



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:58 PM GMT

PDB ID : 1QHG
Title : STRUCTURE OF DNA HELICASE MUTANT WITH ADPNP
Authors : Soultanas, P.; Dillingham, M.S.; Velankar, S.S.; Wigley, D.B.
Deposited on : 1999-05-14
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

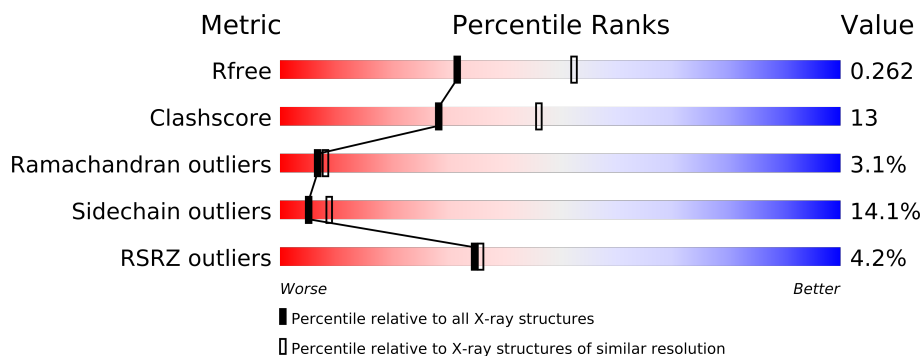
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	724	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	725	-	X
3	ATP	A	726	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5306 atoms, of which 114 are hydrogens and 0 are deuterium.

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.

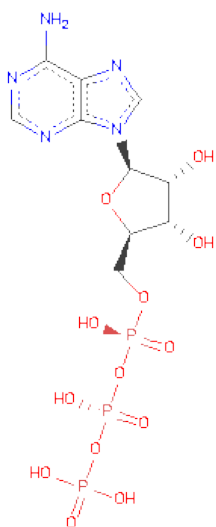
- Molecule 1 is a protein called ATP-DEPENDENT HELICASE PCRA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	622	5149	3186	114	881	948	20	0	0	0

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total 125	O 125	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	138.10Å 138.10Å 111.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 9.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.3 (10.00-2.50) 91.6 (9.99-2.50)	Depositor EDS
R_{merge}	0.61	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , 0.269 0.230 , 0.262	Depositor DCC
R_{free} test set	1763 reflections (4.70%)	DCC
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.2	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37521 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5306	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	4/5119 (0.1%)	1.74	116/6909 (1.7%)

