	0.54
1:D:40:VAL:O	1:D:66:THR:HG22	2.07	0.54
1:E:134:ASN:H	1:E:134:ASN:HD22	1.55	0.54
1:B:102:ARG:HD2	1:B:112:ASN:HB2	1.88	0.54
1:A:102:ARG:CD	1:A:112:ASN:O	2.56	0.54
1:A:125:ARG:HD3	4:A:328:HOH:O	2.08	0.54
1:A:111:ARG:CZ	4:A:415:HOH:O	2.40	0.53
1:E:1:MET:CG	1:E:2:GLU:N	2.71	0.53
1:A:111:ARG:NE	4:A:415:HOH:O	1.99	0.53
1:B:111:ARG:NH2	1:E:148:TYR:O	2.41	0.53
1:D:33:VAL:HG12	1:D:74:VAL:HG12	1.92	0.52
1:D:55:LYS:HB3	1:D:56:PRO:CD	2.40	0.52
2:C:158:ADP:H5'1	2:C:158:ADP:C8	2.40	0.51
1:F:102:ARG:HD3	1:F:112:ASN:O	2.11	0.51
1:A:85:ARG:HD2	1:A:118:ASP:HA	1.93	0.51
1:E:145:ALA:N	4:E:410:HOH:O	2.44	0.51
1:A:20:GLU:CD	4:A:442:HOH:O	2.49	0.51
1:E:1:MET:N	4:E:188:HOH:O	2.43	0.51
1:C:134:ASN:HD22	1:C:135:GLU:N	2.09	0.50
1:E:102:ARG:HD3	1:E:112:ASN:O	2.12	0.50
1:A:15:ARG:HD2	4:B:404:HOH:O	2.10	0.50
1:B:8:ILE:HG13	1:B:73:MET:CE	2.42	0.49
1:F:134:ASN:HD22	1:F:135:GLU:N	2.11	0.49
1:B:8:ILE:HG13	1:B:73:MET:HE2	1.95	0.49
1:A:20:GLU:CG	4:A:442:HOH:O	2.60	0.49
1:F:30:LEU:HB3	1:F:75:VAL:CG1	2.43	0.48
1:B:85:ARG:NE	4:B:417:HOH:O	1.87	0.47
1:D:55:LYS:HB3	1:D:56:PRO:HD2	1.96	0.47
1:E:30:LEU:HB3	1:E:75:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASP:HB3	4:C:169:HOH:O	2.15	0.47
1:C:3:ARG:NH2	4:C:313:HOH:O	2.22	0.47
1:C:33:VAL:HG13	1:C:136:ILE:HG23	1.96	0.47
1:E:29:GLY:HA2	1:E:143:ARG:CZ	2.45	0.47
1:B:30:LEU:HB3	1:B:75:VAL:HG11	1.96	0.46
1:D:142:PRO:HB3	1:E:142:PRO:HB2	1.96	0.46
1:C:92:ASN:HB3	1:C:95:GLU:HG3	1.97	0.46
1:B:33:VAL:HG13	1:B:136:ILE:HG23	1.98	0.46
1:B:107:LEU:HB2	4:B:385:HOH:O	2.16	0.46
1:B:128:ASN:O	4:B:168:HOH:O	2.21	0.45
1:F:46:GLU:HG2	1:F:58:TYR:OH	2.17	0.45
1:B:102:ARG:HD3	1:B:112:ASN:O	2.16	0.45
1:B:107:LEU:N	4:B:385:HOH:O	2.35	0.45
1:C:15:ARG:HD3	1:F:143:ARG:HD2	1.97	0.45
1:E:35:GLY:HA2	1:E:72:ALA:O	2.17	0.45
1:C:60:ASP:CB	4:C:435:HOH:O	2.49	0.45
1:C:46:GLU:HG2	4:C:438:HOH:O	2.17	0.45
1:F:88:ILE:HG12	1:F:114:ILE:HG21	1.98	0.44
4:B:385:HOH:O	1:E:147:LEU:HD23	2.18	0.44
1:A:142:PRO:CB	1:F:142:PRO:HB2	2.47	0.44
4:A:358:HOH:O	1:E:15:ARG:HD2	2.17	0.44
1:B:91:THR:HG22	1:B:109:VAL:HG23	1.99	0.44
1:E:111:ARG:NE	4:E:177:HOH:O	1.98	0.44
1:E:144:ASP:CB	4:E:410:HOH:O	2.66	0.44
1:D:102:ARG:HD2	1:D:112:ASN:HB2	2.00	0.43
1:A:33:VAL:HG13	1:A:136:ILE:CG2	2.48	0.43
1:A:3:ARG:NH1	4:A:395:HOH:O	2.21	0.43
1:E:1:MET:HG2	1:E:2:GLU:N	2.32	0.43
1:A:39:GLN:O	1:A:41:PRO:HD3	2.18	0.43
1:C:102:ARG:CD	1:C:112:ASN:O	2.67	0.43
1:A:78:GLU:CG	4:A:445:HOH:O	2.55	0.42
1:E:10:PRO:HD3	1:E:70:VAL:HG12	2.01	0.42
1:F:55:LYS:HB3	1:F:56:PRO:HD2	2.00	0.42
1:F:43:GLU:O	1:F:47:THR:CG2	2.68	0.42
1:D:142:PRO:CB	1:E:142:PRO:HB2	2.50	0.42
1:E:16:ASN:ND2	1:F:143:ARG:HD3	2.35	0.42
1:F:121:GLU:HB2	4:F:431:HOH:O	2.19	0.42
1:B:27:ARG:HD3	4:B:284:HOH:O	2.21	0.41
1:A:35:GLY:O	1:C:36:LYS:HA	2.21	0.41
1:A:1:MET:HB3	1:A:76:GLU:HG2	2.03	0.41
1:B:6:LEU:HA	1:B:115:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD12	1:A:75:VAL:HG21	2.02	0.41
1:B:88:ILE:O	1:B:102:ARG:HG3	2.21	0.41
1:E:30:LEU:HB3	1:E:75:VAL:HG13	2.03	0.41
1:E:143:ARG:HG3	1:E:147:LEU:CD1	2.46	0.41
1:C:143:ARG:HD2	1:D:15:ARG:HD3	2.04	0.40
1:D:33:VAL:HG13	1:D:136:ILE:HG23	2.02	0.40
1:D:134:ASN:HD22	1:D:134:ASN:C	2.25	0.40
1:E:36:LYS:HE3	1:E:38:MET:SD	2.61	0.40
1:F:107:LEU:HD23	1:F:107:LEU:HA	1.88	0.40
1:A:91:THR:O	1:A:93:PRO:HD3	2.21	0.40

