



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:26 PM UTC

PDB ID : 1QHH / pdb_00001qhh
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)

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

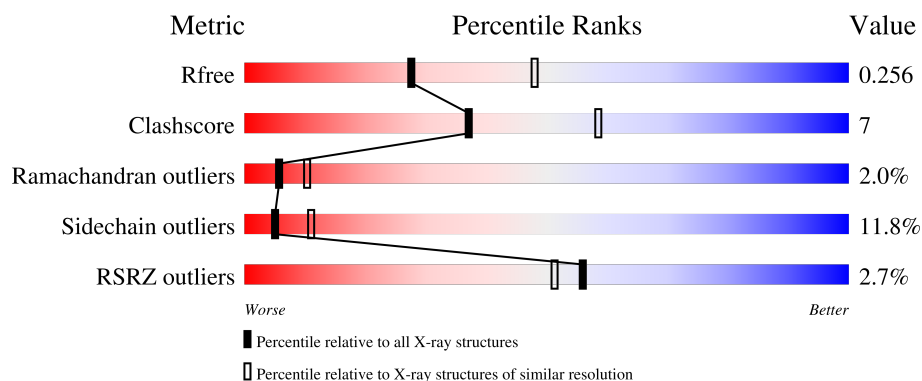
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	167	2% 62% 32% ...
2	B	273	3% 58% 29% 7% ..
3	C	115	2% 63% 20% 5% • 11%
4	D	169	2% 38% 15% •• 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 criteria:

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

2 Entry composition

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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

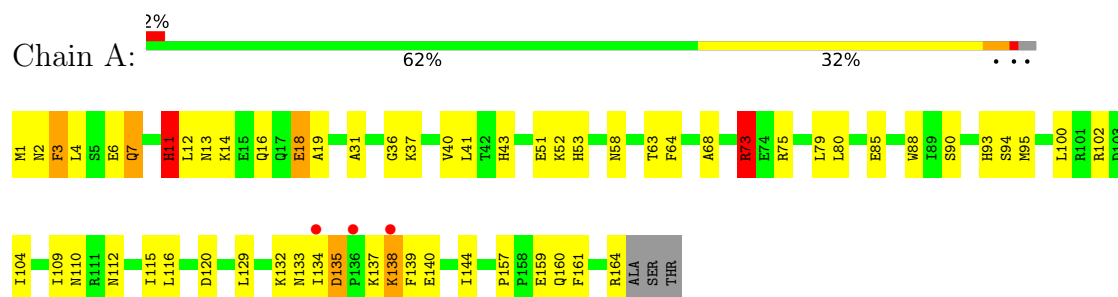
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	46	Total	O	0	0
			46	46		
6	C	3	Total	O	0	0
			3	3		
6	D	13	Total	O	0	0
			13	13		

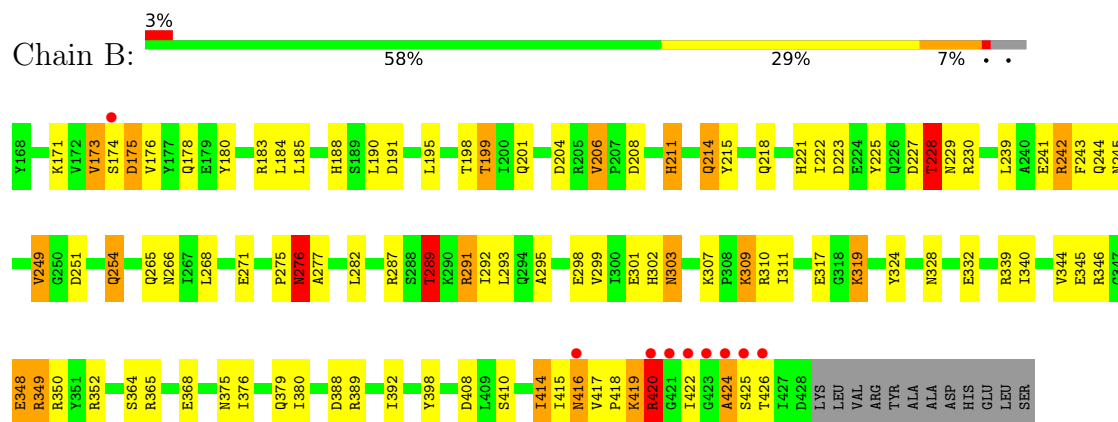
3 Residue-property plots [i](#)