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	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	PHE	CG-CD1	6.72	1.48	1.38
1	A	259	TRP	CG-CD2	-5.34	1.34	1.43
1	A	243	PHE	CB-CG	-5.29	1.42	1.51
1	A	39	ARG	CZ-NH2	-5.09	1.26	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	PHE	CB-CG-CD1	-18.25	108.03	120.80
1	A	647	GLU	O-C-N	15.81	148.00	122.70
1	A	258	ARG	NE-CZ-NH1	15.42	128.01	120.30
1	A	39	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	A	291	ARG	NE-CZ-NH1	15.19	127.89	120.30
1	A	21	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	A	258	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	A	291	ARG	NE-CZ-NH2	-13.43	113.58	120.30
1	A	647	GLU	CA-C-N	-12.87	88.88	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	A	73	ARG	NE-CZ-NH1	10.77	125.68	120.30
1	A	597	MET	CG-SD-CE	-10.70	83.08	100.20
1	A	312	TRP	CD1-CG-CD2	10.10	114.38	106.30
1	A	346	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	601	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	A	70	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	A	312	TRP	CE2-CD2-CG	-8.87	100.20	107.30
1	A	243	PHE	CB-CG-CD2	8.86	127.00	120.80
1	A	259	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	A	88	TRP	CD1-CG-CD2	8.56	113.14	106.30
1	A	242	ARG	CG-CD-NE	8.49	129.63	111.80
1	A	366	VAL	CG1-CB-CG2	-8.34	97.56	110.90
1	A	137	LYS	CA-C-N	-8.31	98.91	117.20
1	A	134	ILE	N-CA-C	8.20	133.13	111.00
1	A	610	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	A	259	TRP	CE2-CD2-CG	-8.17	100.77	107.30
1	A	269	SER	N-CA-C	8.15	133.01	111.00
1	A	605	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	A	70	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	73	ARG	CG-CD-NE	-7.99	95.03	111.80
1	A	350	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	350	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	88	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	602	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	471	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	A	73	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	260	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	287	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	389	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	75	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	257	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	A	471	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	A	242	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	44	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	6	GLU	CA-CB-CG	-6.91	98.20	113.40
1	A	425	SER	N-CA-C	6.90	129.62	111.00
1	A	310	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	270	PHE	CB-CG-CD1	-6.82	116.03	120.80
1	A	310	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	602	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	242	ARG	NH1-CZ-NH2	-6.73	112.00	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	273	ASP	CA-C-N	-6.60	102.68	117.20
1	A	610	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	75	ARG	CG-CD-NE	-6.50	98.14	111.80
1	A	289	THR	N-CA-CB	-6.41	98.13	110.30
1	A	58	ASN	CB-CA-C	-6.40	97.61	110.40
1	A	133	ASN	C-N-CA	6.34	137.54	121.70
1	A	102	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	312	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	75	ARG	CA-CB-CG	-6.21	99.75	113.40
1	A	647	GLU	C-N-CA	-6.20	106.20	121.70
1	A	312	TRP	CG-CD2-CE3	6.16	139.44	133.90
1	A	306	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	225	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	306	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	260	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	95	MET	CA-CB-CG	6.01	123.51	113.30
1	A	243	PHE	O-C-N	5.99	132.29	122.70
1	A	306	ARG	CA-CB-CG	5.99	126.59	113.40
1	A	242	ARG	CA-CB-CG	5.87	126.32	113.40
1	A	346	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	490	LYS	CA-CB-CG	-5.75	100.75	113.40
1	A	411	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	426	THR	N-CA-C	-5.72	95.56	111.00
