



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:39 am BST

PDB ID : 5FM6
Title : Double-heterohexameric rings of full-length Rvb1(ADP)Rvb2(apo)
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Deposited on : 2015-11-02
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

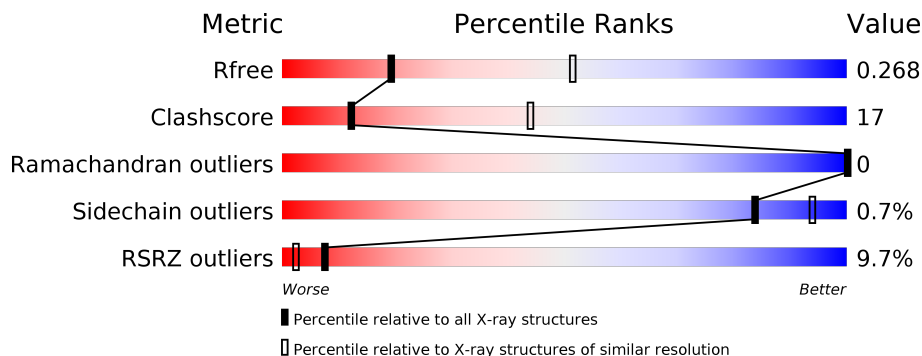
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	464	
2	B	490	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6573 atoms, of which 15 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 RVB1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	426	3280	2057	587	622	5	9	133	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0RYI5
A	0	ALA	-	expression tag	UNP G0RYI5

- Molecule 2 is a protein called RVB2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	419	3241	2029	569	629	2	12	115	0	0

There are 2 discrepancies between the modelled and reference sequences:

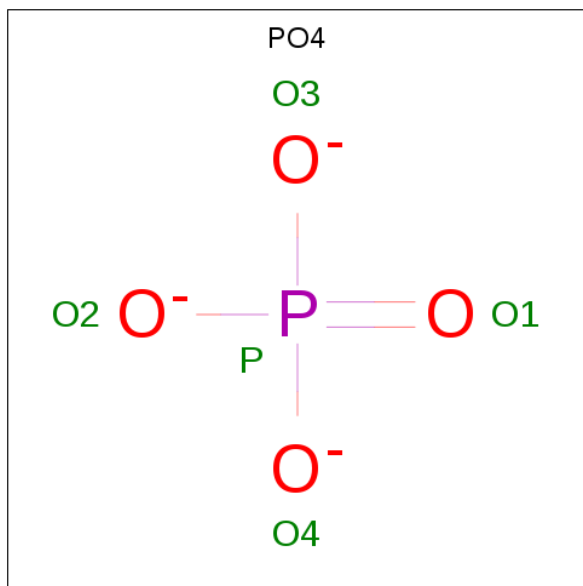
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP G0RYC2
B	0	ALA	-	expression tag	UNP G0RYC2

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
3	A	1	42	10	15	5	10	2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

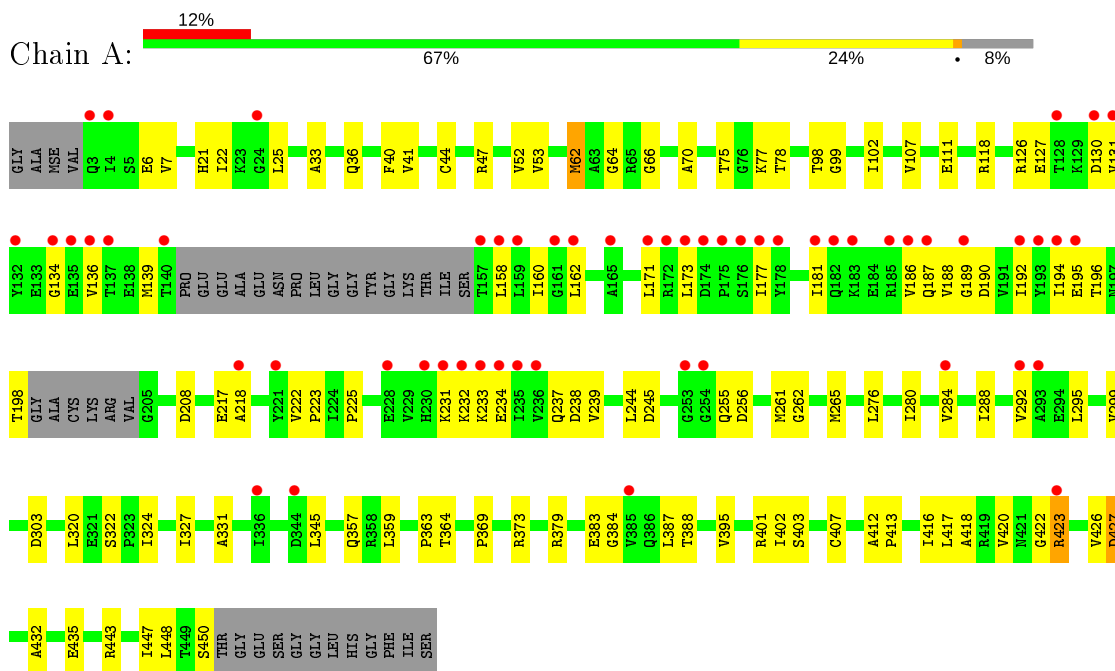


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O P		
4	B	1	5	4 1	0	0
4	B	1	5	4 1	0	0

