



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:15 AM UTC

PDB ID : 4BIY / pdb_00004biy
Title : Crystal structure of CpxAHDC (monoclinic form 2)
Authors : Mechaly, A.E.; Sassoon, N.; Betton, J.M.; Alzari, P.M.
Deposited on : 2013-04-13
Resolution : 3.30 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

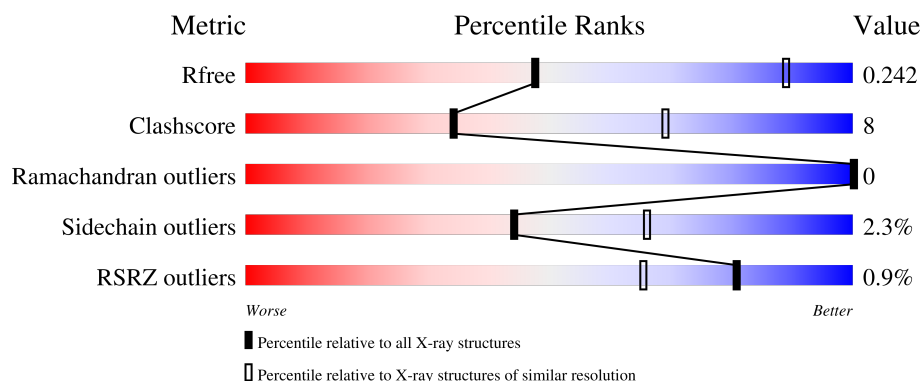
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

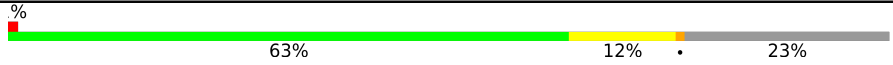
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	298	
1	B	298	
1	C	298	
1	D	298	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	1457	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7134 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 SENSOR PROTEIN CPXA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1797	1125	323	344	5			
1	B	221	Total	C	N	O	S	0	0	0
			1756	1102	316	333	5			
1	C	228	Total	C	N	O	S	0	0	0
			1797	1125	323	344	5			
1	D	216	Total	C	N	O	S	0	0	0
			1710	1070	308	327	5			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	MET	-	expression tag	UNP P0AE82
A	161	GLY	-	expression tag	UNP P0AE82
A	162	SER	-	expression tag	UNP P0AE82
A	163	SER	-	expression tag	UNP P0AE82
A	164	HIS	-	expression tag	UNP P0AE82
A	165	HIS	-	expression tag	UNP P0AE82
A	166	HIS	-	expression tag	UNP P0AE82
A	167	HIS	-	expression tag	UNP P0AE82
A	168	HIS	-	expression tag	UNP P0AE82
A	169	HIS	-	expression tag	UNP P0AE82
A	170	SER	-	expression tag	UNP P0AE82
A	171	SER	-	expression tag	UNP P0AE82
A	172	GLY	-	expression tag	UNP P0AE82
A	173	LEU	-	expression tag	UNP P0AE82
A	174	VAL	-	expression tag	UNP P0AE82
A	175	PRO	-	expression tag	UNP P0AE82
A	176	ARG	-	expression tag	UNP P0AE82
A	177	GLY	-	expression tag	UNP P0AE82
A	178	SER	-	expression tag	UNP P0AE82
A	179	HIS	-	expression tag	UNP P0AE82
A	180	MET	-	expression tag	UNP P0AE82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	expression tag	UNP P0AE82
A	182	ASN	-	expression tag	UNP P0AE82
A	183	LEU	-	expression tag	UNP P0AE82
A	184	TYR	-	expression tag	UNP P0AE82
A	185	PHE	-	expression tag	UNP P0AE82
A	186	GLN	-	expression tag	UNP P0AE82
A	187	GLY	-	expression tag	UNP P0AE82
A	228	VAL	MET	conflict	UNP P0AE82
B	160	MET	-	expression tag	UNP P0AE82
B	161	GLY	-	expression tag	UNP P0AE82
B	162	SER	-	expression tag	UNP P0AE82
B	163	SER	-	expression tag	UNP P0AE82
B	164	HIS	-	expression tag	UNP P0AE82
B	165	HIS	-	expression tag	UNP P0AE82
B	166	HIS	-	expression tag	UNP P0AE82
B	167	HIS	-	expression tag	UNP P0AE82
B	168	HIS	-	expression tag	UNP P0AE82
B	169	HIS	-	expression tag	UNP P0AE82
B	170	SER	-	expression tag	UNP P0AE82
B	171	SER	-	expression tag	UNP P0AE82
B	172	GLY	-	expression tag	UNP P0AE82
B	173	LEU	-	expression tag	UNP P0AE82
B	174	VAL	-	expression tag	UNP P0AE82
B	175	PRO	-	expression tag	UNP P0AE82
B	176	ARG	-	expression tag	UNP P0AE82
B	177	GLY	-	expression tag	UNP P0AE82
B	178	SER	-	expression tag	UNP P0AE82
B	179	HIS	-	expression tag	UNP P0AE82
B	180	MET	-	expression tag	UNP P0AE82
B	181	GLU	-	expression tag	UNP P0AE82
B	182	ASN	-	expression tag	UNP P0AE82
B	183	LEU	-	expression tag	UNP P0AE82
B	184	TYR	-	expression tag	UNP P0AE82
B	185	PHE	-	expression tag	UNP P0AE82
B	186	GLN	-	expression tag	UNP P0AE82
B	187	GLY	-	expression tag	UNP P0AE82
B	228	VAL	MET	conflict	UNP P0AE82
C	160	MET	-	expression tag	UNP P0AE82
C	161	GLY	-	expression tag	UNP P0AE82
C	162	SER	-	expression tag	UNP P0AE82
C	163	SER	-	expression tag	UNP P0AE82
C	164	HIS	-	expression tag	UNP P0AE82

