Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:45 PM GMT

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

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

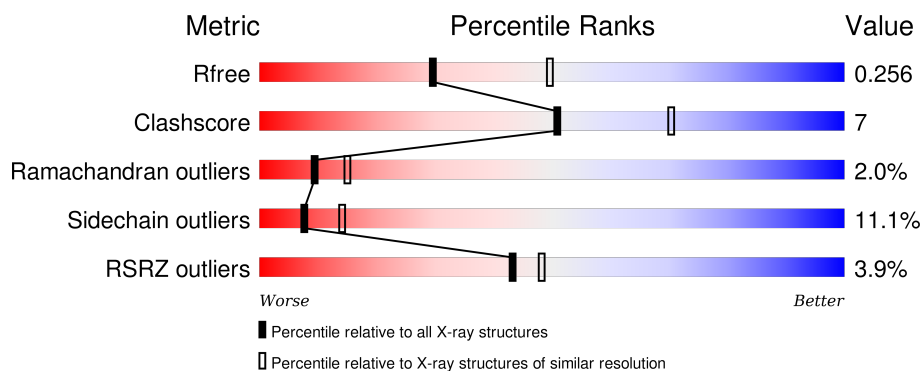|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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   Percentile Ranks   Value

Rfree — 0.256
Clashscore — 7
Ramachandran outliers — 2.0%
Sidechain outliers — 11.1%
RSRZ outliers — 3.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 <=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	167	3% — 68% — 28% — ...
2	B	273	3% — 65% — 24% — ...
3	C	115	7% — 62% — 24% — · — 11%
4	D	169	2% — 42% — 11% — ·· — 43%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ATP	A	700	X	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5291 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 PROTEIN (PCRA (SUBUNIT)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total	C	H	N	O	S	0	0	0
			1330	823	28	238	234	7			

- Molecule 2 is a protein called PROTEIN (PCRA (SUBUNIT)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	261	Total	C	H	N	O	S	0	0	0
			2250	1390	62	388	405	5			

- Molecule 3 is a protein called PROTEIN (PCRA (SUBUNIT)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	102	Total	C	H	N	O	S	0	0	0
			817	510	14	129	162	2			

- Molecule 4 is a protein called PROTEIN (PCRA (SUBUNIT)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	96	Total	C	H	N	O	S	0	0	0
			769	477	10	129	147	6			

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	46	Total 46	O 46	0	0
6	C	3	Total 3	O 3	0	0
6	D	13	Total 13	O 13	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 errors 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.
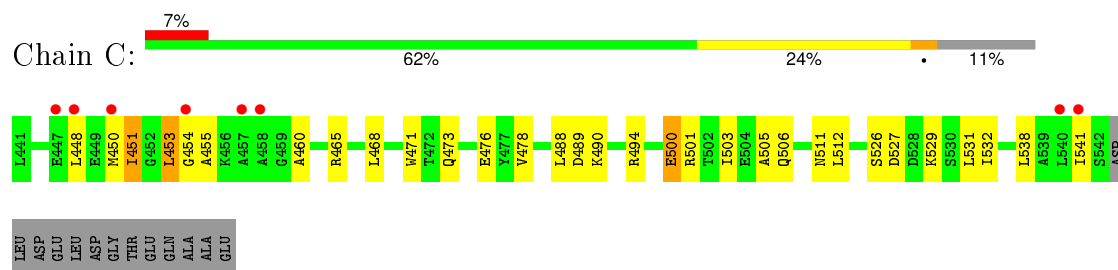
- Molecule 1: PROTEIN (PCRA (SUBUNIT))
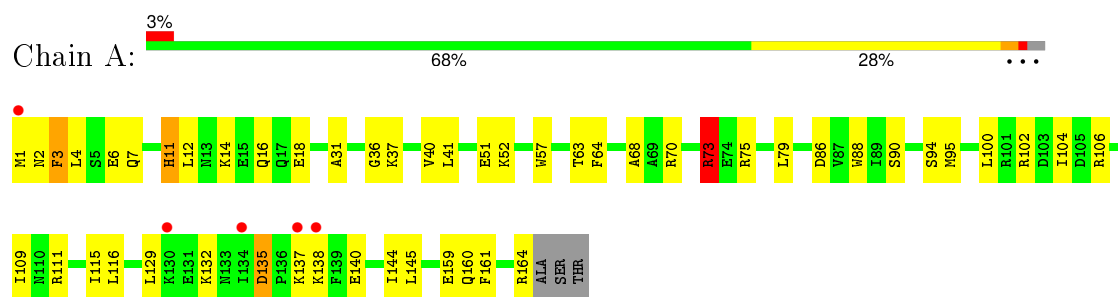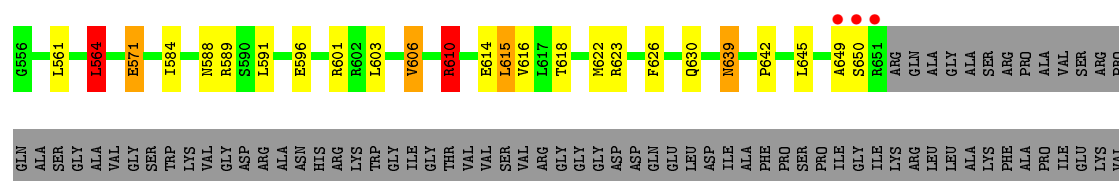

