



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:46 PM UTC

PDB ID : 6DEC / pdb_00006dec
Title : Crystal structure of Bos taurus Arp2/3 complex binding with C-terminus of Homo sapiens SPIN90
Authors : Nolen, B.J.; Luan, Q.
Deposited on : 2018-05-11
Resolution : 4.60 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)
Xtrriage (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

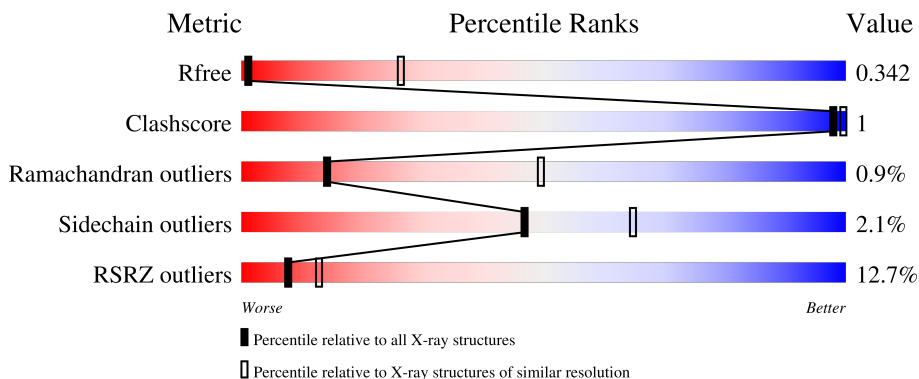
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	418	 8% 88% 6% • 5%
1	H	418	 14% 85% 6% • 8%
2	B	394	 9% 87% 7% 6%
2	I	394	 10% 50% • • 47%
3	C	372	 12% 86% • • 9%

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Mol	Chain	Length	Quality of chain
3	J	372	
4	D	300	
4	K	300	
5	E	178	
5	L	178	
6	F	168	
6	N	168	
7	G	151	
7	O	151	
8	M	455	
8	P	455	
9	Q	6	
10	R	9	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 20563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Actin-related protein 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	398	2010	1202	404	404	0	0	0
1	H	386	1948	1169	389	390	0	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	369	1850	1103	372	375	0	0	0
2	I	209	1030	612	209	209	0	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	339	1757	1070	347	340	0	0	0
3	J	258	1274	758	258	258	0	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	279	1389	830	279	280	0	0	0
4	K	283	1429	855	288	286	0	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	163	Total	C	N	O	0	0	0
			815	488	163	164			
5	L	138	Total	C	N	O	0	0	0
			685	409	138	138			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	165	Total	C	N	O	0	0	0
			829	496	168	165			
6	N	163	Total	C	N	O	0	0	0
			825	496	166	163			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	116	Total	C	N	O	0	0	0
			577	345	116	116			
7	O	132	Total	C	N	O	0	0	0
			648	384	132	132			

- Molecule 8 is a protein called NCK-interacting protein with SH3 domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	329	Total	C	N	O	S	0	0	0
			1638	979	329	329	1			
8	P	328	Total	C	N	O		0	0	0
			1656	995	332	329				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	268	SER	-	expression tag	UNP Q9NZQ3
P	268	SER	-	expression tag	UNP Q9NZQ3

- Molecule 9 is a protein called unidentified.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Q	6	Total	C	N	O	0	0	0
			30	18	6	6			

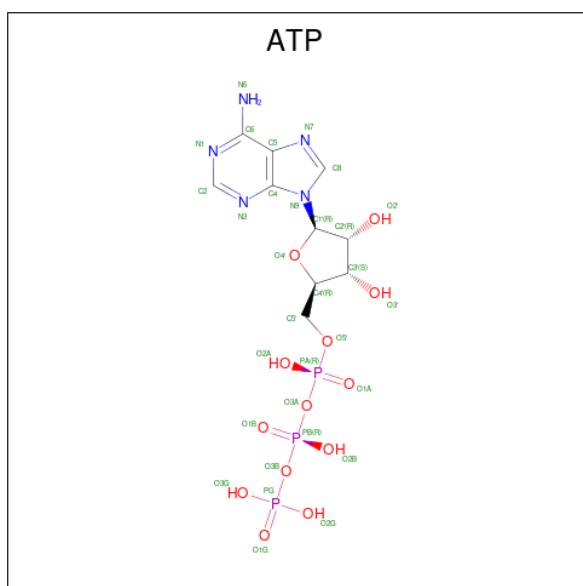
- Molecule 10 is a protein called unidentified.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	R	9	45	27	9	9	0	0	0

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
11	A	1	1	1	0	0
11	B	1	1	1	0	0
11	H	1	1	1	0	0
11	I	1	1	1	0	0

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

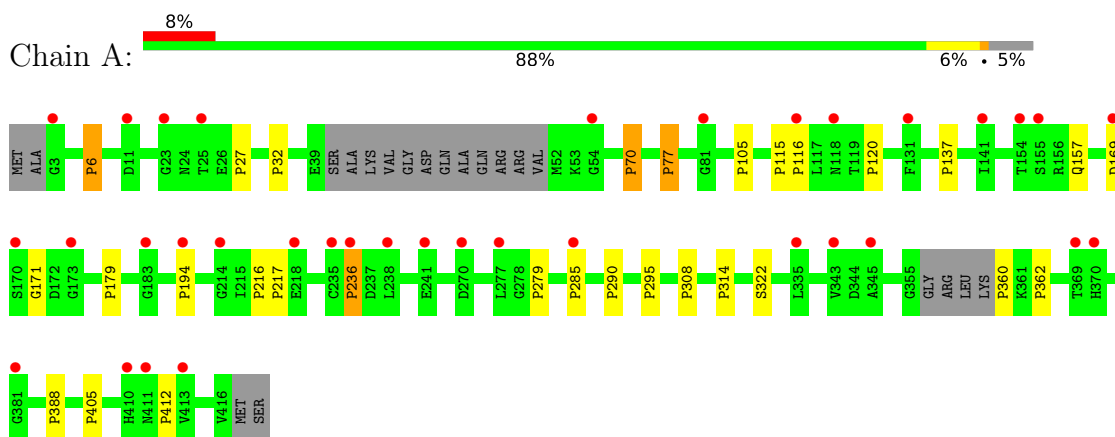


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	A	1	31	10	5	13	3	0	0
12	B	1	31	10	5	13	3	0	0
12	H	1	31	10	5	13	3	0	0
12	I	1	31	10	5	13	3	0	0

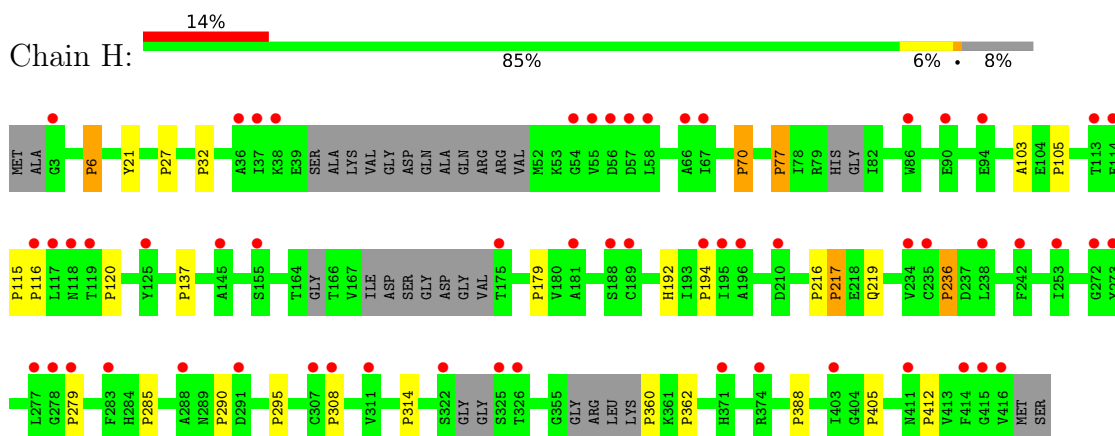
3 Residue-property plots [i](#)

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.

