



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:58 pm BST

PDB ID : 3NCR
Title : GlnK2 from *Archaeoglobus fulgidus*, ADP complex
Authors : Helfmann, S.; Lue, W.; Litz, C.; Andrade, S.L.A.
Deposited on : 2010-06-05
Resolution : 1.44 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

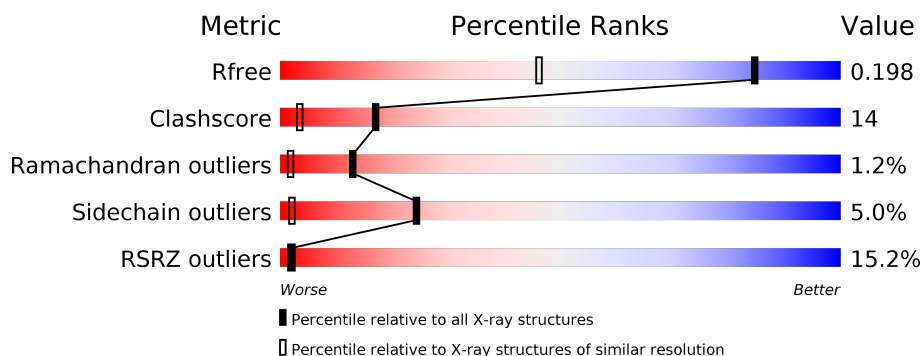
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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 on 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	119	<div> <div>15%</div> <div>74%</div> <div>17%</div> <div>• • 5%</div> </div>
1	B	119	<div> <div>13%</div> <div>73%</div> <div>15%</div> <div>6% 6%</div> </div>
1	C	119	<div> <div>15%</div> <div>80%</div> <div>13%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	C	122	-	X	-	-
6	ACT	B	121	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3204 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 Nitrogen regulatory protein P-II (GlnB-2).

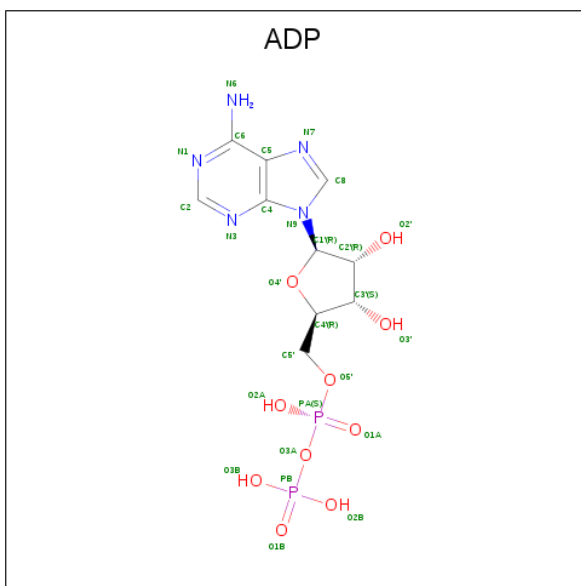
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	22	4	0
			896	566	154	173	3			
1	B	112	Total	C	N	O	S	5	5	0
			883	562	149	167	5			
1	C	116	Total	C	N	O	S	10	3	0
			918	581	160	171	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLU	-	EXPRESSION TAG	UNP O28527
A	114	HIS	-	EXPRESSION TAG	UNP O28527
A	115	HIS	-	EXPRESSION TAG	UNP O28527
A	116	HIS	-	EXPRESSION TAG	UNP O28527
A	117	HIS	-	EXPRESSION TAG	UNP O28527
A	118	HIS	-	EXPRESSION TAG	UNP O28527
A	119	HIS	-	EXPRESSION TAG	UNP O28527
B	113	GLU	-	EXPRESSION TAG	UNP O28527
B	114	HIS	-	EXPRESSION TAG	UNP O28527
B	115	HIS	-	EXPRESSION TAG	UNP O28527
B	116	HIS	-	EXPRESSION TAG	UNP O28527
B	117	HIS	-	EXPRESSION TAG	UNP O28527
B	118	HIS	-	EXPRESSION TAG	UNP O28527
B	119	HIS	-	EXPRESSION TAG	UNP O28527
C	113	GLU	-	EXPRESSION TAG	UNP O28527
C	114	HIS	-	EXPRESSION TAG	UNP O28527
C	115	HIS	-	EXPRESSION TAG	UNP O28527
C	116	HIS	-	EXPRESSION TAG	UNP O28527
C	117	HIS	-	EXPRESSION TAG	UNP O28527
C	118	HIS	-	EXPRESSION TAG	UNP O28527
C	119	HIS	-	EXPRESSION TAG	UNP O28527

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

C₁₀H₁₅N₅O₁₀P₂).