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

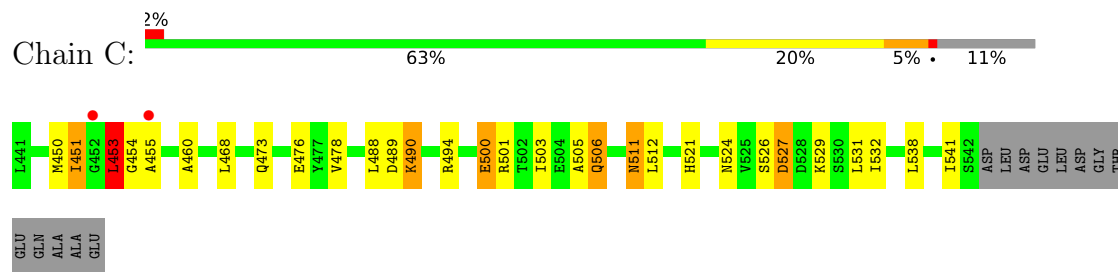
- Molecule 1: PROTEIN (PCRA (SUBUNIT))



- Molecule 2: PROTEIN (PCRA (SUBUNIT))

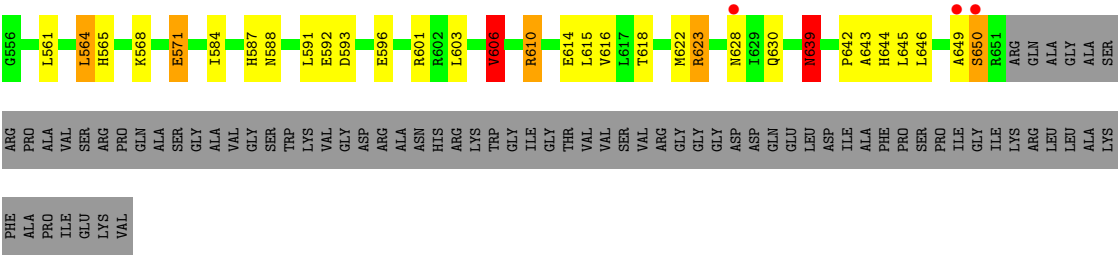


- Molecule 3: PROTEIN (PCRA (SUBUNIT))



- Molecule 4: PROTEIN (PCRA (SUBUNIT))