All (3) 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)
4:B:426:HOH:O	4:E:363:HOH:O[4_455]	1.12	1.08
4:B:172:HOH:O	4:E:364:HOH:O[4_455]	1.28	0.92
1:A:133:GLU:OE1	1:D:86:HIS:ND1[3_544]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	147/157 (94%)	142 (97%)	5 (3%)	0	100	100
1	B	147/157 (94%)	143 (97%)	4 (3%)	0	100	100
1	C	147/157 (94%)	143 (97%)	3 (2%)	1 (1%)	22	21
1	D	147/157 (94%)	144 (98%)	3 (2%)	0	100	100
1	E	147/157 (94%)	144 (98%)	3 (2%)	0	100	100
1	F	147/157 (94%)	143 (97%)	4 (3%)	0	100	100
All	All	882/942 (94%)	859 (97%)	22 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	53	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/135 (94%)	118 (93%)	9 (7%)	14	15
1	B	125/135 (93%)	118 (94%)	7 (6%)	21	23
1	C	125/135 (93%)	121 (97%)	4 (3%)	39	49
1	D	126/135 (93%)	120 (95%)	6 (5%)	25	30
1	E	125/135 (93%)	119 (95%)	6 (5%)	25	30
1	F	125/135 (93%)	119 (95%)	6 (5%)	25	30
All	All	753/810 (93%)	715 (95%)	38 (5%)	24	28

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	47	THR
1	A	61	LEU
1	A	62	ILE
1	A	94	SER
1	A	107	LEU
1	A	124	GLU
1	A	133	GLU
1	A	134	ASN
1	B	1	MET
1	B	7	MET
1	B	33	VAL
1	B	42	MET
1	B	61	LEU
1	B	107	LEU
1	B	134	ASN

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Mol	Chain	Res	Type
1	C	33	VAL
1	C	61	LEU
1	C	107	LEU
1	C	134	ASN
1	D	33	VAL
1	D	47	THR
1	D	61	LEU
1	D	94	SER
1	D	107	LEU
1	D	134	ASN
1	E	33	VAL
1	E	61	LEU
1	E	107	LEU
1	E	121	GLU
1	E	134	ASN
1	E	138	SER
1	F	1	MET
1	F	33	VAL
1	F	47	THR
1	F	61	LEU
1	F	107	LEU
1	F	134	ASN

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	134	ASN
1	B	39	GLN
1	B	134	ASN
1	C	128	ASN
1	C	134	ASN
1	D	16	ASN
1	D	39	GLN
1	D	128	ASN
1	D	134	ASN
1	E	16	ASN
1	E	134	ASN
1	F	53	GLN
1	F	134	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
2	ADP	A	158	3	24,29,29	1.16	2 (8%)	29,45,45	1.28	4 (13%)
2	ADP	B	158	3	24,29,29	0.89	0	29,45,45	1.47	6 (20%)
2	ADP	F	158	3	24,29,29	1.21	2 (8%)	29,45,45	1.62	6 (20%)
2	ADP	E	158	3	24,29,29	0.90	0	29,45,45	1.30	3 (10%)
2	ADP	D	158	3	24,29,29	1.01	1 (4%)	29,45,45	1.49	5 (17%)
2	ADP	C	158	-	24,29,29	1.03	2 (8%)	29,45,45	1.63	9 (31%)