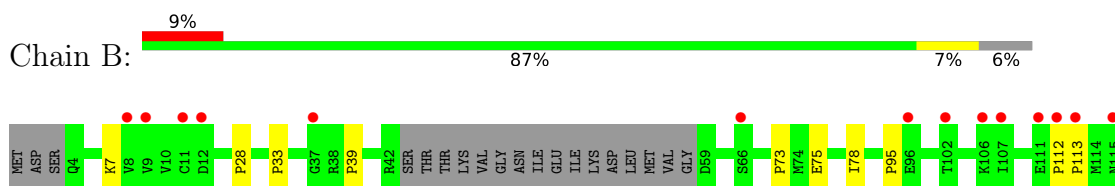
- Molecule 1: Actin-related protein 3

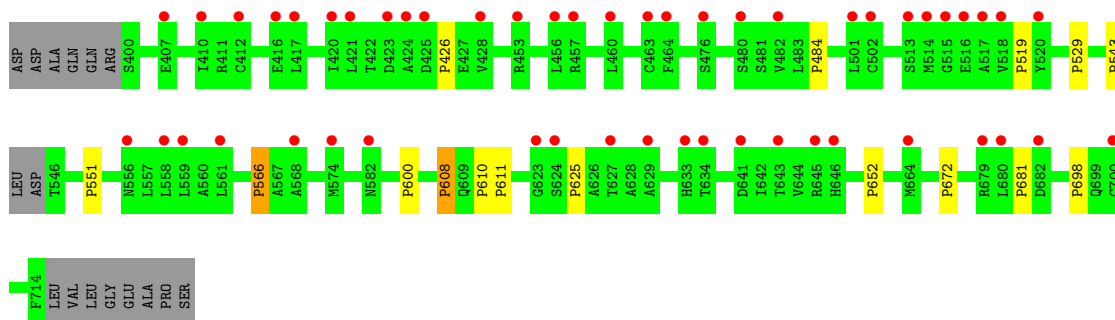


- Molecule 1: Actin-related protein 3

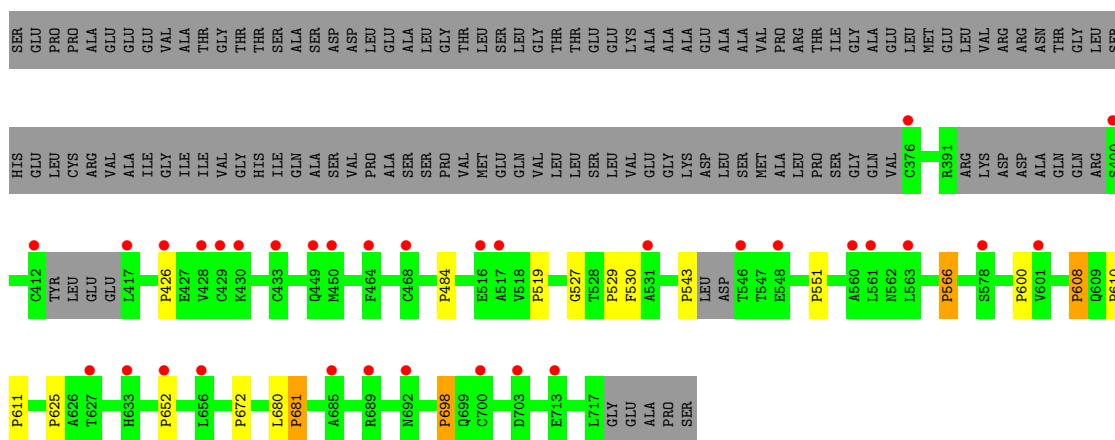


- Molecule 2: Actin-related protein 2





- Molecule 8: NCK-interacting protein with SH3 domain



- Molecule 9: unidentified



There are no outlier residues recorded for this chain.

- Molecule 10: unidentified



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	179.84Å 197.38Å 202.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 4.60 48.94 – 4.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.94-4.60) 94.1 (48.94-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 4.45Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.275 , 0.314 0.317 , 0.342	Depositor DCC
R_{free} test set	1975 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	196.7	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.025 for -h,l,k	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	20563	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, CA

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	0.48	0/2015	1.09	26/2799 (0.9%)
1	H	0.47	0/1947	1.06	26/2699 (1.0%)
2	B	0.46	0/1851	1.00	18/2567 (0.7%)
2	I	0.46	0/1020	0.99	11/1403 (0.8%)
3	C	0.43	0/1772	0.91	14/2466 (0.6%)
3	J	0.41	0/1250	0.94	12/1702 (0.7%)
4	D	0.44	0/1387	0.91	9/1929 (0.5%)
4	K	0.45	0/1432	0.89	9/1994 (0.5%)
5	E	0.41	0/810	0.97	10/1120 (0.9%)
5	L	0.41	0/682	0.89	5/947 (0.5%)
6	F	0.49	0/828	0.94	4/1155 (0.3%)
6	N	0.47	0/824	0.89	4/1147 (0.3%)
7	G	0.46	0/577	0.98	4/800 (0.5%)
7	O	0.43	0/645	0.92	4/891 (0.4%)
8	M	0.44	0/1635	0.98	16/2279 (0.7%)
8	P	0.45	0/1656	0.98	16/2305 (0.7%)
All	All	0.45	0/20331	0.97	188/28203 (0.7%)

There are no bond length outliers.