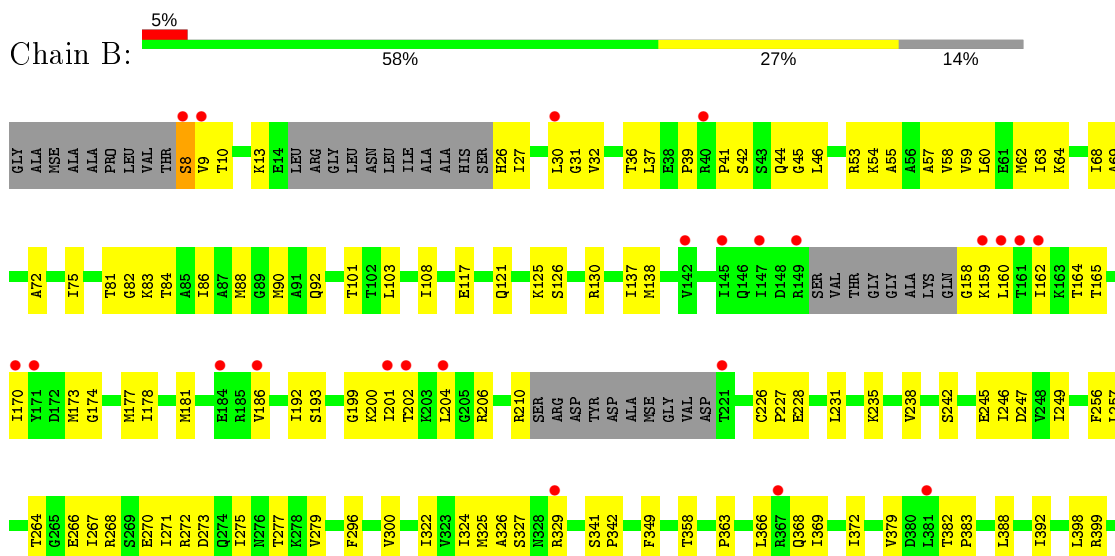
3 Residue-property plots i

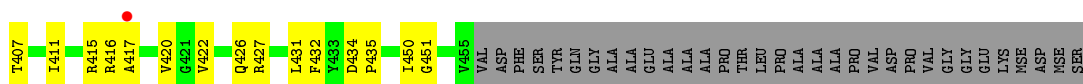
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: RVB1



- Molecule 2: RVB2





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	209.61Å 209.61Å 137.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.63 – 3.00 48.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-3.00) 99.9 (48.63-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.256 0.243 , 0.268	Depositor DCC
R_{free} test set	1170 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	106.2	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6573	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: PO4, ADP

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	0.21	0/3313	0.39	0/4460
2	B	0.22	0/3266	0.41	0/4373
All	All	0.21	0/6579	0.40	0/8833

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	3280	0	3372	104	0
2	B	3241	0	3324	115	0
3	A	27	15	12	1	0
4	B	10	0	0	1	0
All	All	6558	15	6708	215	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 17.