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	ADP	A	158	3	-	2/12/32/32	0/3/3/3
2	ADP	B	158	3	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	F	158	3	-	4/12/32/32	0/3/3/3
2	ADP	E	158	3	-	1/12/32/32	0/3/3/3
2	ADP	D	158	3	-	5/12/32/32	0/3/3/3
2	ADP	C	158	-	-	2/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	158	ADP	C5-C4	3.03	1.48	1.40
2	F	158	ADP	C5-C4	2.95	1.48	1.40
2	F	158	ADP	C2-N3	2.56	1.36	1.32
2	A	158	ADP	C2-N3	2.56	1.36	1.32
2	C	158	ADP	C2-N3	2.49	1.36	1.32
2	A	158	ADP	C5-C4	2.49	1.47	1.40
2	C	158	ADP	C5-C4	2.31	1.47	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	158	ADP	C4-C5-N7	-3.78	105.46	109.40
2	D	158	ADP	N3-C2-N1	-3.77	122.79	128.68
2	E	158	ADP	N3-C2-N1	-3.66	122.96	128.68
2	A	158	ADP	N3-C2-N1	-3.60	123.04	128.68
2	C	158	ADP	N3-C2-N1	-3.27	123.57	128.68
2	B	158	ADP	N3-C2-N1	-3.18	123.72	128.68
2	F	158	ADP	C1'-N9-C4	-3.02	121.33	126.64
2	D	158	ADP	C2-N1-C6	2.98	123.85	118.75
2	F	158	ADP	N3-C2-N1	-2.96	124.05	128.68
2	F	158	ADP	O5'-PA-O1A	2.96	120.62	109.07
2	F	158	ADP	C4-C5-N7	-2.95	106.33	109.40
2	A	158	ADP	C4-C5-N7	-2.92	106.36	109.40
2	C	158	ADP	O4'-C4'-C5'	-2.90	99.83	109.37
2	F	158	ADP	O3A-PB-O1B	-2.68	96.34	111.19
2	D	158	ADP	O3'-C3'-C4'	2.64	118.69	111.05
2	E	158	ADP	O3B-PB-O2B	2.60	117.58	107.64
2	C	158	ADP	PA-O3A-PB	-2.36	124.74	132.83
2	C	158	ADP	O3B-PB-O2B	2.30	116.41	107.64
2	B	158	ADP	C1'-N9-C4	-2.27	122.66	126.64
2	C	158	ADP	C4-C5-N7	-2.24	107.06	109.40
2	A	158	ADP	O3B-PB-O2B	2.18	115.97	107.64
2	C	158	ADP	C1'-N9-C4	-2.17	122.82	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	158	ADP	N6-C6-N1	2.17	123.08	118.57
2	C	158	ADP	O2A-PA-O1A	2.15	122.86	112.24
2	E	158	ADP	C4-C5-N7	-2.08	107.23	109.40
2	B	158	ADP	C5-C6-N6	2.08	123.51	120.35
2	B	158	ADP	O5'-PA-O1A	-2.07	100.99	109.07
2	B	158	ADP	O2A-PA-O1A	2.06	122.42	112.24
2	D	158	ADP	C1'-N9-C4	-2.06	123.03	126.64
2	C	158	ADP	O3A-PB-O1B	-2.05	99.84	111.19
2	A	158	ADP	O4'-C4'-C3'	-2.04	101.07	105.11
2	F	158	ADP	O2B-PB-O1B	2.03	118.63	110.68
2	D	158	ADP	N6-C6-N1	2.00	122.73	118.57

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	158	ADP	C5'-O5'-PA-O2A
2	F	158	ADP	C5'-O5'-PA-O1A
2	F	158	ADP	C5'-O5'-PA-O2A
2	C	158	ADP	O4'-C4'-C5'-O5'
2	C	158	ADP	C3'-C4'-C5'-O5'
2	D	158	ADP	C5'-O5'-PA-O3A
2	D	158	ADP	C5'-O5'-PA-O1A
2	D	158	ADP	PB-O3A-PA-O1A
2	A	158	ADP	PB-O3A-PA-O1A
2	F	158	ADP	C5'-O5'-PA-O3A
2	A	158	ADP	PB-O3A-PA-O2A
2	D	158	ADP	PB-O3A-PA-O2A
2	E	158	ADP	PB-O3A-PA-O2A
2	F	158	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

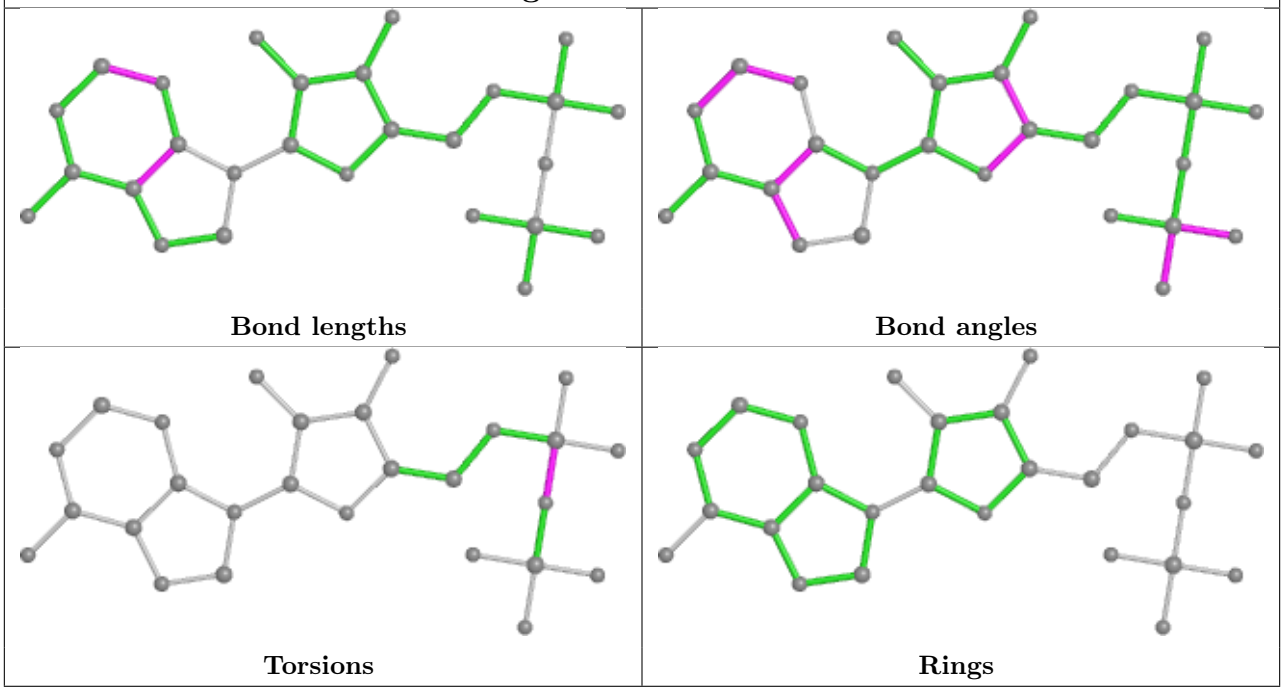
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	158	ADP	2	0

