



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:26 AM UTC

PDB ID : 5A99 / pdb_00005a99
Title : Crystal structure of Operophtera brumata CPV19 polyhedra
Authors : Ji, X.; Axford, D.; Owen, R.; Evans, G.; Ginn, H.M.; Sutton, G.; Stuart, D.I.
Deposited on : 2015-07-17
Resolution : 1.51 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

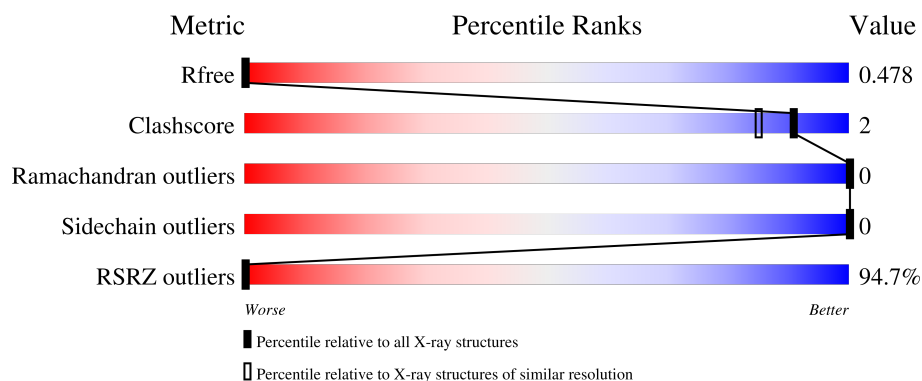
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	248	94% 96% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4299 atoms, of which 1974 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.

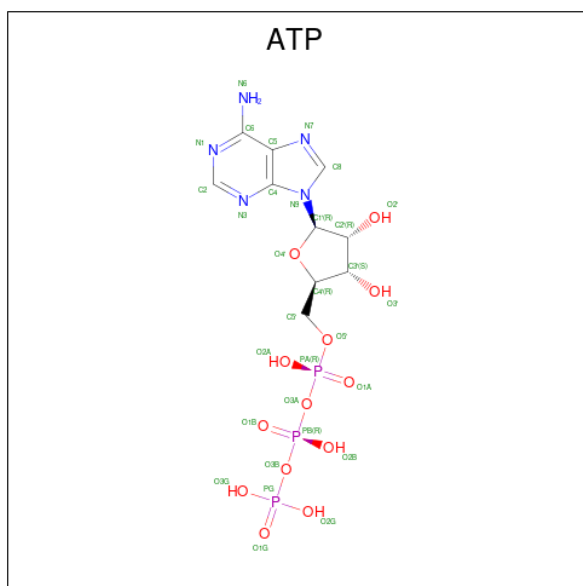
- Molecule 1 is a protein called Polyhedrin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	248	4020	1300	1962	369	382	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	expression tag	UNP Q30C66

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	43	10	12	5	13	3	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