1	A	294	GLN	N-CA-CB	-5.66	100.41	110.60
1	A	236	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	A	575	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	A	111	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	125	MET	CG-SD-CE	-5.57	91.29	100.20
1	A	448	LEU	CA-CB-CG	5.56	128.10	115.30
1	A	26	PRO	N-CD-CG	5.51	111.47	103.20
1	A	243	PHE	CG-CD1-CE1	-5.49	114.76	120.80
1	A	287	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	88	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	A	12	LEU	N-CA-CB	-5.44	99.53	110.40
1	A	76	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	A	320	PRO	CA-N-CD	-5.41	103.93	111.50
1	A	269	SER	CA-CB-OG	-5.40	96.62	111.20
1	A	650	SER	N-CA-C	-5.39	96.44	111.00
1	A	273	ASP	O-C-N	5.35	131.27	122.70
1	A	5	SER	CA-CB-OG	-5.35	96.77	111.20
1	A	273	ASP	N-CA-C	5.34	125.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	C-N-CA	5.34	135.04	121.70
1	A	39	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	A	258	ARG	CB-CG-CD	-5.31	97.78	111.60
1	A	80	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	606	VAL	CA-C-N	5.27	126.74	116.20
1	A	541	ILE	CB-CG1-CD1	5.21	128.50	113.90
1	A	605	TYR	CB-CG-CD1	5.21	124.13	121.00
1	A	242	ARG	CB-CG-CD	-5.20	98.09	111.60
1	A	501	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	243	PHE	CA-C-N	-5.16	105.85	117.20
1	A	58	ASN	CA-CB-CG	5.13	124.68	113.40
1	A	208	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	205	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	243	PHE	CD1-CG-CD2	5.06	124.88	118.30
1	A	352	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	424	ALA	CB-CA-C	-5.05	102.52	110.10
1	A	76	VAL	CA-CB-CG2	5.05	118.47	110.90
1	A	269	SER	CB-CA-C	-5.05	100.51	110.10
1	A	465	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	228	THR	N-CA-CB	-5.04	100.72	110.30
1	A	242	ARG	CD-NE-CZ	5.02	130.63	123.60
1	A	384	LEU	CA-CB-CG	5.01	126.84	115.30
1	A	237	LYS	CB-CG-CD	-5.01	98.58	111.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ASP	Peptide
1	A	215	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	268	LEU	Mainchain
1	A	39	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	585	PHE	Peptide
1	A	610	ARG	Sidechain
1	A	73	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5035	114	4931	128	0
2	A	1	0	0	0	0
3	A	31	0	11	3	0
4	A	125	0	0	12	0
All	All	5192	114	4942	128	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (128) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:GLU:HB2	1:A:623:ARG:NH1	1.21	1.42
1:A:329:GLU:CB	1:A:623:ARG:NH1	1.91	1.31
1:A:329:GLU:CB	1:A:623:ARG:HH11	1.42	1.31
1:A:329:GLU:HB3	1:A:623:ARG:CG	1.73	1.16
1:A:329:GLU:HB3	1:A:623:ARG:HG2	1.29	1.15
1:A:610:ARG:HA	1:A:610:ARG:HE	1.15	1.10
1:A:366:VAL:HG12	4:A:843:HOH:O	1.48	1.08
1:A:571:GLU:OE2	4:A:851:HOH:O	1.71	1.08
1:A:366:VAL:CG1	4:A:843:HOH:O	1.97	1.05
1:A:325:GLU:HG3	4:A:806:HOH:O	1.61	1.00
1:A:329:GLU:HB2	1:A:623:ARG:HH12	1.29	0.96
1:A:329:GLU:HB3	1:A:623:ARG:HG3	1.53	0.88
1:A:329:GLU:HB3	1:A:623:ARG:HH11	1.40	0.85
1:A:350:ARG:HD2	1:A:352:ARG:HH11	1.41	0.85
1:A:610:ARG:HA	1:A:610:ARG:NE	1.91	0.83
1:A:197:MET:O	1:A:201:GLN:HG3	1.81	0.81
1:A:329:GLU:CA	1:A:623:ARG:NH1	2.49	0.76
1:A:297:ASN:HD22	1:A:311:ILE:HG12	1.52	0.75
1:A:451:ILE:HB	1:A:453:LEU:HD23	1.70	0.74
1:A:321:ILE:O	1:A:646:LEU:HD12	1.88	0.73
1:A:287:ARG:HD2	3:A:726:ATP:H5'1	1.69	0.72
1:A:22:THR:HG21	1:A:278:LYS:HE3	1.72	0.71
1:A:308:PRO:O	4:A:764:HOH:O	2.09	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:GLU:HB2	1:A:623:ARG:HH11	0.90	0.71
1:A:578:ILE:O	4:A:731:HOH:O	2.10	0.70
1:A:329:GLU:CB	1:A:623:ARG:HG2	2.18	0.69
1:A:20:VAL:HA	1:A:44:ARG:HG3	1.75	0.69
1:A:350:ARG:HD2	1:A:352:ARG:NH1	2.08	0.69
1:A:226:GLN:NE2	1:A:226:GLN:H	1.92	0.68
1:A:582:GLU:HA	1:A:586:PRO:HD2	1.75	0.68
1:A:328:ASN:HA	1:A:622:MET:O	1.95	0.66
1:A:321:ILE:O	1:A:646:LEU:CD1	2.45	0.65
1:A:590:SER:HA	1:A:596:GLU:HB3	1.78	0.64
1:A:287:ARG:HD2	3:A:726:ATP:C5'	2.28	0.63
1:A:1:MET:HA	1:A:51:GLU:OE1	1.98	0.63
1:A:12:LEU:HB3	1:A:16:GLN:HB2	1.82	0.62
1:A:12:LEU:HA	1:A:16:GLN:OE1	2.01	0.61
1:A:226:GLN:HA	4:A:752:HOH:O	1.99	0.61