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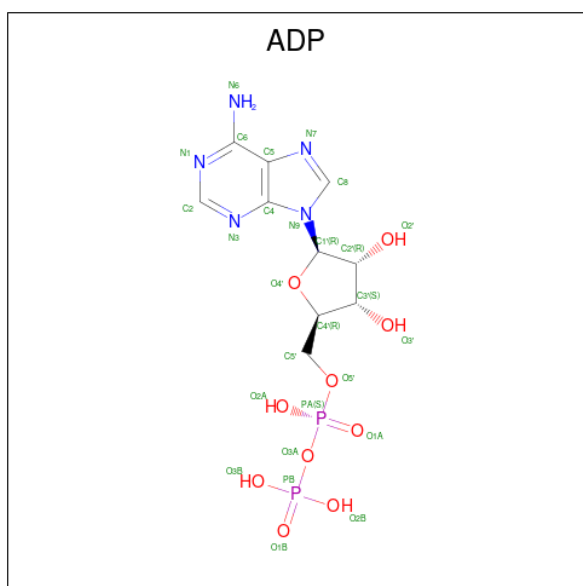
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C	165	HIS	-	expression tag	UNP P0AE82
C	166	HIS	-	expression tag	UNP P0AE82
C	167	HIS	-	expression tag	UNP P0AE82
C	168	HIS	-	expression tag	UNP P0AE82
C	169	HIS	-	expression tag	UNP P0AE82
C	170	SER	-	expression tag	UNP P0AE82
C	171	SER	-	expression tag	UNP P0AE82
C	172	GLY	-	expression tag	UNP P0AE82
C	173	LEU	-	expression tag	UNP P0AE82
C	174	VAL	-	expression tag	UNP P0AE82
C	175	PRO	-	expression tag	UNP P0AE82
C	176	ARG	-	expression tag	UNP P0AE82
C	177	GLY	-	expression tag	UNP P0AE82
C	178	SER	-	expression tag	UNP P0AE82
C	179	HIS	-	expression tag	UNP P0AE82
C	180	MET	-	expression tag	UNP P0AE82
C	181	GLU	-	expression tag	UNP P0AE82
C	182	ASN	-	expression tag	UNP P0AE82
C	183	LEU	-	expression tag	UNP P0AE82
C	184	TYR	-	expression tag	UNP P0AE82
C	185	PHE	-	expression tag	UNP P0AE82
C	186	GLN	-	expression tag	UNP P0AE82
C	187	GLY	-	expression tag	UNP P0AE82
C	228	VAL	MET	conflict	UNP P0AE82
D	160	MET	-	expression tag	UNP P0AE82
D	161	GLY	-	expression tag	UNP P0AE82
D	162	SER	-	expression tag	UNP P0AE82
D	163	SER	-	expression tag	UNP P0AE82
D	164	HIS	-	expression tag	UNP P0AE82
D	165	HIS	-	expression tag	UNP P0AE82
D	166	HIS	-	expression tag	UNP P0AE82
D	167	HIS	-	expression tag	UNP P0AE82
D	168	HIS	-	expression tag	UNP P0AE82
D	169	HIS	-	expression tag	UNP P0AE82
D	170	SER	-	expression tag	UNP P0AE82
D	171	SER	-	expression tag	UNP P0AE82
D	172	GLY	-	expression tag	UNP P0AE82
D	173	LEU	-	expression tag	UNP P0AE82
D	174	VAL	-	expression tag	UNP P0AE82
D	175	PRO	-	expression tag	UNP P0AE82
D	176	ARG	-	expression tag	UNP P0AE82
D	177	GLY	-	expression tag	UNP P0AE82

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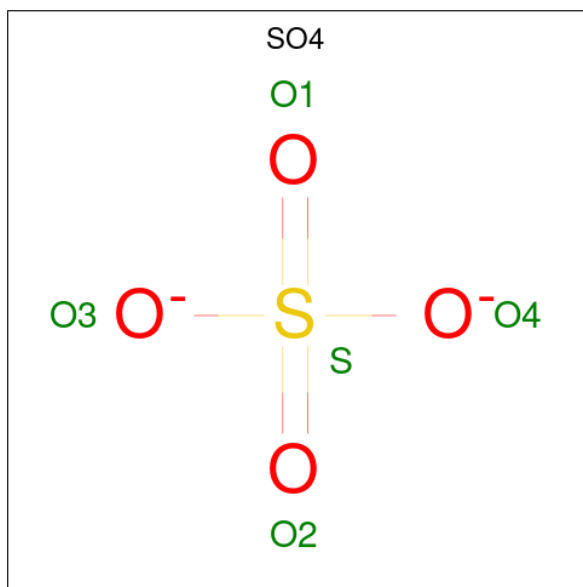
Chain	Residue	Modelled	Actual	Comment	Reference
D	178	SER	-	expression tag	UNP P0AE82
D	179	HIS	-	expression tag	UNP P0AE82
D	180	MET	-	expression tag	UNP P0AE82
D	181	GLU	-	expression tag	UNP P0AE82
D	182	ASN	-	expression tag	UNP P0AE82
D	183	LEU	-	expression tag	UNP P0AE82
D	184	TYR	-	expression tag	UNP P0AE82
D	185	PHE	-	expression tag	UNP P0AE82
D	186	GLN	-	expression tag	UNP P0AE82
D	187	GLY	-	expression tag	UNP P0AE82
D	228	VAL	MET	conflict	UNP P0AE82