All (215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ARG:HD2	2:B:417:ALA:HB2	1.29	1.11
2:B:81:THR:HG21	2:B:358:THR:HB	1.40	0.99
1:A:127:GLU:HB2	1:A:292:VAL:HG13	1.49	0.95
2:B:103:LEU:HD21	2:B:108:ILE:HD11	1.50	0.93
2:B:247:ASP:HB3	2:B:267:ILE:HD13	1.51	0.92
2:B:81:THR:HG22	2:B:82:GLY:H	1.34	0.91
1:A:402:ILE:HG22	1:A:403:SER:H	1.43	0.84
1:A:345:LEU:HD21	2:B:329:ARG:HH22	1.44	0.81
2:B:13:LYS:HD2	2:B:200:LYS:HE3	1.62	0.80
2:B:63:ILE:HD13	2:B:68:ILE:HG21	1.65	0.79
2:B:31:GLY:H	2:B:44:GLN:HG3	1.48	0.78
2:B:81:THR:HG21	2:B:358:THR:CB	2.14	0.78
2:B:31:GLY:N	2:B:44:GLN:HG3	2.01	0.76
2:B:162:ILE:HD11	2:B:192:ILE:HD11	1.69	0.75
1:A:171:LEU:HD23	1:A:173:LEU:HD11	1.69	0.75
2:B:44:GLN:N	2:B:45:GLY:HA2	2.01	0.75
1:A:126:ARG:NH2	1:A:238:ASP:OD1	2.20	0.75
1:A:261:MSE:HE2	1:A:265:MSE:HA	1.68	0.75
2:B:193:SER:HB2	2:B:204:LEU:HD21	1.69	0.75
2:B:13:LYS:CD	2:B:200:LYS:HE3	2.17	0.74
1:A:412:ALA:HB3	1:A:413:PRO:HD3	1.67	0.73
2:B:137:ILE:HD11	2:B:235:LYS:HD2	1.70	0.72
1:A:288:ILE:HD11	1:A:295:LEU:HD23	1.72	0.71
2:B:63:ILE:CD1	2:B:68:ILE:HG12	2.23	0.69
1:A:6:GLU:HG2	1:A:237:GLN:HE22	1.58	0.68
1:A:234:GLU:OE1	1:A:234:GLU:N	2.27	0.68
2:B:341:SER:HB2	2:B:342:PRO:HD2	1.76	0.68
1:A:134:GLY:HA2	1:A:225:PRO:HG2	1.77	0.66
2:B:32:VAL:CG1	2:B:37:LEU:HA	2.26	0.65
1:A:422:GLY:HA2	1:A:423:ARG:HB3	1.79	0.64
1:A:127:GLU:CB	1:A:292:VAL:HG13	2.24	0.64
1:A:261:MSE:HE2	1:A:265:MSE:CA	2.26	0.64
1:A:33:ALA:HB3	1:A:44:CYS:HB3	1.80	0.64
2:B:59:VAL:O	2:B:63:ILE:HG12	1.98	0.63
1:A:423:ARG:HH21	1:A:427:ASP:HB2	1.63	0.63
2:B:268:ARG:NH2	2:B:270:GLU:HG3	2.13	0.63
1:A:195:GLU:HB3	1:A:198:THR:HG23	1.80	0.63
2:B:138:MSE:HE2	2:B:231:LEU:HG	1.81	0.63
2:B:42:SER:HA	2:B:46:LEU:O	1.99	0.62
1:A:383:GLU:N	1:A:384:GLY:HA2	2.14	0.62
2:B:81:THR:CG2	2:B:358:THR:HB	2.24	0.62
1:A:295:LEU:HD11	1:A:324:ILE:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LEU:HD21	2:B:162:ILE:CD1	2.30	0.61
1:A:295:LEU:HD11	1:A:324:ILE:CG2	2.32	0.60
1:A:417:LEU:O	1:A:420:VAL:HG12	2.01	0.60
1:A:217:GLU:HA	1:A:218:ALA:C	2.21	0.60
1:A:418:ALA:O	1:A:422:GLY:N	2.35	0.60
2:B:160:LEU:HD21	2:B:162:ILE:HD12	1.82	0.60
1:A:208:ASP:HB2	1:A:223:PRO:HA	1.83	0.60
1:A:379:ARG:O	1:A:383:GLU:HG2	2.03	0.59
1:A:369:PRO:O	1:A:373:ARG:HG3	2.02	0.59
2:B:325:MSE:HE1	2:B:349:PHE:HE1	1.67	0.59
2:B:55:ALA:O	2:B:59:VAL:HG23	2.03	0.59
2:B:27:ILE:O	2:B:92:GLN:HG3	2.02	0.58
1:A:131:VAL:HG23	1:A:194:ILE:H	1.68	0.58
1:A:98:THR:HG22	1:A:303:ASP:HB3	1.84	0.58
1:A:299:VAL:HG22	1:A:327:ILE:CG2	2.33	0.58
2:B:165:THR:OG1	2:B:228:GLU:HG2	2.03	0.58
1:A:401:ARG:HB3	1:A:402:ILE:HD12	1.85	0.57
2:B:63:ILE:HD13	2:B:68:ILE:HG12	1.86	0.57
1:A:443:ARG:O	1:A:447:ILE:HG12	2.04	0.57
1:A:422:GLY:HA2	1:A:423:ARG:C	2.23	0.57
2:B:81:THR:HG22	2:B:82:GLY:N	2.12	0.57
1:A:36:GLN:HA	1:A:40:PHE:O	2.06	0.56
2:B:206:ARG:HH22	2:B:210:ARG:HB3	1.70	0.56
2:B:206:ARG:NH2	2:B:210:ARG:HB3	2.20	0.56
1:A:432:ALA:O	1:A:435:GLU:HG2	2.05	0.55
1:A:208:ASP:CB	1:A:223:PRO:HA	2.36	0.55
1:A:357:GLN:HG3	2:B:399:ARG:HG2	1.88	0.55
2:B:173:MSE:HB2	2:B:177:MSE:HG2	1.87	0.55
1:A:139:MSE:SE	1:A:188:VAL:HG23	2.56	0.55
1:A:217:GLU:HB2	1:A:218:ALA:HA	1.88	0.55
1:A:130:ASP:HB3	1:A:196:THR:OG1	2.05	0.55
1:A:53:VAL:HG13	1:A:62:MSE:HE2	1.89	0.54