4 Data and refinement statistics

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 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (10.00-2.50) 89.2 (10.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	1862 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	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 3.68% 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 [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	1.00	5/1323 (0.4%)	1.81	26/1783 (1.5%)
2	B	0.97	6/2231 (0.3%)	1.78	51/3016 (1.7%)
3	C	0.80	1/812 (0.1%)	1.65	7/1094 (0.6%)
4	D	1.03	4/772 (0.5%)	1.77	15/1042 (1.4%)
All	All	0.96	16/5138 (0.3%)	1.77	99/6935 (1.4%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	134	ILE	CA-CB	6.73	1.63	1.54
3	C	521	HIS	CD2-NE2	-6.62	1.30	1.37
4	D	644	HIS	CD2-NE2	-6.52	1.30	1.37
2	B	211	HIS	CD2-NE2	-6.05	1.31	1.37
2	B	221	HIS	CD2-NE2	-5.92	1.31	1.37
4	D	565	HIS	CD2-NE2	-5.81	1.31	1.37
2	B	188	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	53	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	43	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	11	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	93	HIS	CD2-NE2	-5.68	1.31	1.37
2	B	211	HIS	CG-ND1	-5.66	1.32	1.38
2	B	302	HIS	CG-ND1	-5.61	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	606	VAL	CA-CB	5.58	1.62	1.54
4	D	587	HIS	CD2-NE2	-5.52	1.31	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	425	SER	N-CA-C	15.52	131.49	109.15
4	D	639	ASN	CA-CB-CG	11.61	124.21	112.60
4	D	591	LEU	O-C-N	11.09	135.62	122.20
1	A	3	PHE	CA-CB-CG	9.83	123.63	113.80
2	B	388	ASP	CA-CB-CG	9.38	121.98	112.60
2	B	254	GLN	OE1-CD-NE2	-9.28	113.32	122.60
2	B	426	THR	N-CA-C	-9.12	93.55	108.41
2	B	289	THR	N-CA-CB	-8.90	97.64	110.36
2	B	276	ASN	OD1-CG-ND2	-8.82	113.78	122.60
1	A	133	ASN	N-CA-C	8.53	121.98	109.69
2	B	191	ASP	CA-CB-CG	8.40	121.00	112.60
2	B	208	ASP	CA-CB-CG	8.01	120.61	112.60
3	C	527	ASP	N-CA-C	-7.78	102.40	111.03
3	C	511	ASN	OD1-CG-ND2	-7.74	114.86	122.60
2	B	416	ASN	OD1-CG-ND2	-7.64	114.96	122.60
2	B	214	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	A	139	PHE	CA-CB-CG	-7.34	106.45	113.80
3	C	506	GLN	OE1-CD-NE2	-6.98	115.62	122.60
2	B	303	ASN	OD1-CG-ND2	-6.94	115.66	122.60
2	B	414	ILE	N-CA-C	6.83	119.46	112.90
2	B	228	THR	N-CA-CB	-6.83	99.93	109.97
1	A	93	HIS	CB-CG-CD2	-6.81	122.35	131.20
2	B	416	ASN	N-CA-C	6.72	120.83	111.56
1	A	110	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	112	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	A	110	ASN	CB-CG-ND2	6.61	126.31	116.40
2	B	244	GLN	OE1-CD-NE2	-6.54	116.06	122.60
4	D	644	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	137	LYS	CA-C-O	6.31	127.48	120.92
1	A	137	LYS	O-C-N	6.26	130.63	122.68
4	D	623	ARG	CA-CB-CG	6.25	126.61	114.10
4	D	646	LEU	N-CA-C	6.24	118.89	108.96
3	C	501	ARG	N-CA-C	6.18	119.95	111.54
1	A	6	GLU	CA-CB-CG	-6.09	101.93	114.10
2	B	301	GLU	CA-CB-CG	-6.02	102.06	114.10
1	A	13	ASN	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ARG	CB-CG-CD	5.97	125.03	111.30
2	B	419	LYS	N-CA-C	-5.97	97.13	108.17
3	C	524	ASN	OD1-CG-ND2	-5.91	116.69	122.60
2	B	319	LYS	O-C-N	-5.89	114.55	121.32
2	B	206	VAL	CA-C-N	5.89	126.30	119.47
2	B	206	VAL	C-N-CA	5.89	126.30	119.47
1	A	85	GLU	CB-CG-CD	5.87	122.57	112.60
4	D	593	ASP	N-CA-C	5.84	119.05	109.76
2	B	307	LYS	CA-C-N	5.83	126.17	119.93
2	B	307	LYS	C-N-CA	5.83	126.17	119.93
2	B	348	GLU	CB-CG-CD	5.82	122.49	112.60
2	B	198	THR	CA-C-O	-5.80	114.28	120.42
2	B	204	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	120	ASP	CA-CB-CG	5.77	118.37	112.60
4	D	565	HIS	CB-CG-CD2	-5.76	123.71	131.20
4	D	606	VAL	CA-C-O	-5.75	114.26	120.47
2	B	379	GLN	OE1-CD-NE2	-5.65	116.95	122.60
2	B	422	ILE	N-CA-C	-5.59	100.43	108.48
1	A	75	ARG	CG-CD-NE	-5.59	99.71	112.00
2	B	310	ARG	CD-NE-CZ	5.57	132.20	124.40
2	B	307	LYS	N-CA-C	-5.53	100.56	109.40
2	B	415	ILE	CB-CA-C	-5.48	103.66	112.16
3	C	506	GLN	CG-CD-NE2	5.48	124.62	116.40
2	B	277	ALA	N-CA-C	5.47	117.79	110.35
2	B	298	GLU	CB-CG-CD	5.46	121.89	112.60
2	B	420	ARG	CA-C-N	5.43	126.01	119.98
2	B	420	ARG	C-N-CA	5.43	126.01	119.98
2	B	254	GLN	CG-CD-NE2	5.39	124.49	116.40
2	B	266	ASN	OD1-CG-ND2	-5.38	117.22	122.60
4	D	643	ALA	N-CA-C	5.37	118.62	111.75
2	B	276	ASN	CB-CG-ND2	5.36	124.45	116.40
2	B	229	ASN	CA-CB-CG	5.35	117.95	112.60
4	D	568	LYS	CB-CG-CD	5.34	123.58	111.30
1	A	19	ALA	N-CA-C	-5.34	104.89	111.40
1	A	75	ARG	CA-CB-CG	-5.30	103.50	114.10
2	B	201	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	157	PRO	CA-C-N	5.27	125.33	119.32
1	A	157	PRO	C-N-CA	5.27	125.33	119.32
1	A	7	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	53	HIS	CB-CG-CD2	-5.25	124.38	131.20
4	D	592	GLU	N-CA-C	5.23	121.95	110.80
2	B	375	ASN	OD1-CG-ND2	-5.22	117.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ARG	CB-CA-C	-5.22	102.66	110.90
2	B	301	GLU	CA-C-O	5.20	125.81	119.05
2	B	173	VAL	CA-C-O	-5.20	115.34	120.85
2	B	376	ILE	N-CA-C	-5.19	102.52	107.76
2	B	392	ILE	N-CA-C	-5.18	105.48	110.72
1	A	18	GLU	CB-CG-CD	5.16	121.37	112.60
4	D	565	HIS	CA-CB-CG	5.13	118.93	113.80
4	D	592	GLU	CA-C-O	-5.12	113.18	120.51
3	C	524	ASN	CB-CG-ND2	5.12	124.08	116.40
2	B	188	HIS	CB-CG-CD2	-5.10	124.57	131.20
2	B	173	VAL	O-C-N	-5.10	116.58	121.83
2	B	266	ASN	CB-CG-ND2	5.07	124.01	116.40
4	D	650	SER	N-CA-C	-5.07	100.00	110.80
1	A	88	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	58	ASN	OD1-CG-ND2	-5.05	117.55	122.60
2	B	309	LYS	CA-CB-CG	5.05	124.19	114.10
1	A	43	HIS	CB-CG-CD2	-5.04	124.64	131.20
4	D	628	ASN	CA-CB-CG	5.02	117.62	112.60
2	B	227	ASP	CA-CB-CG	5.02	117.62	112.60
2	B	310	ARG	CG-CD-NE	-5.01	100.97	112.00
2	B	249	VAL	O-C-N	-5.01	118.03	123.14