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



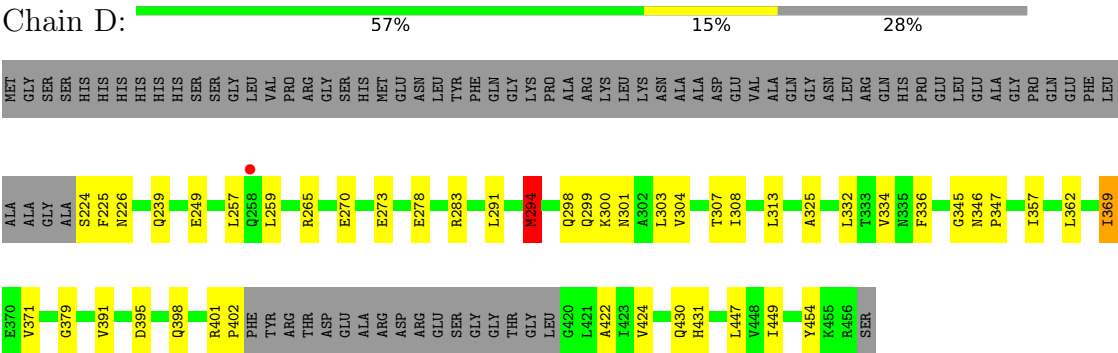
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

● Molecule 1: SENSOR PROTEIN CPXA



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.75Å 139.11Å 114.08Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	47.74 – 3.30 47.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.74-3.30) 98.8 (47.74-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.200 , 0.219 0.219 , 0.242	Depositor DCC
R_{free} test set	1082 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7134	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SO4

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	0.84	2/1827 (0.1%)	1.39	13/2475 (0.5%)
1	B	0.87	0/1786	1.42	15/2418 (0.6%)
1	C	0.79	0/1827	1.42	17/2475 (0.7%)
1	D	0.88	2/1738 (0.1%)	1.44	14/2354 (0.6%)
All	All	0.85	4/7178 (0.1%)	1.42	59/9722 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	294	MET	SD-CE	7.85	1.99	1.79
1	A	236	MET	SD-CE	5.98	1.94	1.79
1	A	252	THR	CA-C	5.60	1.58	1.52
1	D	369	ILE	CG1-CD1	-5.10	1.31	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	PHE	CA-CB-CG	-11.60	102.20	113.80
1	B	418	GLY	CA-C-N	8.22	131.12	120.44
1	B	418	GLY	C-N-CA	8.22	131.12	120.44
1	A	295	SER	N-CA-C	-7.43	103.05	112.93
1	D	334	VAL	CA-C-N	7.13	130.16	120.54
1	D	334	VAL	C-N-CA	7.13	130.16	120.54
1	D	225	PHE	CA-C-N	7.08	135.21	122.46
1	D	225	PHE	C-N-CA	7.08	135.21	122.46
1	D	300	LYS	CA-C-N	7.08	129.77	120.28
1	D	300	LYS	C-N-CA	7.08	129.77	120.28
1	D	379	GLY	N-CA-C	6.96	120.79	110.42
1	C	251	ARG	CA-C-N	6.62	129.05	120.44
1	C	251	ARG	C-N-CA	6.62	129.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	VAL	N-CA-CB	6.24	117.85	110.55
1	D	422	ALA	CA-C-N	5.98	128.10	120.56
1	D	422	ALA	C-N-CA	5.98	128.10	120.56
1	D	336	PHE	CA-CB-CG	-5.93	107.87	113.80
1	C	312	GLN	CA-C-N	5.89	128.64	120.63
1	C	312	GLN	C-N-CA	5.89	128.64	120.63
1	C	236	MET	CA-C-N	5.78	128.29	120.44
1	C	236	MET	C-N-CA	5.78	128.29	120.44
1	B	239	GLN	CA-C-N	5.59	127.78	120.28
1	B	239	GLN	C-N-CA	5.59	127.78	120.28
1	C	422	ALA	CA-C-N	5.58	128.11	120.46
1	C	422	ALA	C-N-CA	5.58	128.11	120.46
1	C	325	ALA	CA-C-N	5.53	127.69	120.28
1	C	325	ALA	C-N-CA	5.53	127.69	120.28
1	B	400	PHE	CA-C-N	5.53	132.20	122.08
1	B	400	PHE	C-N-CA	5.53	132.20	122.08
1	C	220	ALA	CA-C-N	5.46	127.59	120.28
1	C	220	ALA	C-N-CA	5.46	127.59	120.28
1	B	296	ARG	CA-C-N	5.45	127.58	120.28
1	B	296	ARG	C-N-CA	5.45	127.58	120.28
1	D	303	LEU	CA-C-N	5.44	127.79	120.50
1	D	303	LEU	C-N-CA	5.44	127.79	120.50
1	B	266	ARG	CA-C-N	5.43	128.34	120.79
1	B	266	ARG	C-N-CA	5.43	128.34	120.79
1	D	325	ALA	CA-C-N	5.41	127.53	120.28
1	D	325	ALA	C-N-CA	5.41	127.53	120.28
1	A	325	ALA	CA-C-N	5.40	127.51	120.28
1	A	325	ALA	C-N-CA	5.40	127.51	120.28
1	B	359	ARG	CA-C-N	5.36	127.90	120.29
1	B	359	ARG	C-N-CA	5.36	127.90	120.29
1	B	379	GLY	N-CA-C	5.36	118.57	110.75
1	B	325	ALA	CA-C-N	5.35	127.45	120.28
1	B	325	ALA	C-N-CA	5.35	127.45	120.28
1	C	259	LEU	CA-C-N	5.33	125.75	119.94
1	C	259	LEU	C-N-CA	5.33	125.75	119.94
1	A	379	GLY	N-CA-C	5.27	118.44	110.75
1	C	294	MET	CA-C-N	5.26	127.33	120.28
1	C	294	MET	C-N-CA	5.26	127.33	120.28
1	A	359	ARG	CA-C-N	5.06	127.33	120.65
1	A	359	ARG	C-N-CA	5.06	127.33	120.65
1	A	422	ALA	CA-C-N	5.05	127.60	120.42
1	A	422	ALA	C-N-CA	5.05	127.60	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	HIS	CA-C-N	5.05	129.72	122.40
1	A	431	HIS	C-N-CA	5.05	129.72	122.40
1	A	294	MET	CA-C-N	5.04	131.36	122.79
1	A	294	MET	C-N-CA	5.04	131.36	122.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1797	0	1801	23	0
1	B	1756	0	1765	34	0
1	C	1797	0	1801	42	0
1	D	1710	0	1720	36	0
2	A	27	0	12	2	0
2	C	27	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	3	0
3	D	5	0	0	0	0
All	All	7134	0	7111	108	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 8.

