



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:25 am BST

PDB ID : 4PXA
Title : DEAD-box RNA helicase DDX3X Cancer-associated mutant D354V
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Deposited on : 2014-03-22
Resolution : 3.20 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 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

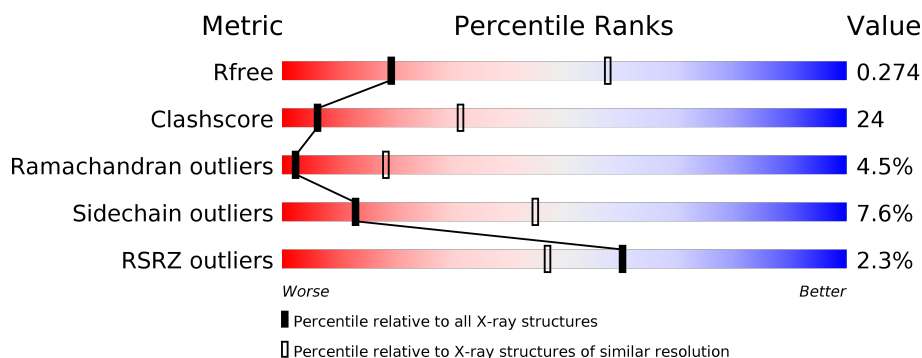
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	467	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>37%</div> <div>5%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3547 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 ATP-dependent RNA helicase DDX3X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3495	2205	611	660	19			

There are 20 discrepancies between the modelled and reference sequences:

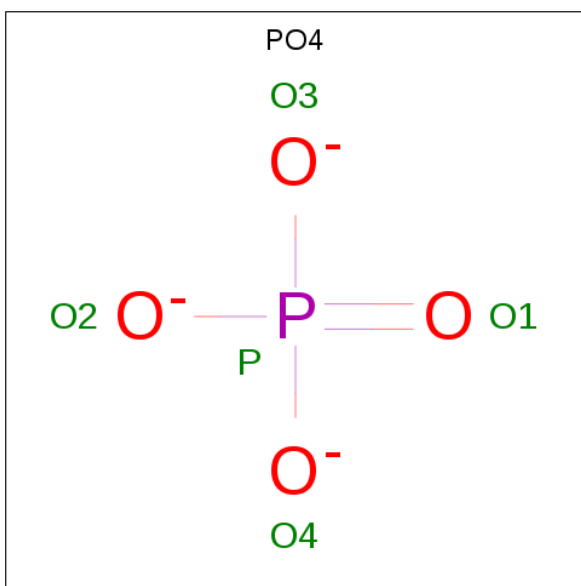
Chain	Residue	Modelled	Actual	Comment	Reference
A	116	MET	-	EXPRESSION TAG	UNP O00571
A	117	GLY	-	EXPRESSION TAG	UNP O00571
A	118	SER	-	EXPRESSION TAG	UNP O00571
A	119	SER	-	EXPRESSION TAG	UNP O00571
A	120	HIS	-	EXPRESSION TAG	UNP O00571
A	121	HIS	-	EXPRESSION TAG	UNP O00571
A	122	HIS	-	EXPRESSION TAG	UNP O00571
A	123	HIS	-	EXPRESSION TAG	UNP O00571
A	124	HIS	-	EXPRESSION TAG	UNP O00571
A	125	HIS	-	EXPRESSION TAG	UNP O00571
A	126	SER	-	EXPRESSION TAG	UNP O00571
A	127	SER	-	EXPRESSION TAG	UNP O00571
A	128	GLY	-	EXPRESSION TAG	UNP O00571
A	129	LEU	-	EXPRESSION TAG	UNP O00571
A	130	VAL	-	EXPRESSION TAG	UNP O00571
A	131	PRO	-	EXPRESSION TAG	UNP O00571
A	132	ARG	-	EXPRESSION TAG	UNP O00571
A	133	GLY	-	EXPRESSION TAG	UNP O00571
A	134	SER	-	EXPRESSION TAG	UNP O00571
A	354	VAL	ASP	ENGINEERED MUTATION	UNP O00571

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.75Å 105.75Å 152.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 3.20 45.85 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.85-3.20) 99.2 (45.85-3.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.206 , 0.271 0.199 , 0.274	Depositor DCC
R_{free} test set	723 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.8	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	0.94	EDS
Total number of atoms	3547	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.40	0/3563	0.63	0/4814