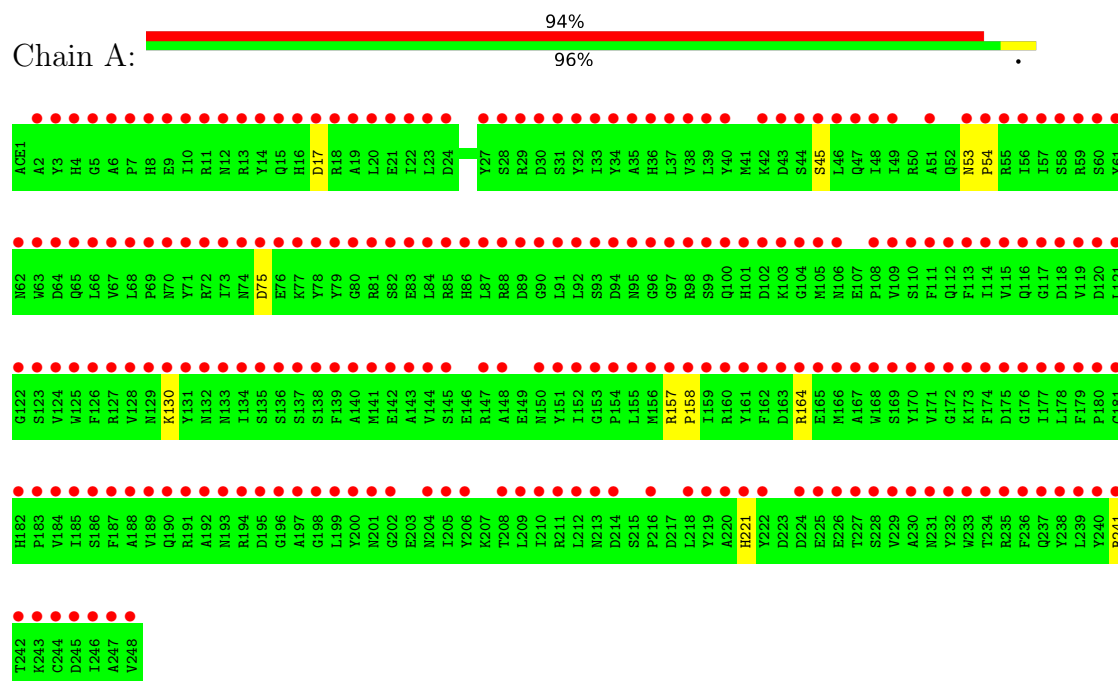
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total 235	O 235	0	0

3 Residue-property plots

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: Polyhedrin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	102.72Å 102.72Å 102.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.94 – 1.51 41.94 – 1.51	Depositor EDS
% Data completeness (in resolution range)	74.0 (41.94-1.51) 74.0 (41.94-1.51)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.228 0.463 , 0.478	Depositor DCC
R_{free} test set	1045 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 174.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.058 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	4299	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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: ACE, ATP, MG

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	0.44	0/2110	0.75	0/2856

There are no bond length outliers.

There are no bond angle outliers.

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	2058	1962	1959	7	2
2	A	31	12	12	0	1
3	A	1	0	0	0	0
4	A	235	0	0	3	1
All	All	2325	1974	1971	7	3

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 2.

All (7) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:NH1	4:A:2040:HOH:O	2.15	0.79
1:A:164:ARG:NH1	4:A:2025:HOH:O	2.20	0.73
1:A:130:LYS:HD2	4:A:2154:HOH:O	2.06	0.56
1:A:53:ASN:CG	1:A:54:PRO:HD2	2.35	0.51
1:A:45:SER:OG	1:A:221:HIS:HE1	1.96	0.48
1:A:75:ASP:OD2	1:A:221:HIS:HD2	1.97	0.48
1:A:157:ARG:HA	1:A:158:PRO:HD3	1.86	0.43

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2042:HOH:O	4:A:2214:HOH:O[22_555]	1.70	0.50
1:A:241:ARG:HH12	2:A:1250:ATP:O1G[2_665]	1.55	0.05
1:A:17:ASP:OD2	1:A:17:ASP:OD2[4_565]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	246/248 (99%)	236 (96%)	10 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	218/218 (100%)	218 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	A	1250	3	32,33,33	1.47	7 (21%)	48,52,52	1.73	10 (20%)