1:A:161:PHE:HD2	1:A:174:SER:HB3	1.65	0.61
1:A:584:ILE:HD11	1:A:630:GLN:HE22	1.64	0.61
1:A:381:VAL:HG12	4:A:835:HOH:O	2.00	0.61
1:A:526:SER:O	1:A:529:LYS:HE2	2.01	0.60
1:A:569:GLY:HA2	3:A:726:ATP:O2G	2.02	0.59
1:A:381:VAL:CG1	4:A:835:HOH:O	2.51	0.59
1:A:229:ASN:ND2	1:A:232:GLN:H	1.99	0.59
1:A:424:ALA:HB1	1:A:460:ALA:HA	1.83	0.59
1:A:125:MET:HE1	1:A:176:VAL:HG21	1.85	0.58
1:A:601:ARG:HD3	1:A:637:PHE:HE1	1.67	0.58
1:A:40:VAL:HG21	1:A:282:LEU:HD21	1.85	0.58
1:A:601:ARG:HD3	1:A:637:PHE:CE1	2.38	0.58
1:A:366:VAL:HG13	4:A:843:HOH:O	1.79	0.58
1:A:290:LYS:NZ	1:A:315:ASN:O	2.37	0.58
1:A:289:THR:HG21	4:A:846:HOH:O	2.04	0.58
1:A:253:ASP:OD1	1:A:306:ARG:HD2	2.03	0.58
1:A:226:GLN:H	1:A:226:GLN:HE21	1.54	0.55
1:A:340:ILE:O	1:A:344:VAL:HG23	2.06	0.55
1:A:297:ASN:HD22	1:A:311:ILE:H	1.53	0.55
1:A:12:LEU:HB3	1:A:16:GLN:CB	2.37	0.55
1:A:31:ALA:O	1:A:251:ASP:HB2	2.07	0.54
1:A:172:VAL:O	1:A:176:VAL:HG12	2.07	0.54
1:A:445:LEU:HD11	1:A:461:LEU:HD22	1.88	0.54
1:A:134:ILE:O	1:A:139:PHE:HB2	2.07	0.54
1:A:610:ARG:CA	1:A:610:ARG:HE	2.05	0.54
1:A:71:GLU:O	1:A:75:ARG:HD2	2.07	0.54
1:A:125:MET:CE	1:A:176:VAL:HG21	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:GLU:HA	1:A:623:ARG:NH1	2.23	0.51
1:A:228:THR:HG23	1:A:233:TYR:HB2	1.92	0.51
1:A:532:ILE:HD12	1:A:532:ILE:H	1.75	0.51
1:A:610:ARG:CA	1:A:610:ARG:NE	2.69	0.50
1:A:389:ARG:HH11	1:A:511:ASN:HD22	1.60	0.50
1:A:289:THR:HG22	1:A:292:ILE:H	1.76	0.50
1:A:195:LEU:O	1:A:199:THR:HG23	2.10	0.50
1:A:61:ALA:HB1	1:A:72:MET:CE	2.41	0.50
1:A:395:ILE:HD13	1:A:488:LEU:HD13	1.94	0.50
1:A:8:LEU:O	1:A:11:HIS:HB2	2.12	0.49
1:A:538:LEU:HA	1:A:541:ILE:HG22	1.93	0.49
1:A:38:THR:HG22	1:A:75:ARG:NH1	2.28	0.48
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.79	0.47
1:A:161:PHE:CD2	1:A:174:SER:HB3	2.47	0.47
1:A:291:ARG:HG3	1:A:645:LEU:HD22	1.97	0.47
1:A:289:THR:HG23	1:A:317:GLU:O	2.14	0.47
1:A:211:HIS:O	1:A:215:TYR:HD1	1.97	0.47
1:A:107:ILE:HA	4:A:777:HOH:O	2.15	0.47
1:A:115:ILE:HA	1:A:190:LEU:O	2.14	0.47
1:A:321:ILE:HB	1:A:646:LEU:HD13	1.96	0.47
1:A:121:GLN:HG2	1:A:145:LEU:HD22	1.97	0.47
1:A:229:ASN:HD22	1:A:232:GLN:HG3	1.77	0.46
1:A:134:ILE:HG23	1:A:139:PHE:CD2	2.49	0.46
1:A:322:LEU:HA	1:A:647:GLU:O	2.14	0.46
1:A:41:LEU:HD13	1:A:249:VAL:HG21	1.97	0.46
1:A:100:LEU:HD22	1:A:104:ILE:HD12	1.98	0.46
1:A:229:ASN:HD21	1:A:232:GLN:H	1.64	0.46
1:A:229:ASN:H	1:A:232:GLN:HE21	1.64	0.45
1:A:121:GLN:HG3	1:A:180:TYR:OH	2.16	0.45
1:A:389:ARG:HH11	1:A:511:ASN:ND2	2.15	0.44
1:A:90:SER:HB2	1:A:94:SER:HB2	2.00	0.44
1:A:387:TYR:HE2	1:A:541:ILE:HD12	1.82	0.44
1:A:29:ILE:HB	1:A:249:VAL:HG22	2.00	0.44
1:A:606:VAL:O	1:A:610:ARG:HD2	2.18	0.44
1:A:73:ARG:O	1:A:77:GLN:HB2	2.18	0.44
1:A:564:LEU:HB3	1:A:603:LEU:HD22	2.00	0.44
1:A:72:MET:O	1:A:76:VAL:HG22	2.17	0.43
1:A:55:ALA:O	1:A:58:ASN:N	2.52	0.43
1:A:500:GLU:HB3	1:A:505:ALA:HB2	2.00	0.43
1:A:18:GLU:OE2	1:A:278:LYS:NZ	2.51	0.43
1:A:140:GLU:HA	1:A:141:PRO:HD2	1.82	0.43
1:A:289:THR:O	1:A:293:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:VAL:O	1:A:484:VAL:HG23	2.19	0.43
1:A:287:ARG:CZ	1:A:571:GLU:HG3	2.48	0.42
1:A:329:GLU:CB	1:A:623:ARG:HG3	2.39	0.42
1:A:410:SER:O	1:A:414:ILE:HG12	2.20	0.42
1:A:324:TYR:HB3	1:A:618:THR:HG22	2.00	0.42
1:A:346:ARG:HD3	1:A:348:GLU:OE2	2.20	0.41
1:A:38:THR:HG22	1:A:75:ARG:HH11	1.85	0.41
1:A:30:MET:HA	1:A:250:GLY:O	2.21	0.41
1:A:599:GLU:OE1	1:A:602:ARG:NH1	2.54	0.41
1:A:110:ASN:HB3	1:A:112:ASN:OD1	2.21	0.41
1:A:352:ARG:HB3	1:A:557:ASP:HA	2.03	0.41
1:A:215:TYR:CE2	1:A:242:ARG:NH2	2.89	0.41
1:A:225:TYR:O	1:A:228:THR:HB	2.21	0.41
1:A:322:LEU:HD23	1:A:323:TYR:N	2.36	0.41
1:A:132:LYS:HB3	1:A:133:ASN:H	1.63	0.41
1:A:4:LEU:O	1:A:8:LEU:HG	2.22	0.40
1:A:585:PHE:O	1:A:585:PHE:CG	2.75	0.40
1:A:387:TYR:OH	1:A:518:VAL:HG11	2.21	0.40
1:A:66:ASN:HA	1:A:66:ASN:HD21	1.77	0.40
1:A:226:GLN:CG	1:A:255:SER:HB3	2.52	0.40
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.92	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	614/724 (85%)	567 (92%)	28 (5%)	19 (3%)	7 8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	134	ILE