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 ⓘ

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	21	0
2	B	2188	62	2168	46	0
3	C	803	14	800	9	0
4	D	759	10	744	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	72	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 (72) 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
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:95:MET:HE1	2:B:239:LEU:HD11	1.83	0.60
1:A:63:THR:HG22	1:A:64:PHE:H	1.67	0.60
1:A:1:MET:H1	1:A:51:GLU:CD	2.10	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:332:GLU:CD	4:D:623:ARG:HH22	2.25	0.44
1:A:31:ALA:O	2:B:251:ASP:HB2	2.18	0.44
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:225:TYR:O	2:B:228:THR:HB	2.18	0.44
2:B:398:TYR:HA	2:B:414:ILE:HD13	1.99	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
2:B:324:TYR:HB3	4:D:618:THR:HG22	2.01	0.43
3:C:489:ASP:OD1	3:C:490:LYS:NZ	2.51	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
1:A:132:LYS:NZ	2:B:175:ASP:OD2	2.53	0.41
2:B:242:ARG:HG3	2:B:243:PHE:N	2.35	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
2:B:211:HIS:O	2:B:215:TYR:HD1	2.03	0.41
4:D:584:ILE:HD11	4:D:630:GLN:NE2	2.35	0.41
2:B:364:SER:O	2:B:368:GLU:HG3	2.20	0.41
3:C:500:GLU:HB3	3:C:505:ALA:HB2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:ALA:O	2:B:299:VAL:HG23	2.20	0.40
1:A:40:VAL:HG21	2:B:282:LEU:HD21	2.02	0.40
1:A:100:LEU:HD22	1:A:104:ILE:HD12	2.04	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%)	6	11
2	B	259/273 (95%)	248 (96%)	7 (3%)	4 (2%)	8	16
3	C	100/115 (87%)	89 (89%)	8 (8%)	3 (3%)	3	5
4	D	94/169 (56%)	86 (92%)	6 (6%)	2 (2%)	5	9
All	All	615/724 (85%)	572 (93%)	31 (5%)	12 (2%)	6	10