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PRO	N-CA-CB	12.44	110.16	103.19
7	G	63	PRO	N-CA-CB	11.49	110.47	102.65
7	O	63	PRO	N-CA-CB	11.13	110.25	102.35
1	A	362	PRO	N-CA-CB	8.97	110.47	103.30
1	A	179	PRO	N-CA-CB	8.68	110.56	103.36
1	H	362	PRO	N-CA-CB	8.64	110.21	103.30
1	H	179	PRO	N-CA-CB	8.63	110.53	103.36
8	M	519	PRO	N-CA-CB	8.51	110.43	103.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	519	PRO	N-CA-CB	8.42	110.35	103.36
3	J	267	PRO	N-CA-CB	8.30	110.25	103.36
6	N	36	PRO	N-CA-CB	8.23	110.60	103.36
1	A	308	PRO	N-CA-CB	8.20	110.47	103.25
3	C	182	PRO	N-CA-CB	8.15	110.53	103.36
8	P	652	PRO	N-CA-CB	8.14	110.52	103.36
2	B	33	PRO	N-CA-CB	8.11	110.50	103.36
8	M	652	PRO	N-CA-CB	8.06	110.45	103.36
6	F	50	PRO	N-CA-CB	8.04	110.47	103.31
1	H	27	PRO	N-CA-CB	8.04	110.35	103.35
4	D	87	PRO	N-CA-CB	8.00	110.43	103.31
3	J	182	PRO	N-CA-CB	7.98	110.38	103.36
6	F	36	PRO	N-CA-CB	7.85	110.27	103.36
3	J	246	PRO	N-CA-CB	7.84	110.62	103.33
3	C	267	PRO	N-CA-CB	7.84	110.14	103.17
1	A	27	PRO	N-CA-CB	7.82	110.60	103.33
1	A	216	PRO	N-CA-CB	7.78	110.63	103.08
6	N	50	PRO	N-CA-CB	7.74	110.20	103.31
6	F	108	PRO	N-CA-CB	7.70	110.62	103.15
3	J	10	PRO	N-CA-CB	7.69	110.48	103.33
7	O	62	PRO	N-CA-CB	7.69	110.54	103.08
1	A	115	PRO	N-CA-CB	7.67	110.53	103.08
1	H	32	PRO	N-CA-CB	7.67	110.59	103.15
5	E	156	PRO	N-CA-CB	7.64	110.45	103.34
1	A	290	PRO	N-CA-CB	7.64	110.57	103.46
1	H	115	PRO	N-CA-CB	7.63	110.48	103.08
2	B	116	PRO	N-CA-CB	7.62	110.42	103.33
1	H	412	PRO	N-CA-CB	7.62	110.41	103.33
7	G	62	PRO	N-CA-CB	7.60	110.45	103.08
3	C	184	PRO	N-CA-CB	7.59	110.54	103.41
8	P	610	PRO	N-CA-CB	7.58	110.43	103.08
1	A	412	PRO	N-CA-CB	7.54	110.34	103.33
1	H	290	PRO	N-CA-CB	7.54	110.47	103.46
5	L	156	PRO	N-CA-CB	7.54	110.35	103.34
3	J	180	PRO	N-CA-CB	7.52	110.33	103.34
4	D	205	PRO	N-CA-CB	7.52	110.38	103.08
2	B	112	PRO	N-CA-CB	7.51	110.36	103.08
1	H	308	PRO	N-CA-CB	7.50	109.98	103.31
1	A	279	PRO	N-CA-CB	7.47	110.68	103.51
4	K	87	PRO	N-CA-CB	7.46	109.95	103.31
8	P	600	PRO	N-CA-CB	7.44	110.27	103.20
1	H	285	PRO	N-CA-CB	7.43	110.26	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	7	PRO	N-CA-CB	7.42	110.39	103.41
8	M	610	PRO	N-CA-CB	7.42	110.28	103.08
1	A	32	PRO	N-CA-CB	7.40	110.33	103.15
4	K	48	PRO	N-CA-CB	7.40	110.22	103.34
1	H	216	PRO	N-CA-CB	7.38	110.24	103.08
1	H	137	PRO	N-CA-CB	7.37	110.59	103.51
6	N	108	PRO	N-CA-CB	7.37	110.30	103.15
4	K	205	PRO	N-CA-CB	7.36	110.22	103.08
2	I	112	PRO	N-CA-CB	7.35	110.21	103.08
1	A	285	PRO	N-CA-CB	7.34	110.18	103.20
1	H	405	PRO	N-CA-CB	7.34	110.56	103.51
3	C	246	PRO	N-CA-CB	7.34	110.16	103.33
8	M	566	PRO	N-CA-CB	7.28	110.89	103.25
8	M	600	PRO	N-CA-CB	7.27	110.10	103.20
8	P	608	PRO	N-CA-CB	7.26	110.87	103.25
8	P	566	PRO	N-CA-CB	7.20	110.81	103.25
3	J	184	PRO	N-CA-CB	7.17	110.39	103.51
3	J	106	PRO	N-CA-CB	7.16	110.39	103.51
4	D	48	PRO	N-CA-CB	7.14	109.98	103.34
2	B	28	PRO	N-CA-CB	7.14	110.45	102.67
8	P	681	PRO	N-CA-CB	7.13	110.74	103.25
1	H	6	PRO	N-CA-CB	7.10	110.71	103.25
3	C	152	PRO	N-CA-CB	7.10	110.33	103.51
8	P	551	PRO	N-CA-CB	7.07	110.79	103.23
5	L	31	PRO	N-CA-CB	7.06	110.67	103.25
1	H	217	PRO	N-CA-CB	7.06	110.66	103.25
5	L	151	PRO	N-CA-CB	7.06	110.28	103.51
1	H	279	PRO	N-CA-CB	7.04	110.27	103.51
5	E	151	PRO	N-CA-CB	7.04	110.26	103.51
2	B	262	PRO	N-CA-CB	7.02	110.62	102.76
8	M	608	PRO	N-CA-CB	7.00	110.60	103.25
4	K	206	PRO	N-CA-CB	6.99	110.59	103.25
1	A	137	PRO	N-CA-CB	6.99	110.22	103.51
1	A	217	PRO	N-CA-CB	6.99	110.22	103.51
2	I	268	PRO	N-CA-CB	6.95	110.18	103.51
7	G	117	PRO	N-CA-CB	6.91	110.50	103.25
8	M	529	PRO	N-CA-CB	6.90	110.49	103.25
8	P	484	PRO	N-CA-CB	6.89	110.49	103.25
2	B	176	PRO	N-CA-CB	6.87	110.35	103.48
7	O	37	PRO	N-CA-CB	6.86	110.45	103.25
5	E	11	PRO	N-CA-CB	6.83	110.54	103.23
3	J	190	PRO	N-CA-CB	6.83	110.42	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	PRO	N-CA-CB	6.82	110.42	103.25
8	P	672	PRO	N-CA-CB	6.82	110.41	103.25
5	E	112	PRO	N-CA-CB	6.81	110.40	103.25
3	C	106	PRO	N-CA-CB	6.80	110.74	103.39
2	I	262	PRO	N-CA-CB	6.80	110.29	102.88
7	O	117	PRO	N-CA-CB	6.79	110.38	103.25
8	P	698	PRO	N-CA-CB	6.79	110.38	103.25
3	C	288	PRO	N-CA-CB	6.78	110.45	103.00
3	C	88	PRO	N-CA-CB	6.76	110.34	103.25
5	E	2	PRO	N-CA-CB	6.76	110.43	103.00
5	E	109	PRO	N-CA-CB	6.75	110.34	103.25
2	I	347	PRO	N-CA-CB	6.74	110.42	103.00
3	J	27	PRO	N-CA-CB	6.73	110.41	103.00
6	N	7	PRO	N-CA-CB	6.73	110.32	103.25
2	B	39	PRO	N-CA-CB	6.72	110.31	103.25
2	B	311	PRO	N-CA-CB	6.72	110.30	103.25
8	M	551	PRO	N-CA-CB	6.71	110.42	103.23
4	D	206	PRO	N-CA-CB	6.71	110.29	103.25
2	I	348	PRO	N-CA-CB	6.69	110.28	103.25
4	D	28	PRO	N-CA-CB	6.69	110.27	103.25
3	C	190	PRO	N-CA-CB	6.67	110.26	103.25
4	K	103	PRO	N-CA-CB	6.67	110.46	102.72
3	C	180	PRO	N-CA-CB	6.67	110.25	103.25
1	H	360	PRO	N-CA-CB	6.67	110.33	103.00
8	M	672	PRO	N-CA-CB	6.66	110.24	103.25
1	A	6	PRO	N-CA-CB	6.66	110.24	103.25
7	G	37	PRO	N-CA-CB	6.65	110.23	103.25
3	J	288	PRO	N-CA-CB	6.65	110.32	103.00
4	D	282	PRO	N-CA-CB	6.64	110.23	103.25
3	J	62	PRO	N-CA-CB	6.64	110.23	103.25
2	B	113	PRO	N-CA-CB	6.64	110.35	103.38
4	D	196	PRO	N-CA-CB	6.64	110.35	103.38
4	K	28	PRO	N-CA-CB	6.64	110.22	103.25
5	E	31	PRO	N-CA-CB	6.64	110.22	103.25
5	L	23	PRO	N-CA-CB	6.64	110.35	103.38
8	P	529	PRO	N-CA-CB	6.63	110.55	103.52
1	A	295	PRO	N-CA-CB	6.63	110.72	103.23
5	E	104	PRO	N-CA-CB	6.63	110.21	103.25
5	E	106	PRO	N-CA-CB	6.62	110.21	103.25
1	A	360	PRO	N-CA-CB	6.62	110.28	103.00
1	A	236	PRO	N-CA-CB	6.62	110.20	103.25
3	J	88	PRO	N-CA-CB	6.62	110.40	102.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	176	PRO	N-CA-CB	6.61	110.19	103.25
8	P	543	PRO	N-CA-CB	6.61	110.27	103.00
8	M	426	PRO	N-CA-CB	6.61	110.19	103.25
1	A	388	PRO	N-CA-CB	6.60	110.51	103.52
8	M	484	PRO	N-CA-CB	6.60	110.18	103.25
1	H	236	PRO	N-CA-CB	6.59	110.17	103.25
3	C	27	PRO	N-CA-CB	6.59	110.17	103.25
1	A	70	PRO	N-CA-CB	6.59	110.17	103.25
3	C	140	PRO	N-CA-CB	6.58	110.16	103.25
2	B	348	PRO	N-CA-CB	6.58	110.50	103.52
1	A	405	PRO	N-CA-CB	6.58	109.82	103.51
2	I	311	PRO	N-CA-CB	6.58	110.23	103.00
4	K	196	PRO	N-CA-CB	6.56	110.27	103.38
8	M	611	PRO	N-CA-CB	6.56	110.13	103.25
1	A	77	PRO	N-CA-CB	6.55	110.13	103.25
4	D	103	PRO	N-CA-CB	6.52	110.28	102.72
1	H	295	PRO	N-CA-CB	6.51	110.58	103.23
1	H	70	PRO	N-CA-CB	6.51	110.08	103.25
2	B	95	PRO	N-CA-CB	6.48	110.06	103.25
2	I	113	PRO	N-CA-CB	6.47	110.05	103.25
1	A	120	PRO	N-CA-CB	6.45	110.66	103.44
8	P	426	PRO	N-CA-CB	6.44	110.02	103.25
2	I	314	PRO	N-CA-CB	6.44	110.41	103.33
2	I	116	PRO	N-CA-CB	6.43	110.49	103.23
2	B	268	PRO	N-CA-CB	6.42	109.99	103.25
1	H	388	PRO	N-CA-CB	6.39	110.29	103.52
8	M	698	PRO	N-CA-CB	6.38	109.94	103.25
4	K	282	PRO	N-CA-CB	6.37	109.94	103.25
2	B	314	PRO	N-CA-CB	6.35	110.03	103.23
1	H	194	PRO	N-CA-CB	6.35	109.92	103.25
8	M	543	PRO	N-CA-CB	6.34	109.98	103.00
2	I	247	PRO	N-CA-CB	6.34	110.24	103.52
3	C	62	PRO	N-CA-CB	6.29	109.85	103.25
1	H	77	PRO	N-CA-CB	6.27	109.84	103.25
4	K	229	PRO	N-CA-CB	6.27	110.16	103.39
1	A	116	PRO	N-CA-CB	6.26	110.45	103.44
2	B	247	PRO	N-CA-CB	6.20	110.38	103.44
8	P	625	PRO	N-CA-CB	6.19	110.14	103.33
8	M	681	PRO	N-CA-CB	6.18	109.73	103.25
1	A	194	PRO	N-CA-CB	6.17	109.73	103.25
2	B	73	PRO	N-CA-CB	6.17	110.35	103.44
1	A	314	PRO	N-CA-CB	6.16	110.34	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	625	PRO	N-CA-CB	6.14	110.08	103.33
1	H	314	PRO	N-CA-CB	6.13	110.30	103.44
1	H	120	PRO	N-CA-CB	6.08	110.25	103.44
4	D	229	PRO	N-CA-CB	6.06	109.94	103.39
1	H	105	PRO	N-CA-CB	5.94	110.09	103.44
1	H	116	PRO	N-CA-CB	5.92	110.07	103.44
1	A	105	PRO	N-CA-CB	5.92	110.07	103.44
5	L	33	PRO	N-CA-CB	5.79	110.62	103.15
5	E	33	PRO	N-CA-CB	5.67	110.46	103.15
3	C	10	PRO	N-CA-CB	5.37	110.08	103.15
2	B	369	ASP	CB-CA-C	-5.28	110.47	116.54
8	P	611	PRO	N-CA-CB	5.25	110.35	103.42

There are no chirality outliers.

There are no planarity outliers.

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	2010	0	906	2	0
1	H	1948	0	873	3	0
2	B	1850	0	839	4	0
2	I	1030	0	449	1	0
3	C	1757	0	843	3	0
3	J	1274	0	551	5	0
4	D	1389	0	632	0	0
4	K	1429	0	663	3	0
5	E	815	0	349	0	0
5	L	685	0	291	0	0
6	F	829	0	371	0	0
6	N	825	0	370	1	0
7	G	577	0	282	0	0
7	O	648	0	311	0	0
8	M	1638	0	737	0	0
8	P	1656	0	760	1	0
9	Q	30	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	R	45	0	11	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
12	A	31	0	12	1	0
12	B	31	0	12	0	0
12	H	31	0	12	0	0
12	I	31	0	12	0	0
All	All	20563	0	9294	21	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 1.

All (21) 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)
3:J:224:SER:O	3:J:242:SER:N	2.30	0.65
4:K:2:ILE:O	4:K:254:HIS:NE2	2.26	0.60
2:B:222:TYR:CZ	2:B:259:PHE:HB3	2.42	0.54
2:B:241:VAL:HA	2:B:255:GLY:HA2	1.90	0.53
4:K:250:TYR:OH	6:N:160:VAL:O	2.24	0.52
3:C:247:LEU:HA	3:C:262:GLY:HA3	1.92	0.51
3:J:270:PHE:HA	3:J:282:GLY:H	1.75	0.51
3:C:261:ALA:HB2	3:C:267:PRO:HA	1.93	0.49
3:J:125:PHE:HA	3:J:132:TRP:HA	1.95	0.49
3:J:79:TRP:HA	3:J:88:PRO:HA	1.96	0.47
3:C:270:PHE:HA	3:C:282:GLY:H	1.81	0.46
8:P:527:GLY:O	8:P:530:PHE:N	2.48	0.45
1:A:169:ASP:HA	1:A:322:SER:O	2.18	0.44
1:H:21:TYR:CE1	4:K:36:ALA:HB3	2.52	0.44
1:A:171:GLY:HA3	12:A:502:ATP:O1G	2.19	0.43
2:B:75:GLU:N	2:B:78:ILE:O	2.51	0.43
3:J:69:THR:O	3:J:77:TYR:N	2.51	0.43
2:B:222:TYR:CE1	2:B:259:PHE:HB3	2.56	0.41
1:H:21:TYR:OH	1:H:103:ALA:HB2	2.21	0.41
2:I:185:ALA:O	2:I:189:ILE:N	2.42	0.40
1:H:217:PRO:C	1:H:219:GLN:H	2.29	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	392/418 (94%)	374 (95%)	13 (3%)	5 (1%)	9	41
1	H	372/418 (89%)	355 (95%)	13 (4%)	4 (1%)	11	45
2	B	365/394 (93%)	337 (92%)	25 (7%)	3 (1%)	16	53
2	I	189/394 (48%)	180 (95%)	7 (4%)	2 (1%)	11	45
3	C	333/372 (90%)	305 (92%)	24 (7%)	4 (1%)	10	42
3	J	210/372 (56%)	202 (96%)	7 (3%)	1 (0%)	24	63
4	D	273/300 (91%)	268 (98%)	5 (2%)	0	100	100
4	K	281/300 (94%)	275 (98%)	6 (2%)	0	100	100
5	E	151/178 (85%)	141 (93%)	4 (3%)	6 (4%)	2	18
5	L	132/178 (74%)	131 (99%)	1 (1%)	0	100	100
6	F	163/168 (97%)	160 (98%)	3 (2%)	0	100	100
6	N	159/168 (95%)	154 (97%)	4 (2%)	1 (1%)	21	58
7	G	114/151 (76%)	112 (98%)	1 (1%)	1 (1%)	14	49
7	O	126/151 (83%)	123 (98%)	2 (2%)	1 (1%)	16	53
8	M	323/455 (71%)	311 (96%)	10 (3%)	2 (1%)	21	58
8	P	320/455 (70%)	307 (96%)	8 (2%)	5 (2%)	7	37
All	All	3903/4872 (80%)	3735 (96%)	133 (3%)	35 (1%)	14	49