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Mol	Chain	Res	Type
1	A	135	ASP
1	A	453	LEU
1	A	455	ALA
1	A	56	PRO
1	A	269	SER
1	A	424	ALA
1	A	454	GLY
1	A	649	ALA
1	A	650	SER
1	A	138	LYS
1	A	586	PRO
1	A	131	GLU
1	A	169	TYR
1	A	346	ARG
1	A	420	ARG
1	A	540	LEU
1	A	541	ILE

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	540/618 (87%)	464 (86%)	76 (14%)	5 9

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	PHE
1	A	7	GLN
1	A	18	GLU
1	A	39	ARG
1	A	52	LYS
1	A	56	PRO
1	A	63	THR
1	A	70	ARG
1	A	72	MET
1	A	73	ARG

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Mol	Chain	Res	Type
1	A	79	LEU
1	A	80	LEU
1	A	129	LEU
1	A	130	LYS
1	A	159	GLU
1	A	171	LYS
1	A	175	ASP
1	A	178	GLN
1	A	183	ARG
1	A	199	THR
1	A	206	VAL
1	A	222	ILE
1	A	226	GLN
1	A	228	THR
1	A	229	ASN
1	A	242	ARG
1	A	243	PHE
1	A	268	LEU
1	A	278	LYS
1	A	287	ARG
1	A	289	THR
1	A	293	LEU
1	A	301	GLU
1	A	339	ARG
1	A	345	GLU
1	A	349	ARG
1	A	352	ARG
1	A	365	ARG
1	A	366	VAL
1	A	388	ASP
1	A	408	ASP
1	A	416	ASN
1	A	419	LYS
1	A	450	MET
1	A	451	ILE
1	A	467	GLN
1	A	468	LEU
1	A	478	VAL
1	A	488	LEU
1	A	494	ARG
1	A	500	GLU
1	A	503	ILE

