



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2026 – 12:16 PM EDT

PDB ID : 36ZL / pdb_000036zl
Title : Structure of Bacteroides thetaiotaomicron ATP:cob(I)alamin adenosyltransferase (ATR or BtuR, BT2760) bound to cob(II)alamin and ATP
Authors : Mascarenhas, R.; Maurya, B.
Deposited on : 2026-07-07
Resolution : 2.20 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

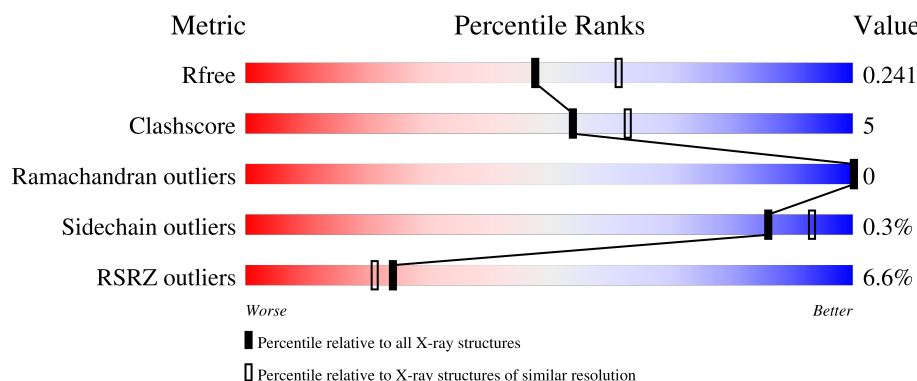
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	187	2% 88% 10% .
1	B	187	6% 70% 12% 19%
1	C	187	6% 91% 9% .
1	D	187	3% 87% 10% .
1	E	187	8% 78% 9% 13%

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Mol	Chain	Length	Quality of chain
1	F	187	

2 Entry composition [i](#)

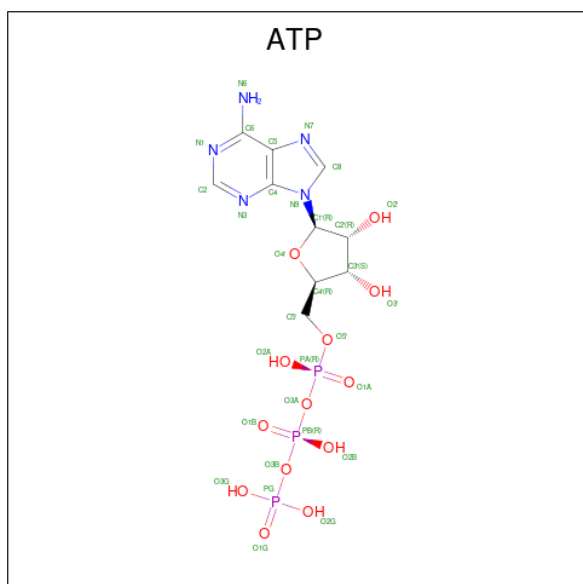
There are 8 unique types of molecules in this entry. The entry contains 8311 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Corrinoid adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1432	901	250	276	5			
1	B	152	Total	C	N	O	S	0	0	0
			1192	755	203	229	5			
1	C	186	Total	C	N	O	S	0	0	0
			1455	915	254	280	6			
1	D	180	Total	C	N	O	S	0	0	0
			1411	891	242	273	5			
1	E	162	Total	C	N	O	S	0	0	0
			1282	804	225	248	5			
1	F	144	Total	C	N	O	S	0	0	0
			1150	730	198	217	5			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

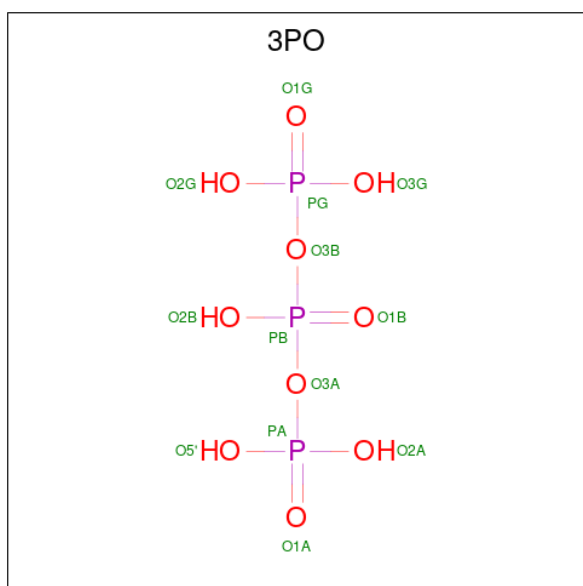


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		

- Molecule 4 is TRIPHOSPHATE (CCD ID: 3PO) (formula: $\text{H}_5\text{O}_{10}\text{P}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			13	10	3		
4	E	1	Total	O	P	0	0
			13	10	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

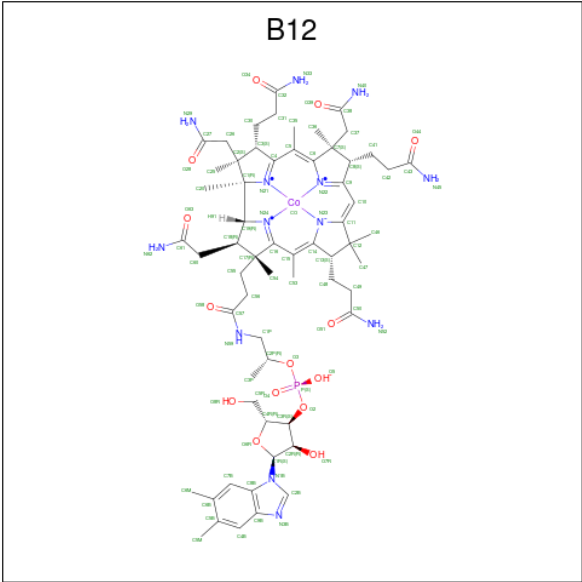
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
7	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

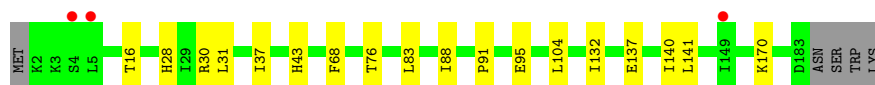
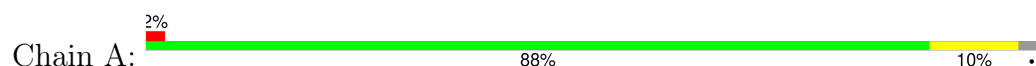
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	18	Total	O	0	0
			18	18		
8	B	9	Total	O	0	0
			9	9		
8	C	20	Total	O	0	0
			20	20		
8	D	18	Total	O	0	0
			18	18		
8	E	6	Total	O	0	0
			6	6		
8	F	2	Total	O	0	0
			2	2		

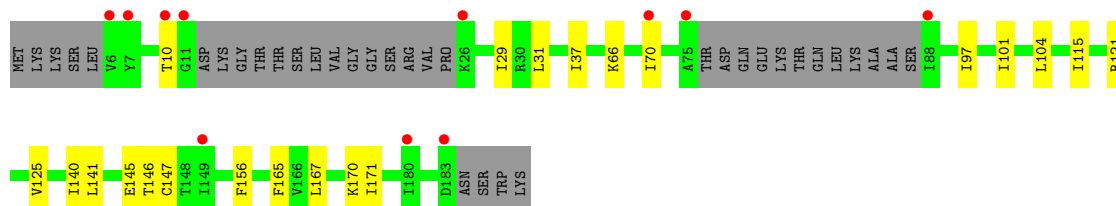
3 Residue-property plots [i](#)

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.

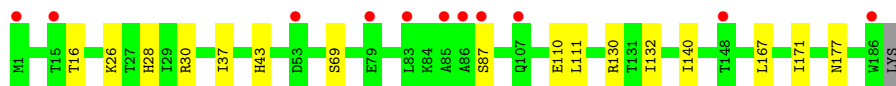
• Molecule 1: Corrinoide adenosyltransferase



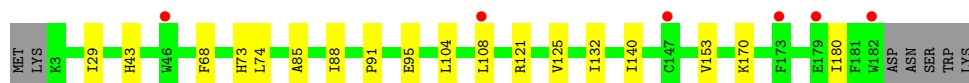
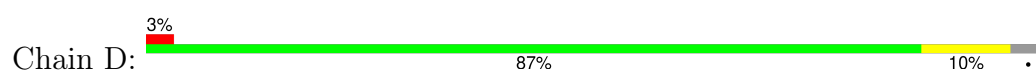
• Molecule 1: Corrinoide adenosyltransferase



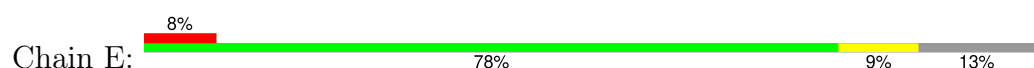
• Molecule 1: Corrinoide adenosyltransferase