- Molecule 2: PROTEIN (PCRA (SUBUNIT))
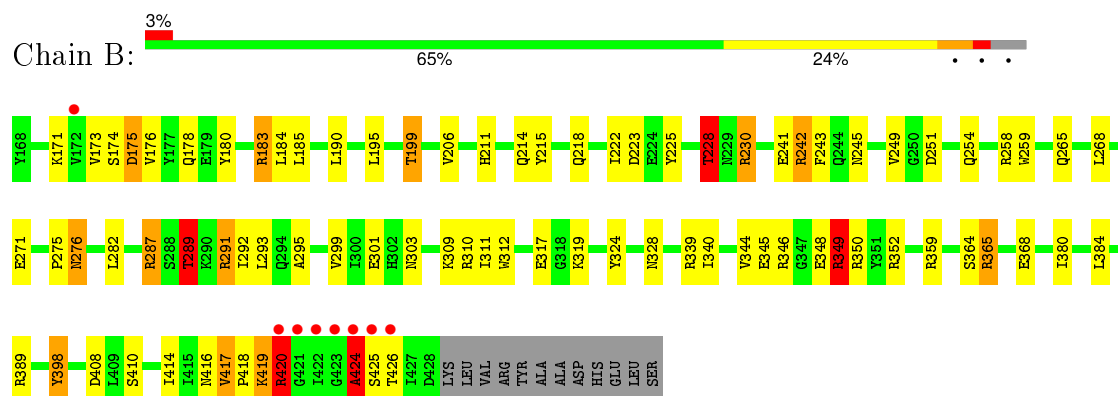
- Molecule 3: PROTEIN (PCRA (SUBUNIT))

- Molecule 4: PROTEIN (PCRA (SUBUNIT))

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	138.94Å 138.94Å 111.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 19.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (10.00-2.50) 92.1 (19.78-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.00 (at 2.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.228 , 0.285 0.209 , 0.256	Depositor DCC
R_{free} test set	1845 reflections (4.88%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 80.0	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.51$, $<L^2> = 0.34$	Xtriage
Outliers	0 of 42105 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5291	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.80	0/1323	1.49	17/1783 (1.0%)
2	B	0.81	0/2231	1.51	30/3016 (1.0%)
3	C	0.72	0/812	1.34	5/1094 (0.5%)
4	D	0.85	0/772	1.50	7/1042 (0.7%)
All	All	0.80	0/5138	1.48	59/6935 (0.9%)