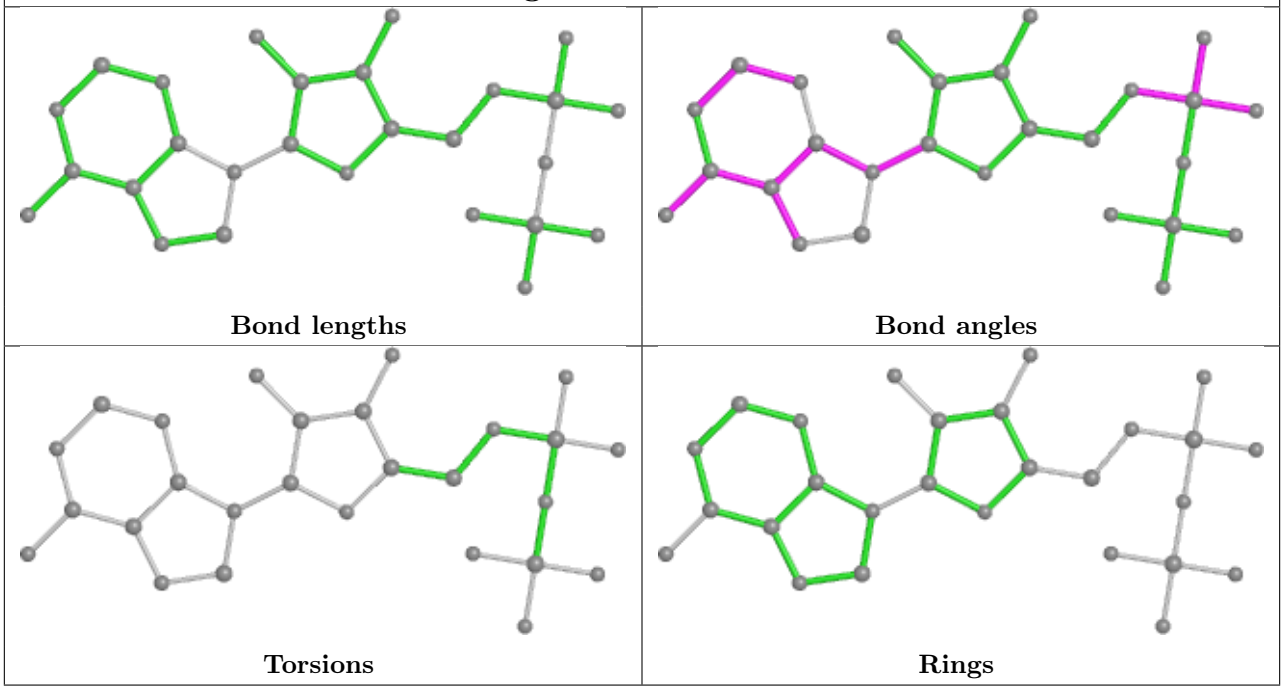
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