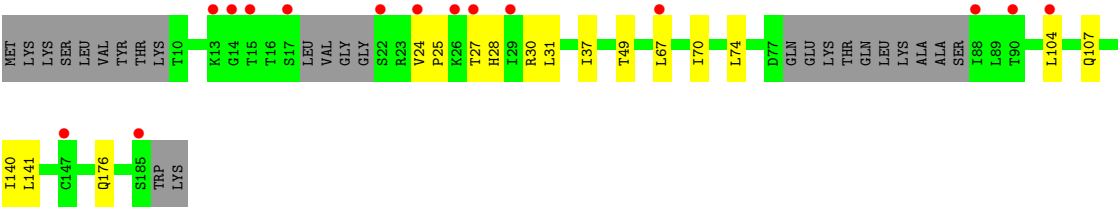


• Molecule 1: Corrinoide adenosyltransferase

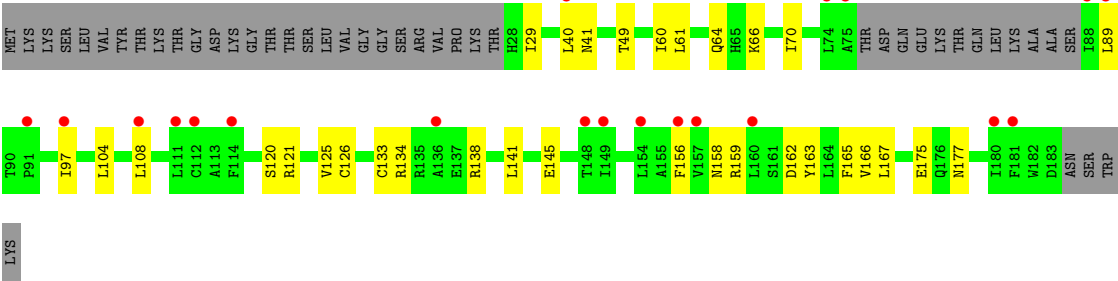


• Molecule 1: Corrinoide adenosyltransferase





● Molecule 1: Corrionid adenosyltransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.22Å 81.86Å 111.18Å 90.00° 102.78° 90.00°	Depositor
Resolution (Å)	45.20 – 2.20 45.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.20-2.20) 98.9 (45.20-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.20Å)	Xtriage
Refinement program	PHENIX (2.0_5936: ???)	Depositor
R, R_{free}	0.204 , 0.241 0.205 , 0.241	Depositor DCC
R_{free} test set	2795 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8311	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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: K, ATP, B12, SO4, MG, 3PO

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	0.24	0/1456	0.46	0/1973
1	B	0.20	0/1211	0.37	0/1642
1	C	0.21	0/1479	0.41	0/2003
1	D	0.21	0/1435	0.42	0/1945
1	E	0.22	0/1303	0.45	0/1765
1	F	0.14	0/1171	0.35	0/1588
All	All	0.21	0/8055	0.41	0/10916

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	1432	0	1419	9	0
1	B	1192	0	1154	11	0
1	C	1455	0	1443	10	0
1	D	1411	0	1400	12	0
1	E	1282	0	1247	11	0
1	F	1150	0	1122	22	0
2	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	B	13	0	0	0	0
4	E	13	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	C	5	0	0	0	0
6	F	5	0	0	0	0
7	C	91	0	88	7	0
7	E	91	0	88	5	0
8	A	18	0	0	0	0
8	B	9	0	0	0	0
8	C	20	0	0	0	0
8	D	18	0	0	0	0
8	E	6	0	0	0	0
8	F	2	0	0	0	0
All	All	8311	0	7997	80	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 5.

All (80) 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:C:37:ILE:HD11	1:C:140:ILE:HD11	1.71	0.71
1:D:29:ILE:H	1:D:29:ILE:HD12	1.60	0.66
1:E:104:LEU:HA	1:E:107:GLN:HE22	1.62	0.65
7:C:204:B12:H531	7:C:204:B12:H543	1.79	0.64
7:E:202:B12:H543	7:E:202:B12:H531	1.80	0.62
1:B:66:LYS:O	1:B:70:ILE:HG13	2.00	0.61
1:D:91:PRO:O	1:D:95:GLU:HG3	2.02	0.59
1:E:28:HIS:HB3	1:E:31:LEU:HD23	1.84	0.59
1:A:104:LEU:HD22	1:A:170:LYS:HD2	1.85	0.58
7:C:204:B12:H351	7:C:204:B12:H362	1.84	0.58
1:A:16:THR:HG21	1:A:31:LEU:HD21	1.85	0.58
1:D:108:LEU:HD21	1:D:170:LYS:HA	1.84	0.57
1:F:29:ILE:HD12	1:F:29:ILE:H	1.69	0.57
7:E:202:B12:H362	7:E:202:B12:H351	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:SER:HB3	1:F:177:ASN:ND2	2.20	0.56
1:E:37:ILE:HG23	1:E:67:LEU:HD12	1.87	0.56
1:B:37:ILE:HD11	1:B:140:ILE:HD11	1.87	0.56
1:F:126:CYS:SG	1:F:167:LEU:HD22	2.47	0.55
1:A:137:GLU:O	1:A:141:LEU:HD13	2.08	0.53
7:C:204:B12:H8	7:C:204:B12:N40	2.24	0.53
1:F:66:LYS:O	1:F:70:ILE:HG13	2.10	0.52
1:A:68:PHE:HA	7:C:204:B12:H522	1.74	0.52
1:D:121:ARG:HA	1:F:49:THR:HG21	1.92	0.52
1:F:60:ILE:O	1:F:64:GLN:HG3	2.10	0.51
1:C:130:ARG:HD2	7:C:204:B12:H402	1.75	0.51
1:F:121:ARG:O	1:F:125:VAL:HG23	2.10	0.51
7:C:204:B12:H8	7:C:204:B12:H401	1.75	0.50
7:E:202:B12:H251	7:E:202:B12:H291	1.75	0.50
1:D:68:PHE:HA	7:E:202:B12:H522	1.75	0.50
7:E:202:B12:H59	7:E:202:B12:H5R2	1.76	0.50
1:B:167:LEU:O	1:B:171:ILE:HG13	2.11	0.49
1:F:141:LEU:O	1:F:145:GLU:HG3	2.11	0.49
1:D:180:ILE:HD13	1:F:61:LEU:HD11	1.94	0.49
1:B:141:LEU:O	1:B:145:GLU:HG3	2.13	0.48
1:F:104:LEU:O	1:F:108:LEU:HD23	2.13	0.48
1:F:158:ASN:HD22	1:F:159:ARG:NH1	2.11	0.47
1:C:110:GLU:HG3	1:E:176:GLN:OE1	2.14	0.47
1:C:28:HIS:CE1	1:C:30:ARG:HG3	2.49	0.47
1:B:97:ILE:HD11	1:B:156:PHE:CE2	2.50	0.47
1:A:76:THR:HG21	1:A:83:LEU:HD12	1.97	0.47
1:F:97:ILE:HD11	1:F:156:PHE:CE2	2.51	0.46
1:A:91:PRO:O	1:A:95:GLU:HG3	2.15	0.46
1:F:175:GLU:HB2	1:F:177:ASN:ND2	2.31	0.45
1:D:73:HIS:CD2	1:D:153:VAL:HG21	2.52	0.45
1:B:29:ILE:HD11	1:B:146:THR:HG21	1.97	0.45
1:E:28:HIS:CE1	1:E:30:ARG:HG3	2.51	0.45
1:F:89:LEU:HD12	1:F:89:LEU:HA	1.81	0.45
1:C:69:SER:HB3	1:C:87:SER:HA	1.98	0.45
1:D:85:ALA:HA	1:D:88:ILE:HD12	1.98	0.45
1:E:70:ILE:O	1:E:74:LEU:HG	2.17	0.45
1:D:43:HIS:CE1	1:D:132:ILE:HD13	2.51	0.45
1:C:16:THR:HB	1:C:26:LYS:HE3	1.98	0.44
1:F:163:TYR:CZ	1:F:167:LEU:HD12	2.53	0.44
1:B:115:ILE:HD11	1:B:165:PHE:CZ	2.52	0.43
1:B:97:ILE:O	1:B:101:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:LEU:O	1:F:41:ASN:CB	2.66	0.43
1:A:28:HIS:CE1	1:A:30:ARG:HG3	2.54	0.43
1:D:104:LEU:HD22	1:D:170:LYS:HE3	2.01	0.43
1:E:49:THR:HG21	1:F:121:ARG:HA	2.00	0.43
1:C:43:HIS:CE1	1:C:132:ILE:HD13	2.54	0.42
1:E:25:PRO:C	1:E:27:THR:H	2.27	0.42
1:A:43:HIS:CE1	1:A:132:ILE:HD13	2.55	0.42
1:B:146:THR:HG23	1:B:147:CYS:SG	2.59	0.41
1:E:24:VAL:HG21	1:E:31:LEU:HD21	2.02	0.41
1:A:37:ILE:HD11	1:A:140:ILE:HD11	2.02	0.41
1:B:121:ARG:O	1:B:125:VAL:HG23	2.20	0.41
1:B:104:LEU:HG	1:B:170:LYS:HD2	2.03	0.41
1:E:141:LEU:HA	1:E:141:LEU:HD23	1.88	0.41
1:C:177:ASN:HD22	1:C:177:ASN:HA	1.75	0.41
1:E:37:ILE:HD11	1:E:140:ILE:HD11	2.02	0.41
1:C:167:LEU:O	1:C:171:ILE:HG13	2.20	0.41
1:D:74:LEU:HD11	1:D:140:ILE:HG12	2.02	0.41
1:F:40:LEU:HD22	1:F:133:CYS:HA	2.03	0.41
1:F:134:ARG:O	1:F:138:ARG:HG3	2.20	0.41
1:F:162:ASP:O	1:F:166:VAL:HG23	2.21	0.41
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.81	0.40
1:D:121:ARG:O	1:D:125:VAL:HG23	2.21	0.40
1:F:158:ASN:HD22	1:F:159:ARG:HH12	1.68	0.40
7:C:204:B12:H301	7:C:204:B12:H203	2.04	0.40
1:F:165:PHE:C	1:F:165:PHE:CD1	2.99	0.40

There are no symmetry-related clashes.