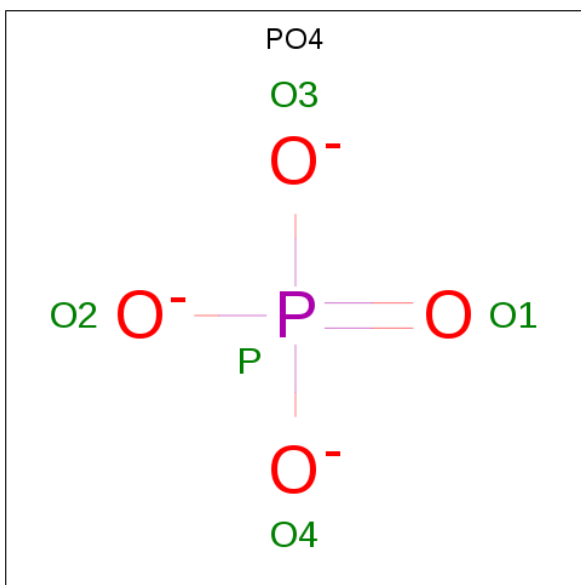


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 7 is water.

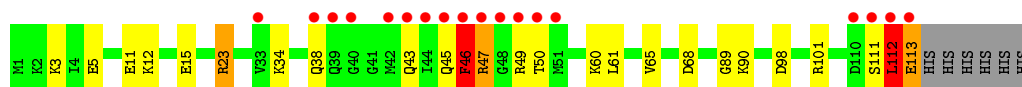
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total	O	0	0
			139	139		
7	B	132	Total	O	0	0
			132	132		
7	C	123	Total	O	0	0
			123	123		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

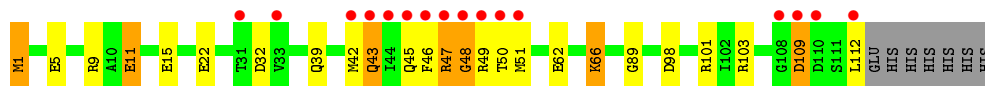
- Molecule 1: Nitrogen regulatory protein P-II (GlnB-2)

Chain A: 




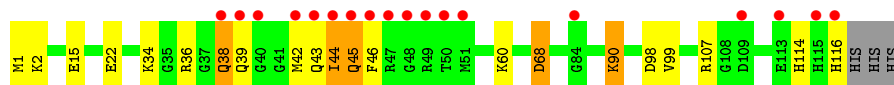
- Molecule 1: Nitrogen regulatory protein P-II (GlnB-2)

Chain B: 



- Molecule 1: Nitrogen regulatory protein P-II (GlnB-2)

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.83Å 123.83Å 125.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 1.44 39.62 – 1.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.62-1.44) 99.2 (39.62-1.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.157 , 0.200 0.155 , 0.198	Depositor DCC
R_{free} test set	4358 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.005 for -l,-k,-h 0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3204	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACT, PO4, ADP, CL

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	1.59	3/911 (0.3%)	1.18	8/1221 (0.7%)
1	B	1.53	3/904 (0.3%)	1.15	7/1211 (0.6%)
1	C	1.59	7/939 (0.7%)	1.11	3/1258 (0.2%)
All	All	1.57	13/2754 (0.5%)	1.15	18/3690 (0.5%)

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	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15[A]	GLU	CD-OE1	8.96	1.35	1.25
1	C	15[B]	GLU	CD-OE1	8.96	1.35	1.25
1	A	3	LYS	CD-CE	-7.97	1.31	1.51
1	B	5	GLU	CD-OE1	7.25	1.33	1.25
1	B	11	GLU	CG-CD	5.81	1.60	1.51
1	A	65	VAL	CB-CG1	5.67	1.64	1.52
1	C	107	ARG	CB-CG	-5.59	1.37	1.52
1	C	60	LYS	CE-NZ	5.57	1.62	1.49
1	B	62	GLU	CD-OE2	5.41	1.31	1.25
1	C	2	LYS	CE-NZ	-5.35	1.35	1.49
1	A	113	GLU	CD-OE1	-5.32	1.19	1.25
1	C	90	LYS	CD-CE	5.04	1.63	1.51
1	C	99	VAL	CB-CG1	5.01	1.63	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CB-CG-OD2	8.85	126.26	118.30
1	B	98	ASP	CB-CG-OD1	8.45	125.90	118.30
1	B	9	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	C	36	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	68	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	23	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	B	109	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	46	PHE	N-CA-C	6.53	128.64	111.00
1	B	98	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	23	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	32	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	112	LEU	CB-CA-C	5.65	120.94	110.20
1	A	68	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	98	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	112	LEU	CB-CG-CD1	5.36	120.11	111.00
1	B	15	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	C	107	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	B	9	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	896	0	928	27	1
1	B	883	0	928	36	1
1	C	918	0	954	15	3
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	2	0
3	A	1	0	0	0	0
4	A	10	0	0	1	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	4	0	3	9	0
6	C	4	0	3	0	0
7	A	139	0	0	14	3
7	B	132	0	0	5	2
7	C	123	0	0	5	2
All	All	3204	0	2852	78	7