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	PRO
1	A	157	GLN
3	C	140	PRO
5	E	108	GLU
5	E	112	PRO
8	M	608	PRO

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Mol	Chain	Res	Type
8	P	608	PRO
1	A	70	PRO
3	C	27	PRO
3	C	190	PRO
5	E	104	PRO
8	P	681	PRO
2	B	7	LYS
5	E	109	PRO
1	H	70	PRO
1	H	77	PRO
3	J	190	PRO
2	I	348	PRO
8	P	680	LEU
8	P	698	PRO
1	A	236	PRO
5	E	103	PHE
8	M	566	PRO
1	H	236	PRO
8	P	566	PRO
6	N	6	ARG
1	A	6	PRO
2	B	346	ASP
1	H	6	PRO
2	B	385	VAL
5	E	111	PHE
3	C	62	PRO
7	G	37	PRO
7	O	37	PRO
2	I	176	PRO

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	8/363 (2%)	8 (100%)	0	100	100
1	H	7/363 (2%)	6 (86%)	1 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	6/345 (2%)	6 (100%)	0	100	100
3	C	10/313 (3%)	10 (100%)	0	100	100
4	D	1/264 (0%)	1 (100%)	0	100	100
4	K	5/264 (2%)	5 (100%)	0	100	100
5	E	1/159 (1%)	1 (100%)	0	100	100
6	F	1/155 (1%)	1 (100%)	0	100	100
6	N	2/155 (1%)	2 (100%)	0	100	100
7	G	1/123 (1%)	1 (100%)	0	100	100
8	M	1/392 (0%)	1 (100%)	0	100	100
8	P	5/392 (1%)	5 (100%)	0	100	100
All	All	48/3288 (2%)	47 (98%)	1 (2%)	47	65

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	192	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
12	ATP	B	502	11	32,33,33	1.44	5 (15%)	48,52,52	1.74	9 (18%)
12	ATP	I	502	11	32,33,33	1.43	5 (15%)	48,52,52	1.74	9 (18%)
12	ATP	H	502	11	32,33,33	1.41	4 (12%)	48,52,52	1.78	9 (18%)
12	ATP	A	502	11	32,33,33	1.41	4 (12%)	48,52,52	1.76	9 (18%)

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
12	ATP	B	502	11	-	6/22/38/38	0/3/3/3
12	ATP	I	502	11	-	2/22/38/38	0/3/3/3
12	ATP	H	502	11	-	3/22/38/38	0/3/3/3
12	ATP	A	502	11	-	1/22/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	502	ATP	C5-C4	4.82	1.47	1.39
12	H	502	ATP	C5-C4	4.80	1.47	1.39
12	A	502	ATP	C5-C4	4.79	1.47	1.39
12	I	502	ATP	C5-C4	4.71	1.47	1.39
12	A	502	ATP	C5-C6	2.83	1.48	1.41
12	B	502	ATP	C5-C6	2.82	1.48	1.41
12	H	502	ATP	C5-C6	2.78	1.48	1.41
12	I	502	ATP	C5-C6	2.74	1.48	1.41
12	B	502	ATP	C8-N7	2.43	1.36	1.31
12	A	502	ATP	C8-N7	2.41	1.36	1.31
12	I	502	ATP	C8-N7	2.40	1.36	1.31
12	H	502	ATP	C8-N7	2.35	1.36	1.31
12	B	502	ATP	PB-O3B	2.27	1.62	1.59
12	H	502	ATP	C5-N7	-2.23	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	502	ATP	C5-N7	-2.22	1.35	1.39
12	A	502	ATP	C5-N7	-2.21	1.35	1.39
12	B	502	ATP	C5-N7	-2.18	1.35	1.39
12	I	502	ATP	PB-O3B	2.01	1.61	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	502	ATP	C5-C4-N3	-6.02	118.43	126.72
12	A	502	ATP	C5-C4-N3	-5.89	118.60	126.72
12	I	502	ATP	C5-C4-N3	-5.81	118.72	126.72
12	B	502	ATP	C5-C4-N3	-5.69	118.88	126.72
12	H	502	ATP	N3-C4-N9	4.74	135.23	127.17
12	A	502	ATP	N3-C4-N9	4.56	134.93	127.17
12	I	502	ATP	N3-C4-N9	4.54	134.88	127.17
12	B	502	ATP	N3-C4-N9	4.37	134.60	127.17
12	H	502	ATP	C2-N3-C4	3.75	120.99	111.83
12	I	502	ATP	C2-N3-C4	3.74	120.97	111.83
12	B	502	ATP	C2-N3-C4	3.72	120.92	111.83
12	A	502	ATP	C2-N3-C4	3.72	120.91	111.83
12	B	502	ATP	C4-C5-N7	-3.61	106.45	110.58
12	H	502	ATP	C4-C5-N7	-3.58	106.48	110.58
12	A	502	ATP	C4-C5-N7	-3.57	106.50	110.58
12	I	502	ATP	C4-C5-N7	-3.52	106.56	110.58
12	B	502	ATP	N3-C2-N1	-3.41	123.43	128.58
12	I	502	ATP	N3-C2-N1	-3.29	123.59	128.58
12	A	502	ATP	N3-C2-N1	-3.21	123.72	128.58
12	H	502	ATP	N3-C2-N1	-3.21	123.73	128.58
12	I	502	ATP	C4-N9-C8	2.61	108.48	105.74
12	H	502	ATP	C5-N7-C8	2.60	107.54	103.45
12	B	502	ATP	C5-N7-C8	2.59	107.52	103.45
12	A	502	ATP	C5-N7-C8	2.55	107.46	103.45
12	I	502	ATP	C5-N7-C8	2.55	107.45	103.45
12	H	502	ATP	C4-N9-C8	2.53	108.39	105.74
12	A	502	ATP	C4-N9-C8	2.48	108.34	105.74
12	B	502	ATP	C4-N9-C8	2.47	108.33	105.74
12	B	502	ATP	C6-C5-N7	2.27	136.47	132.09
12	A	502	ATP	C3'-C2'-C1'	2.25	105.71	101.46
12	H	502	ATP	C3'-C2'-C1'	2.19	105.61	101.46
12	I	502	ATP	C3'-C2'-C1'	2.18	105.58	101.46
12	I	502	ATP	C6-C5-N7	2.16	136.25	132.09
12	A	502	ATP	C6-C5-N7	2.09	136.12	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	502	ATP	C6-C5-N7	2.05	136.04	132.09
12	B	502	ATP	C2-N1-C6	2.01	122.04	118.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