1:A:345:LEU:CD2	2:B:329:ARG:HH22	2.15	0.54
2:B:174:GLY:O	2:B:178:ILE:HG13	2.07	0.54
1:A:75:THR:HB	1:A:364:THR:HB	1.89	0.54
1:A:402:ILE:HG22	1:A:403:SER:N	2.17	0.54
2:B:181:MSE:HE3	2:B:186:VAL:HG11	1.89	0.54
2:B:63:ILE:HD11	2:B:68:ILE:HG12	1.90	0.54
2:B:83:LYS:NZ	2:B:327:SER:O	2.41	0.53
2:B:256:PHE:CE2	2:B:257:LEU:HG	2.44	0.53
2:B:164:THR:HG23	2:B:231:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:CD1	1:A:295:LEU:HD23	2.38	0.53
2:B:382:THR:HG23	2:B:383:PRO:HD2	1.90	0.53
2:B:415:ARG:O	2:B:416:ARG:HB2	2.09	0.53
1:A:171:LEU:HD23	1:A:173:LEU:CD1	2.37	0.53
1:A:402:ILE:HD12	1:A:402:ILE:H	1.74	0.53
1:A:53:VAL:HG13	1:A:62:MSE:CE	2.40	0.52
1:A:136:VAL:CG1	1:A:188:VAL:HG22	2.40	0.52
1:A:107:VAL:HG12	1:A:111:GLU:HB2	1.93	0.51
1:A:402:ILE:N	1:A:402:ILE:HD12	2.25	0.51
1:A:131:VAL:HG13	1:A:231:LYS:HB3	1.92	0.51
1:A:64:GLY:HA2	1:A:320:LEU:O	2.12	0.50
2:B:31:GLY:HA2	2:B:44:GLN:HG2	1.94	0.50
2:B:86:ILE:O	2:B:90:MSE:HG3	2.10	0.50
2:B:173:MSE:CB	2:B:177:MSE:HG2	2.42	0.50
1:A:295:LEU:O	1:A:295:LEU:HD12	2.11	0.50
1:A:383:GLU:HB2	1:A:384:GLY:HA2	1.92	0.50
2:B:30:LEU:O	2:B:53:ARG:HD2	2.12	0.50
1:A:208:ASP:N	1:A:222:VAL:O	2.45	0.49
2:B:379:VAL:HG13	2:B:420:VAL:HG21	1.93	0.49
2:B:60:LEU:O	2:B:64:LYS:HG3	2.13	0.49
2:B:181:MSE:HG2	2:B:201:ILE:HG12	1.94	0.49
2:B:82:GLY:O	2:B:86:ILE:HG13	2.12	0.49
1:A:134:GLY:CA	1:A:225:PRO:HG2	2.43	0.49
1:A:448:LEU:HD12	1:A:448:LEU:O	2.12	0.49
2:B:101:THR:HG22	2:B:126:SER:HB3	1.94	0.49
1:A:99:GLY:O	1:A:102:ILE:HG12	2.13	0.49
2:B:101:THR:CG2	2:B:126:SER:HB3	2.42	0.49
2:B:117:GLU:OE2	2:B:272:ARG:NH2	2.46	0.49
1:A:177:ILE:O	1:A:181:ILE:HG12	2.13	0.48
1:A:78:THR:HB	3:A:501:ADP:O2A	2.12	0.48
2:B:121:GLN:O	2:B:125:LYS:HG3	2.12	0.48
1:A:195:GLU:HB3	1:A:198:THR:CG2	2.44	0.48
2:B:32:VAL:HA	2:B:39:PRO:HA	1.93	0.48
2:B:54:LYS:O	2:B:58:VAL:HG23	2.13	0.48
1:A:186:VAL:O	1:A:187:GLN:HG3	2.13	0.48
2:B:450:ILE:HG23	2:B:451:GLY:N	2.29	0.48
2:B:434:ASP:HB2	2:B:435:PRO:HD2	1.96	0.48
2:B:170:ILE:N	2:B:170:ILE:HD12	2.29	0.47
2:B:9:VAL:HG23	2:B:10:THR:N	2.27	0.47
2:B:158:GLY:O	2:B:159:LYS:HG3	2.13	0.47
2:B:44:GLN:N	2:B:45:GLY:CA	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD21	1:A:192:ILE:HD11	1.96	0.47
2:B:256:PHE:CD2	2:B:257:LEU:HG	2.50	0.47
2:B:388:LEU:HD21	2:B:426:GLN:HG2	1.95	0.47
1:A:134:GLY:HA2	1:A:225:PRO:CG	2.45	0.47
2:B:366:LEU:HD23	2:B:398:LEU:HD13	1.97	0.47
2:B:41:PRO:HA	2:B:53:ARG:HH22	1.80	0.47
1:A:387:LEU:HD23	1:A:387:LEU:H	1.79	0.47
2:B:247:ASP:CB	2:B:267:ILE:HD13	2.34	0.47
1:A:127:GLU:HG3	1:A:292:VAL:HG22	1.97	0.46
2:B:382:THR:CG2	2:B:383:PRO:HD2	2.45	0.46
2:B:8:SER:HB2	2:B:9:VAL:H	1.53	0.46
1:A:276:LEU:O	1:A:280:ILE:HG12	2.14	0.46
2:B:271:ILE:O	2:B:275:ILE:HG12	2.14	0.46
1:A:131:VAL:HA	1:A:194:ILE:O	2.15	0.46
1:A:77:LYS:HD2	1:A:331:ALA:HB1	1.97	0.46
2:B:27:ILE:H	2:B:88:MSE:CE	2.27	0.46
2:B:264:THR:OG1	2:B:266:GLU:OE1	2.29	0.46
1:A:25:LEU:O	1:A:47:ARG:HD2	2.16	0.46
1:A:70:ALA:O	1:A:363:PRO:HA	2.16	0.46
2:B:245:GLU:O	2:B:249:ILE:HG13	2.15	0.46
2:B:407:THR:O	2:B:411:ILE:HG13	2.16	0.46
1:A:412:ALA:O	1:A:416:ILE:HG12	2.16	0.45
1:A:36:GLN:HG2	1:A:41:VAL:HG22	1.97	0.45
2:B:325:MSE:HE1	2:B:349:PHE:CE1	2.50	0.45
2:B:193:SER:CB	2:B:204:LEU:HD21	2.43	0.45
1:A:262:GLY:O	1:A:265:MSE:HG2	2.17	0.45