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 14.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLN:O	1:B:46:PHE:CD1	1.86	1.27
1:B:45:GLN:O	1:B:46:PHE:HD1	0.93	1.22
1:A:61:LEU:HD22	7:A:411:HOH:O	1.41	1.20
1:C:34:LYS:HE3	7:C:415:HOH:O	1.55	1.05
1:B:1[B]:MET:SD	1:B:109:ASP:OD2	2.14	1.05
1:A:113:GLU:OE2	1:C:38:GLN:NE2	1.89	1.04
7:A:269:HOH:O	6:B:121:ACT:H3	1.60	0.98
1:B:103:ARG:HE	6:B:121:ACT:CH3	1.76	0.98
1:C:114:HIS:HD2	1:C:116:HIS:H	1.14	0.94
1:B:101:ARG:HD3	6:B:121:ACT:OXT	1.68	0.94
1:B:103:ARG:HE	6:B:121:ACT:H2	1.30	0.93
1:A:61:LEU:HD13	7:A:411:HOH:O	1.69	0.92
1:C:114:HIS:CD2	1:C:116:HIS:H	1.88	0.89
1:B:22[A]:GLU:HG3	7:B:319:HOH:O	1.74	0.86
1:B:43:GLN:HE21	1:B:50:THR:HG21	1.41	0.84
1:A:113:GLU:HG3	1:A:113:GLU:O	1.75	0.84
1:C:68:ASP:OD1	1:C:114:HIS:NE2	2.10	0.83
1:B:46:PHE:C	1:B:47:ARG:HG2	2.00	0.82
7:A:269:HOH:O	6:B:121:ACT:CH3	2.20	0.81
1:A:112:LEU:HB3	1:A:113:GLU:HA	1.68	0.75
1:A:101:ARG:HG3	1:A:111:SER:HB2	1.68	0.74
1:B:1[B]:MET:SD	1:B:112:LEU:HD12	2.28	0.74
1:A:23:ARG:HD2	7:A:161:HOH:O	1.88	0.73
1:B:66:LYS:HD3	7:B:137:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:CG	1:A:113:GLU:O	2.29	0.73
1:A:61:LEU:CD2	7:A:411:HOH:O	2.12	0.73
1:B:11:GLU:OE1	7:B:218:HOH:O	2.07	0.73
1:B:1[B]:MET:SD	1:B:112:LEU:CD1	2.80	0.69
1:B:47:ARG:O	1:B:48:GLY:C	2.29	0.68
1:C:114:HIS:HE1	7:C:272:HOH:O	1.75	0.68
1:C:114:HIS:CE1	7:C:272:HOH:O	2.48	0.67
1:B:103:ARG:NE	6:B:121:ACT:H2	2.08	0.66
1:B:47:ARG:C	1:B:49:ARG:N	2.45	0.65
1:B:47:ARG:O	1:B:49:ARG:N	2.30	0.65
1:A:23:ARG:NH1	7:A:396:HOH:O	2.30	0.65
1:A:61:LEU:CD1	7:A:411:HOH:O	2.33	0.63
1:A:112:LEU:CB	1:A:113:GLU:HA	2.27	0.62
1:A:60[A]:LYS:NZ	4:A:122:PO4:O1	2.29	0.61
1:B:103:ARG:HE	6:B:121:ACT:H1	1.63	0.61
1:A:89:GLY:HA2	2:A:120:ADP:H5'1	1.82	0.61
1:A:61:LEU:CG	7:A:411:HOH:O	2.44	0.59
1:B:1[B]:MET:CE	1:B:112:LEU:CD1	2.79	0.59
1:B:43:GLN:HE21	1:B:50:THR:CG2	2.13	0.59
1:A:90:LYS:NZ	7:A:288:HOH:O	2.36	0.59
7:A:288:HOH:O	1:B:101:ARG:HG3	2.00	0.59
1:B:1[B]:MET:CE	1:B:112:LEU:HD11	2.35	0.57
1:B:46:PHE:O	1:B:49:ARG:CB	2.54	0.56
1:A:12:LYS:NZ	1:A:15:GLU:OE1	2.33	0.56
1:C:1[A]:MET:HE1	1:C:98:ASP:HA	1.90	0.54
1:B:1[B]:MET:SD	1:B:112:LEU:HD11	2.48	0.54
1:C:44:ILE:HG23	1:C:45:GLN:H	1.73	0.54
1:A:34:LYS:HE2	7:B:354:HOH:O	2.08	0.53
1:B:66:LYS:HE2	1:B:109:ASP:O	2.09	0.53
1:C:90:LYS:NZ	2:C:120:ADP:N7	2.54	0.52
1:A:38:GLN:NE2	7:A:190:HOH:O	2.42	0.52
1:A:47:ARG:O	1:A:47:ARG:HG2	2.11	0.50
1:B:1[B]:MET:HE1	1:B:112:LEU:HG	1.94	0.49
1:B:103:ARG:NE	6:B:121:ACT:CH3	2.61	0.49
1:B:22[B]:GLU:CD	7:B:138:HOH:O	2.52	0.47
1:B:1[B]:MET:CG	1:B:109:ASP:OD2	2.62	0.47
1:B:66:LYS:HD2	1:B:112:LEU:HD12	1.96	0.47
1:A:113:GLU:C	2:C:120:ADP:HN61	2.19	0.45
1:A:113:GLU:HG2	1:C:38:GLN:OE1	2.15	0.45
1:C:44:ILE:CG2	1:C:45:GLN:N	2.80	0.45
1:A:101:ARG:NE	1:A:111:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HE2	2:A:120:ADP:N7	2.32	0.44
1:B:1[B]:MET:HE3	1:B:112:LEU:HD11	1.99	0.44
1:C:68:ASP:OD1	1:C:114:HIS:CE1	2.70	0.44
1:B:89:GLY:HA2	2:B:120:ADP:H5'1	2.01	0.43
1:C:34:LYS:CE	7:C:415:HOH:O	2.34	0.42
1:A:11[A]:GLU:HG3	7:A:179:HOH:O	2.18	0.42
1:A:23:ARG:CZ	7:A:396:HOH:O	2.66	0.42
1:B:47:ARG:C	1:B:49:ARG:H	2.20	0.41
1:B:46:PHE:C	1:B:47:ARG:CG	2.72	0.41
1:B:42:MET:C	1:B:43:GLN:HG3	2.41	0.41
1:B:103:ARG:NE	6:B:121:ACT:H1	2.34	0.41
1:C:39:GLN:NE2	7:C:160:HOH:O	2.53	0.40
1:A:5:GLU:OE1	1:A:60[B]:LYS:HE2	2.22	0.40