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	180/187 (96%)	179 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	146/187 (78%)	144 (99%)	2 (1%)	0	100	100
1	C	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
1	D	178/187 (95%)	178 (100%)	0	0	100	100
1	E	156/187 (83%)	155 (99%)	1 (1%)	0	100	100
1	F	140/187 (75%)	139 (99%)	1 (1%)	0	100	100
All	All	984/1122 (88%)	975 (99%)	9 (1%)	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	158/167 (95%)	157 (99%)	1 (1%)	78	89
1	B	129/167 (77%)	127 (98%)	2 (2%)	55	71
1	C	160/167 (96%)	160 (100%)	0	100	100
1	D	156/167 (93%)	156 (100%)	0	100	100
1	E	142/167 (85%)	142 (100%)	0	100	100
1	F	126/167 (75%)	126 (100%)	0	100	100
All	All	871/1002 (87%)	868 (100%)	3 (0%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ILE
1	B	10	THR
1	B	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	C	177	ASN
1	D	158	ASN
1	F	64	GLN
1	F	158	ASN
1	F	177	ASN

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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	201	5	32,33,33	0.68	2 (6%)	48,52,52	0.46	0
2	ATP	D	201	5	32,33,33	0.72	2 (6%)	48,52,52	0.47	0
4	3PO	B	201	-	10,12,12	2.43	1 (10%)	17,20,20	2.00	7 (41%)
7	B12	C	204	-	94,101,101	1.11	6 (6%)	149,166,166	1.63	25 (16%)
2	ATP	C	201	5	32,33,33	0.34	0	48,52,52	0.33	0
6	SO4	C	203	-	4,4,4	0.70	0	6,6,6	0.24	0
6	SO4	F	201	-	4,4,4	0.68	0	6,6,6	0.18	0
4	3PO	E	201	-	10,12,12	2.44	1 (10%)	17,20,20	2.04	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	B12	E	202	-	94,101,101	1.12	6 (6%)	149,166,166	1.68	32 (21%)

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	201	5	-	3/22/38/38	0/3/3/3
2	ATP	D	201	5	-	8/22/38/38	0/3/3/3
4	3PO	B	201	-	-	3/12/12/12	-
7	B12	C	204	-	-	9/56/223/223	0/3/11/11
2	ATP	C	201	5	-	3/22/38/38	0/3/3/3
4	3PO	E	201	-	-	5/12/12/12	-
7	B12	E	202	-	-	13/56/223/223	0/3/11/11

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	201	3PO	PB-O3A	-7.35	1.51	1.59
4	B	201	3PO	PB-O3A	-7.18	1.51	1.59
7	C	204	B12	C14-N23	3.44	1.39	1.35
7	E	202	B12	C35-C5	3.17	1.57	1.50
7	E	202	B12	C14-N23	2.97	1.39	1.35
7	E	202	B12	C54-C17	2.96	1.59	1.54
7	C	204	B12	C54-C17	2.95	1.59	1.54
7	C	204	B12	C35-C5	2.84	1.56	1.50
2	A	201	ATP	PB-O3B	-2.69	1.56	1.59
2	D	201	ATP	PB-O3B	-2.55	1.56	1.59
2	D	201	ATP	PA-O3A	2.50	1.62	1.59
7	E	202	B12	C19-N24	-2.37	1.46	1.49
7	E	202	B12	C48-C13	2.31	1.59	1.54
7	C	204	B12	C2B-N1B	-2.24	1.33	1.37
7	C	204	B12	C30-C3	2.10	1.59	1.54
7	E	202	B12	C6B-C5B	2.10	1.46	1.40
2	A	201	ATP	PA-O3A	-2.10	1.57	1.59
7	C	204	B12	C6B-C5B	2.02	1.45	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	204	B12	C54-C17-C18	-6.58	103.55	112.99
7	E	202	B12	C54-C17-C18	-5.43	105.20	112.99
7	E	202	B12	C18-C17-C16	4.87	106.56	100.69
7	E	202	B12	C19-N24-C16	4.85	112.59	107.29
7	C	204	B12	C18-C17-C16	4.74	106.41	100.69
7	C	204	B12	C19-N24-C16	4.73	112.46	107.29
7	C	204	B12	C9-N22-C6	4.69	110.92	105.28
7	E	202	B12	C9-N22-C6	4.21	110.35	105.28
7	C	204	B12	C13-C14-C15	-4.13	118.03	124.32
7	E	202	B12	C17-C16-N24	-3.86	105.27	111.17
4	E	201	3PO	O2G-PG-O3B	3.65	116.87	104.64
4	B	201	3PO	O2G-PG-O3B	3.57	116.62	104.64
7	C	204	B12	C17-C16-N24	-3.54	105.77	111.17
7	E	202	B12	C13-C14-C15	-3.41	119.12	124.32
7	C	204	B12	C1-C19-C18	-3.34	116.49	121.90
7	C	204	B12	C16-C15-C14	-3.33	116.19	121.26
7	E	202	B12	C1P-N59-C57	-3.31	115.58	122.69
7	C	204	B12	C1P-N59-C57	-3.24	115.74	122.69
7	E	202	B12	C9B-C8B-N1B	3.21	106.73	105.30
7	E	202	B12	C54-C17-C16	-3.17	95.96	112.41
7	E	202	B12	C56-C55-C17	-3.07	109.66	115.58
7	E	202	B12	C1-C19-C18	-3.04	116.98	121.90
7	C	204	B12	C2P-C1P-N59	-3.03	108.47	112.92
7	E	202	B12	O6R-C1R-N1B	-3.01	102.30	108.09
7	E	202	B12	C7B-C8B-C9B	2.98	126.04	122.47
7	E	202	B12	C15-C16-N24	2.97	126.65	122.42
7	C	204	B12	C54-C17-C16	-2.91	97.31	112.41
7	C	204	B12	C15-C16-N24	2.88	126.53	122.42
7	E	202	B12	C5M-C5B-C6B	-2.85	114.94	120.76
7	E	202	B12	C16-C15-C14	-2.85	116.92	121.26
7	E	202	B12	C55-C17-C16	2.83	122.14	116.59
4	E	201	3PO	O3G-PG-O2G	2.82	118.39	107.80
4	B	201	3PO	O3G-PG-O2G	2.82	118.39	107.80
7	C	204	B12	C55-C17-C18	2.75	116.37	111.12
7	C	204	B12	C5M-C5B-C6B	-2.75	115.15	120.76
7	C	204	B12	C7B-C8B-C9B	2.64	125.64	122.47
7	E	202	B12	C48-C13-C12	-2.63	108.99	116.52
7	E	202	B12	C13-C14-N23	2.63	112.66	109.09
4	E	201	3PO	O5'-PA-O2A	2.62	117.64	107.80
7	C	204	B12	C56-C55-C17	-2.60	110.56	115.58
4	E	201	3PO	O2B-PB-O3A	2.60	114.29	107.27
7	C	204	B12	O28-C27-N29	-2.56	115.70	122.53
7	E	202	B12	C4B-C5B-C6B	2.51	123.37	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	204	B12	C55-C17-C16	2.48	121.45	116.59
7	E	202	B12	C53-C15-C16	2.48	124.58	120.36
7	C	204	B12	C9B-C8B-N1B	2.45	106.39	105.30
7	E	202	B12	C1-C2-C3	-2.44	98.53	101.60
7	E	202	B12	C8B-C9B-N3B	-2.43	107.37	110.00
7	E	202	B12	C48-C13-C14	2.43	114.55	108.51
7	E	202	B12	C2P-C1P-N59	-2.41	109.38	112.92
4	B	201	3PO	O2B-PB-O3A	2.40	113.77	107.27
7	E	202	B12	O28-C27-N29	-2.40	116.11	122.53
7	C	204	B12	C4B-C5B-C6B	2.40	123.20	119.69
7	E	202	B12	C18-C19-N24	2.38	105.91	102.33
7	C	204	B12	C18-C19-N24	2.38	105.91	102.33
4	B	201	3PO	O5'-PA-O2A	2.36	116.66	107.80
7	E	202	B12	C35-C5-C4	-2.35	112.04	116.79
7	C	204	B12	C2-C1-C19	-2.34	114.98	118.61
7	C	204	B12	C8B-C9B-N3B	-2.27	107.54	110.00
7	E	202	B12	O2-C3R-C2R	2.23	119.69	111.68
4	E	201	3PO	O3B-PG-O1G	-2.13	99.84	111.04
7	E	202	B12	C2R-C1R-N1B	2.13	118.58	113.30
7	E	202	B12	C7B-C8B-N1B	-2.11	127.23	131.39
7	E	202	B12	C9B-C4B-C5B	-2.10	116.93	120.83
4	B	201	3PO	O3G-PG-O1G	-2.10	102.64	110.83
7	C	204	B12	O2-C3R-C2R	2.10	119.21	111.68
4	B	201	3PO	O3B-PG-O1G	-2.10	100.00	111.04
4	E	201	3PO	O3G-PG-O1G	-2.08	102.73	110.83
7	C	204	B12	C13-C14-N23	2.05	111.86	109.09
4	B	201	3PO	O2B-PB-O1B	-2.01	103.10	112.44

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201	ATP	PB-O3B-PG-O2G
2	D	201	ATP	C5'-O5'-PA-O1A
2	D	201	ATP	C5'-O5'-PA-O3A
4	E	201	3PO	PB-O3B-PG-O2G
7	C	204	B12	C1P-C2P-O3-P
7	C	204	B12	C2P-O3-P-O4
7	E	202	B12	C1P-C2P-O3-P
7	E	202	B12	C3P-C2P-O3-P
7	E	202	B12	C2P-O3-P-O2
7	E	202	B12	C14-C13-C48-C49