1:A:188:VAL:HA	1:A:189:GLY:HA2	1.55	0.45
1:A:423:ARG:HH21	1:A:427:ASP:CB	2.30	0.45
2:B:32:VAL:HG13	2:B:37:LEU:HA	1.99	0.45
1:A:52:VAL:HB	2:B:432:PHE:HZ	1.82	0.45
1:A:134:GLY:HA2	1:A:225:PRO:HD2	1.99	0.45
1:A:280:ILE:O	1:A:284:VAL:HG23	2.17	0.45
1:A:66:GLY:O	1:A:359:LEU:HA	2.17	0.45
2:B:63:ILE:HD13	2:B:68:ILE:CG2	2.43	0.45
1:A:130:ASP:HA	1:A:232:LYS:HA	1.97	0.45
1:A:322:SER:OG	1:A:324:ILE:HD12	2.17	0.45
1:A:136:VAL:HG12	1:A:188:VAL:HG22	1.99	0.45
2:B:63:ILE:CD1	2:B:68:ILE:HG21	2.42	0.44
2:B:26:HIS:HB3	2:B:88:MSE:HE1	1.99	0.44
2:B:322:ILE:HD12	2:B:322:ILE:N	2.32	0.44
1:A:388:THR:HG23	1:A:426:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ILE:HG21	2:B:398:LEU:HD21	1.99	0.44
2:B:202:THR:O	2:B:204:LEU:HD22	2.17	0.43
1:A:130:ASP:HB3	1:A:196:THR:HG1	1.81	0.43
2:B:422:VAL:O	2:B:426:GLN:HG3	2.18	0.43
2:B:434:ASP:HB2	2:B:435:PRO:CD	2.48	0.43
2:B:72:ALA:HB1	2:B:325:MSE:HE2	2.00	0.43
2:B:173:MSE:SE	2:B:177:MSE:HG2	2.68	0.43
2:B:296:PHE:HA	2:B:324:ILE:O	2.18	0.43
2:B:37:LEU:HD22	2:B:57:ALA:HB1	2.00	0.43
2:B:275:ILE:O	2:B:279:VAL:HG23	2.18	0.43
2:B:32:VAL:HG13	2:B:37:LEU:C	2.37	0.43
1:A:126:ARG:HA	1:A:126:ARG:HD3	1.74	0.43
2:B:388:LEU:O	2:B:392:ILE:HG13	2.18	0.43
2:B:300:VAL:HG21	2:B:325:MSE:SE	2.68	0.43
1:A:231:LYS:HE3	1:A:233:LYS:HD2	1.99	0.43
2:B:75:ILE:CG2	2:B:83:LYS:HB3	2.49	0.43
1:A:422:GLY:CA	1:A:423:ARG:C	2.88	0.43
2:B:242:SER:O	2:B:246:ILE:HG13	2.19	0.43
2:B:75:ILE:O	2:B:326:ALA:HA	2.19	0.43
1:A:136:VAL:O	1:A:188:VAL:HG13	2.19	0.42
1:A:118:ARG:HH21	1:A:245:ASP:CG	2.22	0.42
1:A:7:VAL:HG21	1:A:244:LEU:HD23	2.02	0.42
2:B:130:ARG:HG3	2:B:238:VAL:HG13	1.99	0.42
2:B:226:CYS:HA	2:B:227:PRO:HD3	1.88	0.42
1:A:118:ARG:NH2	1:A:245:ASP:OD1	2.48	0.42
1:A:21:HIS:CE1	1:A:379:ARG:HD3	2.55	0.42
2:B:450:ILE:HG23	2:B:451:GLY:H	1.85	0.42
2:B:68:ILE:HG23	2:B:69:ALA:N	2.34	0.42
2:B:363:PRO:HA	2:B:366:LEU:HD12	2.02	0.42
1:A:387:LEU:HD23	1:A:387:LEU:N	2.34	0.42
1:A:395:VAL:O	1:A:407:CYS:HB2	2.20	0.42
2:B:273:ASP:O	2:B:277:THR:HG23	2.20	0.42
1:A:136:VAL:HG23	1:A:190:ASP:O	2.20	0.41
1:A:158:LEU:CD1	1:A:160:ILE:HG13	2.50	0.41
2:B:103:LEU:HD21	2:B:108:ILE:CD1	2.35	0.41
1:A:6:GLU:HG2	1:A:237:GLN:NE2	2.30	0.41
2:B:427:ARG:O	2:B:431:LEU:HG	2.20	0.41
2:B:27:ILE:H	2:B:88:MSE:HE2	1.85	0.41
1:A:160:ILE:HB	1:A:173:LEU:HD13	2.01	0.41
1:A:231:LYS:CE	1:A:233:LYS:HD2	2.51	0.41
1:A:255:GLN:HG3	1:A:256:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLY:O	2:B:201:ILE:HD12	2.20	0.41
2:B:84:THR:OG1	4:B:501:PO4:O2	2.38	0.41
1:A:7:VAL:HG23	1:A:239:VAL:HG11	2.03	0.41
2:B:36:THR:O	2:B:37:LEU:HB2	2.20	0.41
2:B:58:VAL:O	2:B:62:MSE:HG3	2.21	0.41
2:B:75:ILE:HG21	2:B:83:LYS:CB	2.51	0.41
1:A:383:GLU:HB2	1:A:384:GLY:CA	2.51	0.41
1:A:22:ILE:HD12	1:A:40:PHE:CE2	2.57	0.40
2:B:368:GLN:O	2:B:372:ILE:HG13	2.22	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	420/464 (90%)	400 (95%)	20 (5%)	0	100	100
2	B	411/490 (84%)	400 (97%)	11 (3%)	0	100	100
All	All	831/954 (87%)	800 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	351/367 (96%)	347 (99%)	4 (1%)	73	90
2	B	354/386 (92%)	353 (100%)	1 (0%)	92	97
All	All	705/753 (94%)	700 (99%)	5 (1%)	84	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	MSE
1	A	423	ARG
1	A	427	ASP
1	A	450	SER
2	B	8	SER