All (7) 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)
1:C:46:PHE:CE2	7:A:388:HOH:O[16_555]	1.72	0.48
1:A:47:ARG:NH1	1:C:22:GLU:OE1[16_555]	1.82	0.38
7:C:415:HOH:O	7:C:415:HOH:O[16_555]	1.93	0.27
1:B:51:MET:CE	7:B:277:HOH:O[16_555]	2.01	0.19
1:C:46:PHE:CZ	7:A:320:HOH:O[16_555]	2.05	0.15
7:B:181:HOH:O	7:B:409:HOH:O[16_555]	2.17	0.03
7:A:402:HOH:O	7:C:222:HOH:O[16_555]	2.18	0.02

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	115/119 (97%)	111 (96%)	2 (2%)	2 (2%)	9 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	114/119 (96%)	108 (95%)	4 (4%)	2 (2%)	8	1
1	C	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
All	All	345/357 (97%)	333 (96%)	8 (2%)	4 (1%)	13	2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	47	ARG
1	B	47	ARG
1	B	48	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/100 (97%)	92 (95%)	5 (5%)	23	2
1	B	96/100 (96%)	91 (95%)	5 (5%)	23	2
1	C	100/100 (100%)	95 (95%)	5 (5%)	24	2
All	All	293/300 (98%)	278 (95%)	15 (5%)	24	2

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	45	GLN
1	A	46	PHE
1	A	49	ARG
1	A	50	THR
1	B	1[A]	MET
1	B	1[B]	MET
1	B	39	GLN
1	B	43	GLN
1	B	66	LYS

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Mol	Chain	Res	Type
1	C	38	GLN
1	C	42	MET
1	C	43	GLN
1	C	44	ILE
1	C	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	GLN
1	C	45	GLN
1	C	114	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	120	5	24,29,29	1.32	3 (12%)	29,45,45	1.32	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	122	-	4,4,4	1.58	1 (25%)	6,6,6	1.78	2 (33%)
4	PO4	C	122	-	4,4,4	2.25	2 (50%)	6,6,6	2.13	3 (50%)
2	ADP	C	120	5	24,29,29	1.22	2 (8%)	29,45,45	1.13	1 (3%)
4	PO4	B	122	-	4,4,4	1.42	0	6,6,6	1.02	0
6	ACT	C	121	-	1,3,3	1.12	0	0,3,3	0.00	-
2	ADP	B	120	5	24,29,29	1.21	3 (12%)	29,45,45	1.69	4 (13%)
4	PO4	A	123	-	4,4,4	1.53	1 (25%)	6,6,6	2.61	2 (33%)
6	ACT	B	121	-	1,3,3	0.52	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	120	5	-	3/12/32/32	0/3/3/3
2	ADP	A	120	5	-	3/12/32/32	0/3/3/3
2	ADP	B	120	5	-	3/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	122	PO4	P-O3	-3.39	1.44	1.54
2	A	120	ADP	PB-O3B	-2.61	1.44	1.54
2	B	120	ADP	C5-C4	2.58	1.47	1.40
4	A	123	PO4	P-O2	-2.54	1.47	1.54
2	B	120	ADP	O4'-C1'	2.53	1.44	1.41
4	C	122	PO4	P-O2	-2.43	1.47	1.54
2	A	120	ADP	PA-O2A	-2.40	1.44	1.55
2	C	120	ADP	PA-O2A	-2.29	1.44	1.55
2	A	120	ADP	PB-O2B	-2.26	1.46	1.54
2	C	120	ADP	PB-O2B	-2.21	1.46	1.54
2	B	120	ADP	C2-N3	2.13	1.35	1.32
4	A	122	PO4	P-O1	2.08	1.55	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	123	PO4	O4-P-O2	5.06	124.21	107.97
2	B	120	ADP	N3-C2-N1	-4.94	120.96	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	ADP	C2-N1-C6	4.08	125.73	118.75
2	C	120	ADP	C4-C5-N7	-3.86	105.37	109.40
4	C	122	PO4	O3-P-O2	3.70	119.84	107.97
2	B	120	ADP	N6-C6-N1	3.50	125.84	118.57
2	A	120	ADP	C4-C5-N7	-3.41	105.84	109.40
2	A	120	ADP	N3-C2-N1	-3.30	123.52	128.68
4	A	122	PO4	O4-P-O3	3.06	117.78	107.97
4	A	123	PO4	O3-P-O2	-2.98	98.39	107.97
2	A	120	ADP	C2-N1-C6	2.79	123.53	118.75
4	C	122	PO4	O4-P-O2	-2.64	99.49	107.97
4	C	122	PO4	O4-P-O3	-2.49	99.97	107.97
2	B	120	ADP	C1'-N9-C4	-2.22	122.75	126.64
4	A	122	PO4	O2-P-O1	-2.06	103.35	110.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	120	ADP	C5'-O5'-PA-O2A
2	C	120	ADP	C5'-O5'-PA-O2A
2	B	120	ADP	C5'-O5'-PA-O2A
2	A	120	ADP	C5'-O5'-PA-O3A
2	C	120	ADP	C5'-O5'-PA-O3A
2	B	120	ADP	C5'-O5'-PA-O3A
2	A	120	ADP	C5'-O5'-PA-O1A
2	C	120	ADP	C5'-O5'-PA-O1A
2	B	120	ADP	C5'-O5'-PA-O1A