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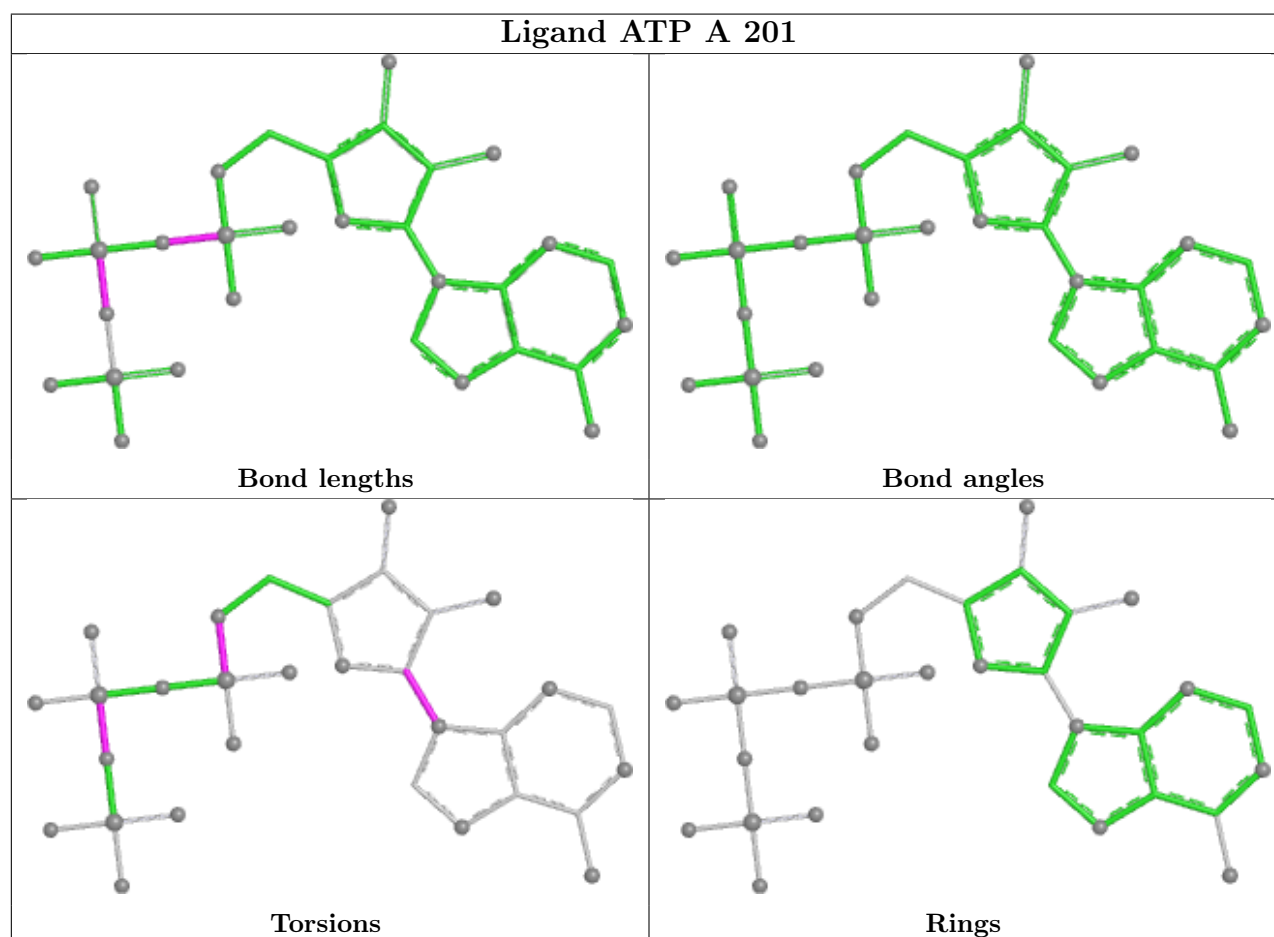
Mol	Chain	Res	Type	Atoms
7	E	202	B12	C2-C26-C27-O28
7	E	202	B12	C2-C26-C27-N29
7	C	204	B12	C14-C13-C48-C49
7	E	202	B12	C3R-C4R-C5R-O8R
7	E	202	B12	O6R-C4R-C5R-O8R
7	C	204	B12	C3P-C2P-O3-P
7	C	204	B12	C3-C30-C31-C32
4	E	201	3PO	PB-O3B-PG-O1G
4	B	201	3PO	PB-O3B-PG-O2G
7	C	204	B12	C48-C49-C50-O51
7	E	202	B12	C48-C49-C50-O51
7	E	202	B12	C2P-O3-P-O4
7	E	202	B12	C48-C49-C50-N52
4	E	201	3PO	PA-O3A-PB-O3B
7	C	204	B12	C48-C49-C50-N52
2	A	201	ATP	C5'-O5'-PA-O3A
2	C	201	ATP	C5'-O5'-PA-O3A
2	D	201	ATP	C5'-O5'-PA-O2A
7	C	204	B12	C2P-O3-P-O2
2	D	201	ATP	PG-O3B-PB-O2B
7	E	202	B12	C42-C41-C8-C9
2	C	201	ATP	PB-O3B-PG-O1G
7	C	204	B12	C18-C60-C61-O63
2	D	201	ATP	PB-O3B-PG-O3G
2	D	201	ATP	C2'-C1'-N9-C8
2	C	201	ATP	PG-O3B-PB-O2B
4	E	201	3PO	PA-O3A-PB-O1B
4	B	201	3PO	PB-O3B-PG-O1G
7	E	202	B12	C55-C56-C57-O58
2	A	201	ATP	C2'-C1'-N9-C8
2	A	201	ATP	PG-O3B-PB-O2B
2	D	201	ATP	PG-O3B-PB-O1B
4	B	201	3PO	PA-O3A-PB-O2B
4	E	201	3PO	PA-O3A-PB-O2B

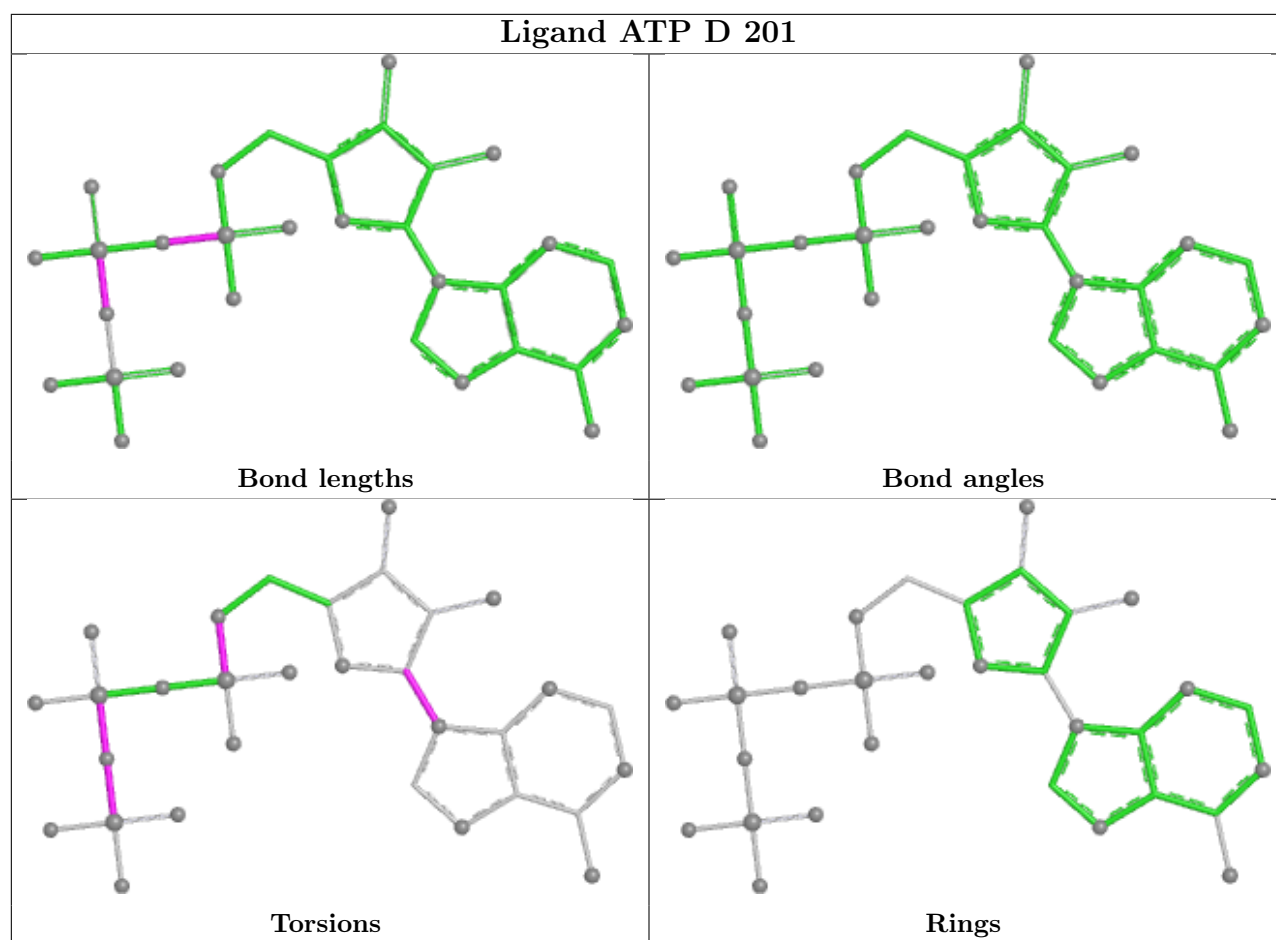
There are no ring outliers.