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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
4	PO4	B	501	-	4,4,4	0.93	0	6,6,6	0.36	0
4	PO4	B	502	-	4,4,4	0.90	0	6,6,6	0.40	0
3	ADP	A	501	-	24,29,29	0.65	0	29,45,45	0.65	1 (3%)

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
3	ADP	A	501	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	501	ADP	C5-C6-N6	2.20	123.69	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	O4'-C4'-C5'-O5'
3	A	501	ADP	C3'-C4'-C5'-O5'
3	A	501	ADP	PA-O3A-PB-O1B
3	A	501	ADP	PA-O3A-PB-O2B
3	A	501	ADP	PA-O3A-PB-O3B

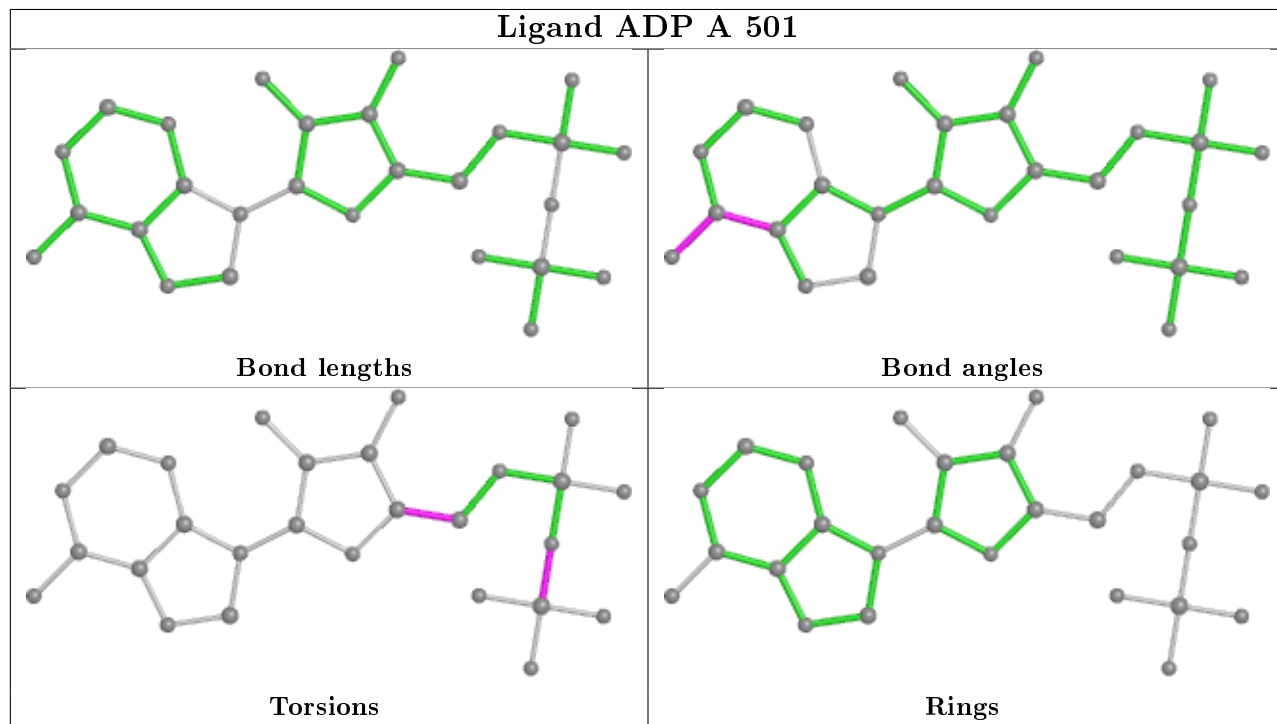
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	PO4	1	0
3	A	501	ADP	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](#)