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
2	ATP	A	1250	3	-	4/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ATP	C5-C4	4.83	1.47	1.39
2	A	1250	ATP	PA-O3A	2.63	1.62	1.59
2	A	1250	ATP	C8-N7	2.44	1.36	1.31
2	A	1250	ATP	C5-C6	2.37	1.47	1.41
2	A	1250	ATP	C5-N7	-2.29	1.34	1.39
2	A	1250	ATP	PB-O3A	2.16	1.61	1.59
2	A	1250	ATP	C4-N9	-2.08	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ATP	C5-C4-N3	-5.55	119.07	126.72
2	A	1250	ATP	N3-C4-N9	4.86	135.43	127.17
2	A	1250	ATP	C2-N3-C4	3.56	120.52	111.83
2	A	1250	ATP	N3-C2-N1	-3.47	123.33	128.58
2	A	1250	ATP	C4-N9-C8	3.31	109.21	105.74
2	A	1250	ATP	C4-C5-N7	-2.70	107.50	110.58
2	A	1250	ATP	C5-N7-C8	2.21	106.92	103.45
2	A	1250	ATP	N9-C8-N7	-2.17	110.86	113.94
2	A	1250	ATP	O3G-PG-O2G	2.08	115.62	107.80
2	A	1250	ATP	C2-N1-C6	2.04	122.07	118.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

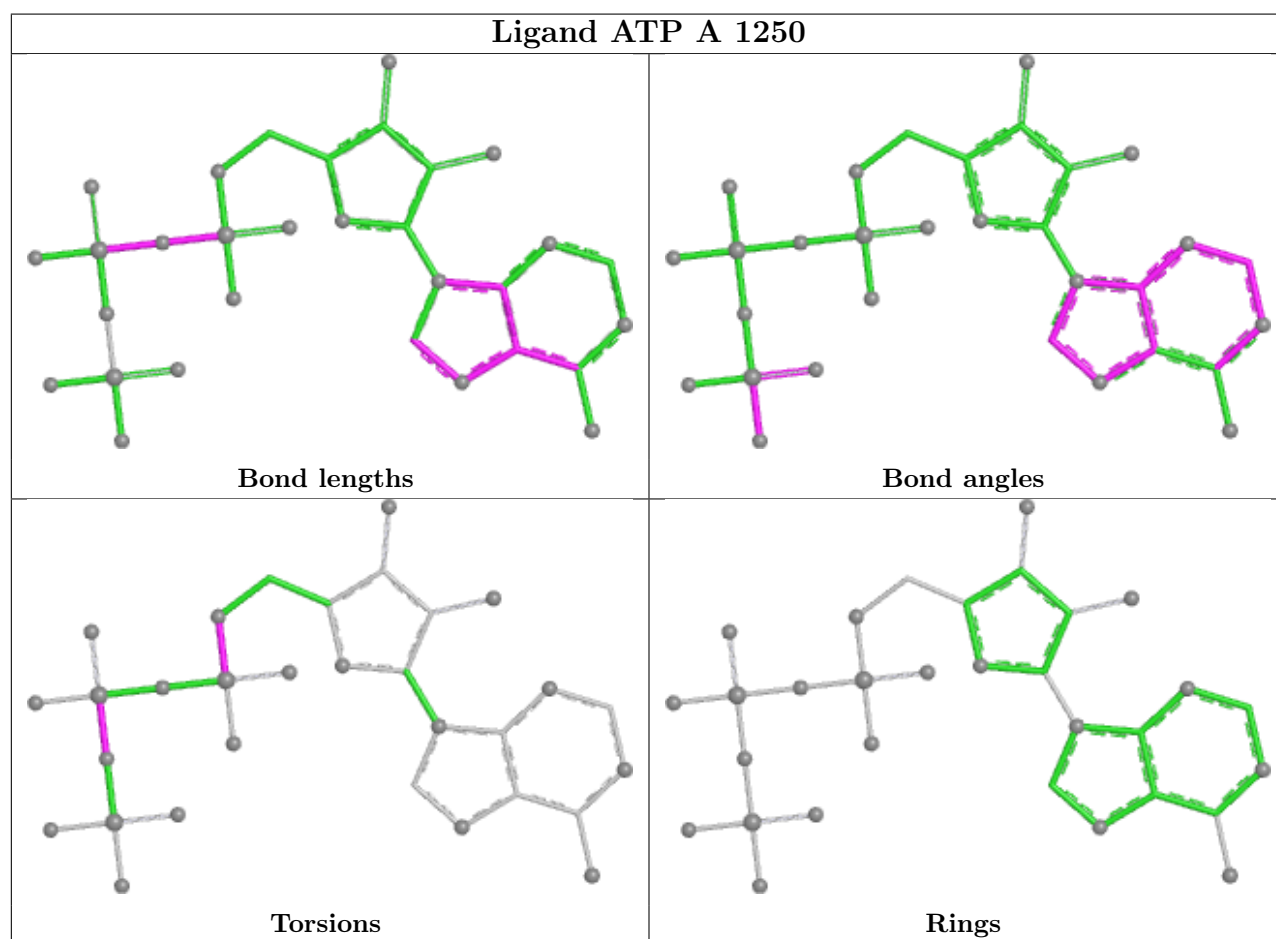
Mol	Chain	Res	Type	Atoms
2	A	1250	ATP	C5'-O5'-PA-O1A
2	A	1250	ATP	C5'-O5'-PA-O2A
2	A	1250	ATP	C5'-O5'-PA-O3A
2	A	1250	ATP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1250	ATP	0	1