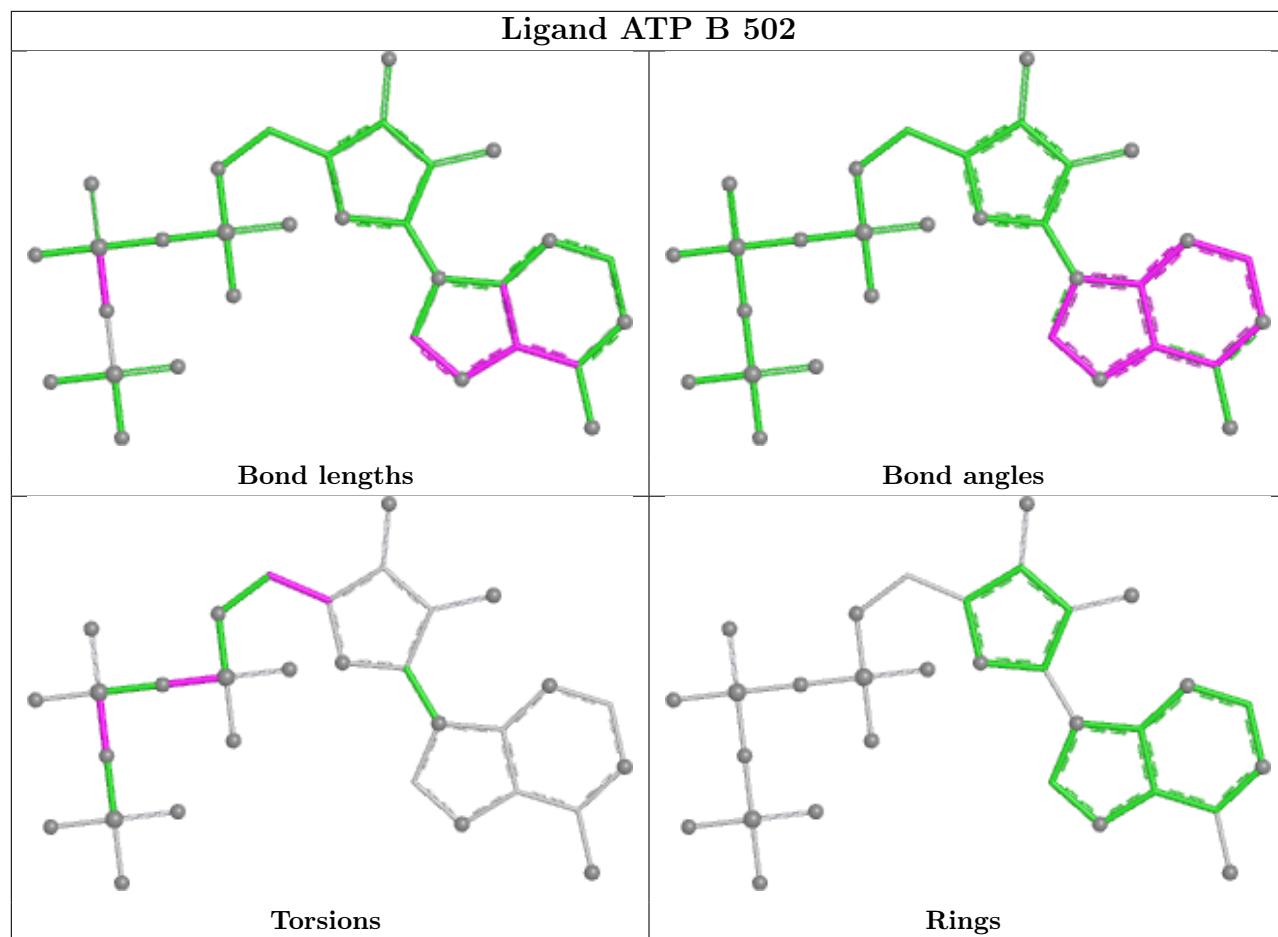
Mol	Chain	Res	Type	Atoms
12	B	502	ATP	O4'-C4'-C5'-O5'
12	B	502	ATP	C3'-C4'-C5'-O5'
12	B	502	ATP	PG-O3B-PB-O1B
12	B	502	ATP	PG-O3B-PB-O2B
12	B	502	ATP	PB-O3A-PA-O1A
12	H	502	ATP	PB-O3A-PA-O1A
12	H	502	ATP	PB-O3A-PA-O2A
12	A	502	ATP	C2'-C1'-N9-C8
12	B	502	ATP	PB-O3A-PA-O2A
12	I	502	ATP	PB-O3A-PA-O2A
12	H	502	ATP	C3'-C4'-C5'-O5'
12	I	502	ATP	PB-O3A-PA-O1A

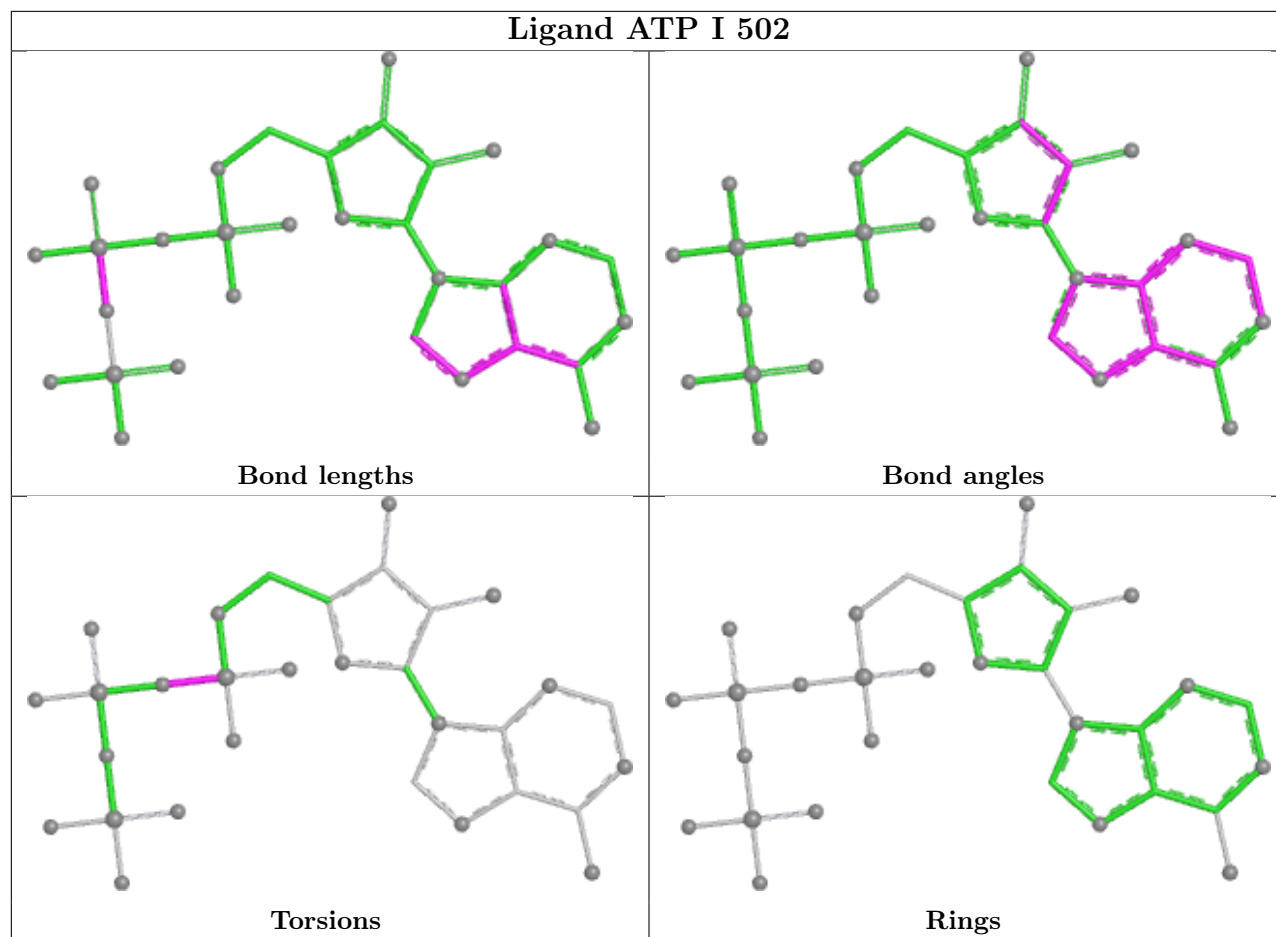
There are no ring outliers.

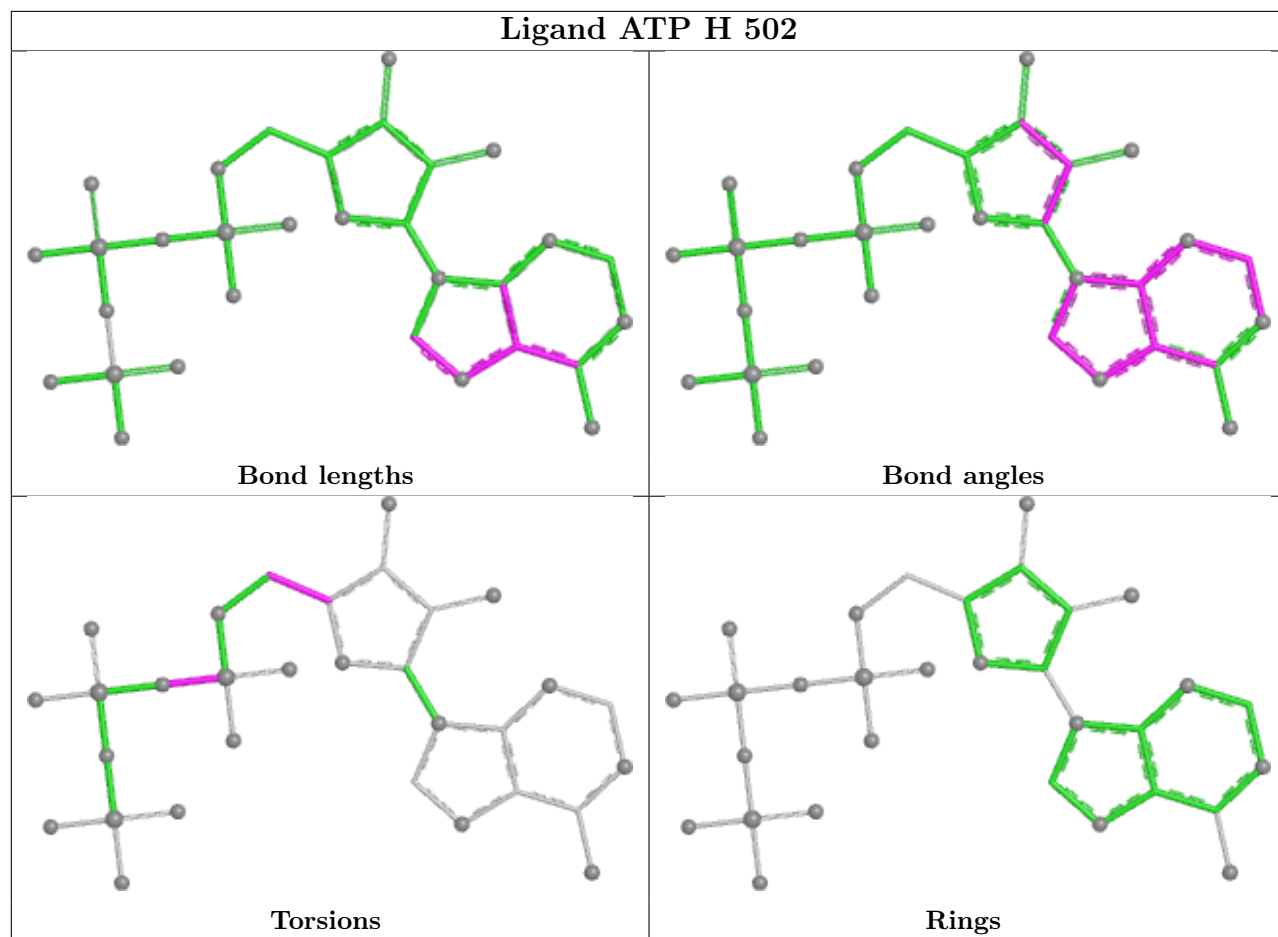
1 monomer is involved in 1 short contact:

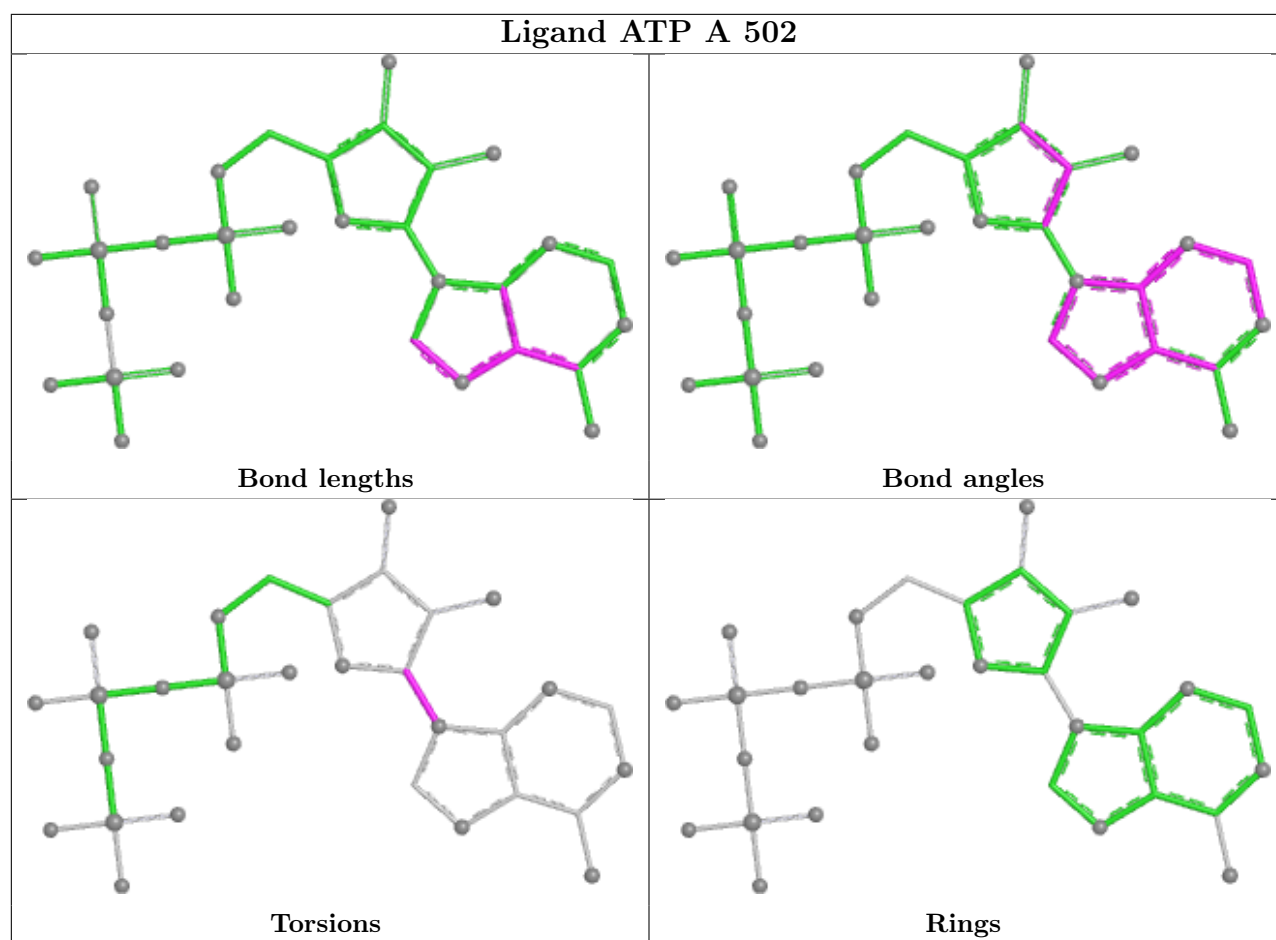
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	502	ATP	1	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	19:MET	C	21:ALA	N	4.49

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	398/418 (95%)	0.63	35 (8%) 15 19	76, 138, 200, 295	0
1	H	386/418 (92%)	0.82	57 (14%) 5 11	82, 157, 246, 311	0
2	B	369/394 (93%)	0.51	37 (10%) 12 17	66, 155, 253, 296	0
2	I	209/394 (53%)	1.03	41 (19%) 3 7	121, 215, 330, 447	0
3	C	339/372 (91%)	0.68	45 (13%) 7 12	78, 140, 193, 229	0
3	J	258/372 (69%)	1.14	48 (18%) 3 8	140, 245, 321, 379	0
4	D	279/300 (93%)	0.77	39 (13%) 6 12	71, 219, 342, 423	0
4	K	283/300 (94%)	0.43	15 (5%) 32 31	76, 146, 213, 256	0
5	E	163/178 (91%)	0.80	20 (12%) 8 13	117, 178, 251, 281	0
5	L	138/178 (77%)	0.90	17 (12%) 8 13	145, 242, 330, 351	0
6	F	165/168 (98%)	0.53	9 (5%) 30 30	58, 118, 203, 233	0
6	N	163/168 (97%)	0.78	25 (15%) 5 11	78, 156, 224, 288	0
7	G	116/151 (76%)	0.73	17 (14%) 6 11	90, 179, 281, 305	0
7	O	132/151 (87%)	0.95	17 (12%) 7 12	142, 248, 305, 333	0
8	M	329/455 (72%)	1.01	58 (17%) 4 9	102, 202, 289, 315	0
8	P	328/455 (72%)	0.58	33 (10%) 12 17	71, 156, 277, 312	0
9	Q	0/6	-	-	-	-
10	R	0/9	-	-	-	-
All	All	4055/4887 (82%)	0.75	513 (12%) 8 13	58, 172, 284, 447	0

All (513) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	85	CYS	8.7
3	J	327	ASN	8.4
8	M	380	GLN	7.6