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	2

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	610	ARG	NE-CZ-NH1	11.28	125.94	120.30
4	D	610	ARG	NE-CZ-NH2	-10.16	115.22	120.30
4	D	589	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	88	TRP	CD1-CG-CD2	9.34	113.77	106.30
2	B	310	ARG	NE-CZ-NH2	-9.17	115.71	120.30
2	B	312	TRP	CD1-CG-CD2	8.12	112.80	106.30
4	D	591	LEU	O-C-N	8.07	135.62	122.70
2	B	258	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	88	TRP	CE2-CD2-CG	-7.72	101.13	107.30
2	B	425	SER	N-CA-C	7.59	131.49	111.00
2	B	359	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	57	TRP	CD1-CG-CD2	7.32	112.16	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	471	TRP	CD1-CG-CD2	7.27	112.12	106.30
2	B	230	ARG	NE-CZ-NH1	7.23	123.92	120.30
2	B	312	TRP	CE2-CD2-CG	-7.12	101.60	107.30
2	B	259	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	A	57	TRP	CE2-CD2-CG	-7.06	101.65	107.30
2	B	258	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	137	LYS	CA-C-N	-7.00	101.80	117.20
3	C	471	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	A	3	PHE	CB-CG-CD2	-6.85	116.00	120.80
2	B	287	ARG	NE-CZ-NH2	-6.85	116.88	120.30
2	B	183	ARG	NE-CZ-NH2	-6.78	116.91	120.30
3	C	465	ARG	NE-CZ-NH2	-6.74	116.93	120.30
3	C	501	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	B	259	TRP	CE2-CD2-CG	-6.69	101.95	107.30
2	B	310	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	B	289	THR	N-CA-CB	-6.66	97.64	110.30
2	B	349	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	B	426	THR	N-CA-C	-6.46	93.55	111.00
2	B	310	ARG	CD-NE-CZ	6.14	132.20	123.60
2	B	291	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	B	359	ARG	NE-CZ-NH1	6.06	123.33	120.30
3	C	448	LEU	CA-CB-CG	6.02	129.14	115.30
4	D	623	ARG	CA-CB-CG	6.00	126.61	113.40
1	A	111	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	88	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	3	PHE	CB-CG-CD1	5.88	124.92	120.80
1	A	106	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	75	ARG	CG-CD-NE	-5.76	99.71	111.80
2	B	398	TYR	CB-CG-CD1	-5.75	117.55	121.00
2	B	312	TRP	CG-CD1-NE1	-5.56	104.54	110.10
2	B	228	THR	N-CA-CB	-5.46	99.93	110.30
4	D	564	LEU	CA-CB-CG	5.33	127.56	115.30
2	B	365	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	145	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	95	MET	CA-CB-CG	5.26	122.25	113.30
1	A	6	GLU	CA-CB-CG	-5.21	101.93	113.40
2	B	424	ALA	CB-CA-C	-5.17	102.34	110.10
1	A	73	ARG	CB-CG-CD	5.17	125.03	111.60
2	B	310	ARG	CG-CD-NE	-5.16	100.97	111.80
2	B	301	GLU	CA-CB-CG	-5.15	102.06	113.40
4	D	615	LEU	CA-CB-CG	5.14	127.12	115.30
2	B	419	LYS	N-CA-C	-5.14	97.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ARG	CD-NE-CZ	5.12	130.77	123.60
1	A	86	ASP	CB-CG-OD1	5.08	122.87	118.30
2	B	384	LEU	CA-CB-CG	5.08	126.99	115.30
2	B	417	VAL	CA-CB-CG2	-5.01	103.38	110.90
2	B	312	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ASP	Peptide
1	A	73	ARG	Sidechain