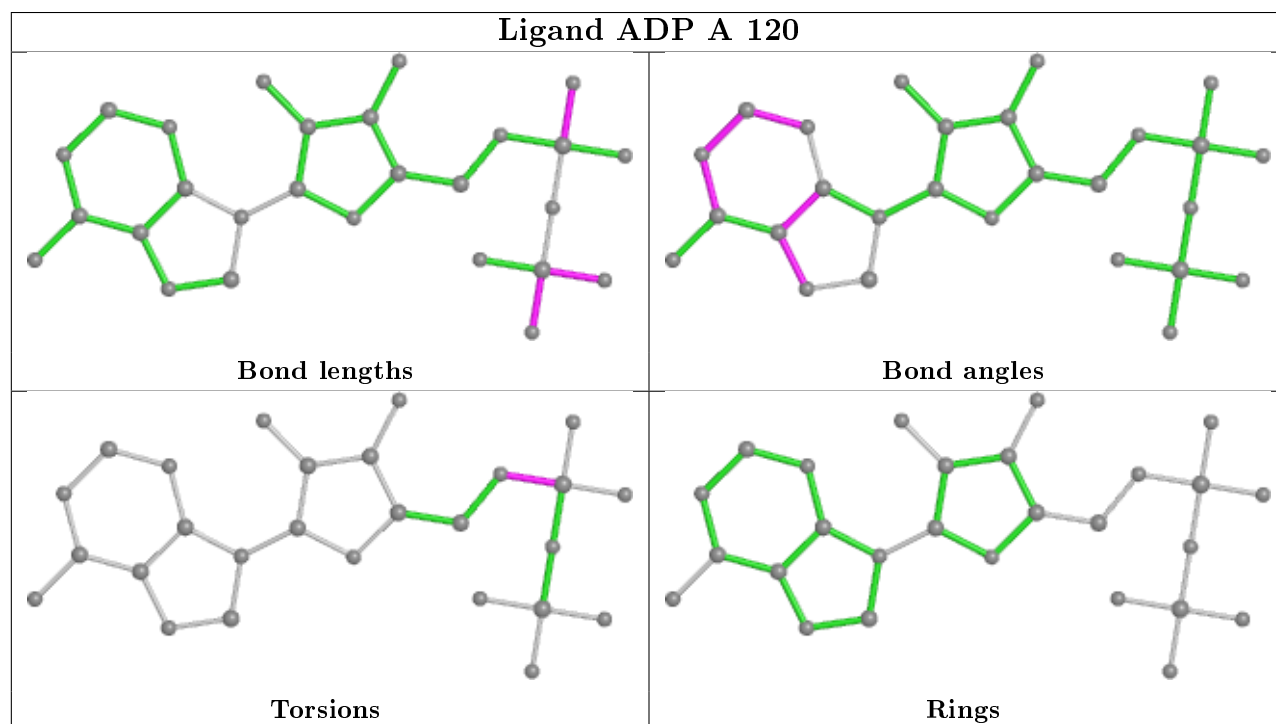
There are no ring outliers.