2 monomers are involved in 12 short contacts:

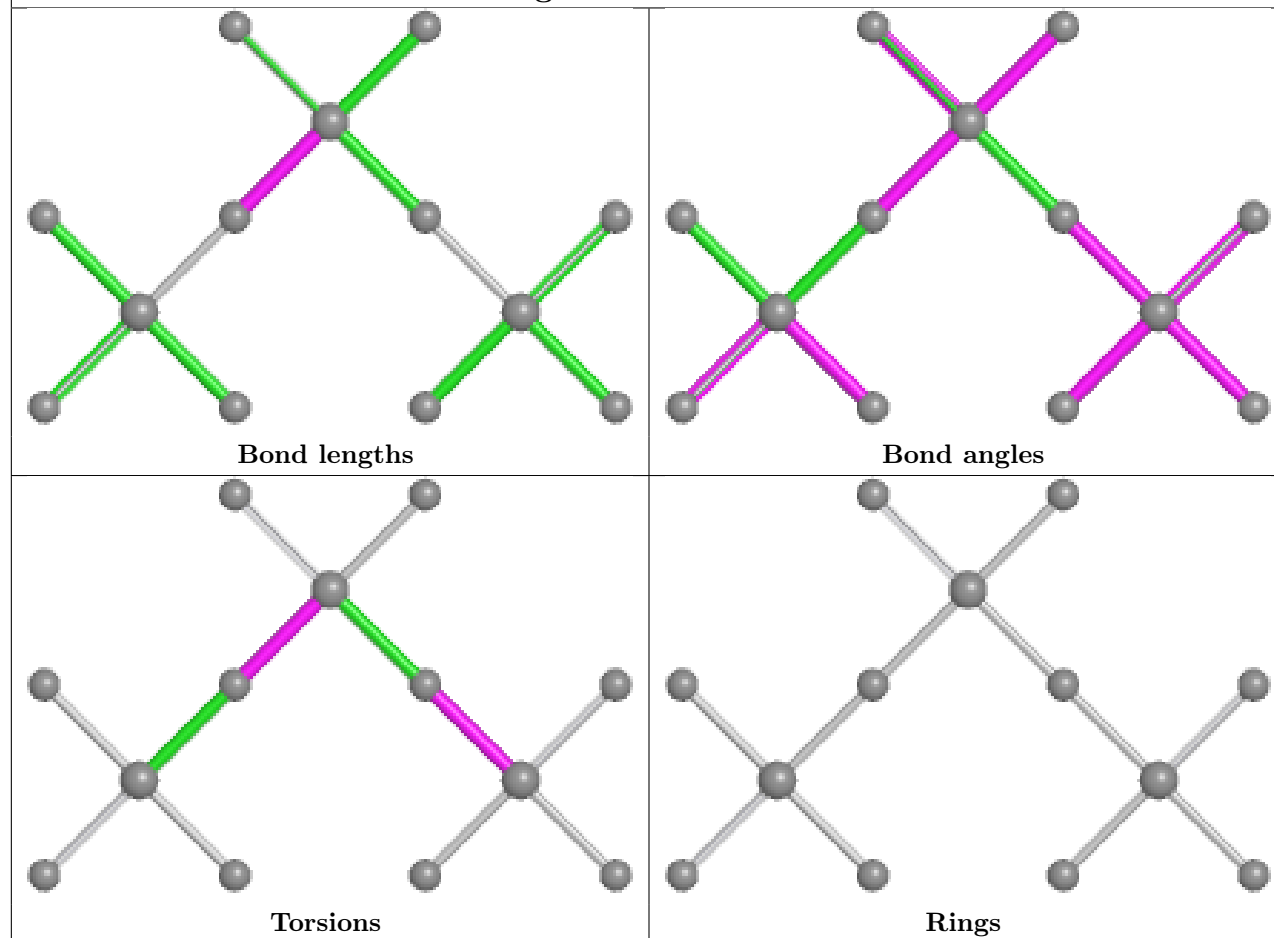
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	204	B12	7	0
7	E	202	B12	5	0

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.