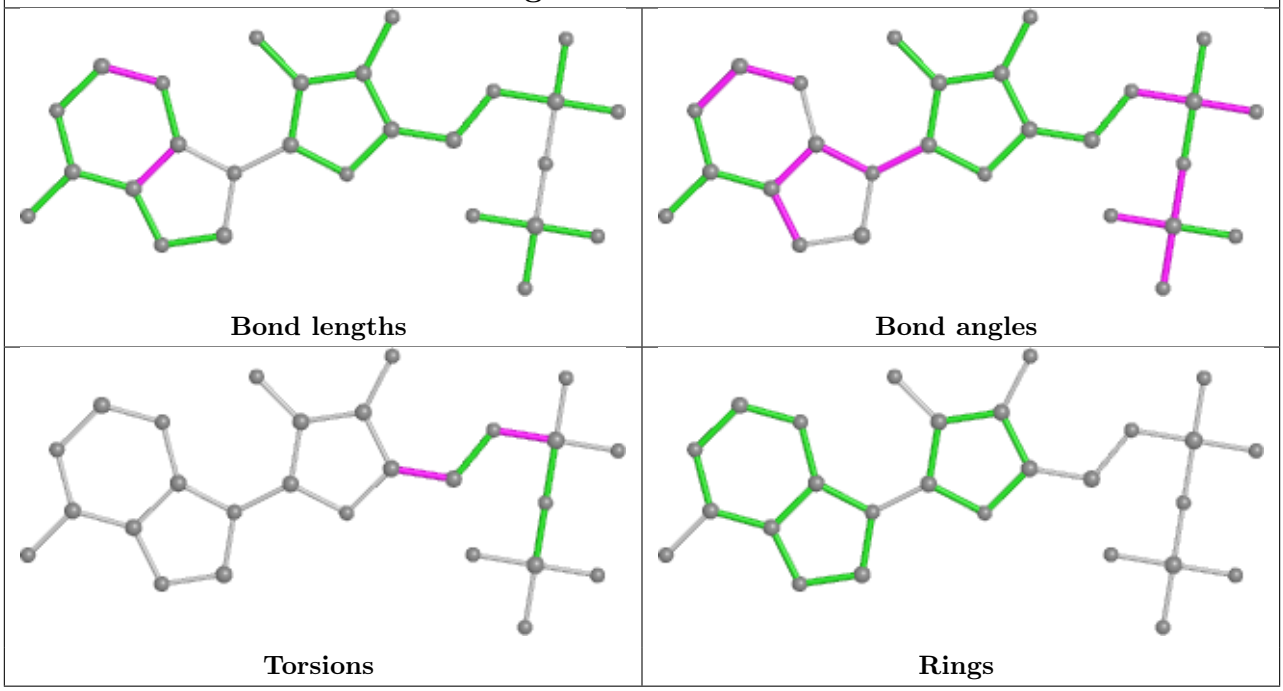
Ligand ADP A 158



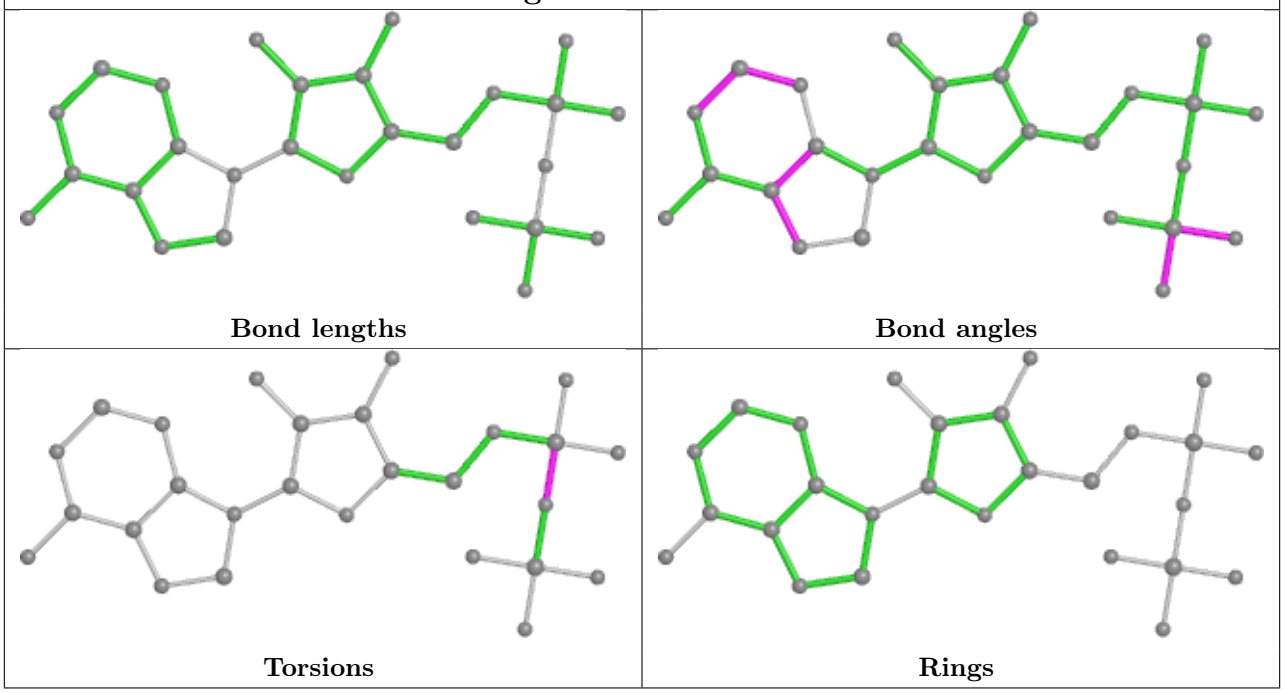
Ligand ADP B 158



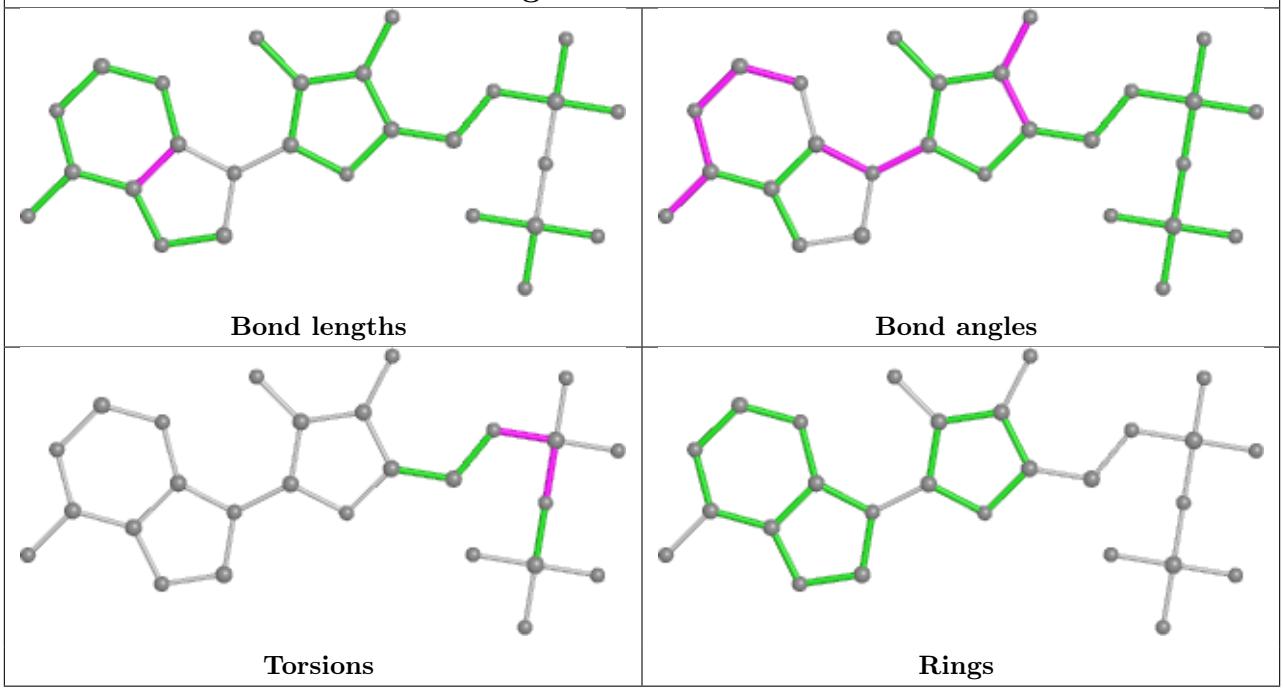
Ligand ADP F 158



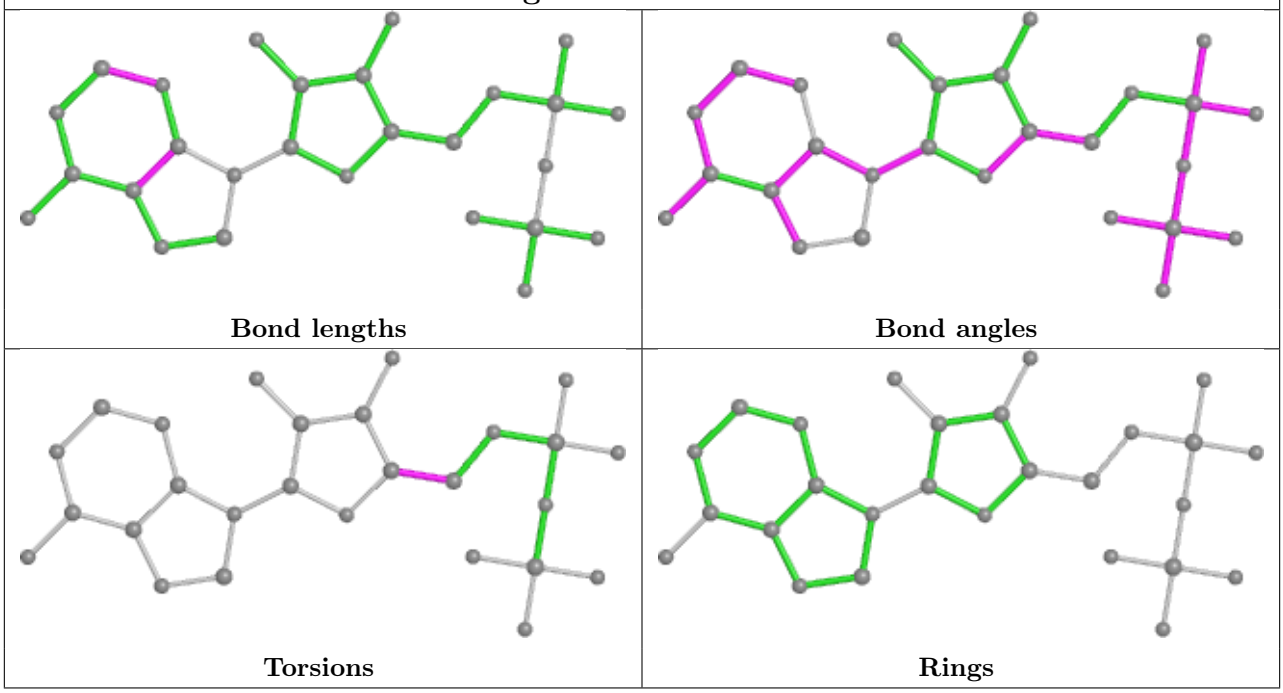
Ligand ADP E 158



Ligand ADP D 158



Ligand ADP C 158



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	149/157 (94%)	-0.38	0	100	100	8, 15, 29, 36	0
1	B	149/157 (94%)	-0.55	0	100	100	7, 16, 29, 34	0
1	C	149/157 (94%)	-0.37	0	100	100	8, 17, 30, 36	0
1	D	149/157 (94%)	-0.38	2 (1%)	77	75	8, 17, 30, 36	0
1	E	149/157 (94%)	-0.51	2 (1%)	77	75	6, 16, 28, 35	0
1	F	149/157 (94%)	-0.30	4 (2%)	54	52	8, 17, 31, 38	0
All	All	894/942 (94%)	-0.41	8 (0%)	84	83	6, 16, 30, 38	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	148	TYR	3.8
1	E	147	LEU	3.0
1	F	53	GLN	2.8