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 ⓘ

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	247/248 (99%)	4.53	234 (94%) 0 0	10, 15, 26, 36	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	9.6
1	A	115	VAL	9.2
1	A	87	LEU	8.8
1	A	40	TYR	8.8
1	A	164	ARG	8.7
1	A	10	ILE	8.6
1	A	3	TYR	8.1
1	A	66	LEU	8.0
1	A	91	LEU	7.9
1	A	37	LEU	7.7
1	A	54	PRO	7.4
1	A	84	LEU	7.3
1	A	139	PHE	7.2
1	A	236	PHE	7.1
1	A	128	VAL	7.1
1	A	222	TYR	7.0
1	A	171	VAL	7.0
1	A	197	ALA	7.0
1	A	22	ILE	7.0
1	A	188	ALA	6.9
1	A	192	ALA	6.9
1	A	246	ILE	6.9
1	A	151	TYR	6.9
1	A	114	ILE	6.9
1	A	23	LEU	6.7
1	A	14	TYR	6.7
1	A	77	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	123	SER	6.5
1	A	196	GLY	6.5
1	A	144	VAL	6.4
1	A	73	ILE	6.3
1	A	166	MET	6.3
1	A	32	TYR	6.3
1	A	75	ASP	6.3
1	A	210	ILE	6.3
1	A	229	VAL	6.3
1	A	227	THR	6.2
1	A	20	LEU	6.2
1	A	68	LEU	6.2
1	A	189	VAL	6.1
1	A	33	ILE	6.1
1	A	198	GLY	6.1
1	A	208	THR	6.0
1	A	240	TYR	6.0
1	A	168	TRP	5.9
1	A	16	HIS	5.9
1	A	5	GLY	5.9
1	A	46	LEU	5.9
1	A	63	TRP	5.9
1	A	82	SER	5.9
1	A	51	ALA	5.8
1	A	219	TYR	5.8
1	A	157	ARG	5.8
1	A	119	VAL	5.8
1	A	7	PRO	5.7
1	A	161	TYR	5.7
1	A	69	PRO	5.7
1	A	34	TYR	5.7
1	A	244	CYS	5.6
1	A	28	SER	5.6
1	A	155	LEU	5.6
1	A	103	LYS	5.6
1	A	130	LYS	5.6
1	A	218	LEU	5.5
1	A	19	ALA	5.4
1	A	79	TYR	5.4
1	A	183	PRO	5.4
1	A	140	ALA	5.4
1	A	243	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	71	TYR	5.3
1	A	200	TYR	5.3
1	A	121	LEU	5.3
1	A	206	TYR	5.3
1	A	74	ASN	5.2
1	A	108	PRO	5.2
1	A	134	ILE	5.2
1	A	141	MET	5.2
1	A	174	PHE	5.2
1	A	158	PRO	5.2
1	A	61	TYR	5.2
1	A	49	ILE	5.2
1	A	181	CYS	5.2
1	A	228	SER	5.1
1	A	18	ARG	5.1
1	A	97	GLY	5.1
1	A	124	VAL	5.1
1	A	170	TYR	5.1
1	A	125	TRP	5.0
1	A	45	SER	5.0
1	A	152	ILE	5.0
1	A	29	ARG	5.0
1	A	148	ALA	5.0
1	A	180	PRO	4.9
1	A	60	SER	4.9
1	A	72	ARG	4.9
1	A	111	PHE	4.9
1	A	131	TYR	4.9
1	A	12	ASN	4.9
1	A	44	SER	4.8
1	A	27	TYR	4.8
1	A	247	ALA	4.8
1	A	163	ASP	4.8
1	A	232	TYR	4.8
1	A	62	ASN	4.8
1	A	92	LEU	4.7
1	A	80	GLY	4.7
1	A	117	GLY	4.7
1	A	160	ARG	4.7
1	A	248	VAL	4.7
1	A	154	PRO	4.7
1	A	234	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	233	TRP	4.6