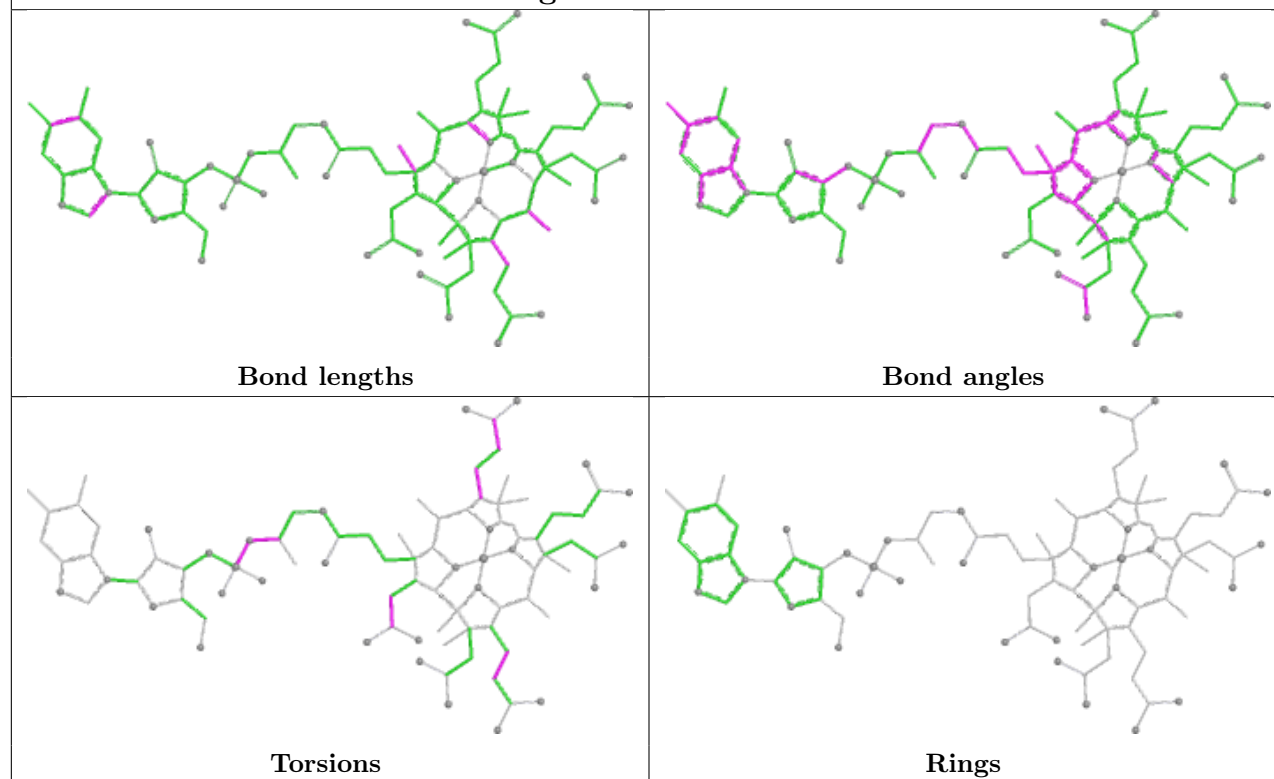


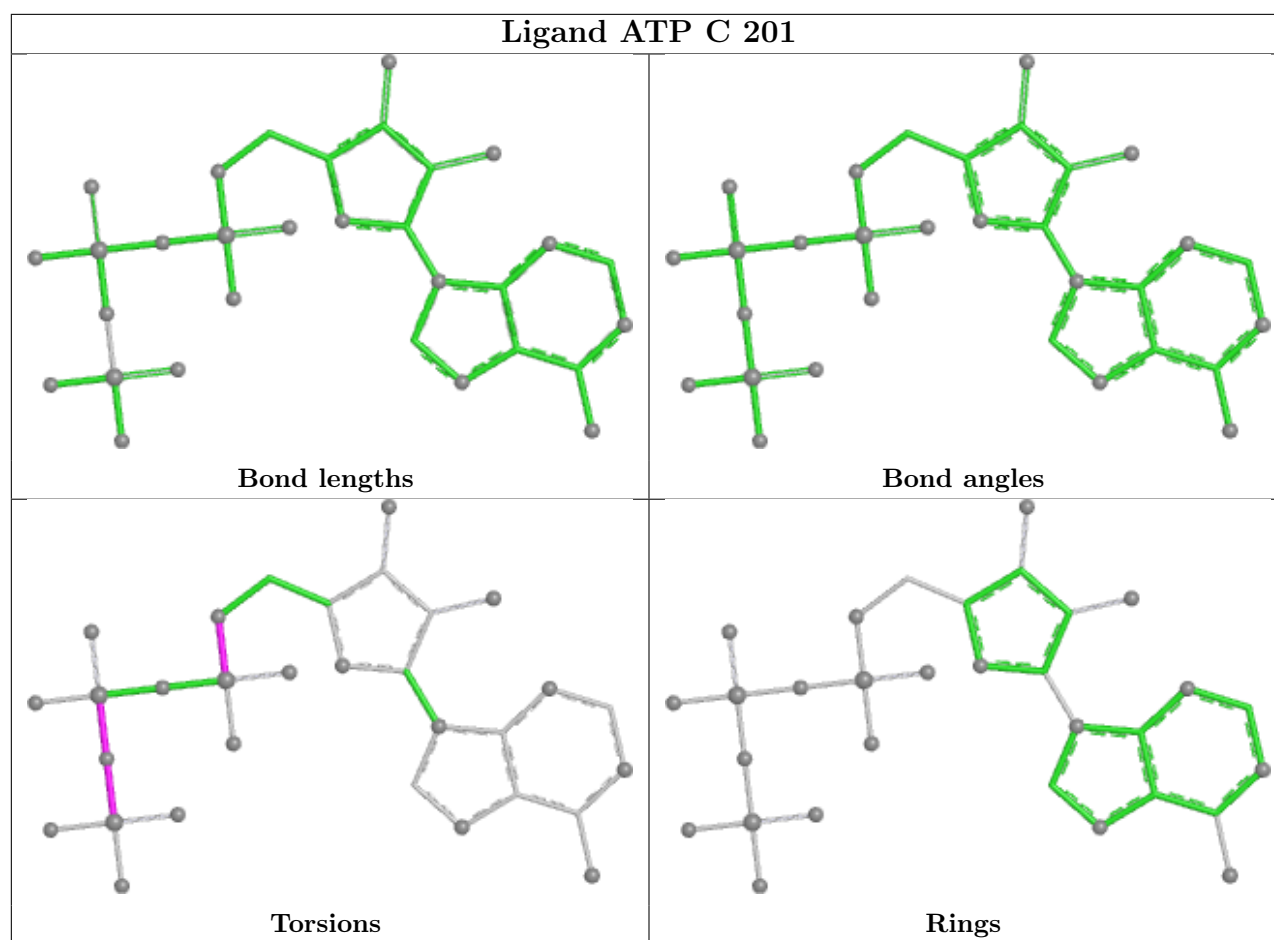


Ligand 3PO B 201

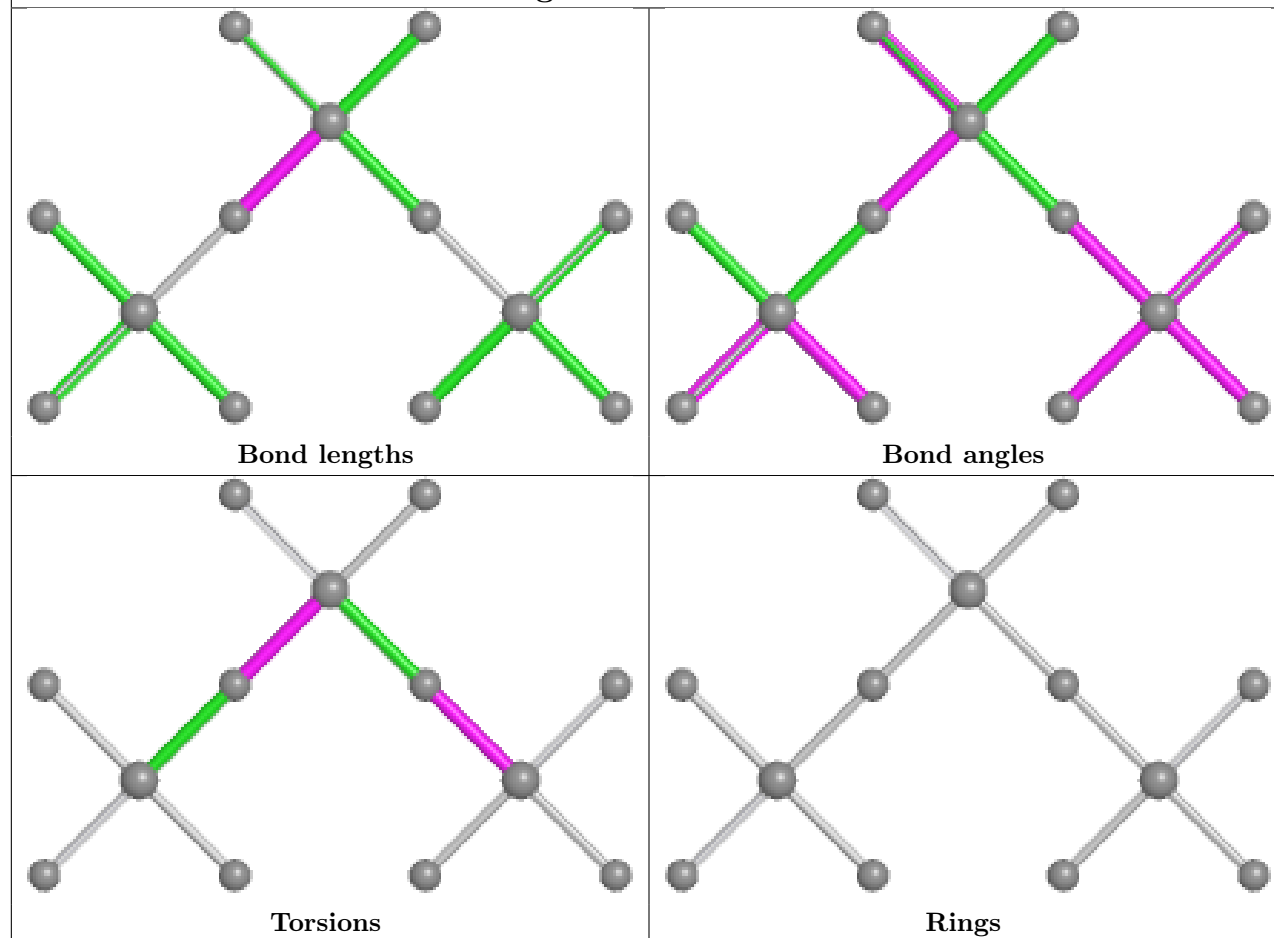


Ligand B12 C 204

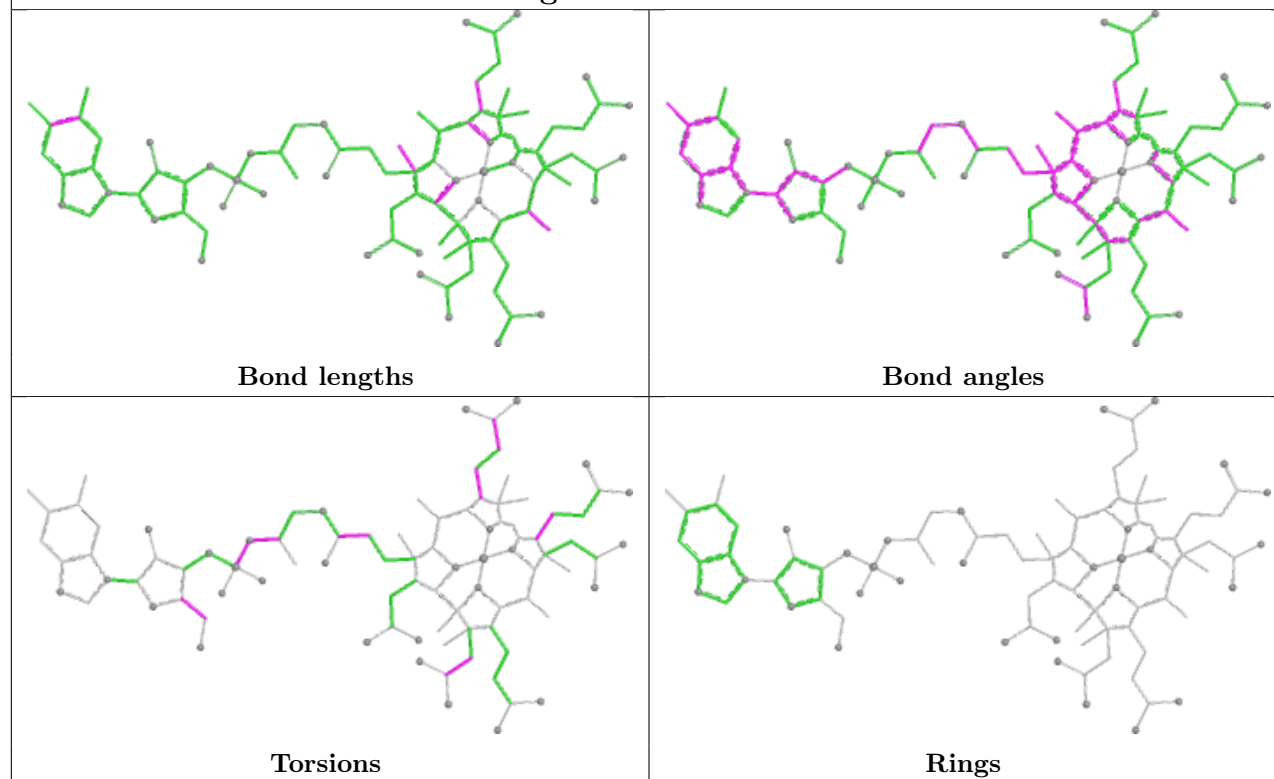




Ligand 3PO E 201



Ligand B12 E 202



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	182/187 (97%)	0.28	3 (1%) 70 67	42, 60, 91, 113	0
1	B	152/187 (81%)	0.50	11 (7%) 21 18	42, 66, 107, 154	0
1	C	186/187 (99%)	0.39	11 (5%) 28 25	42, 69, 125, 157	0
1	D	180/187 (96%)	0.33	6 (3%) 49 46	45, 65, 130, 157	0
1	E	162/187 (86%)	0.74	15 (9%) 14 12	50, 82, 142, 170	0
1	F	144/187 (77%)	1.04	20 (13%) 6 5	70, 110, 142, 167	0
All	All	1006/1122 (89%)	0.53	66 (6%) 24 21	42, 73, 135, 170	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	TRP	4.3
1	B	7	TYR	3.5
1	C	15	THR	3.4
1	B	88	ILE	3.4
1	E	104	LEU	3.3
1	F	88	ILE	3.2
1	B	11	GLY	3.1
1	F	74	LEU	3.0
1	C	83	LEU	3.0
1	C	86	ALA	3.0
1	F	154	LEU	2.9
1	E	17	SER	2.8
1	B	6	VAL	2.8
1	B	75	ALA	2.8
1	F	148	THR	2.7
1	C	87	SER	2.7
1	B	70	ILE	2.7
1	F	112	CYS	2.7
1	A	149	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	75	ALA	2.6
1	F	89	LEU	2.5
1	F	156	PHE	2.5
1	F	157	VAL	2.5
1	C	85	ALA	2.5
1	E	90	THR	2.4
1	E	24	VAL	2.4
1	E	14	GLY	2.4
1	F	180	ILE	2.4
1	B	10	THR	2.4
1	B	149	ILE	2.4
1	F	149	ILE	2.4
1	F	108	LEU	2.4
1	F	136	ALA	2.4
1	E	22	SER	2.3
1	F	114	PHE	2.3
1	E	67	LEU	2.3
1	B	26	LYS	2.3
1	D	182	TRP	2.3
1	E	26	LYS	2.3
1	F	91	PRO	2.3
1	E	15	THR	2.3
1	D	108	LEU	2.3
1	C	107	GLN	2.3
1	E	147	CYS	2.2
1	D	179	GLU	2.2
1	E	185	SER	2.2
1	F	97	ILE	2.2
1	B	183	ASP	2.2
1	E	88	ILE	2.2
1	D	46	TRP	2.2
1	F	181	PHE	2.2
1	A	4	SER	2.2
1	C	148	THR	2.2
1	A	5	LEU	2.1
1	C	1	MET	2.1
1	D	147	CYS	2.1
1	F	160	LEU	2.1
1	C	53	ASP	2.1
1	D	173	PHE	2.1
1	E	27	THR	2.1
1	E	13	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	111	LEU	2.1
1	B	180	ILE	2.0
1	C	79	GLU	2.0
1	F	40	LEU	2.0
1	E	29	ILE	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](#)