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	417/464 (89%)	0.80	56 (13%) 3 1	72, 101, 169, 198	33 (7%)
2	B	407/490 (83%)	0.60	24 (5%) 22 7	68, 97, 131, 154	28 (6%)
All	All	824/954 (86%)	0.70	80 (9%) 7 2	68, 99, 154, 198	61 (7%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	THR	9.6
1	A	181	ILE	6.7
1	A	231	LYS	6.6
1	A	159	LEU	6.6
1	A	137	THR	5.6
1	A	175	PRO	5.5
1	A	182	GLN	5.4
1	A	192	ILE	5.3
1	A	194	ILE	5.3
1	A	186	VAL	5.0
1	A	140	THR	5.0
1	A	178	TYR	4.9
1	A	131	VAL	4.9
1	A	158	LEU	4.5
2	B	145	ILE	4.4
1	A	173	LEU	4.1
1	A	230	HIS	4.0
1	A	221	TYR	3.9
1	A	171	LEU	3.9
1	A	176	SER	3.8
2	B	204	LEU	3.8
1	A	165	ALA	3.8
2	B	162	ILE	3.7
1	A	183	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	134	GLY	3.6
1	A	195	GLU	3.4
1	A	292	VAL	3.4
2	B	147	ILE	3.3
1	A	189	GLY	3.3
1	A	336	ILE	3.2
1	A	128	THR	3.1
2	B	160	LEU	3.1
1	A	235	ILE	3.1
1	A	3	GLN	3.1
1	A	174	ASP	3.0
1	A	172	ARG	3.0
1	A	228	GLU	3.0
1	A	232	LYS	3.0
1	A	236	VAL	3.0
1	A	177	ILE	3.0
1	A	254	GLY	2.9
2	B	171	TYR	2.9
1	A	193	TYR	2.9
2	B	170	ILE	2.9
2	B	40	ARG	2.9
2	B	417	ALA	2.8
1	A	344	ASP	2.8
1	A	423	ARG	2.7
1	A	234	GLU	2.7
1	A	185	ARG	2.7
1	A	284	VAL	2.7
1	A	4	ILE	2.6
1	A	218	ALA	2.5
1	A	162	LEU	2.5
2	B	221	THR	2.5
1	A	135	GLU	2.4
2	B	202	THR	2.4
1	A	24	GLY	2.4
1	A	132	TYR	2.4
2	B	381	LEU	2.4
2	B	367	ARG	2.4
1	A	233	LYS	2.3
2	B	149	ARG	2.3
2	B	30	LEU	2.3
2	B	329	ARG	2.3
1	A	136	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	142	VAL	2.2
2	B	161	THR	2.2
2	B	9	VAL	2.2
2	B	184	GLU	2.2
1	A	293	ALA	2.2
2	B	8	SER	2.2
2	B	201	ILE	2.1
2	B	186	VAL	2.1
1	A	161	GLY	2.1
1	A	130	ASP	2.1
2	B	159	LYS	2.1
1	A	187	GLN	2.1
1	A	253	GLY	2.0
1	A	385	VAL	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](#)