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	1302	28	1356	20	0
2	B	2188	62	2168	44	0
3	C	803	14	800	9	0
4	D	759	10	744	16	0
5	A	31	0	11	2	0
6	A	32	0	0	1	0
6	B	46	0	0	1	0
6	C	3	0	0	0	0
6	D	13	0	0	1	0
All	All	5177	114	5079	70	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 7.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:THR:HG21	6:B:731:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:VAL:HA	2:B:176:VAL:HG12	1.69	0.73
4:D:639:ASN:HB3	6:D:779:HOH:O	1.96	0.66
2:B:328:ASN:HA	4:D:622:MET:O	1.96	0.65
2:B:291:ARG:HG3	4:D:645:LEU:HD22	1.80	0.63
3:C:451:ILE:HB	3:C:453:LEU:HD23	1.80	0.62
1:A:41:LEU:HD13	2:B:249:VAL:HG21	1.81	0.61
2:B:389:ARG:HH11	3:C:511:ASN:HD21	1.49	0.61
1:A:63:THR:HG22	1:A:64:PHE:H	1.67	0.60
2:B:410:SER:O	2:B:414:ILE:HG12	2.03	0.57
3:C:526:SER:O	3:C:529:LYS:HE2	2.04	0.57
4:D:564:LEU:HB3	4:D:603:LEU:HD22	1.85	0.57
2:B:350:ARG:HD2	2:B:352:ARG:HH11	1.69	0.57
2:B:424:ALA:HB1	3:C:460:ALA:HA	1.88	0.56
2:B:289:THR:HG22	2:B:292:ILE:H	1.70	0.55
2:B:340:ILE:O	2:B:344:VAL:HG23	2.07	0.55
2:B:319:LYS:HD2	4:D:614:GLU:HG2	1.90	0.54
1:A:1:MET:H1	1:A:51:GLU:CD	2.10	0.53
2:B:414:ILE:HA	2:B:417:VAL:HG12	1.91	0.53
2:B:214:GLN:HB3	2:B:242:ARG:HG2	1.90	0.53
1:A:36:GLY:HA3	5:A:700:ATP:H8	1.74	0.52
2:B:271:GLU:O	2:B:275:PRO:HA	2.09	0.52
2:B:389:ARG:HH11	3:C:511:ASN:ND2	2.08	0.52
2:B:348:GLU:O	2:B:349:ARG:HD3	2.10	0.51
1:A:115:ILE:HA	2:B:190:LEU:O	2.10	0.50
1:A:161:PHE:HD2	2:B:174:SER:HB3	1.77	0.49
2:B:251:ASP:OD1	2:B:309:LYS:NZ	2.46	0.49
2:B:418:PRO:HG2	2:B:420:ARG:HG3	1.95	0.49
1:A:37:LYS:HE2	2:B:223:ASP:OD1	2.13	0.49
2:B:276:ASN:ND2	2:B:276:ASN:H	2.10	0.48
4:D:606:VAL:O	4:D:610:ARG:HD2	2.13	0.47
2:B:287:ARG:HD2	4:D:571:GLU:HG2	1.97	0.47
1:A:2:ASN:HD22	1:A:4:LEU:H	1.64	0.46
5:A:700:ATP:O1G	4:D:610:ARG:NH2	2.48	0.46
1:A:63:THR:HG21	1:A:68:ALA:HB1	1.98	0.46
3:C:538:LEU:HA	3:C:541:ILE:HG22	1.98	0.46
2:B:195:LEU:O	2:B:199:THR:HG23	2.16	0.46
2:B:303:ASN:ND2	4:D:601:ARG:HE	2.13	0.46
4:D:642:PRO:HG2	4:D:645:LEU:CD1	2.46	0.45
1:A:102:ARG:NH1	6:A:758:HOH:O	2.48	0.45
2:B:242:ARG:NH1	2:B:243:PHE:CE2	2.85	0.45
1:A:31:ALA:O	2:B:251:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLN:O	2:B:245:ASN:HB2	2.17	0.44
2:B:287:ARG:HD2	4:D:571:GLU:CG	2.48	0.44
1:A:104:ILE:HG12	1:A:109:ILE:HB	1.99	0.44
2:B:398:TYR:HA	2:B:414:ILE:HD13	1.99	0.44
2:B:225:TYR:O	2:B:228:THR:HB	2.18	0.44
1:A:90:SER:HB2	1:A:94:SER:HB2	2.00	0.43
3:C:532:ILE:H	3:C:532:ILE:HD12	1.84	0.43
3:C:489:ASP:OD1	3:C:490:LYS:NZ	2.51	0.43
2:B:324:TYR:HB3	4:D:618:THR:HG22	2.01	0.43
2:B:289:THR:HG23	2:B:317:GLU:O	2.18	0.42
2:B:380:ILE:HD13	4:D:561:LEU:HB2	2.01	0.42
2:B:242:ARG:HG3	2:B:243:PHE:N	2.35	0.41
1:A:132:LYS:NZ	2:B:175:ASP:OD2	2.53	0.41
4:D:584:ILE:HD11	4:D:630:GLN:HE22	1.85	0.41
2:B:254:GLN:HG2	4:D:606:VAL:HG12	2.03	0.41
1:A:140:GLU:O	1:A:144:ILE:HG13	2.20	0.41
4:D:584:ILE:HD11	4:D:630:GLN:NE2	2.35	0.41
2:B:211:HIS:O	2:B:215:TYR:HD1	2.03	0.41
3:C:500:GLU:HB3	3:C:505:ALA:HB2	2.03	0.41
2:B:364:SER:O	2:B:368:GLU:HG3	2.20	0.41
1:A:12:LEU:HB3	1:A:16:GLN:HB2	2.03	0.41
1:A:63:THR:HG22	1:A:64:PHE:N	2.34	0.41
2:B:180:TYR:O	2:B:184:LEU:HD13	2.21	0.41
2:B:291:ARG:HB2	2:B:317:GLU:O	2.21	0.40
1:A:160:GLN:O	1:A:164:ARG:NH1	2.55	0.40
2:B:295:ALA:O	2:B:299:VAL:HG23	2.20	0.40
1:A:100:LEU:HD22	1:A:104:ILE:HD12	2.04	0.40
1:A:40:VAL:HG21	2:B:282:LEU:HD21	2.02	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	162/167 (97%)	149 (92%)	10 (6%)	3 (2%)	10	16
2	B	259/273 (95%)	248 (96%)	7 (3%)	4 (2%)	13	22
3	C	100/115 (87%)	89 (89%)	8 (8%)	3 (3%)	5	7
4	D	94/169 (56%)	86 (92%)	6 (6%)	2 (2%)	9	14
All	All	615/724 (85%)	572 (93%)	31 (5%)	12 (2%)	9	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
2	B	424	ALA
3	C	453	LEU
3	C	455	ALA
1	A	138	LYS
2	B	346	ARG
3	C	454	GLY
4	D	649	ALA
4	D	650	SER
1	A	11	HIS
2	B	241	GLU
2	B	420	ARG