1	D	54	GLY	2.7
1	D	149	GLU	2.7
1	F	148	TYR	2.4
1	F	1	MET	2.3
1	F	56	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 monosaccharides in this entry.

6.4 Ligands (i)

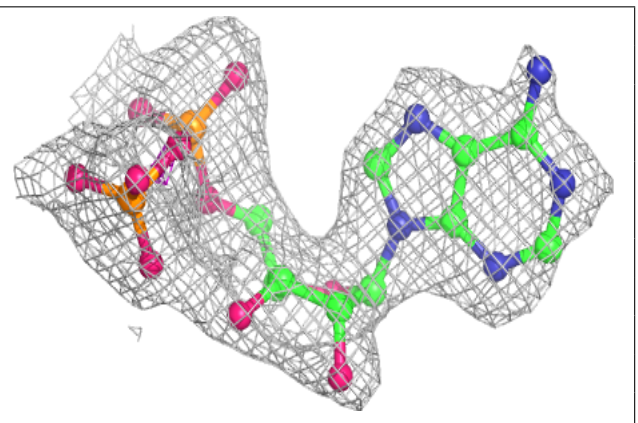
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

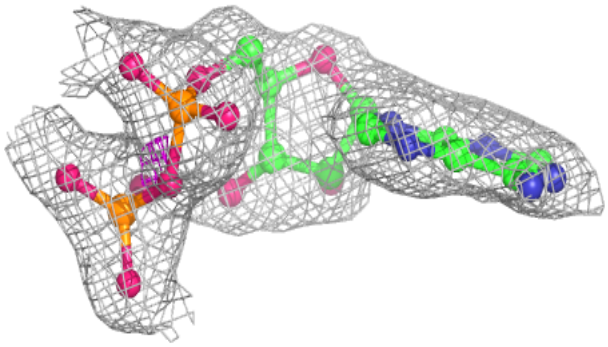
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	159	1/1	0.82	0.08	43,43,43,43	0
3	MG	A	159	1/1	0.86	0.18	48,48,48,48	0
2	ADP	F	158	27/27	0.93	0.14	27,38,43,44	0
3	MG	D	159	1/1	0.95	0.05	40,40,40,40	0
2	ADP	D	158	27/27	0.95	0.11	21,29,36,37	0
3	MG	E	159	1/1	0.96	0.05	24,24,24,24	0
2	ADP	C	158	27/27	0.96	0.15	23,33,37,38	0
3	MG	B	159	1/1	0.98	0.08	2,2,2,2	0
2	ADP	E	158	27/27	0.98	0.08	8,13,17,18	0
2	ADP	A	158	27/27	0.98	0.11	18,22,24,25	0
2	ADP	B	158	27/27	0.98	0.07	9,14,21,22	0