1	A	159	ILE	4.6
1	A	4	HIS	4.6
1	A	47	GLN	4.6
1	A	9	GLU	4.5
1	A	6	ALA	4.5
1	A	235	ARG	4.5
1	A	101	HIS	4.5
1	A	165	GLU	4.5
1	A	67	VAL	4.5
1	A	133	ASN	4.5
1	A	64	ASP	4.5
1	A	241	ARG	4.5
1	A	126	PHE	4.4
1	A	209	LEU	4.4
1	A	177	ILE	4.4
1	A	212	LEU	4.4
1	A	53	ASN	4.4
1	A	179	PHE	4.4
1	A	2	ALA	4.3
1	A	83	GLU	4.3
1	A	191	ARG	4.3
1	A	220	ALA	4.3
1	A	113	PHE	4.3
1	A	238	TYR	4.2
1	A	201	ASN	4.2
1	A	81	ARG	4.2
1	A	143	ALA	4.2
1	A	78	TYR	4.1
1	A	70	ASN	4.1
1	A	30	ASP	4.1
1	A	38	VAL	4.1
1	A	39	LEU	4.1
1	A	162	PHE	4.0
1	A	35	ALA	4.0
1	A	175	ASP	4.0
1	A	58	SER	4.0
1	A	187	PHE	4.0
1	A	216	PRO	4.0
1	A	118	ASP	3.9
1	A	48	ILE	3.9
1	A	176	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	86	HIS	3.9
1	A	184	VAL	3.9
1	A	231	ASN	3.9
1	A	57	ILE	3.8
1	A	225	GLU	3.8
1	A	182	HIS	3.8
1	A	205	ILE	3.7
1	A	239	LEU	3.7
1	A	85	ARG	3.7
1	A	138	SER	3.7
1	A	109	VAL	3.6
1	A	104	GLY	3.6
1	A	76	GLU	3.6
1	A	136	SER	3.6
1	A	169	SER	3.6
1	A	145	SER	3.6
1	A	224	ASP	3.6
1	A	89	ASP	3.6
1	A	135	SER	3.6
1	A	245	ASP	3.6
1	A	100	GLN	3.6
1	A	242	THR	3.5
1	A	221	HIS	3.5
1	A	237	GLN	3.5
1	A	94	ASP	3.5
1	A	167	ALA	3.5
1	A	17	ASP	3.5
1	A	214	ASP	3.5
1	A	185	ILE	3.5
1	A	21	GLU	3.5
1	A	226	GLU	3.4
1	A	90	GLY	3.4
1	A	8	HIS	3.4
1	A	95	ASN	3.4
1	A	31	SER	3.3
1	A	15	GLN	3.3
1	A	132	ASN	3.3
1	A	102	ASP	3.3
1	A	147	ARG	3.3
1	A	199	LEU	3.3
1	A	195	ASP	3.3
1	A	13	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	11	ARG	3.2
1	A	194	ARG	3.2
1	A	204	ASN	3.2
1	A	137	SER	3.2
1	A	202	GLY	3.2
1	A	173	LYS	3.1
1	A	116	GLN	3.1
1	A	59	ARG	3.1
1	A	88	ARG	3.0
1	A	110	SER	3.0
1	A	65	GLN	3.0
1	A	156	MET	3.0
1	A	150	ASN	2.9
1	A	96	GLY	2.9
1	A	56	ILE	2.9
1	A	211	ARG	2.9
1	A	36	HIS	2.9
1	A	105	MET	2.8
1	A	127	ARG	2.8
1	A	112	GLN	2.8
1	A	153	GLY	2.8
1	A	93	SER	2.7
1	A	230	ALA	2.6
1	A	99	SER	2.6
1	A	122	GLY	2.6
1	A	186	SER	2.6
1	A	190	GLN	2.5
1	A	142	GLU	2.4
1	A	42	LYS	2.4
1	A	213	ASN	2.4
1	A	24	ASP	2.4
1	A	106	ASN	2.4
1	A	172	GLY	2.3
1	A	120	ASP	2.3
1	A	193	ASN	2.3
1	A	55	ARG	2.2
1	A	98	ARG	2.2
1	A	43	ASP	2.0
1	A	129	ASN	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](#)

