



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 05:31 AM EDT

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 : unknown
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

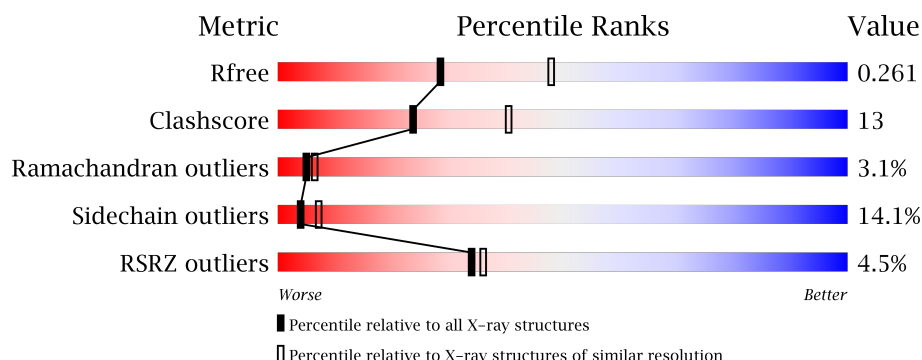
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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. 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	724	<div> <div>4%</div> <div>53%</div> <div>25%</div> <div>6%</div> <div>14%</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
3	ATP	A	726	X	-	-	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 deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- 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: $C_{10}H_{16}N_5O_{13}P_3$).



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

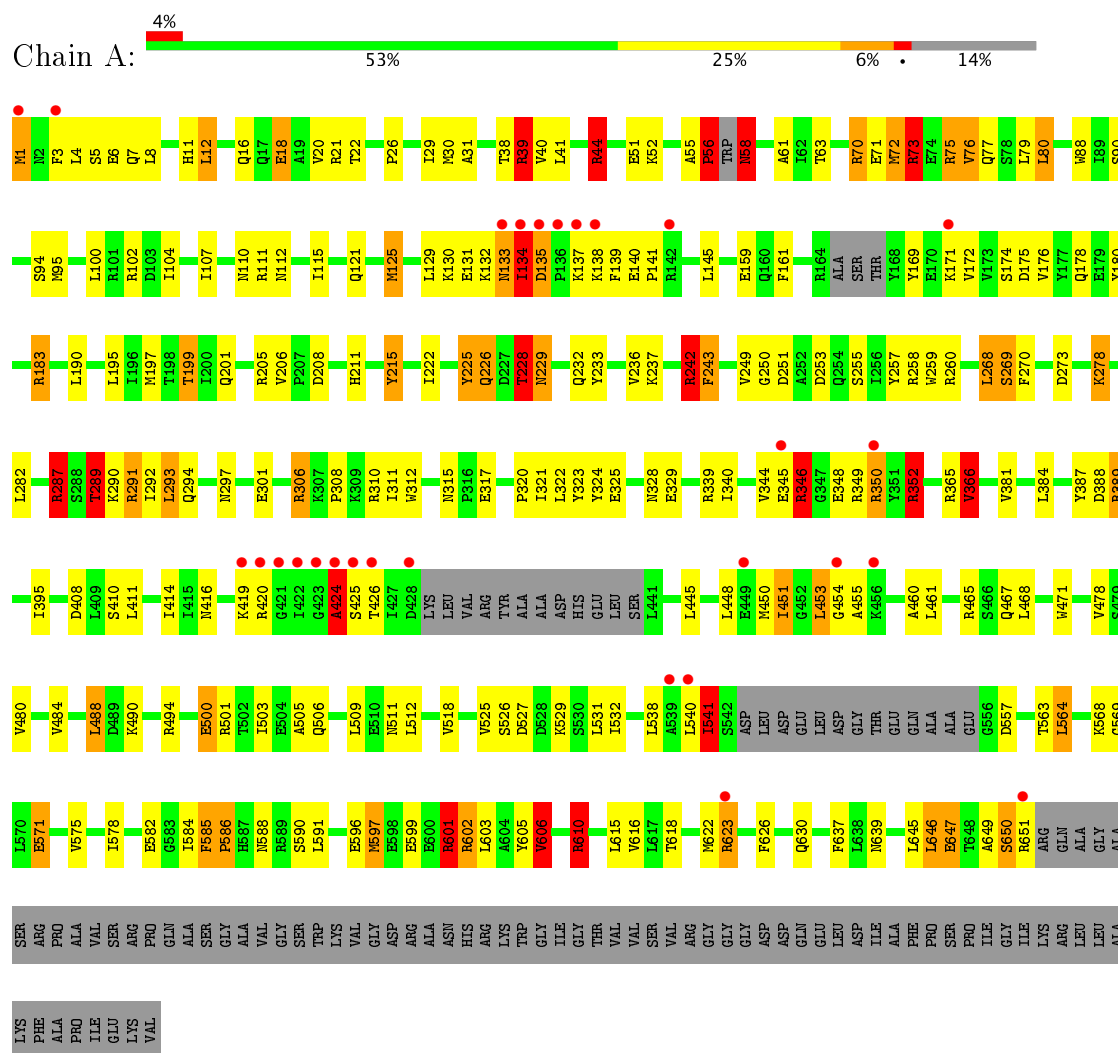
- Molecule 4 is water.