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Mol	Chain	Res	Type	RSRZ
2	I	167	CYS	7.5
1	H	54	GLY	7.4
2	I	225	TYR	6.6
2	I	123	ILE	6.5
2	I	119	ASN	6.4
6	F	46	LEU	6.2
8	P	531	ALA	6.1
8	M	623	GLY	6.0
3	C	175	GLU	6.0
1	H	308	PRO	5.9
8	P	468	CYS	5.7
3	J	99	ALA	5.6
3	J	51	HIS	5.6
3	J	255	GLU	5.5
4	D	231	HIS	5.4
1	H	415	GLY	5.3
3	J	98	ALA	5.3
8	P	426	PRO	5.2
1	H	322	SER	5.2
3	J	95	ILE	5.1
4	D	139	GLU	5.1
2	B	383	VAL	5.1
5	L	51	ALA	5.0
1	H	94	GLU	5.0
2	I	121	GLU	5.0
8	M	376	CYS	4.9
2	I	117	THR	4.8
5	E	104	PRO	4.8
3	J	185	TRP	4.8
4	D	208	GLU	4.8
2	I	120	ARG	4.6
1	H	55	VAL	4.6
2	I	278	VAL	4.6
1	H	279	PRO	4.6
4	D	155	GLU	4.6
3	J	213	ASN	4.5
1	A	118	ASN	4.5
8	P	428	VAL	4.5
8	M	514	MET	4.5
1	H	189	CYS	4.5
6	N	5	LEU	4.4
6	F	19	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	176	VAL	4.4
6	N	142	ILE	4.4
1	H	175	THR	4.4
1	H	234	VAL	4.4
1	A	411	ASN	4.3
5	E	126	ASP	4.3
8	M	517	ALA	4.3
1	H	194	PRO	4.2
3	C	111	PHE	4.2
2	B	102	THR	4.2
8	P	412	CYS	4.2
8	P	517	ALA	4.1
3	C	132	TRP	4.1
4	D	227	LEU	4.1
3	J	210	PHE	4.1
4	D	229	PRO	4.1
6	N	51	VAL	4.1
5	E	109	PRO	4.0
5	E	153	ASN	4.0
4	D	232	THR	4.0
2	B	158	ASP	4.0
8	P	546	THR	4.0
3	J	263	HIS	4.0
4	D	125	PHE	4.0
7	G	36	GLY	3.9
5	E	127	GLU	3.9
8	M	420	ILE	3.9
1	H	311	VAL	3.9
2	I	176	PRO	3.9
4	K	231	HIS	3.9
6	N	55	ARG	3.9
8	M	457	ARG	3.9
4	D	226	VAL	3.9
2	I	358	GLY	3.8
8	M	453	ARG	3.8
1	A	116	PRO	3.8
7	O	100	LYS	3.8
5	L	25	ARG	3.8
7	O	95	VAL	3.8
8	M	558	LEU	3.8
1	H	118	ASN	3.7
8	M	377	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
8	P	700	CYS	3.7
1	H	145	ALA	3.7
1	H	325	SER	3.7
2	B	11	CYS	3.7
8	M	633	HIS	3.7
2	I	166	ILE	3.7
6	N	79	ALA	3.7
3	C	100	ARG	3.7
3	J	34	ILE	3.7
6	F	3	ALA	3.7
2	I	159	SER	3.6
2	B	117	THR	3.6
5	E	86	ASN	3.6
5	E	173	LEU	3.6
3	C	353	GLY	3.6
3	C	371	ILE	3.6
3	J	15	ALA	3.6
4	D	124	VAL	3.6
1	H	403	ILE	3.6
2	B	66	SER	3.6
7	O	79	VAL	3.6
8	M	456	LEU	3.6
5	E	39	THR	3.6
8	M	407	GLU	3.6
1	A	170	SER	3.5
2	B	115	ASN	3.5
8	M	480	SER	3.5
1	A	236	PRO	3.5
8	M	646	HIS	3.5
8	M	513	SER	3.5
7	O	103	VAL	3.5
3	C	24	ALA	3.5
6	N	34	ASN	3.5
4	K	236	ALA	3.5
3	C	14	HIS	3.5
3	C	25	ILE	3.5
3	J	123	CYS	3.5
3	J	272	TYR	3.5
5	E	129	MET	3.4
2	I	203	ALA	3.4
2	I	302	VAL	3.4
7	O	99	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	3.4
7	O	51	MET	3.4
3	C	187	SER	3.4
5	L	48	TYR	3.4
8	M	378	ASP	3.4
4	K	214	ALA	3.3
1	A	81	GLY	3.3
6	N	7	PRO	3.3
1	A	277	LEU	3.3
8	M	424	ALA	3.3
1	H	414	PHE	3.3
7	O	150	THR	3.3
1	H	238	LEU	3.3
2	I	141	GLN	3.3
3	J	260	ALA	3.3
5	L	45	ALA	3.3
8	M	425	ASP	3.3
3	C	26	CYS	3.2
3	C	109	LYS	3.2
1	A	169	ASP	3.2
5	E	7	SER	3.2
4	D	126	GLU	3.2
2	I	142	ALA	3.2
1	H	36	ALA	3.2
5	E	108	GLU	3.2
1	A	131	PHE	3.2
2	I	235	LEU	3.2
3	C	112	ALA	3.2
1	A	23	GLY	3.2
2	B	157	VAL	3.2
4	D	211	ASP	3.2
2	B	207	SER	3.1
1	H	273	TYR	3.1
8	P	464	PHE	3.1
2	I	143	VAL	3.1
2	B	107	ILE	3.1
8	P	685	ALA	3.1
3	C	59	ASP	3.1
8	M	516	GLU	3.1
3	C	214	GLY	3.1
8	M	412	CYS	3.1
5	E	10	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
7	G	104	ASP	3.1
2	I	224	GLY	3.1
8	M	556	ASN	3.1
3	J	342	CYS	3.1
8	M	463	CYS	3.1
8	M	417	LEU	3.0
3	J	249	ALA	3.0
2	B	206	HIS	3.0
8	P	400	SER	3.0
1	A	235	CYS	3.0
1	H	307	CYS	3.0
1	H	411	ASN	3.0
3	J	153	ASN	3.0
3	C	16	TRP	3.0
6	N	106	ARG	3.0
3	J	50	GLU	3.0
4	K	235	SER	3.0
4	D	233	ASN	3.0
3	C	150	TRP	3.0
5	E	67	THR	3.0
8	M	384	VAL	3.0
1	H	291	ASP	2.9
8	M	682	ASP	2.9
7	G	95	VAL	2.9
3	J	134	CYS	2.9
2	I	238	THR	2.9
3	C	27	PRO	2.9
6	F	32	ARG	2.9
3	C	331	GLN	2.9
2	B	307	SER	2.9
8	M	643	THR	2.9
3	J	232	ASP	2.9
2	I	288	ALA	2.9
2	I	124	VAL	2.9
6	F	79	ALA	2.9
4	K	39	ASP	2.9
8	M	624	SER	2.9
2	I	177	HIS	2.9
2	I	335	GLU	2.9
8	M	416	GLU	2.9
4	D	142	ALA	2.9
3	J	230	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	111	HIS	2.9
3	J	36	GLU	2.9
7	O	14	VAL	2.9
7	O	151	VAL	2.9
8	P	652	PRO	2.9
3	J	346	CYS	2.9
3	J	348	THR	2.9
1	H	3	GLY	2.9
8	P	692	ASN	2.9
2	B	113	PRO	2.8
8	M	629	ALA	2.8
1	A	155	SER	2.8
8	P	376	CYS	2.8
4	D	86	ASN	2.8
5	L	122	ASN	2.8
1	H	155	SER	2.8
3	J	214	GLY	2.8
4	D	122	ALA	2.8
6	N	103	ILE	2.8
6	N	141	GLU	2.8
8	P	429	CYS	2.8
7	G	50	ASN	2.8
7	G	55	LEU	2.8
7	G	42	VAL	2.8
6	N	50	PRO	2.8
7	G	93	LYS	2.8
3	C	325	HIS	2.8
3	C	5	SER	2.8
7	G	53	ALA	2.7
1	H	116	PRO	2.7
3	C	92	ILE	2.7
3	J	204	TRP	2.7
4	K	159	ASP	2.7
1	A	3	GLY	2.7
1	H	277	LEU	2.7
8	M	460	LEU	2.7
1	H	195	ILE	2.7
2	B	123	ILE	2.7
4	D	194	THR	2.7
5	L	143	ARG	2.7
1	A	270	ASP	2.7
7	G	88	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	45	GLU	2.7
6	N	70	VAL	2.7
3	J	69	THR	2.7
7	G	119	ASP	2.7
2	B	37	GLY	2.7
1	A	410	HIS	2.7
6	N	29	VAL	2.7
7	G	52	THR	2.7
4	D	105	SER	2.7
1	A	381	GLY	2.7
3	J	35	TYR	2.7
3	J	172	TYR	2.7
4	D	8	ASN	2.7
3	C	347	THR	2.7
3	C	210	PHE	2.7
4	D	215	ALA	2.6
4	D	249	ASP	2.6
7	O	58	ALA	2.6
8	M	679	ARG	2.6
4	D	7	ASN	2.6
3	J	114	GLY	2.6
8	M	390	ALA	2.6
1	H	374	ARG	2.6
2	B	8	VAL	2.6
8	M	423	ASP	2.6
2	I	256	GLY	2.6
2	B	276	VAL	2.6
3	C	334	VAL	2.6
4	K	258	SER	2.6
8	P	417	LEU	2.6
3	J	104	TRP	2.6
2	I	234	ALA	2.6
4	D	246	THR	2.6
7	G	62	PRO	2.6
3	C	185	TRP	2.6
1	H	272	GLY	2.6
2	B	119	ASN	2.6
1	H	288	ALA	2.6
3	C	216	ARG	2.6
6	N	6	ARG	2.6
8	M	482	VAL	2.6
2	I	174	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	K	213	ASP	2.6
8	P	560	ALA	2.6
1	A	369	THR	2.5
2	I	308	THR	2.5
8	M	634	THR	2.5
3	C	355	SER	2.5
5	L	172	SER	2.5
3	C	116	GLY	2.5
1	H	56	ASP	2.5
4	D	39	ASP	2.5
1	A	194	PRO	2.5
1	A	285	PRO	2.5
4	D	10	ILE	2.5
4	D	5	GLU	2.5
8	M	379	GLN	2.5
8	P	703	ASP	2.5
3	C	96	ASN	2.5
5	L	78	CYS	2.5
8	M	582	ASN	2.5
1	H	86	TRP	2.5
2	B	308	THR	2.5
3	J	264	ASP	2.5
5	L	74	TYR	2.5
8	M	641	ASP	2.5
1	A	173	GLY	2.5
1	H	181	ALA	2.5
8	P	578	SER	2.5
2	I	347	PRO	2.5
8	M	428	VAL	2.5
8	M	645	ARG	2.5
3	C	209	CYS	2.5
3	J	4	HIS	2.5
5	E	43	ASP	2.5
5	E	51	ALA	2.5
4	D	193	HIS	2.5
6	N	21	CYS	2.4
8	M	559	LEU	2.4
8	P	713	GLU	2.4
4	D	173	ASP	2.4
8	M	664	MET	2.4
1	H	196	ALA	2.4
7	O	149	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	211	GLU	2.4
5	L	27	GLN	2.4
4	D	248	ARG	2.4
2	B	106	LYS	2.4
1	H	117	LEU	2.4
4	D	212	THR	2.4
1	H	67	ILE	2.4
1	A	370	HIS	2.4
4	D	145	HIS	2.4
1	A	25	THR	2.4
2	B	379	GLN	2.4
8	M	574	MET	2.4
2	I	118	LYS	2.4
1	H	66	ALA	2.4
3	J	223	ASP	2.4
3	C	211	SER	2.4
3	J	340	ALA	2.4
4	K	257	CYS	2.4
5	E	47	TYR	2.4
7	O	111	TYR	2.4
1	H	38	LYS	2.4
1	A	218	GLU	2.4
8	P	656	LEU	2.4
1	A	214	GLY	2.4
5	L	174	SER	2.4
3	J	227	CYS	2.4
5	E	12	ASP	2.4
3	C	188	LYS	2.4
5	L	79	LEU	2.4
6	N	24	ASN	2.4
7	G	61	ASN	2.4
2	B	96	GLU	2.3
7	O	12	ARG	2.3
8	P	450	MET	2.3
5	L	86	ASN	2.3
3	J	256	SER	2.3
1	H	57	ASP	2.3
2	B	112	PRO	2.3
8	M	502	CYS	2.3
8	P	433	CYS	2.3
4	K	260	ALA	2.3
6	F	120	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
8	M	568	ALA	2.3
1	H	58	LEU	2.3
2	I	287	GLN	2.3
2	I	354	VAL	2.3
8	M	464	PHE	2.3
2	B	367	ASP	2.3
1	H	235	CYS	2.3
3	C	91	VAL	2.3
3	C	102	VAL	2.3
5	L	80	LYS	2.3
2	B	159	SER	2.3
3	J	115	SER	2.3
1	A	141	ILE	2.3
3	C	152	PRO	2.3
1	A	413	VAL	2.3
3	C	70	CYS	2.3
4	K	146	TYR	2.3
1	H	37	ILE	2.3
2	I	307	SER	2.3
1	A	345	ALA	2.3
7	G	58	ALA	2.3
8	P	563	LEU	2.3
1	H	278	GLY	2.2
2	B	116	PRO	2.2
6	N	18	ALA	2.2
2	I	244	TYR	2.2
1	A	335	LEU	2.2
7	O	80	LEU	2.2
2	I	243	SER	2.2
8	M	476	SER	2.2
1	H	210	ASP	2.2
2	B	111	GLU	2.2
5	L	40	ASP	2.2
1	H	253	ILE	2.2
4	D	242	ASN	2.2
8	M	680	LEU	2.2
1	A	183	GLY	2.2
7	G	151	VAL	2.2
2	B	120	ARG	2.2
4	K	108	SER	2.2
2	B	297	PHE	2.2
7	G	99	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	9	ARG	2.2
7	O	107	MET	2.2
1	H	283	PHE	2.2
8	P	430	LYS	2.2
8	M	515	GLY	2.2
8	P	627	THR	2.2
8	P	601	VAL	2.2
2	B	180	ARG	2.2
7	O	31	GLY	2.2
5	E	2	PRO	2.2
6	N	120	ASN	2.2
2	I	212	THR	2.2
2	I	303	LEU	2.2
8	M	421	LEU	2.2
1	A	343	VAL	2.2
4	K	124	VAL	2.2
6	N	28	GLN	2.2
8	P	449	GLN	2.2
2	I	236	GLU	2.2
1	A	54	GLY	2.1
6	N	36	PRO	2.1
7	G	57	ALA	2.1
7	O	90	ASP	2.1
3	J	56	THR	2.1
6	N	33	HIS	2.1
3	J	5	SER	2.1
4	D	82	SER	2.1
2	I	328	ARG	2.1
1	H	90	GLU	2.1
8	P	516	GLU	2.1
8	P	548	GLU	2.1
6	N	25	PHE	2.1
3	C	17	ASN	2.1
2	B	9	VAL	2.1
2	I	200	ARG	2.1
3	C	103	ARG	2.1
6	N	8	TYR	2.1
3	C	229	ALA	2.1
3	C	241	ALA	2.1
3	J	209	CYS	2.1
4	D	209	LEU	2.1
2	B	12	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	154	THR	2.1
4	K	128	TYR	2.1
3	J	171	ALA	2.1
8	P	689	ARG	2.1
8	M	520	TYR	2.1
8	P	633	HIS	2.1
3	J	12	SER	2.1
3	J	242	SER	2.1
6	F	158	ARG	2.1
8	M	700	CYS	2.1
8	M	627	THR	2.1
5	L	138	GLN	2.1
3	C	42	TRP	2.1
1	H	416	VAL	2.1
8	M	518	VAL	2.1
4	D	238	ASP	2.1
1	H	125	TYR	2.1
3	J	320	GLY	2.1
1	A	241	GLU	2.1
2	B	348	PRO	2.1
5	L	130	ARG	2.0
6	N	105	ARG	2.0
3	C	149	ASP	2.0
8	P	561	LEU	2.0
1	H	371	HIS	2.0
8	M	410	ILE	2.0
1	H	119	THR	2.0
2	I	284	ASN	2.0
2	B	295	SER	2.0
3	C	115	SER	2.0
8	M	501	LEU	2.0
1	A	11	ASP	2.0
4	D	174	ASP	2.0
5	E	64	ALA	2.0
6	N	19	ALA	2.0
1	H	113	THR	2.0
1	H	114	GLU	2.0
3	J	198	SER	2.0
8	M	561	LEU	2.0
2	B	166	ILE	2.0
2	B	165	HIS	2.0
4	K	238	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	J	250	VAL	2.0
1	H	326	THR	2.0
1	H	188	SER	2.0
4	D	166	SER	2.0
6	F	43	SER	2.0
1	H	242	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