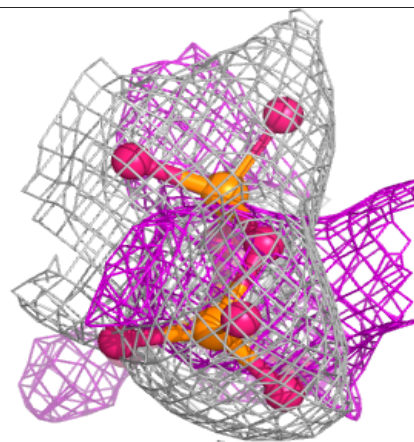
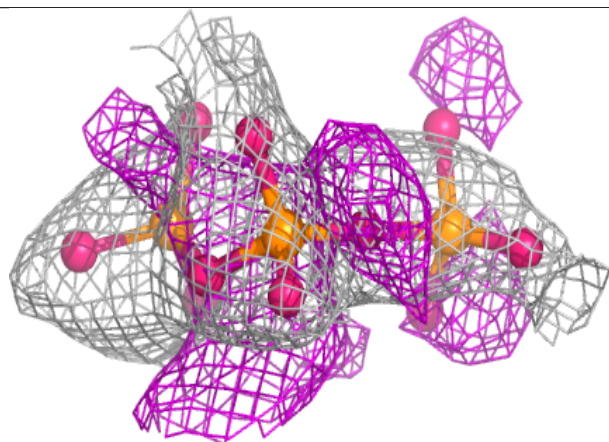
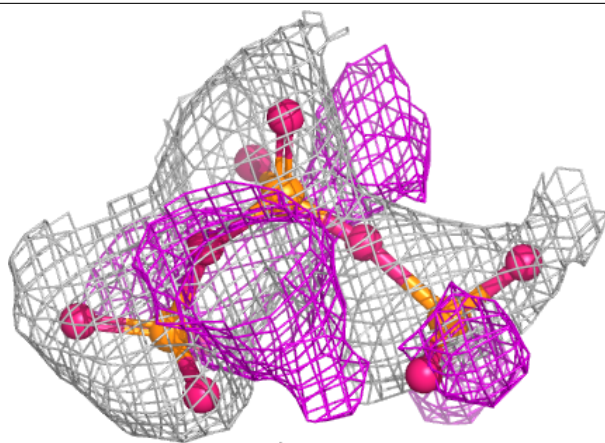
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	3PO	B	201	13/13	0.42	0.13	113,124,131,133	0
4	3PO	E	201	13/13	0.57	0.10	122,127,132,132	0
5	MG	E	203	1/1	0.81	0.08	49,49,49,49	0
6	SO4	F	201	5/5	0.85	0.09	88,90,98,99	0
2	ATP	D	201	31/31	0.90	0.10	42,50,58,65	0
6	SO4	C	203	5/5	0.93	0.09	46,50,53,55	0
2	ATP	C	201	31/31	0.93	0.08	57,67,73,74	0
7	B12	E	202	91/91	0.95	0.09	41,48,55,62	0
7	B12	C	204	91/91	0.96	0.09	42,57,68,73	0
2	ATP	A	201	31/31	0.96	0.07	45,51,55,55	0
5	MG	B	202	1/1	0.97	0.08	65,65,65,65	0
3	K	A	202	1/1	0.98	0.06	52,52,52,52	0
3	K	D	202	1/1	0.98	0.19	60,60,60,60	0
5	MG	C	202	1/1	1.00	0.02	49,49,49,49	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.

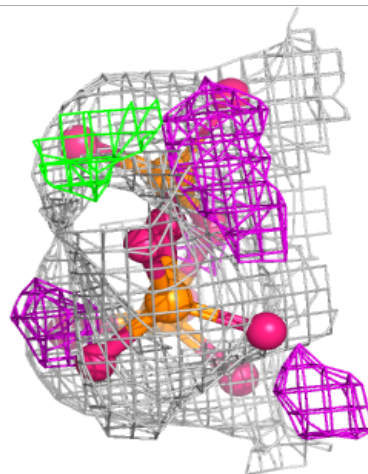
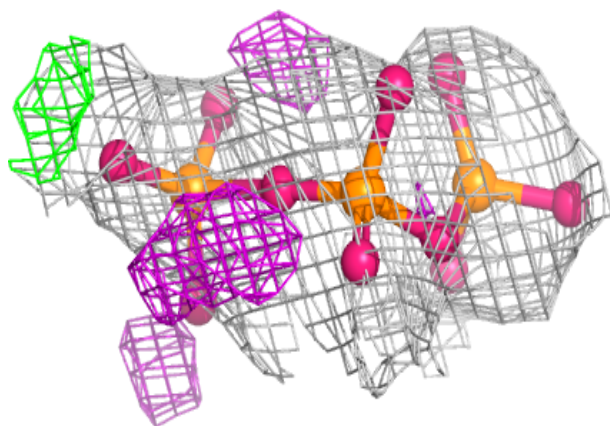
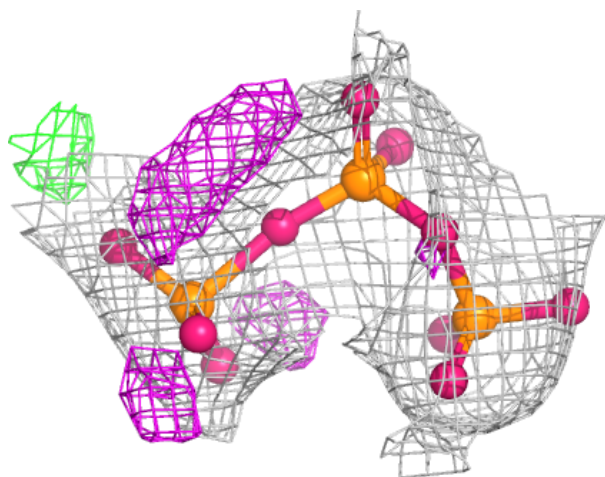
Electron density around 3PO B 201:

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



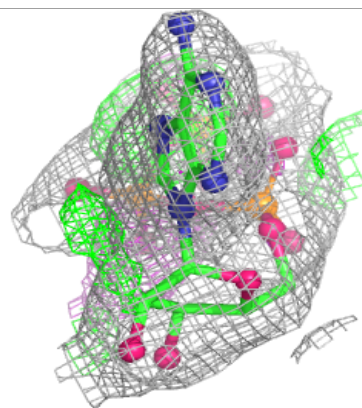
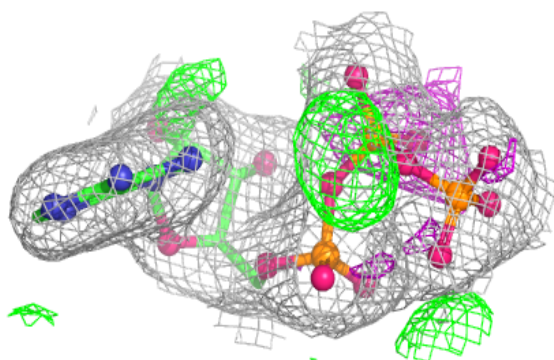
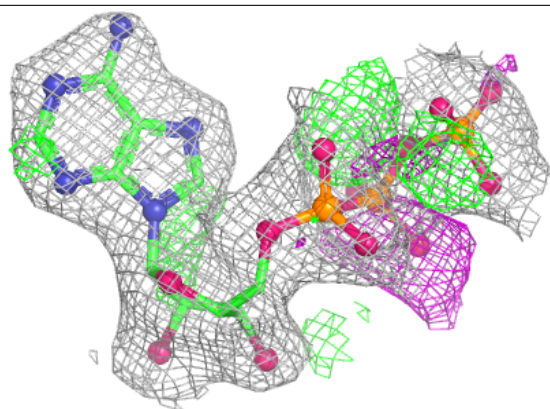
Electron density around 3PO E 201:

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

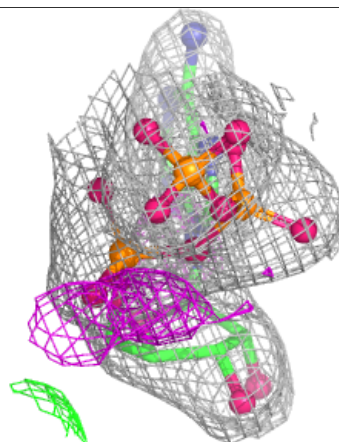
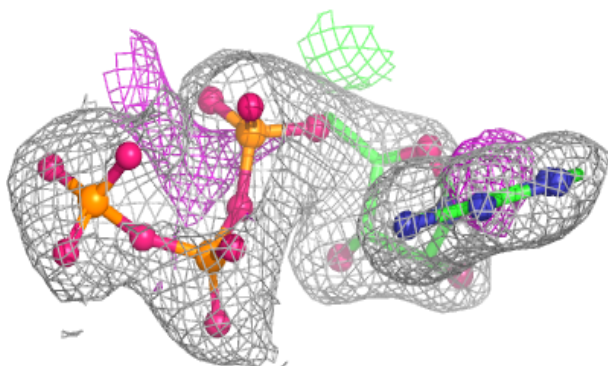
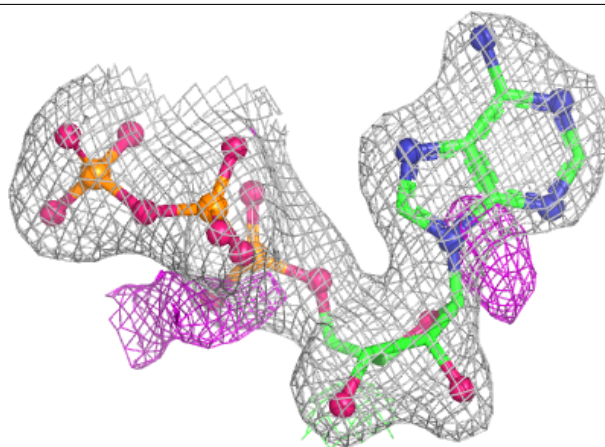