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

3 Residue-property plots

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: ATP-DEPENDENT HELICASE PCRA



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 , 0.261	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 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	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.

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, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 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	5035	114	5045	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	5056	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (128) 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: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: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
1:A:329:GLU:HB2	1:A:623:ARG:HH11	0.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:ASN:HD21	1:A:311:ILE:H	1.41	0.66
1:A:321:ILE:O	1:A:646:LEU:CD1	2.45	0.65
1:A:297:ASN:HD21	1:A:311:ILE:HG12	1.60	0.64
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:584:ILE:HD11	1:A:630:GLN:HE22	1.62	0.62
1:A:12:LEU:HA	1:A:16:GLN:OE1	2.01	0.61
1:A:161:PHE:HD2	1:A:174:SER:HB3	1.65	0.61
1:A:226:GLN:HA	4:A:752:HOH:O	1.99	0.61
1:A:381:VAL:HG12	4:A:835:HOH:O	2.00	0.61
1:A:389:ARG:HH11	1:A:511:ASN:HD21	1.49	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:229:ASN:ND2	1:A:232:GLN:H	1.99	0.59
1:A:381:VAL:CG1	4:A:835:HOH:O	2.51	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:40:VAL:HG21	1:A:282:LEU:HD21	1.85	0.58
1:A:601:ARG:HD3	1:A:637:PHE:HE1	1.67	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	1.53	0.56
1:A:229:ASN:HD21	1:A:232:GLN:HG3	1.69	0.56
1:A:340:ILE:O	1:A:344:VAL:HG23	2.06	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	1:A:532:ILE:HD12	1.75	0.51
1:A:610:ARG:CA	1:A:610:ARG:NE	2.69	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:395:ILE:HD13	1:A:488:LEU:HD13	1.94	0.50
1:A:61:ALA:HB1	1:A:72:MET:CE	2.41	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:107:ILE:HA	4:A:777:HOH:O	2.15	0.47
1:A:211:HIS:O	1:A:215:TYR:HD1	1.97	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:H	1.63	0.46
1:A:134:ILE:HG23	1:A:139:PHE:CD2	2.49	0.46
1:A:297:ASN:ND2	1:A:311:ILE:HG12	2.29	0.46
1:A:100:LEU:HD22	1:A:104:ILE:HD12	1.98	0.46
1:A:41:LEU:HD13	1:A:249:VAL:HG21	1.97	0.46
1:A:322:LEU:HA	1:A:647:GLU:O	2.14	0.46
1:A:121:GLN:HG3	1:A:180:TYR:OH	2.16	0.45
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:55:ALA:O	1:A:58:ASN:N	2.52	0.43
1:A:72:MET:O	1:A:76:VAL:HG22	2.17	0.43
1:A:500:GLU:HB3	1:A:505:ALA:HB2	2.00	0.43
1:A:140:GLU:HA	1:A:141:PRO:HD2	1.82	0.43
1:A:18:GLU:OE2	1:A:278:LYS:NZ	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:O	1:A:293:LEU:HD22	2.18	0.43
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:389:ARG:HH11	1:A:511:ASN:ND2	2.15	0.42
1:A:229:ASN:H	1:A:232:GLN:HE21	1.66	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:110:ASN:HB3	1:A:112:ASN:OD1	2.21	0.41
1:A:599:GLU:OE1	1:A:602:ARG:NH1	2.54	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:132:LYS:HB3	1:A:133:ASN:H	1.63	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: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: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 [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	614/724 (85%)	567 (92%)	28 (5%)	19 (3%)	5 6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	134	ILE
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%)	4 7