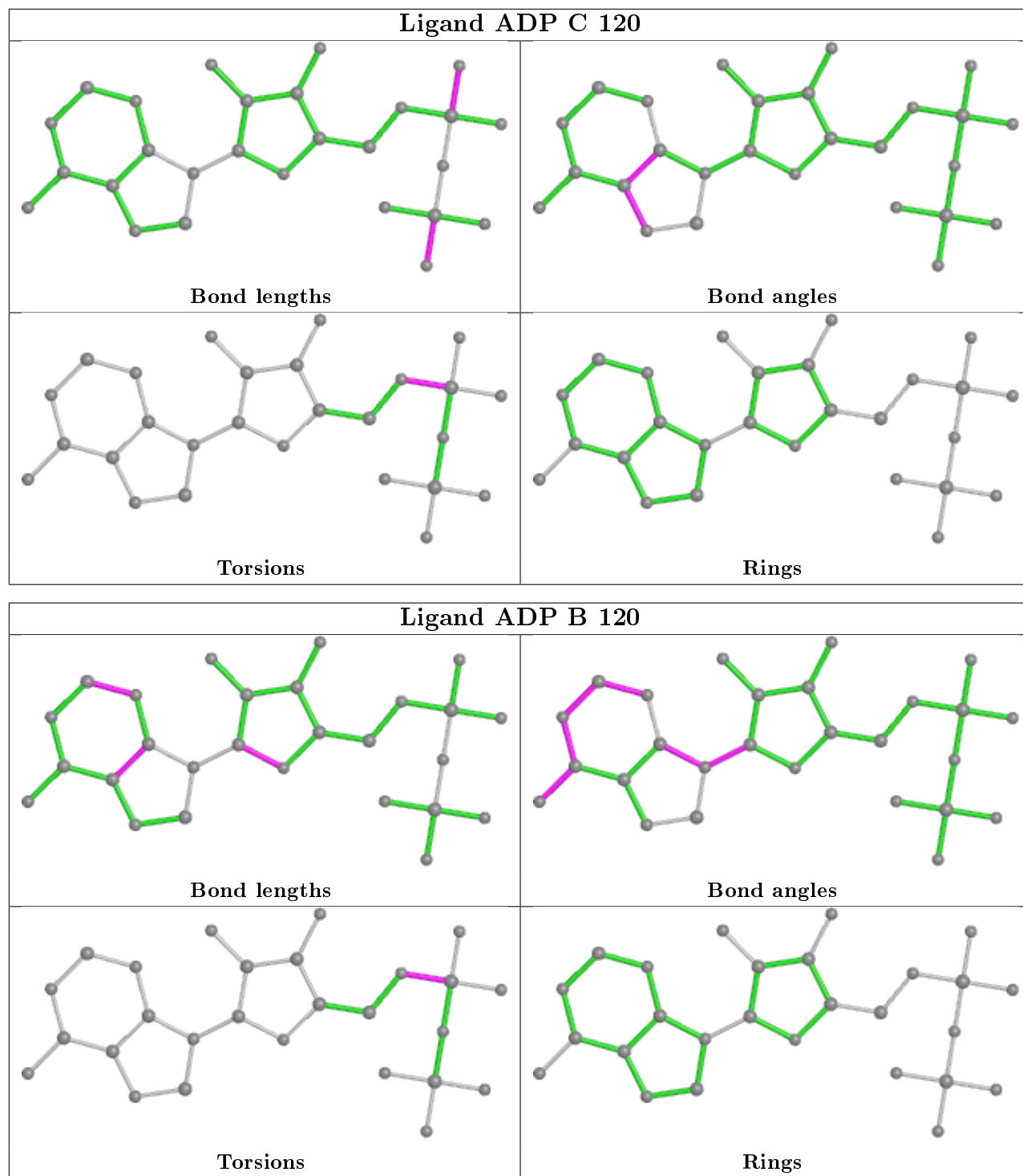
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	120	ADP	2	0
4	A	122	PO4	1	0
2	C	120	ADP	2	0
2	B	120	ADP	1	0
6	B	121	ACT	9	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	113/119 (94%)	0.45	18 (15%) 1 2	13, 21, 63, 80	6 (5%)
1	B	112/119 (94%)	0.65	16 (14%) 2 2	13, 19, 60, 82	1 (0%)
1	C	116/119 (97%)	0.63	18 (15%) 2 2	13, 22, 64, 87	3 (2%)
All	All	341/357 (95%)	0.58	52 (15%) 2 2	13, 21, 63, 87	10 (2%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	PHE	12.8
1	B	48	GLY	10.2
1	C	50	THR	9.9
1	C	46	PHE	9.7
1	A	50	THR	8.3
1	B	47	ARG	8.0
1	A	46	PHE	7.4
1	C	47	ARG	7.4
1	A	45	GLN	7.3
1	A	48	GLY	7.2
1	A	47	ARG	7.1
1	C	44	ILE	7.0
1	C	48	GLY	7.0
1	A	49	ARG	5.9
1	B	45	GLN	5.9
1	A	44	ILE	5.7
1	C	45	GLN	5.7
1	B	50	THR	5.6
1	C	116	HIS	5.6
1	B	110	ASP	5.4
1	C	49	ARG	5.1
1	C	51[A]	MET	4.6
1	B	44	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	110	ASP	4.5
1	B	49	ARG	4.4
1	A	112	LEU	4.2
1	A	43	GLN	4.1
1	B	109	ASP	3.9
1	C	43	GLN	3.9
1	B	43	GLN	3.5
1	A	51	MET	3.3
1	C	40	GLY	3.3
1	A	40	GLY	2.9
1	C	39	GLN	2.8
1	C	42	MET	2.8
1	B	112	LEU	2.7
1	B	33	VAL	2.7
1	A	111	SER	2.7
1	C	115	HIS	2.6
1	B	108	GLY	2.5
1	A	42	MET	2.5
1	C	38	GLN	2.4
1	B	31	THR	2.3
1	B	51	MET	2.3
1	A	39	GLN	2.3
1	A	33	VAL	2.2
1	A	38	GLN	2.2
1	C	113	GLU	2.1
1	A	113	GLU	2.0
1	C	84	GLY	2.0
1	C	109	ASP	2.0
1	B	42	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