All (108) 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:236:MET:HE1	1:D:239:GLN:CD	1.90	0.95
1:C:236:MET:HE1	1:D:239:GLN:OE1	1.69	0.92
1:C:236:MET:HG3	1:C:303:LEU:HD11	1.49	0.91
1:C:236:MET:HE1	1:D:239:GLN:NE2	1.85	0.90
1:C:446:ARG:NH2	3:C:1457:SO4:O4	2.03	0.90
1:C:236:MET:CE	1:D:239:GLN:HE22	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LEU:HD22	1:B:423:ILE:HD11	1.63	0.79
1:C:236:MET:HE1	1:D:239:GLN:HE22	1.49	0.78
1:D:308:ILE:HD11	1:D:347:PRO:HG3	1.67	0.77
1:C:235:MET:SD	1:D:299:GLN:HA	2.25	0.76
1:A:357:ILE:HD11	1:A:424:VAL:HG11	1.66	0.76
1:A:234:ARG:NH1	1:B:432:ARG:HE	1.86	0.73
1:C:441:PRO:HG2	3:C:1457:SO4:O1	1.88	0.72
1:C:232:LEU:O	1:C:236:MET:HG2	1.88	0.72
1:C:254:LEU:HD22	1:C:288:ILE:HD12	1.77	0.66
1:A:234:ARG:HH12	1:B:432:ARG:HE	1.42	0.66
1:B:363:ARG:HH22	1:B:418:GLY:HA2	1.65	0.62
1:A:254:LEU:HD22	1:A:288:ILE:HD12	1.82	0.61
1:B:265:ARG:HH22	1:B:275:GLU:HG3	1.65	0.61
1:C:253:PRO:HB3	1:D:283:ARG:HD3	1.83	0.61
1:A:294:MET:HG2	1:A:417:THR:HG21	1.83	0.60
1:C:236:MET:HE2	1:D:239:GLN:HE22	1.64	0.60
1:A:357:ILE:HD13	1:A:449:ILE:HD11	1.84	0.59
1:C:265:ARG:HH22	1:C:275:GLU:HG3	1.69	0.57
1:B:400:PHE:O	1:B:401:ARG:HG3	2.04	0.57
1:C:277:ILE:HG23	1:D:257:LEU:HG	1.87	0.57
1:A:246:ILE:HG13	1:B:291:LEU:HD13	1.87	0.56
1:C:227:GLN:HE21	1:D:430:GLN:HE22	1.54	0.56
1:B:357:ILE:HD11	1:B:424:VAL:HG11	1.88	0.56
1:A:265:ARG:HH22	1:A:275:GLU:HG3	1.71	0.55
1:B:401:ARG:HB2	1:B:404:TYR:OH	2.07	0.55
1:B:395:ASP:O	1:B:399:ILE:HG23	2.07	0.55
1:B:289:ASN:O	1:B:293:VAL:HG23	2.06	0.54
1:C:236:MET:CE	1:D:239:GLN:OE1	2.50	0.54
1:C:233:GLU:HG2	1:C:303:LEU:HD12	1.89	0.54
1:A:251:ARG:NH2	1:A:289:ASN:OD1	2.38	0.53
1:C:357:ILE:HD13	1:C:449:ILE:HD11	1.90	0.53
1:B:419:LEU:HD22	1:B:423:ILE:CD1	2.37	0.53
1:D:265:ARG:HH11	1:D:270:GLU:HG2	1.74	0.53
1:C:242:LEU:HD21	1:D:294:MET:HB2	1.91	0.52
1:B:365:SER:HB3	1:B:386:ASP:HB2	1.91	0.52
1:D:357:ILE:HD13	1:D:449:ILE:HD11	1.91	0.52
1:B:359:ARG:HA	1:B:362:LEU:HD12	1.91	0.51
1:C:239:GLN:HG3	1:D:298:GLN:OE1	2.11	0.51
1:C:402:PRO:HD2	1:D:249:GLU:HG3	1.92	0.51
1:C:264:LEU:HD13	1:D:273:GLU:HB2	1.93	0.51
1:D:398:GLN:HE22	1:D:401:ARG:HH11	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG23	1:B:257:LEU:HG	1.92	0.50
1:A:405:ARG:HG3	2:A:501:ADP:O3'	2.12	0.49
1:D:301:ASN:HB3	1:D:346:ASN:HD21	1.78	0.49
1:C:244:SER:HB2	1:C:295:SER:HB3	1.94	0.48
1:B:346:ASN:HD22	1:B:349:ALA:H	1.60	0.48
1:B:346:ASN:ND2	1:B:349:ALA:H	2.12	0.48
1:B:357:ILE:HD13	1:B:449:ILE:HD11	1.95	0.47
1:B:391:VAL:CG1	1:B:395:ASP:HB2	2.45	0.47
1:B:419:LEU:HD13	1:B:423:ILE:CD1	2.45	0.47
1:A:364:TYR:OH	2:A:501:ADP:H2'	2.15	0.47
1:C:227:GLN:HE21	1:D:430:GLN:NE2	2.14	0.46
1:C:364:TYR:OH	2:C:501:ADP:H2'	2.16	0.46
1:C:336:PHE:CD2	1:C:336:PHE:N	2.83	0.46
1:D:308:ILE:HG21	1:D:313:LEU:HD13	1.98	0.46
1:B:266:ARG:HH12	1:C:227:GLN:C	2.23	0.46
1:B:346:ASN:HD22	1:B:349:ALA:HB2	1.80	0.46
1:C:256:ARG:HH12	1:D:283:ARG:CZ	2.29	0.46
1:C:290:ASP:HB2	1:C:403:PHE:CD1	2.49	0.46