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 ⓘ

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%)	128 (91%)	13 (9%)	8	19
2	B	233/243 (96%)	207 (89%)	26 (11%)	6	12
3	C	86/96 (90%)	70 (81%)	16 (19%)	1	3
4	D	82/136 (60%)	73 (89%)	9 (11%)	6	13
All	All	542/618 (88%)	478 (88%)	64 (12%)	5	11

All (64) 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	80	LEU
1	A	116	LEU
1	A	129	LEU
1	A	138	LYS
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

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Mol	Chain	Res	Type
2	B	265	GLN
2	B	268	LEU
2	B	276	ASN
2	B	289	THR
2	B	291	ARG
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	453	LEU
3	C	468	LEU
3	C	473	GLN
3	C	476	GLU
3	C	478	VAL
3	C	488	LEU
3	C	490	LYS
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	639	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	112	ASN
2	B	181	GLN
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	587	HIS
4	D	630	GLN
4	D	644	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 oligosaccharides 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	-	32,33,33	2.70	11 (34%)	48,52,52	3.17	17 (35%)

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	6/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	ATP	PA-O3A	-8.17	1.50	1.59
5	A	700	ATP	PB-O3A	-8.17	1.50	1.59
5	A	700	ATP	C6-N6	4.90	1.46	1.34
5	A	700	ATP	C8-N7	3.91	1.39	1.31
5	A	700	ATP	C5-C4	-3.43	1.33	1.39
5	A	700	ATP	C2-N1	2.51	1.38	1.33
5	A	700	ATP	PG-O2G	-2.22	1.46	1.54
5	A	700	ATP	O4'-C1'	2.21	1.47	1.42
5	A	700	ATP	C5-C6	-2.15	1.35	1.41
5	A	700	ATP	C2-N3	2.05	1.37	1.33
5	A	700	ATP	C5-N7	-2.02	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	ATP	C6-C5-C4	10.52	131.55	117.18
5	A	700	ATP	C5-C4-N3	-7.72	116.09	126.72
5	A	700	ATP	C6-C5-N7	-7.71	117.22	132.09
5	A	700	ATP	O4'-C1'-N9	5.96	119.53	108.09
5	A	700	ATP	O3G-PG-O3B	5.54	123.23	104.64
5	A	700	ATP	O3'-C3'-C4'	5.36	126.48	111.08
5	A	700	ATP	N3-C4-N9	4.55	134.91	127.17
5	A	700	ATP	O3'-C3'-C2'	3.93	124.41	111.82
5	A	700	ATP	O5'-C5'-C4'	3.77	121.83	108.99
5	A	700	ATP	N9-C8-N7	-3.46	109.03	113.94
5	A	700	ATP	C2'-C3'-C4'	3.26	108.90	102.61
5	A	700	ATP	C5-C4-N9	2.93	109.00	105.81
5	A	700	ATP	O4'-C4'-C3'	-2.86	99.48	105.15
5	A	700	ATP	O2B-PB-O3B	2.78	114.80	107.27
5	A	700	ATP	C3'-C2'-C1'	-2.47	96.79	101.46
5	A	700	ATP	O4'-C4'-C5'	2.43	117.13	109.33
5	A	700	ATP	O2B-PB-O3A	-2.02	101.82	107.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	700	ATP	C3'

All (6) torsion outliers are listed below:

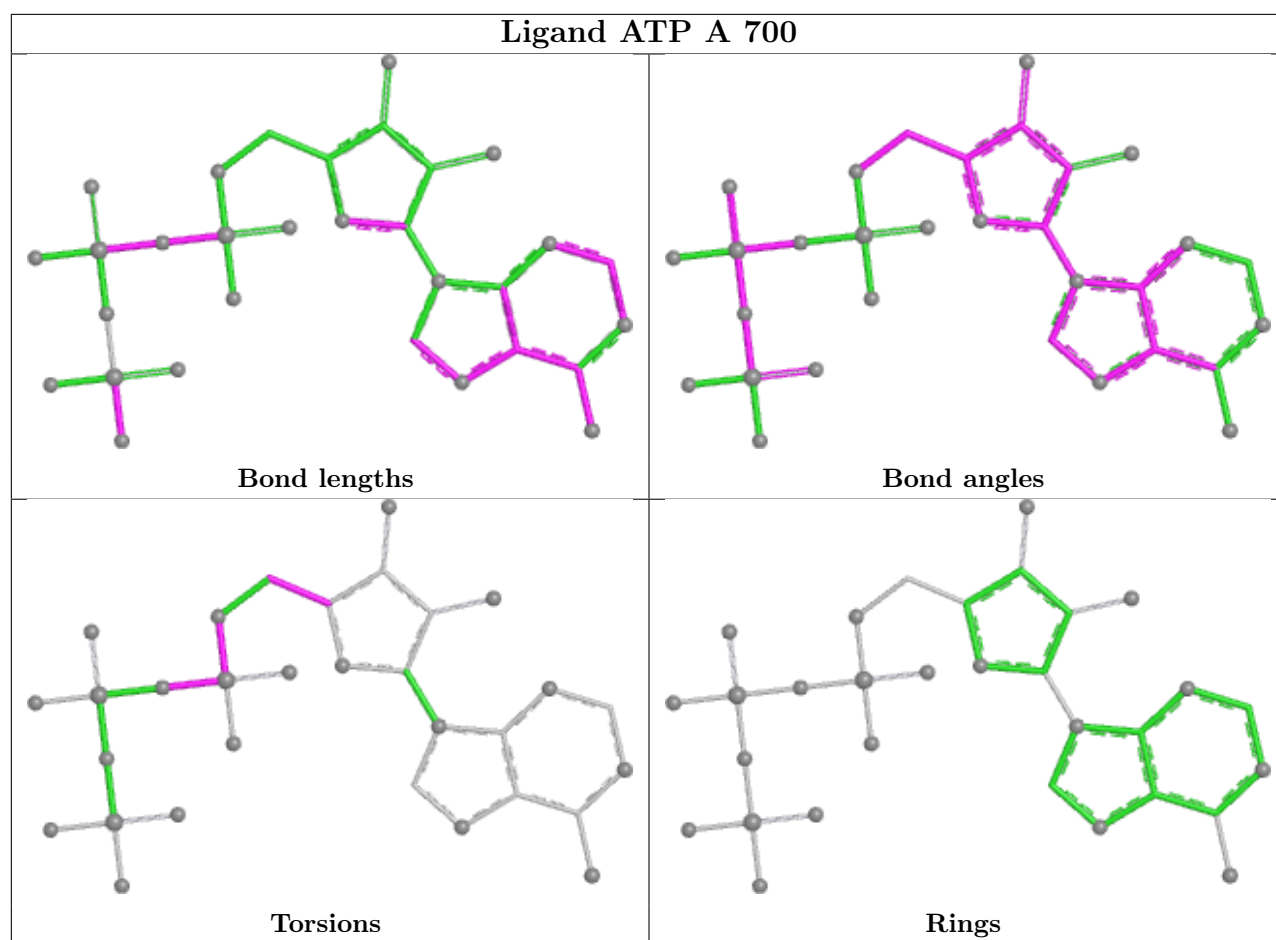
Mol	Chain	Res	Type	Atoms
5	A	700	ATP	C5'-O5'-PA-O1A
5	A	700	ATP	C5'-O5'-PA-O2A
5	A	700	ATP	C5'-O5'-PA-O3A
5	A	700	ATP	C3'-C4'-C5'-O5'
5	A	700	ATP	PB-O3A-PA-O1A
5	A	700	ATP	O4'-C4'-C5'-O5'