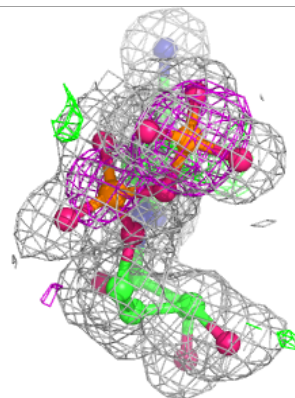
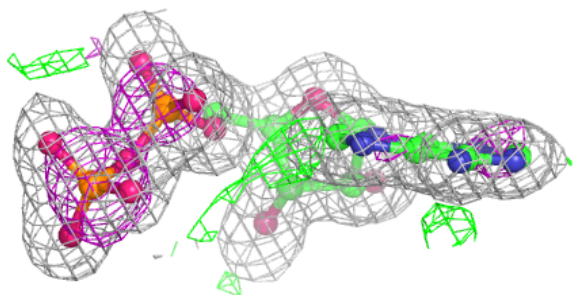
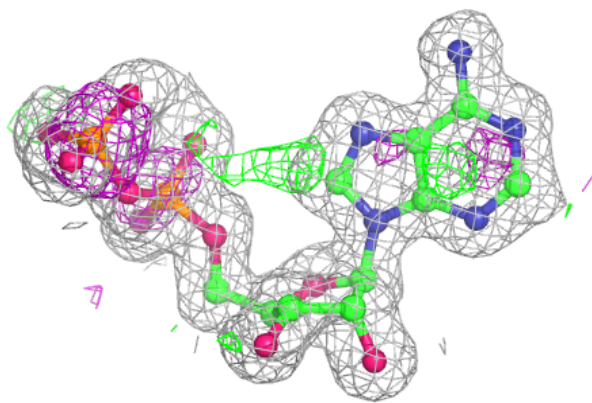
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	B	121	4/4	0.86	0.18	50,51,51,51	0
4	PO4	A	123	5/5	0.94	0.22	36,42,51,52	0
2	ADP	C	120	27/27	0.94	0.08	15,19,31,35	0
5	MG	C	123	1/1	0.94	0.14	67,67,67,67	1
2	ADP	A	120	27/27	0.95	0.07	15,18,30,34	0
5	MG	A	124	1/1	0.96	0.08	49,49,49,49	1
6	ACT	C	121	4/4	0.97	0.10	40,41,44,45	0
5	MG	B	123	1/1	0.97	0.40	41,41,41,41	1
2	ADP	B	120	27/27	0.98	0.06	12,16,21,23	0
4	PO4	B	122	5/5	0.99	0.05	23,24,28,29	0
4	PO4	C	122	5/5	0.99	0.07	30,32,41,42	0
3	CL	A	121	1/1	1.00	0.11	15,15,15,15	0
4	PO4	A	122	5/5	1.00	0.05	20,27,29,37	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.