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	70	ARG
1	A	72	MET
1	A	73	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	494	ARG
1	A	500	GLU
1	A	503	ILE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	630	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	27,33,33	1.63	7 (25%)	25,52,52	3.17	10 (40%)

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	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	726	ATP	C5-C4	-3.33	1.33	1.40
3	A	726	ATP	PG-O2G	-2.00	1.46	1.54
3	A	726	ATP	C2-N1	2.32	1.38	1.33
3	A	726	ATP	C8-N7	2.44	1.39	1.34
3	A	726	ATP	C2-N3	2.53	1.36	1.32
3	A	726	ATP	C6-N6	2.95	1.46	1.34
3	A	726	ATP	PG-O3B	3.40	1.65	1.60

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	726	ATP	C4'-O4'-C1'	-11.67	97.35	109.77
3	A	726	ATP	C1'-N9-C4	-3.57	120.46	126.64
3	A	726	ATP	C5-C6-N1	-2.02	113.60	119.70
3	A	726	ATP	C5-C6-N6	2.12	124.79	120.47
3	A	726	ATP	C4-C5-N7	2.54	111.86	109.41
3	A	726	ATP	O5'-PA-O1A	2.63	119.86	109.25
3	A	726	ATP	O5'-C5'-C4'	2.64	118.35	109.00
3	A	726	ATP	O2'-C2'-C1'	2.95	120.85	111.61
3	A	726	ATP	C5'-C4'-C3'	3.40	128.23	115.29
3	A	726	ATP	O4'-C4'-C3'	5.10	115.30	105.17

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	726	ATP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	622/724 (85%)	-0.37	28 (4%) 34 36	0, 27, 70, 99	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	ILE	7.9
1	A	422	ILE	6.2
1	A	135	ASP	5.9
1	A	133	ASN	5.3
1	A	421	GLY	4.7
1	A	423	GLY	4.6
1	A	424	ALA	4.1
1	A	3	PHE	3.9
1	A	456	LYS	3.7
1	A	171	LYS	3.6
1	A	651	ARG	3.4
1	A	540	LEU	3.2
1	A	420	ARG	3.2
1	A	539	ALA	3.2
1	A	138	LYS	3.0
1	A	449	GLU	3.0
1	A	137	LYS	3.0
1	A	136	PRO	2.9
1	A	426	THR	2.9
1	A	425	SER	2.8
1	A	419	LYS	2.8
1	A	623	ARG	2.5
1	A	454	GLY	2.4
1	A	142	ARG	2.3
1	A	1	MET	2.3
1	A	350	ARG	2.2
1	A	345	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	428	ASP	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ATP	A	726	31/31	0.87	0.23	2.56	11,47,72,75	0
2	MG	A	725	1/1	0.67	0.39	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.