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Mol	Chain	Res	Type
1	A	506	GLN
1	A	512	LEU
1	A	525	VAL
1	A	527	ASP
1	A	531	LEU
1	A	541	ILE
1	A	563	THR
1	A	564	LEU
1	A	568	LYS
1	A	571	GLU
1	A	588	ASN
1	A	591	LEU
1	A	597	MET
1	A	601	ARG
1	A	606	VAL
1	A	610	ARG
1	A	615	LEU
1	A	616	VAL
1	A	623	ARG
1	A	626	PHE
1	A	639	ASN
1	A	646	LEU
1	A	651	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	66	ASN
1	A	214	GLN
1	A	226	GLN
1	A	229	ASN
1	A	232	GLN
1	A	244	GLN
1	A	297	ASN
1	A	315	ASN
1	A	467	GLN
1	A	511	ASN
1	A	524	ASN
1	A	630	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	726	2	33,33,33	2.21	10 (30%)	52,52,52	3.51	20 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	726	2	1/1/7/7	0/22/38/38	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	726	ATP	PB-O3A	-6.33	1.48	1.59
3	A	726	ATP	PA-O3A	-6.32	1.48	1.59
3	A	726	ATP	C6-N6	3.45	1.46	1.35
3	A	726	ATP	C5-C4	-3.33	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	726	ATP	PG-O3B	3.08	1.65	1.60
3	A	726	ATP	C8-N9	2.37	1.40	1.36
3	A	726	ATP	C8-N7	2.35	1.39	1.34
3	A	726	ATP	PG-O2G	-2.22	1.46	1.54
3	A	726	ATP	C2-N1	2.21	1.38	1.33
3	A	726	ATP	C2-N3	2.14	1.36	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	726	ATP	O4'-C1'-N9	13.94	121.41	108.44
3	A	726	ATP	C4'-O4'-C1'	-11.42	97.35	109.75
3	A	726	ATP	C6-C5-C4	7.50	131.02	117.25
3	A	726	ATP	N3-C4-N9	5.12	134.67	125.43
3	A	726	ATP	O4'-C4'-C3'	5.00	115.30	105.17
3	A	726	ATP	O3A-PB-O3B	4.87	111.56	101.66
3	A	726	ATP	C5-C4-N3	-4.12	116.74	125.70
3	A	726	ATP	C6-C5-N7	-3.72	117.12	131.34
3	A	726	ATP	C1'-N9-C4	-3.57	120.46	126.64
3	A	726	ATP	C8-N9-C1'	3.39	133.06	126.38
3	A	726	ATP	C5'-C4'-C3'	3.25	128.23	115.21
3	A	726	ATP	O4'-C1'-C2'	3.23	111.72	106.77
3	A	726	ATP	O2'-C2'-C1'	3.18	120.85	111.23
3	A	726	ATP	C2'-C1'-N9	2.95	120.83	113.27
3	A	726	ATP	C3'-C2'-C1'	-2.81	96.51	100.91
3	A	726	ATP	O3G-PG-O3B	2.75	118.21	105.14
3	A	726	ATP	C4-C5-N7	2.73	111.86	109.52
3	A	726	ATP	O5'-PA-O1A	2.68	119.86	109.37
3	A	726	ATP	O5'-C5'-C4'	2.57	118.35	108.94
3	A	726	ATP	N7-C8-N9	-2.02	108.65	114.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	726	ATP	C4'

There are no torsion outliers.

There are no ring outliers.

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	622/724 (85%)	-0.34	26 (4%) 35 36	0, 27, 70, 99	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	ILE	7.9
1	A	422	ILE	6.1
1	A	135	ASP	5.9
1	A	133	ASN	5.0
1	A	423	GLY	4.8
1	A	421	GLY	4.7
1	A	3	PHE	3.7
1	A	456	LYS	3.5
1	A	420	ARG	3.4
1	A	171	LYS	3.3
1	A	651	ARG	3.2
1	A	424	ALA	3.2
1	A	539	ALA	3.0
1	A	426	THR	2.9
1	A	449	GLU	2.9
1	A	136	PRO	2.7
1	A	138	LYS	2.6
1	A	419	LYS	2.6
1	A	623	ARG	2.6
1	A	540	LEU	2.6
1	A	137	LYS	2.5
1	A	1	MET	2.3
1	A	425	SER	2.3
1	A	592	GLU	2.2
1	A	142	ARG	2.2
1	A	650	SER	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	725	1/1	0.38	5.15	56,56,56,56	0
3	ATP	A	726	31/31	0.23	2.71	11,47,72,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.