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

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 [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%)	-0.26	3 (1%) 67 64	14, 34, 77, 91	0
2	B	261/273 (95%)	-0.35	9 (3%) 48 43	14, 32, 72, 100	0
3	C	102/115 (88%)	0.09	2 (1%) 65 61	20, 51, 81, 90	0
4	D	96/169 (56%)	-0.51	3 (3%) 51 47	15, 27, 64, 85	0
All	All	623/724 (86%)	-0.28	17 (2%) 56 51	14, 34, 78, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	650	SER	5.1
1	A	134	ILE	4.2
4	D	649	ALA	3.9
2	B	421	GLY	3.7
2	B	420	ARG	3.2
2	B	425	SER	3.2
3	C	452	GLY	3.0
2	B	424	ALA	2.8
2	B	423	GLY	2.8
2	B	416	ASN	2.7
2	B	174	SER	2.5
2	B	422	ILE	2.4
1	A	136	PRO	2.3
2	B	426	THR	2.3
4	D	628	ASN	2.2
1	A	138	LYS	2.2
3	C	455	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](#)

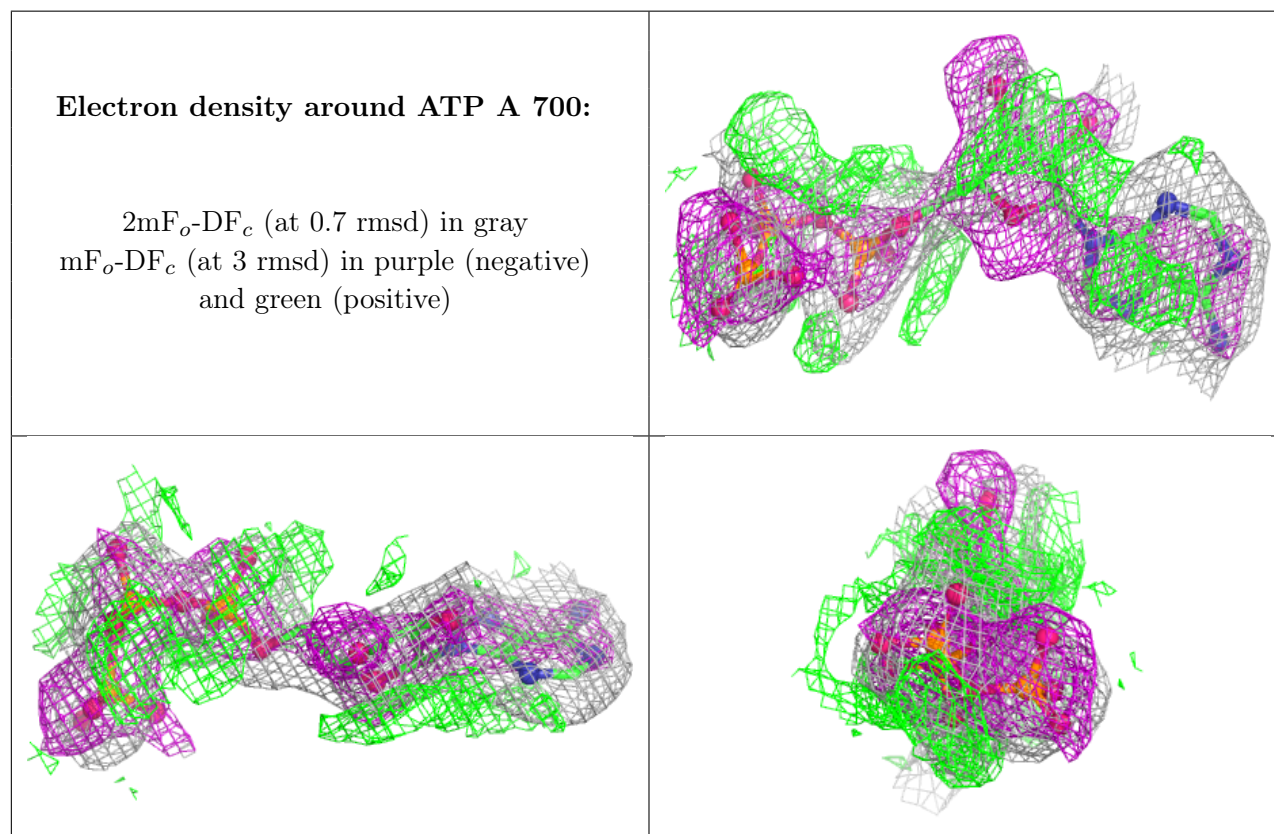
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ATP	A	700	31/31	0.83	0.12	2,11,40,48	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.