Electron density around ATP D 201:

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

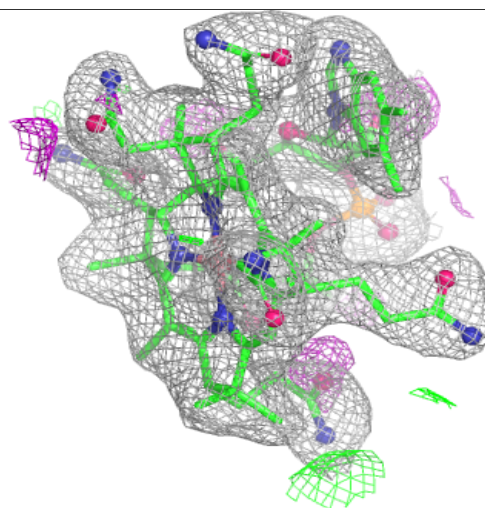
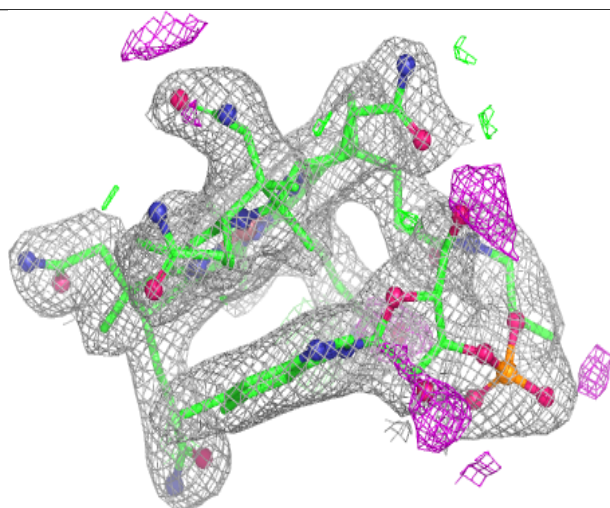
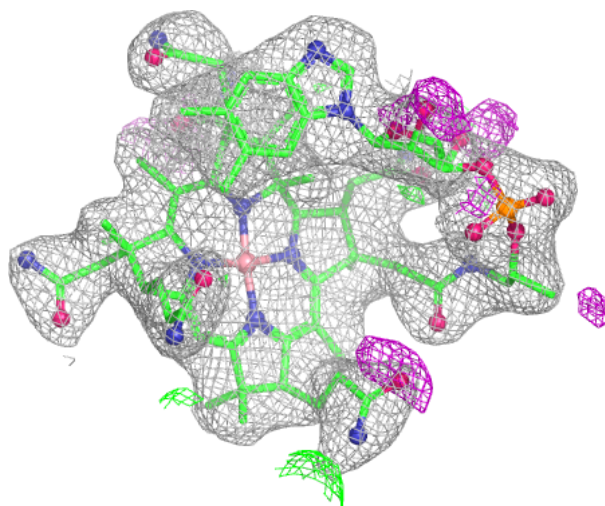
**Electron density around ATP C 201:**

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



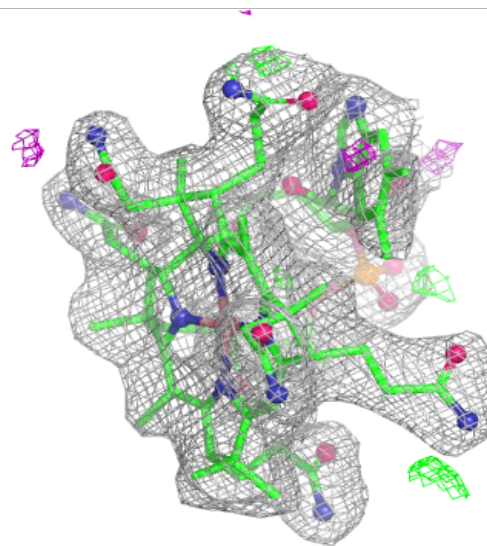
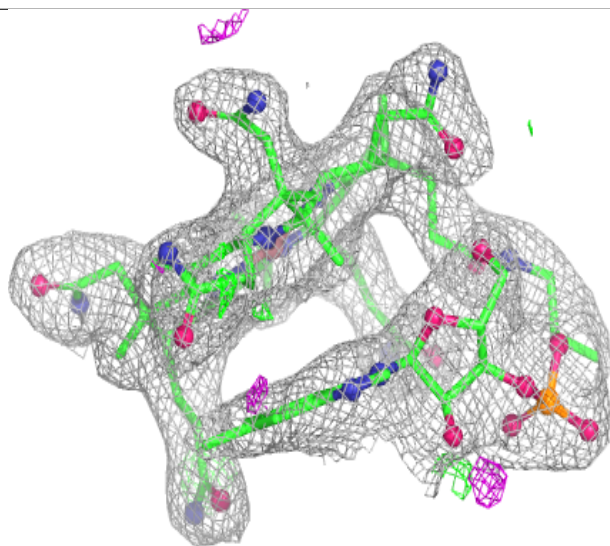
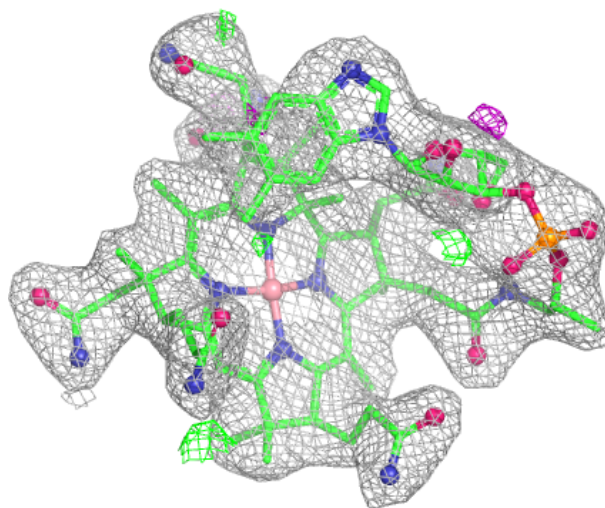
Electron density around B12 E 202:

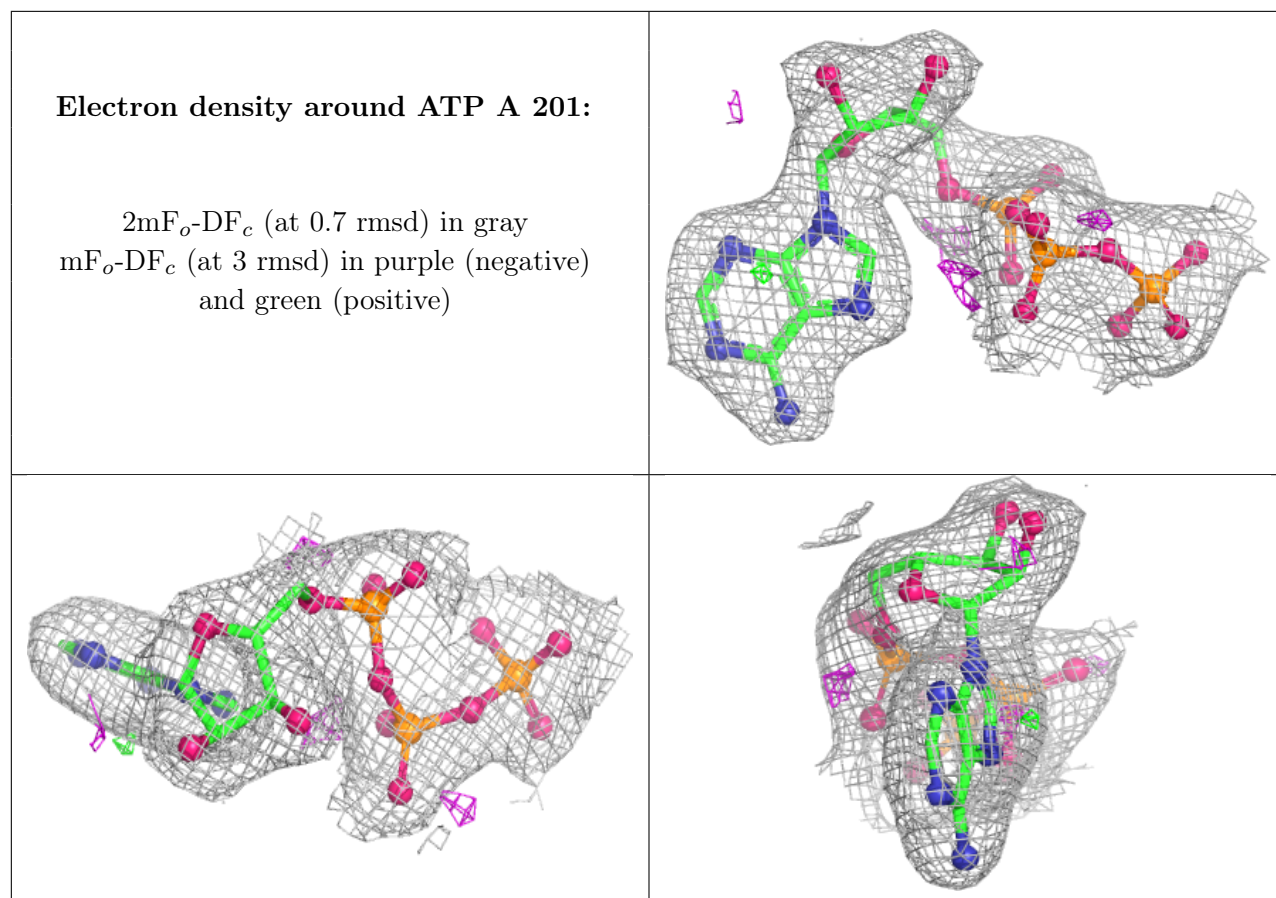
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B12 C 204:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.