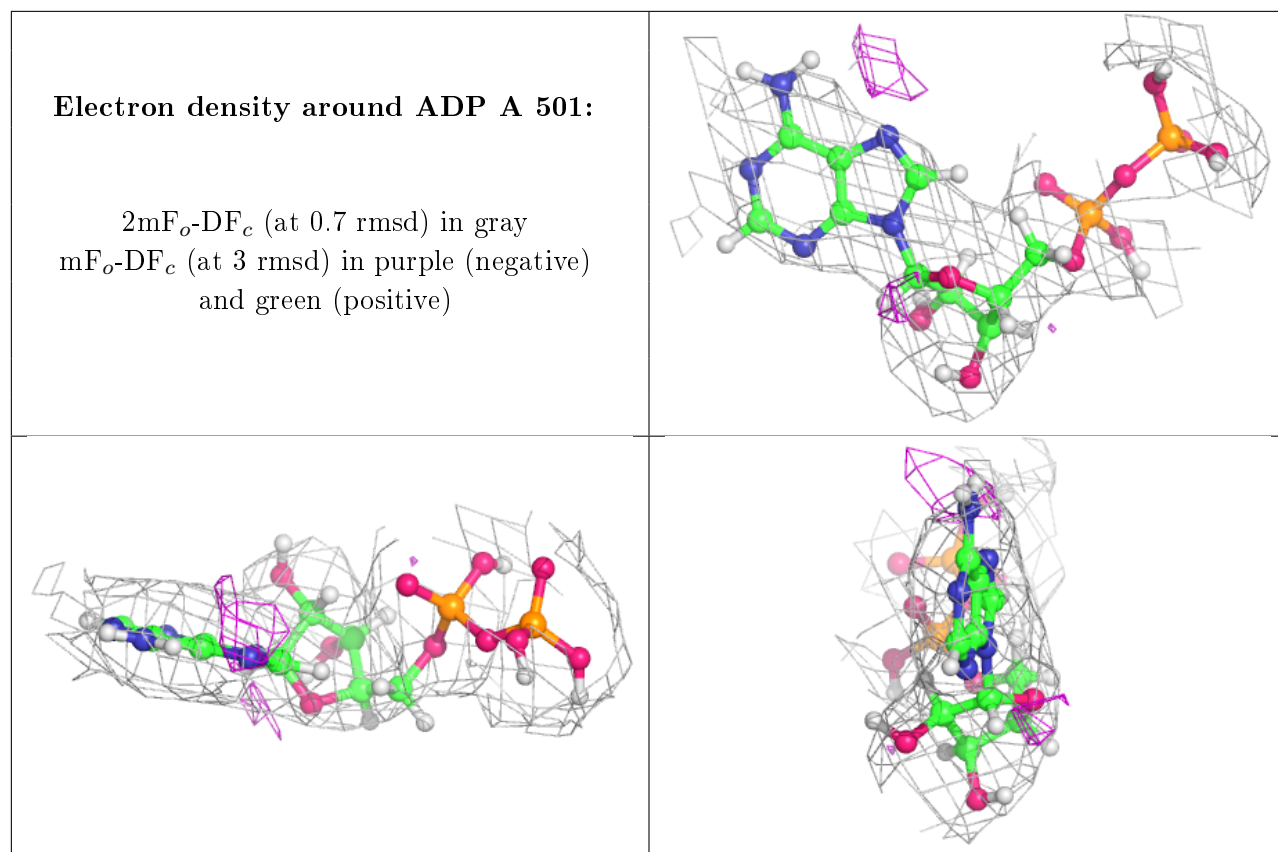
There are no carbohydrates in this entry.

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	PO4	B	502	5/5	0.90	0.21	99,101,103,104	0
4	PO4	B	501	5/5	0.93	0.23	87,91,94,95	0
3	ADP	A	501	27/27	0.97	0.20	72,93,113,119	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.