1:A:434:TRP:HB3	1:C:397:GLU:CD	2.40	0.45
1:B:404:TYR:HB2	1:B:420:GLY:HA2	1.98	0.45
1:D:357:ILE:HD11	1:D:424:VAL:HG11	1.98	0.45
1:A:267:ARG:HD3	1:B:273:GLU:CD	2.41	0.45
1:D:362:LEU:HA	1:D:369:ILE:HD11	1.99	0.45
1:D:224:SER:C	1:D:226:ASN:H	2.25	0.45
1:B:364:TYR:HB2	1:B:386:ASP:OD2	2.17	0.45
1:C:291:LEU:HD13	1:C:403:PHE:HZ	1.82	0.45
1:A:405:ARG:HH11	1:A:418:GLY:N	2.15	0.44
1:C:290:ASP:HB2	1:C:403:PHE:CE1	2.53	0.44
1:B:419:LEU:CD2	1:B:423:ILE:HD11	2.42	0.43
1:D:391:VAL:CG1	1:D:395:ASP:HB2	2.49	0.43
1:B:373:PHE:CE2	1:B:382:ILE:HG12	2.52	0.43
1:A:398:GLN:HG3	1:A:401:ARG:HH11	1.84	0.43
1:C:244:SER:CB	1:C:295:SER:HB3	2.49	0.43
1:D:398:GLN:HE22	1:D:401:ARG:NH1	2.16	0.43
1:C:246:ILE:HG13	1:D:291:LEU:HD13	2.01	0.43
1:A:357:ILE:CD1	1:A:424:VAL:HG11	2.43	0.42
1:B:346:ASN:HD22	1:B:349:ALA:CB	2.32	0.42
1:D:307:THR:HG23	1:D:454:TYR:HD2	1.85	0.42
1:B:391:VAL:HG13	1:B:395:ASP:HB2	2.01	0.42
1:C:300:LYS:HG2	1:C:301:ASN:H	1.84	0.42
1:C:357:ILE:HG23	1:C:447:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLU:CG	1:C:303:LEU:HD12	2.50	0.42
1:C:391:VAL:CG1	1:C:395:ASP:HB2	2.50	0.42
1:A:419:LEU:O	1:A:423:ILE:HD12	2.20	0.41
1:B:332:LEU:HD11	1:B:371:VAL:HG23	2.02	0.41
1:A:299:GLN:HE21	1:A:302:ALA:HB2	1.85	0.41
1:C:441:PRO:CG	3:C:1457:SO4:O1	2.64	0.41
1:D:345:GLY:HA3	1:D:431:HIS:CD2	2.55	0.41
1:B:364:TYR:HB3	1:B:389:PRO:HD2	2.02	0.41
1:D:332:LEU:HD11	1:D:371:VAL:HG23	2.02	0.41
1:D:357:ILE:HG23	1:D:447:LEU:HD13	2.03	0.41
1:A:291:LEU:HD13	1:A:403:PHE:HZ	1.86	0.41
1:D:401:ARG:HA	1:D:402:PRO:HD2	1.94	0.41
1:B:454:TYR:HE2	1:B:456:ARG:HE	1.68	0.41
1:A:289:ASN:O	1:A:293:VAL:HG23	2.21	0.40
1:C:335:ASN:HB2	1:C:336:PHE:CD2	2.56	0.40
1:A:241:ARG:NH2	1:B:429:GLN:OE1	2.54	0.40
1:C:236:MET:CE	1:D:239:GLN:NE2	2.56	0.40
1:A:424:VAL:O	1:A:428:ILE:HG12	2.22	0.40
1:D:301:ASN:HB3	1:D:346:ASN:ND2	2.37	0.40
1:B:363:ARG:NH2	1:B:418:GLY:HA2	2.32	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	224/298 (75%)	213 (95%)	11 (5%)	0	100	100
1	B	217/298 (73%)	209 (96%)	8 (4%)	0	100	100
1	C	224/298 (75%)	217 (97%)	7 (3%)	0	100	100
1	D	212/298 (71%)	206 (97%)	6 (3%)	0	100	100
All	All	877/1192 (74%)	845 (96%)	32 (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	195/251 (78%)	191 (98%)	4 (2%)	47	67
1	B	192/251 (76%)	186 (97%)	6 (3%)	35	60
1	C	195/251 (78%)	191 (98%)	4 (2%)	47	67
1	D	188/251 (75%)	184 (98%)	4 (2%)	47	67
All	All	770/1004 (77%)	752 (98%)	18 (2%)	44	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	A	278	GLU
1	A	398	GLN
1	A	405	ARG
1	B	259	LEU
1	B	275	GLU
1	B	278	GLU
1	B	294	MET
1	B	399	ILE
1	B	405	ARG
1	C	239	GLN
1	C	278	GLU
1	C	307	THR
1	C	382	ILE
1	D	259	LEU
1	D	278	GLU
1	D	294	MET
1	D	304	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	299	GLN
1	A	335	ASN
1	A	348	ASN
1	A	430	GLN
1	B	227	GLN
1	B	240	GLN
1	B	258	GLN
1	B	346	ASN
1	C	226	ASN
1	C	301	ASN
1	C	335	ASN
1	C	348	ASN
1	D	240	GLN
1	D	289	ASN
1	D	301	ASN
1	D	430	GLN