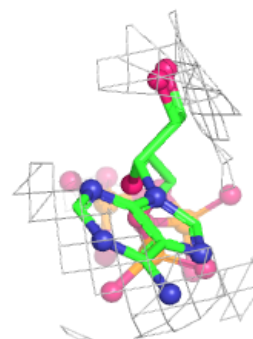
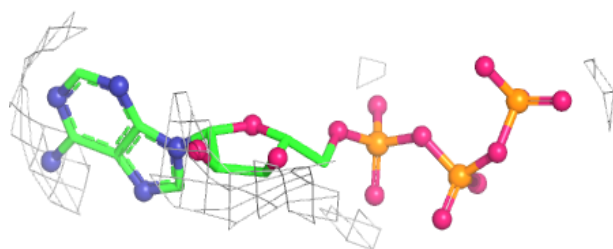
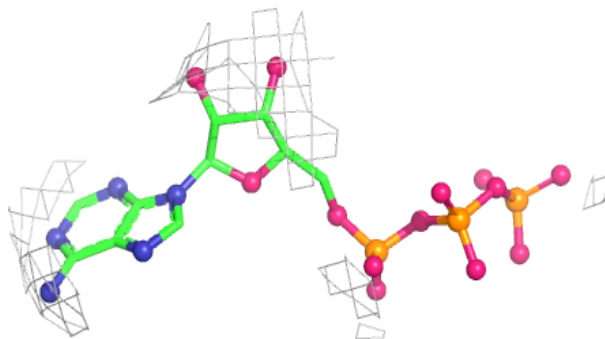
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	ATP	I	502	31/31	0.78	0.11	177,240,301,313	0
12	ATP	H	502	31/31	0.80	0.20	129,147,198,226	0
11	CA	I	501	1/1	0.87	0.10	301,301,301,301	0
12	ATP	B	502	31/31	0.89	0.14	100,117,145,151	0
12	ATP	A	502	31/31	0.90	0.14	106,119,162,181	0
11	CA	H	501	1/1	0.93	0.31	144,144,144,144	0
11	CA	A	501	1/1	0.96	0.26	87,87,87,87	0
11	CA	B	501	1/1	0.97	0.17	116,116,116,116	0

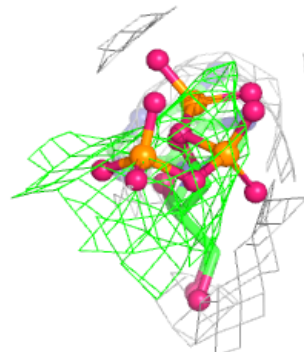
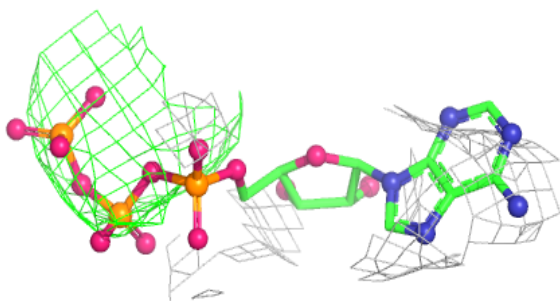
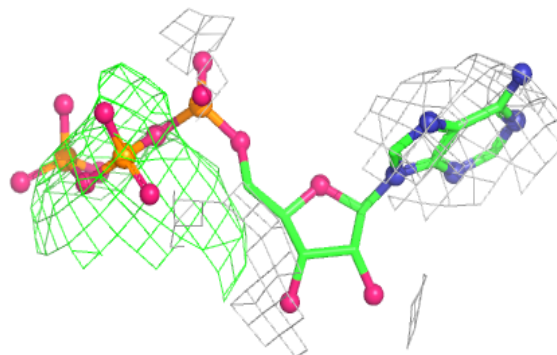
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP I 502:

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

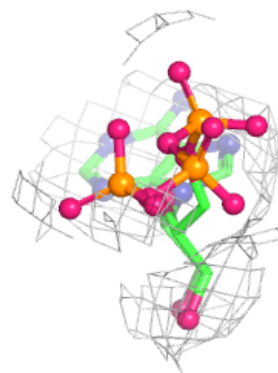
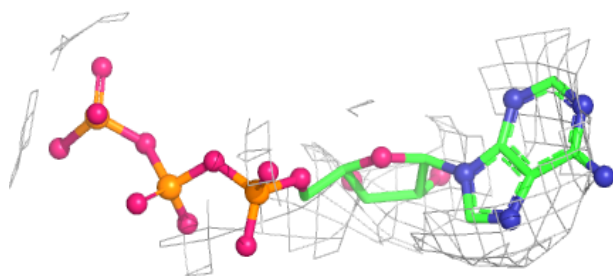
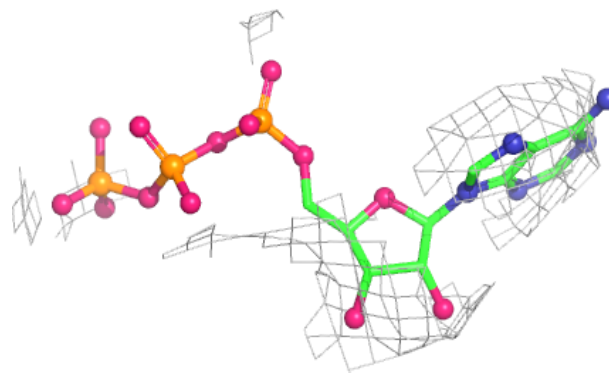
**Electron density around ATP H 502:**

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

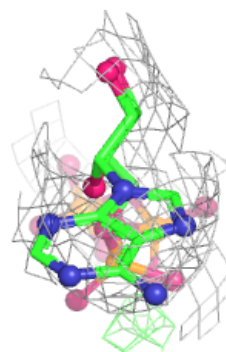
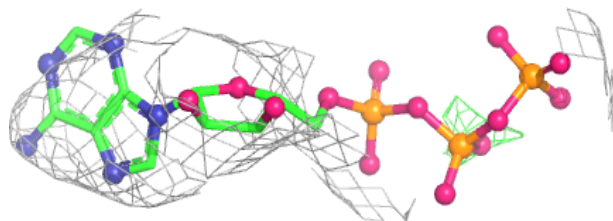
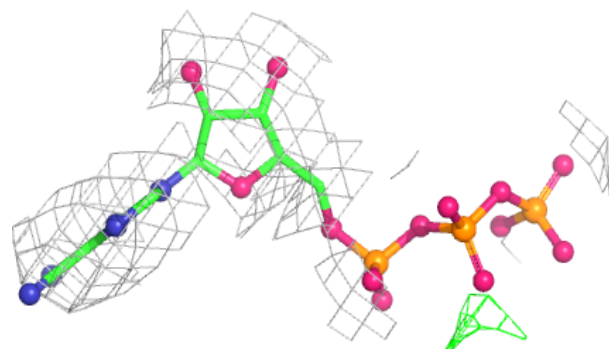


Electron density around ATP B 502:

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

**Electron density around ATP A 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.