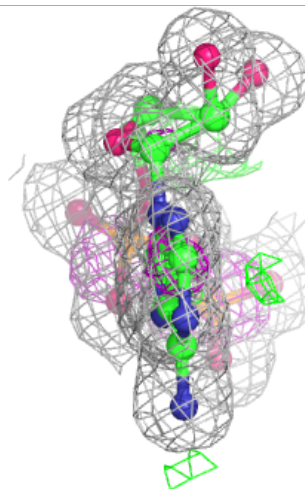
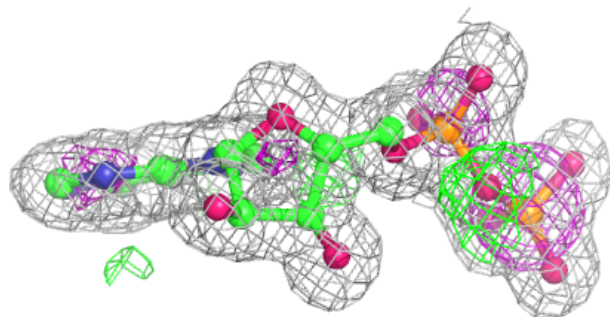
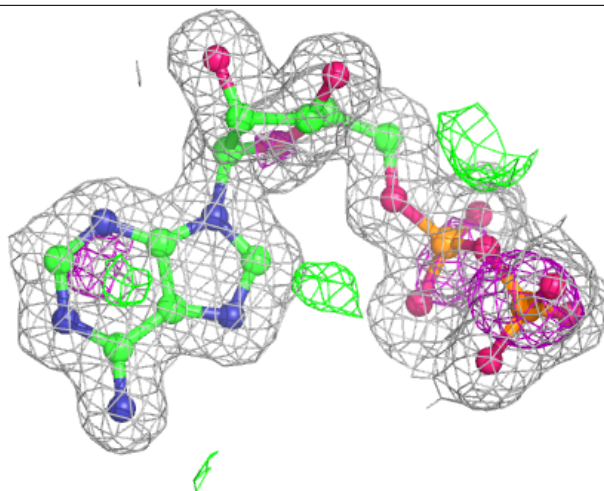
Electron density around ADP C 120:

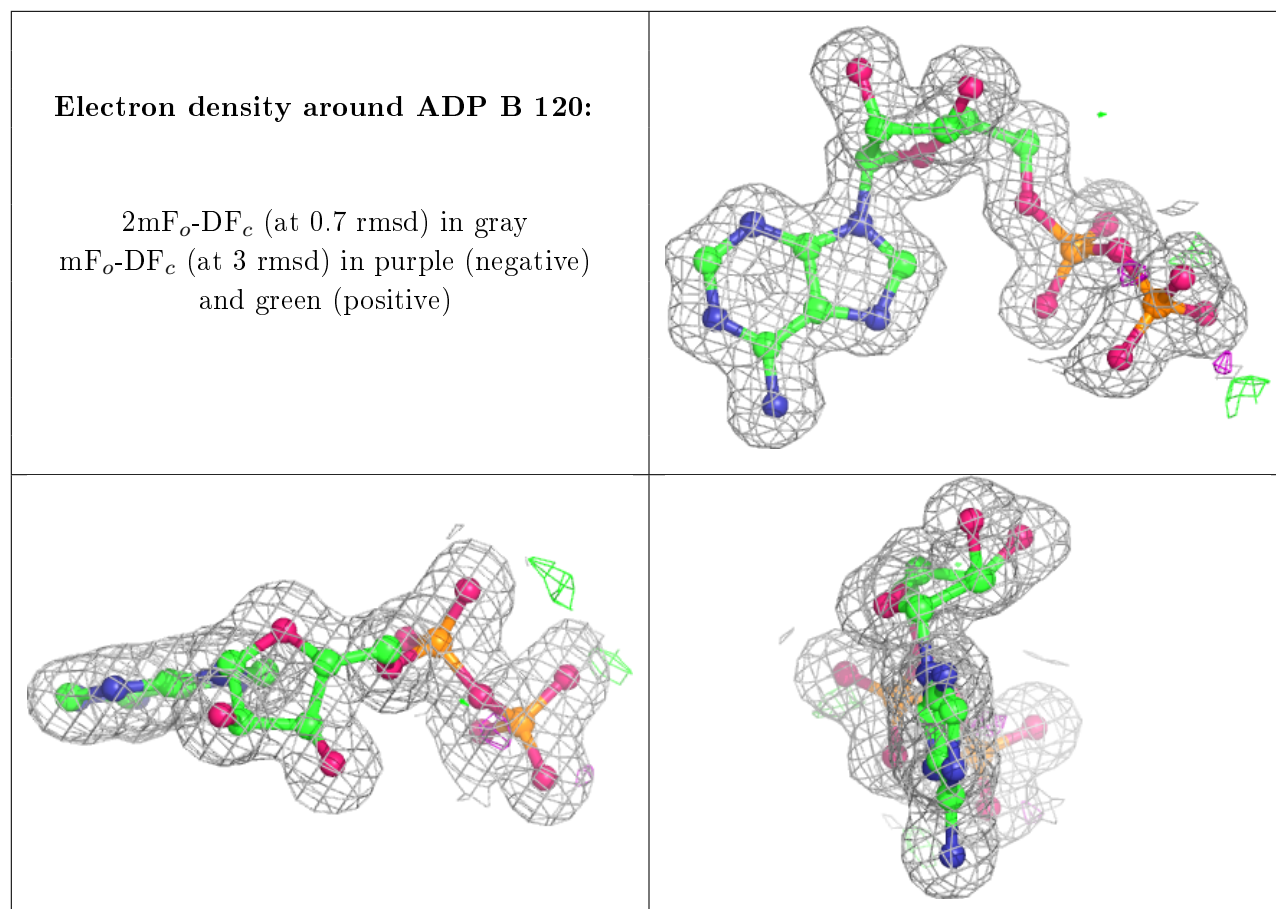
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 120:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.