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	1457	-	4,4,4	0.47	0	6,6,6	0.74	0
3	SO4	B	1457	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	A	1457	-	4,4,4	0.39	0	6,6,6	0.34	0
2	ADP	C	501	-	28,29,29	0.37	0	43,45,45	0.53	0
3	SO4	D	1457	-	4,4,4	0.49	0	6,6,6	0.92	0
2	ADP	A	501	-	28,29,29	0.39	0	43,45,45	0.53	0

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	ADP	A	501	-	-	2/16/32/32	0/3/3/3
2	ADP	C	501	-	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ADP	PB-O3A-PA-O2A
2	C	501	ADP	PB-O3A-PA-O2A
2	C	501	ADP	PB-O3A-PA-O1A
2	A	501	ADP	PB-O3A-PA-O1A

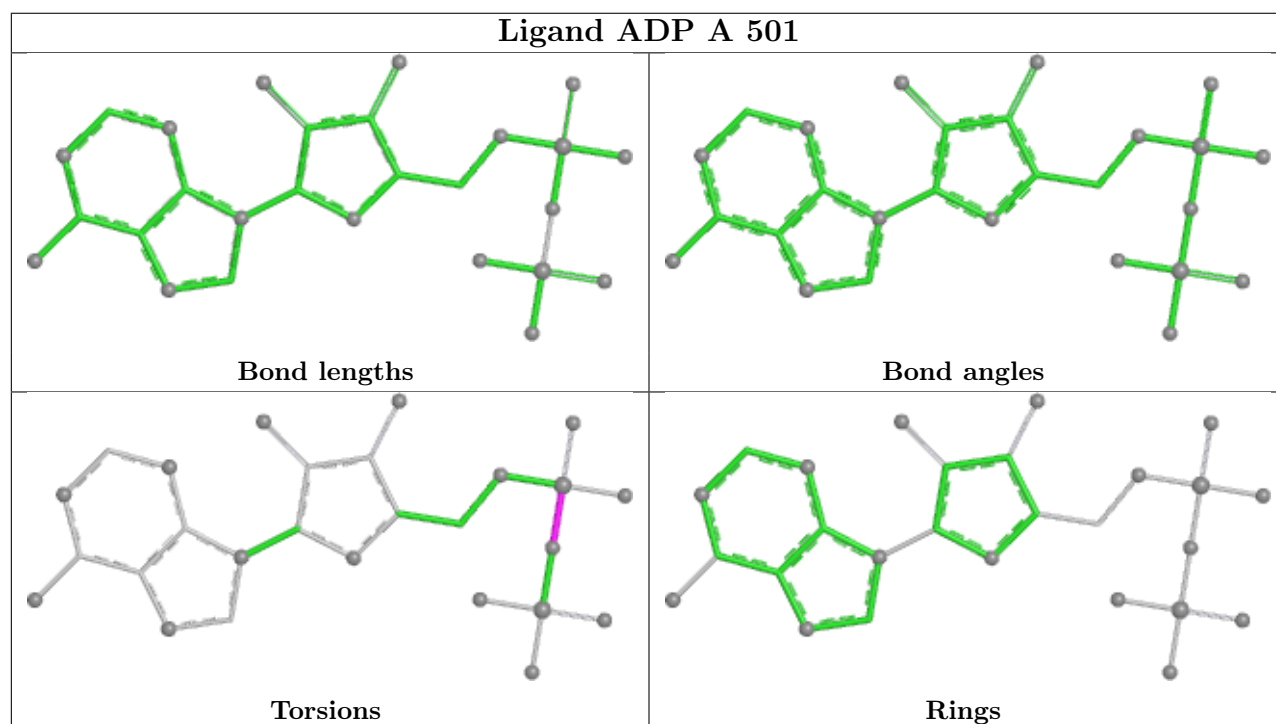
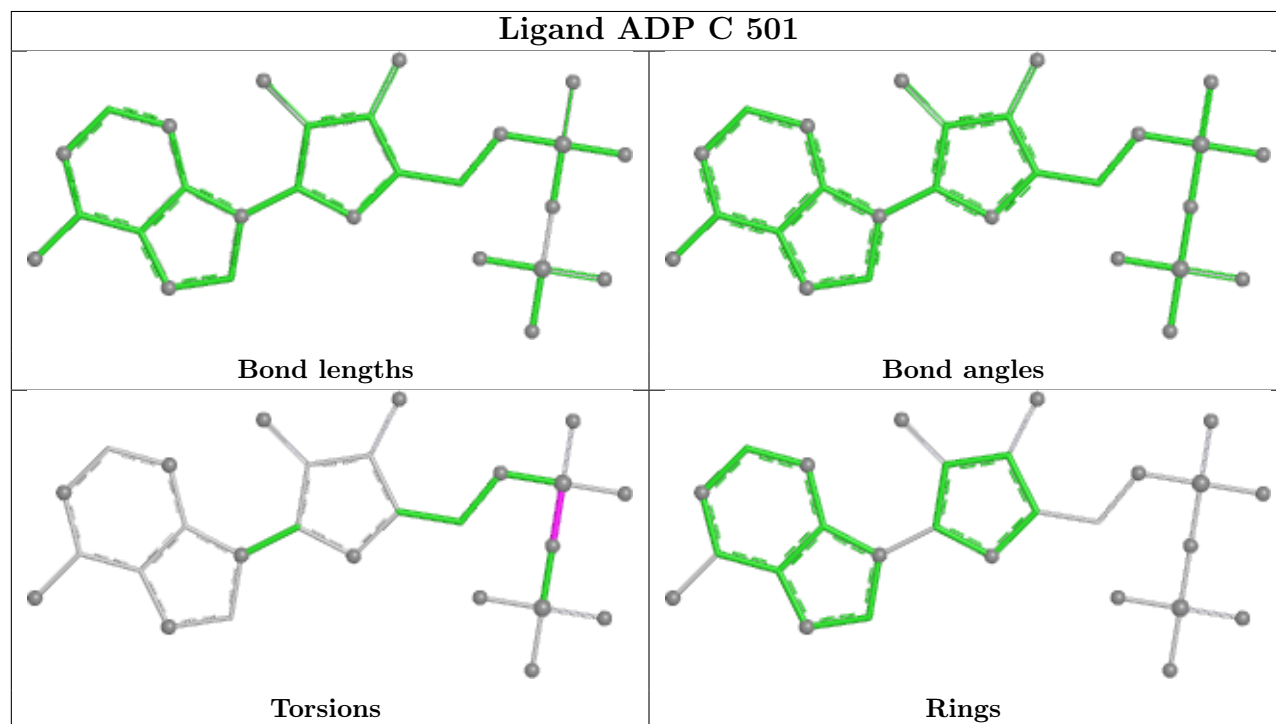
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1457	SO4	3	0
2	C	501	ADP	1	0
2	A	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/298 (76%)	-0.09	3 (1%) 75 56	60, 92, 137, 161	0
1	B	221/298 (74%)	-0.06	2 (0%) 81 65	48, 98, 155, 193	0
1	C	228/298 (76%)	-0.05	2 (0%) 81 65	70, 105, 150, 182	0
1	D	216/298 (72%)	0.06	1 (0%) 87 76	55, 132, 189, 225	0
All	All	893/1192 (74%)	-0.03	8 (0%) 81 65	48, 103, 164, 225	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	LEU	3.4
1	A	294	MET	3.1
1	A	225	PHE	2.5
1	D	258	GLN	2.3
1	B	402	PRO	2.2
1	C	403	PHE	2.1
1	C	371	VAL	2.1
1	B	335	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