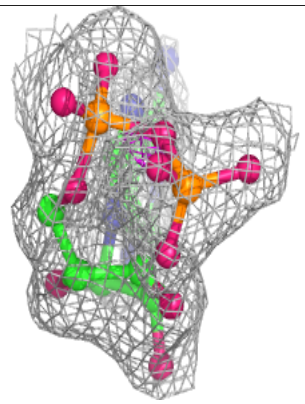
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP F 158:

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

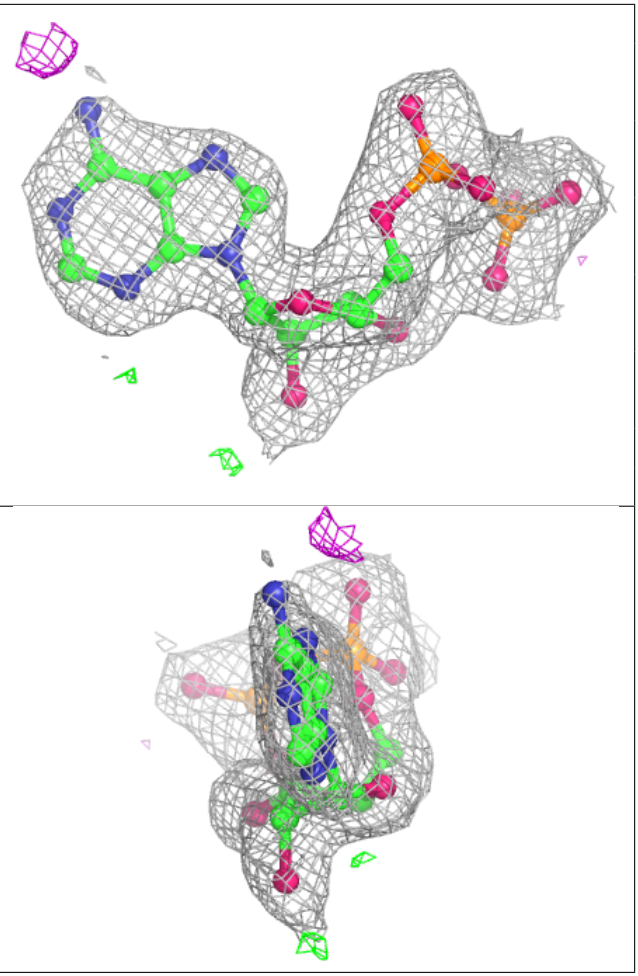






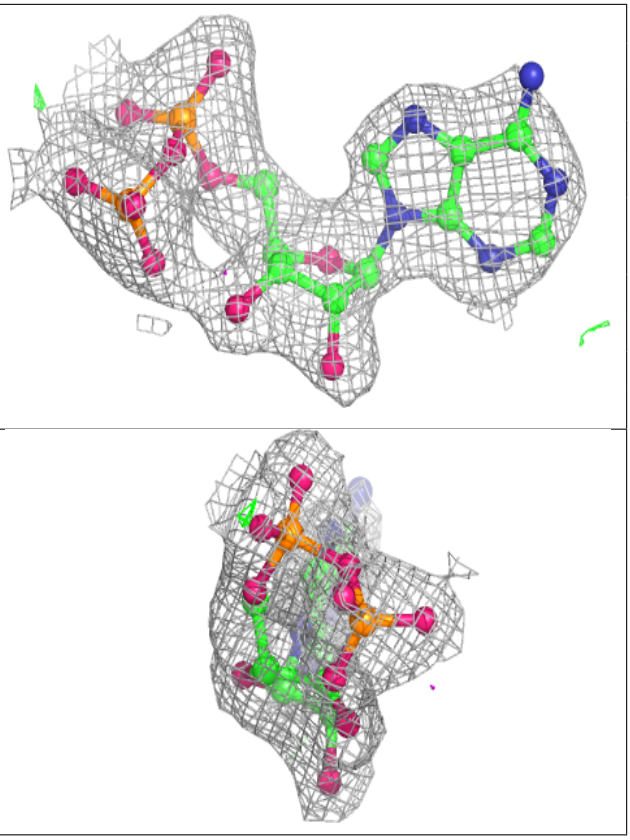
Electron density around ADP D 158:

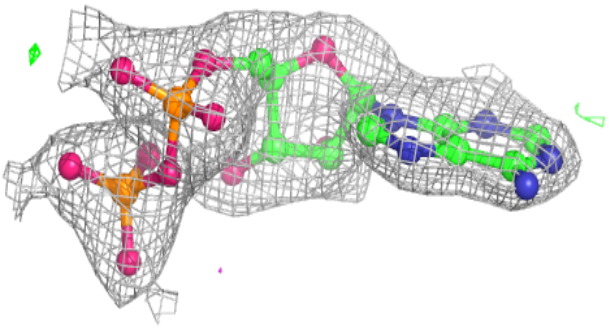
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP C 158:

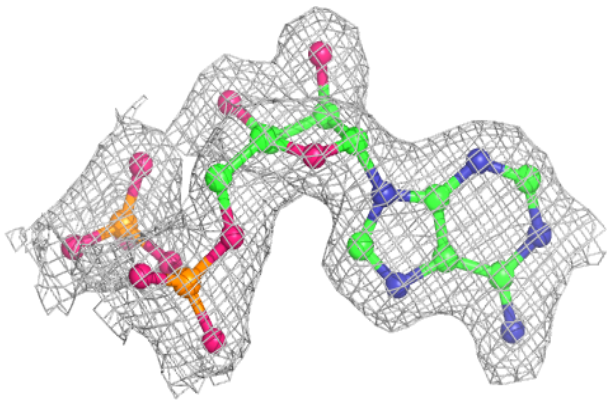
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

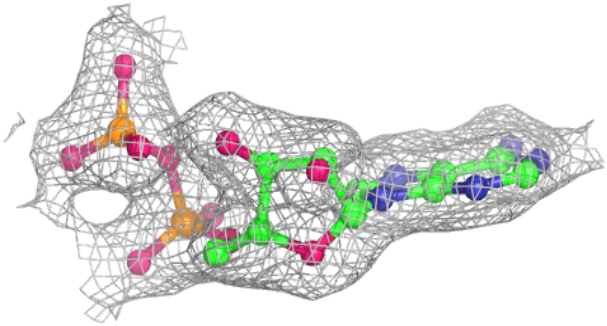


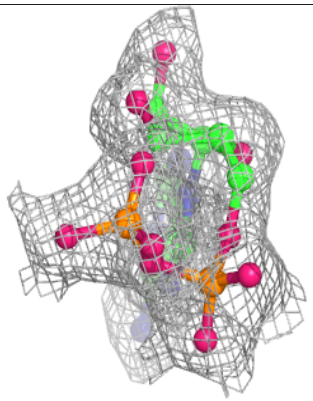


Electron density around ADP E 158:

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

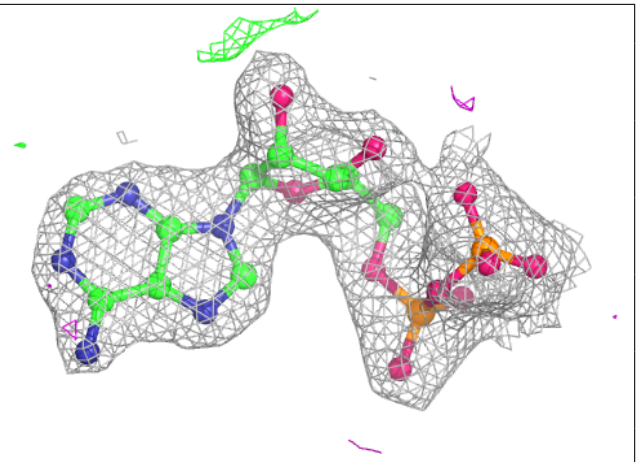


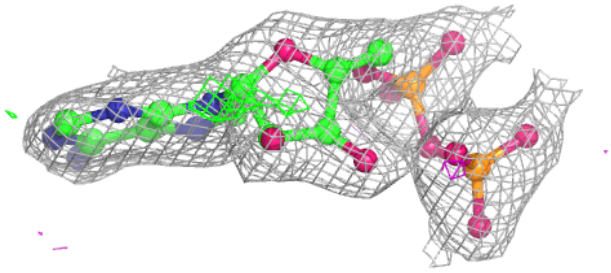


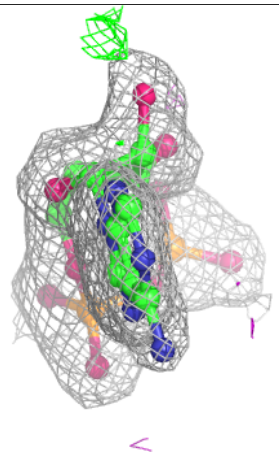


Electron density around ADP A 158:

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

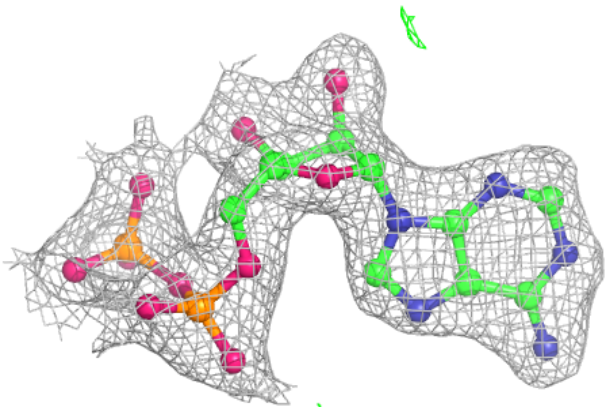


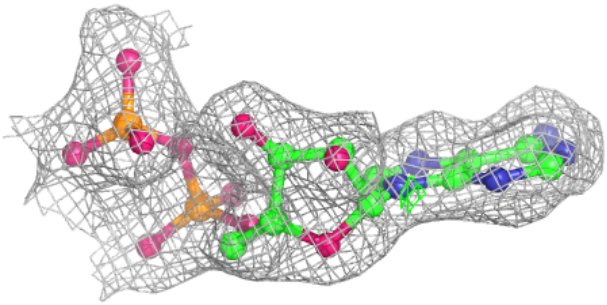


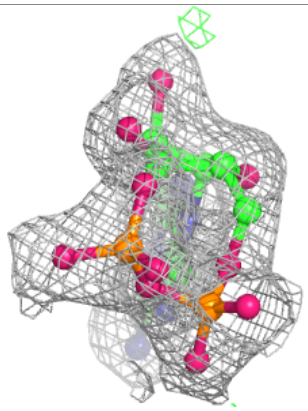


Electron density around ADP B 158:

$2mF_o$-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.