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	141/143 (99%)	130 (92%)	11 (8%)	16	29
2	B	233/243 (96%)	208 (89%)	25 (11%)	8	15
3	C	86/96 (90%)	72 (84%)	14 (16%)	3	5
4	D	82/136 (60%)	72 (88%)	10 (12%)	6	11
All	All	542/618 (88%)	482 (89%)	60 (11%)	8	14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	7	GLN
1	A	11	HIS
1	A	14	LYS
1	A	18	GLU
1	A	52	LYS
1	A	73	ARG
1	A	79	LEU
1	A	116	LEU
1	A	129	LEU
1	A	159	GLU
2	B	171	LYS
2	B	175	ASP
2	B	178	GLN
2	B	183	ARG
2	B	185	LEU
2	B	199	THR
2	B	206	VAL
2	B	222	ILE
2	B	228	THR
2	B	230	ARG
2	B	242	ARG
2	B	265	GLN
2	B	268	LEU
2	B	276	ASN
2	B	289	THR
2	B	293	LEU
2	B	311	ILE
2	B	339	ARG
2	B	345	GLU
2	B	349	ARG
2	B	365	ARG
2	B	408	ASP
2	B	416	ASN
2	B	419	LYS
2	B	420	ARG
3	C	450	MET
3	C	451	ILE
3	C	468	LEU
3	C	473	GLN
3	C	476	GLU
3	C	478	VAL
3	C	488	LEU