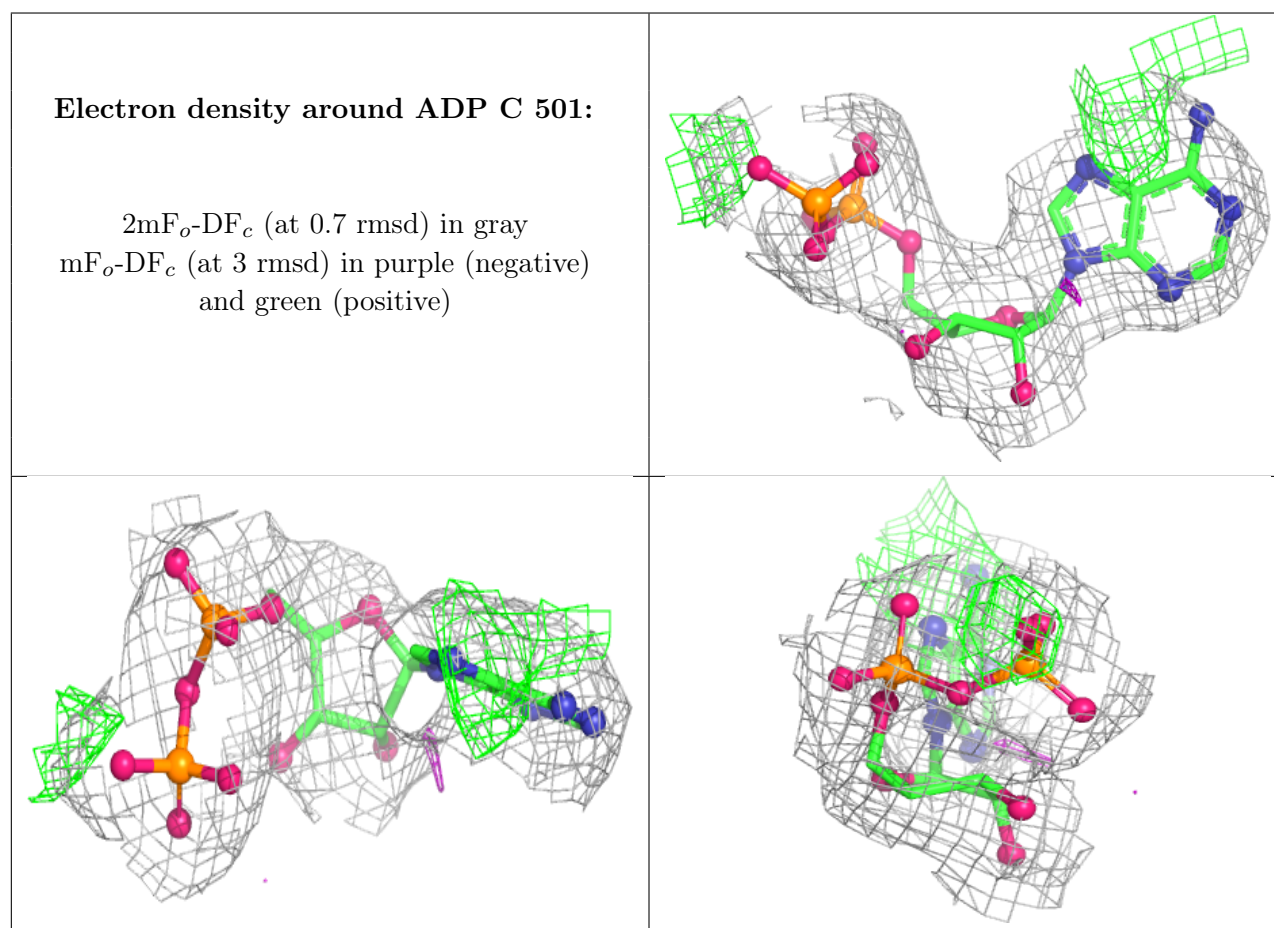
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

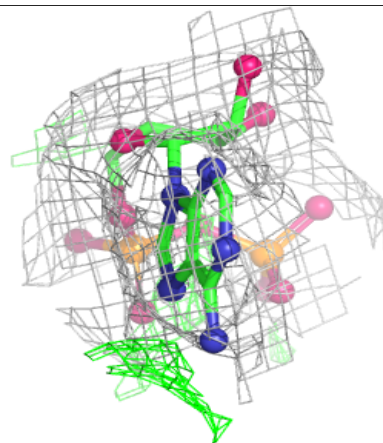
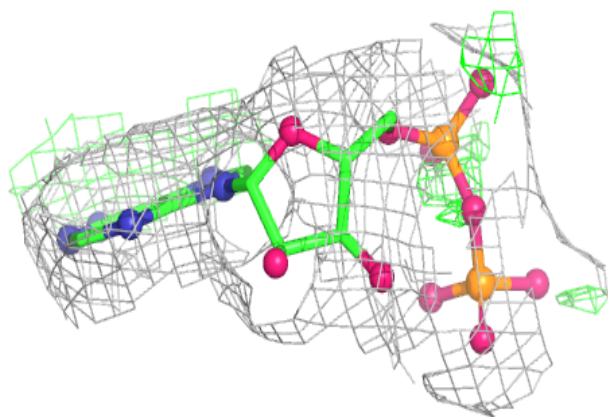
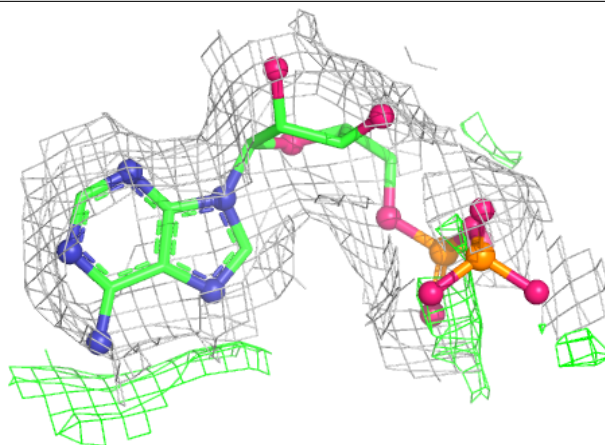
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	1457	5/5	0.54	0.10	210,210,210,212	0
3	SO4	C	1457	5/5	0.67	0.10	228,229,229,230	0
3	SO4	A	1457	5/5	0.89	0.09	101,102,103,105	0
2	ADP	C	501	27/27	0.92	0.10	86,92,100,101	0
3	SO4	B	1457	5/5	0.95	0.06	104,106,106,106	0
2	ADP	A	501	27/27	0.96	0.07	71,77,87,89	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 ADP A 501:

$2mF_o - DF_c$ (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.