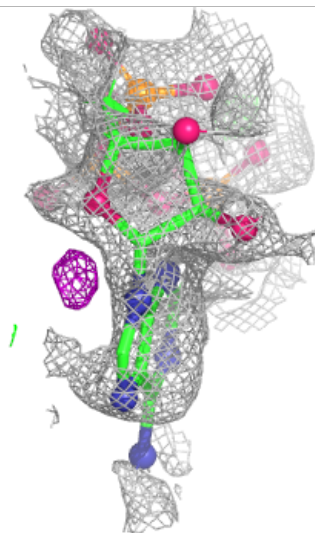
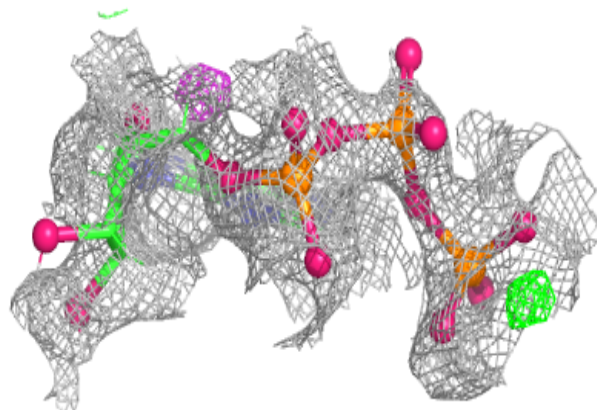
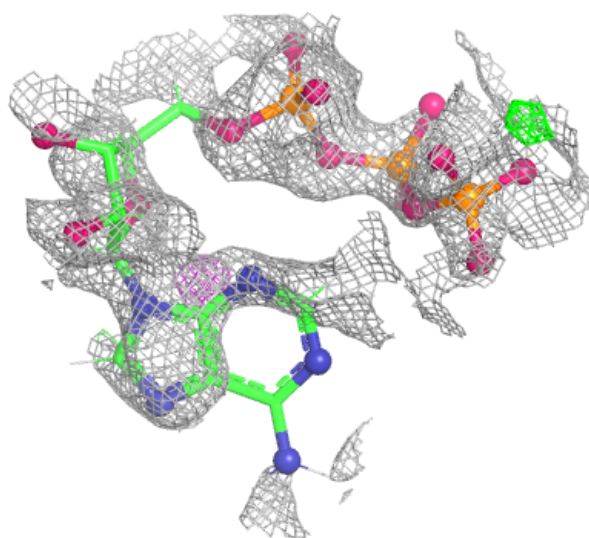
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	A	1250	31/31	0.65	0.22	12,19,29,34	0
3	MG	A	1251	1/1	0.76	0.12	17,17,17,17	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 A 1250:

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.