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Mol	Chain	Res	Type
3	C	494	ARG
3	C	500	GLU
3	C	503	ILE
3	C	506	GLN
3	C	512	LEU
3	C	527	ASP
3	C	531	LEU
4	D	564	LEU
4	D	571	GLU
4	D	588	ASN
4	D	596	GLU
4	D	606	VAL
4	D	610	ARG
4	D	615	LEU
4	D	616	VAL
4	D	626	PHE
4	D	639	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	112	ASN
2	B	232	GLN
2	B	276	ASN
2	B	303	ASN
2	B	315	ASN
2	B	416	ASN
3	C	511	ASN
4	D	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	#$|Z| > 2$
5	ATP	A	700	-	24,33,33	1.91	7 (29%)	31,52,52	2.53	13 (41%)

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
5	ATP	A	700	-	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)
5	A	700	ATP	C5-C4	-3.34	1.33	1.40
5	A	700	ATP	PG-O2G	-2.27	1.46	1.54
5	A	700	ATP	C2-N1	2.37	1.38	1.33
5	A	700	ATP	C8-N7	2.39	1.39	1.34
5	A	700	ATP	C2-N3	3.05	1.37	1.32
5	A	700	ATP	C6-N6	3.81	1.46	1.34
5	A	700	ATP	O4'-C1'	4.66	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	ATP	PB-O3B-PG	-4.20	118.59	132.67
5	A	700	ATP	O4'-C4'-C3'	-2.81	99.48	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	700	ATP	C1'-N9-C4	-2.32	123.45	126.94
5	A	700	ATP	N3-C2-N1	-2.26	127.16	128.89
5	A	700	ATP	O2B-PB-O3B	2.14	114.80	105.09
5	A	700	ATP	O4'-C4'-C5'	2.18	117.13	109.32
5	A	700	ATP	C2'-C3'-C4'	3.06	108.90	102.61
5	A	700	ATP	O5'-C5'-C4'	3.45	121.83	109.12
5	A	700	ATP	O3A-PA-O5'	3.77	112.94	102.94
5	A	700	ATP	O3'-C3'-C2'	3.87	124.41	111.83
5	A	700	ATP	O3G-PG-O3B	4.00	123.23	105.09
5	A	700	ATP	O3'-C3'-C4'	5.14	126.48	111.05
5	A	700	ATP	O4'-C1'-N9	5.46	119.53	108.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	700	ATP	C3'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	ATP	2	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 (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	164/167 (98%)	-0.34	5 (3%)	54	59	14, 34, 80, 91	0
2	B	261/273 (95%)	-0.34	8 (3%)	52	57	14, 32, 72, 100	0
3	C	102/115 (88%)	-0.04	8 (7%)	16	17	20, 51, 81, 90	0
4	D	96/169 (56%)	-0.49	3 (3%)	52	57	15, 27, 64, 85	0
All	All	623/724 (86%)	-0.32	24 (3%)	43	48	14, 34, 79, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	ILE	10.2
2	B	421	GLY	9.0
4	D	650	SER	8.6
2	B	424	ALA	6.3
2	B	423	GLY	5.6
1	A	134	ILE	3.7
2	B	420	ARG	3.7
1	A	1	MET	3.4
2	B	426	THR	3.3
3	C	450	MET	3.2
3	C	540	LEU	3.2
1	A	130	LYS	3.2
3	C	454	GLY	3.1
4	D	651	ARG	3.1
4	D	649	ALA	2.9
3	C	457	ALA	2.9
1	A	137	LYS	2.9
2	B	425	SER	2.8
3	C	541	ILE	2.6
3	C	447	GLU	2.3
3	C	448	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	138	LYS	2.2
2	B	172	VAL	2.2
3	C	458	ALA	2.1

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
5	ATP	A	700	31/31	0.90	0.22	<mark>2.89</mark>	2,11,40,48	0

6.5 Other polymers (i)

There are no such residues in this entry.