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

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	3495	0	3484	171	0
2	A	27	0	12	3	0
3	A	25	0	0	0	0
All	All	3547	0	3496	171	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 24.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HA	1:A:527:HIS:HB2	1.37	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:HZ	1:A:202:ARG:HH12	1.21	0.85
1:A:176:PRO:HB3	1:A:216:GLU:OE1	1.78	0.82
1:A:471:ILE:HG13	1:A:495:LEU:HD21	1.62	0.82
1:A:552:ILE:O	1:A:552:ILE:HG12	1.80	0.80
1:A:351:ARG:HG2	1:A:351:ARG:HH11	1.45	0.80
1:A:160:PHE:HE2	1:A:202:ARG:HH22	1.29	0.79
1:A:354:VAL:HA	1:A:527:HIS:CB	2.11	0.77
1:A:269:SER:HB3	1:A:319:LEU:HD12	1.65	0.76
1:A:458:GLU:HG3	1:A:470:SER:HB2	1.66	0.75
1:A:351:ARG:HH21	1:A:534:ARG:NH2	1.84	0.74
1:A:439:GLY:O	1:A:441:ASP:N	2.21	0.74
1:A:168:VAL:HG22	1:A:405:VAL:HG12	1.73	0.70
1:A:202:ARG:HB2	1:A:202:ARG:NH1	2.07	0.70
1:A:405:VAL:HG23	1:A:405:VAL:O	1.92	0.69
1:A:487:PHE:CE1	1:A:495:LEU:HB2	2.26	0.69
1:A:478:ARG:HH11	1:A:478:ARG:HG2	1.57	0.68
1:A:274:PRO:HD2	1:A:278:LEU:HD23	1.73	0.68
1:A:414:ASN:HD21	1:A:537:ASN:C	1.98	0.68
1:A:159:ASN:O	1:A:163:TYR:HD2	1.78	0.67
1:A:160:PHE:HZ	1:A:202:ARG:NH1	1.93	0.66
1:A:461:LEU:O	1:A:466:TYR:HB2	1.97	0.65
1:A:295:VAL:HG13	1:A:318:HIS:HB2	1.79	0.65
1:A:373:LYS:HD2	1:A:398:ASP:HB2	1.77	0.65
1:A:351:ARG:HG2	1:A:351:ARG:NH1	2.10	0.64
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.79	0.63
1:A:514:ILE:HG22	1:A:542:THR:HB	1.80	0.63
1:A:513:VAL:O	1:A:541:ALA:HA	1.99	0.63
1:A:550:ILE:HD12	1:A:553:THR:OG1	1.99	0.63
1:A:309:GLN:OE1	1:A:326:ARG:NH1	2.33	0.62
1:A:435:LEU:O	1:A:438:THR:HB	2.00	0.61
1:A:479:ASP:O	1:A:482:GLU:HB2	2.01	0.60
1:A:421:TRP:HA	1:A:545:PHE:O	2.01	0.60
1:A:159:ASN:HD22	1:A:163:TYR:HE2	1.47	0.60
1:A:168:VAL:HG13	1:A:405:VAL:HG12	1.83	0.59
1:A:575:ALA:O	1:A:576:TYR:HB2	2.01	0.59
1:A:184:ASP:O	1:A:185:VAL:HG13	2.01	0.59
1:A:438:THR:O	1:A:440:LYS:HD3	2.03	0.58
1:A:480:ARG:O	1:A:484:LEU:HD13	2.04	0.58
1:A:257:ASN:O	1:A:259:ARG:N	2.37	0.57
1:A:310:ILE:O	1:A:314:GLU:HG2	2.05	0.57
1:A:200:TYR:OH	2:A:601:ADP:H2'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ARG:HB3	1:A:505:LEU:HD21	1.85	0.57
1:A:191:ILE:O	1:A:195:ILE:HG13	2.05	0.56
1:A:356:GLY:HA3	1:A:503:ARG:HD2	1.86	0.56
1:A:472:HIS:O	1:A:480:ARG:HD3	2.06	0.56
1:A:226:THR:HA	2:A:601:ADP:O2B	2.06	0.56
1:A:502:ALA:HA	1:A:505:LEU:HD12	1.86	0.56
1:A:538:LEU:HD23	1:A:539:GLY:O	2.05	0.56
1:A:402:PHE:CE2	1:A:404:ALA:HB2	2.42	0.55
1:A:351:ARG:HE	1:A:534:ARG:HH21	1.54	0.55
1:A:531:ARG:HH11	1:A:531:ARG:HG2	1.72	0.55
1:A:508:SER:O	1:A:509:ASN:CB	2.54	0.54
1:A:443:LEU:CD2	1:A:493:PRO:HA	2.36	0.54
1:A:471:ILE:HG13	1:A:495:LEU:CD2	2.36	0.54
1:A:327:LEU:HD23	1:A:364:ILE:HD13	1.89	0.54
1:A:370:MET:HG3	1:A:371:PRO:HD2	1.89	0.54
1:A:443:LEU:HD12	1:A:509:ASN:O	2.08	0.54
1:A:257:ASN:C	1:A:259:ARG:H	2.12	0.53
1:A:148:GLN:NE2	1:A:148:GLN:HA	2.23	0.53
1:A:301:TYR:H	1:A:309:GLN:HE22	1.55	0.53
1:A:414:ASN:HD21	1:A:538:LEU:N	2.06	0.52
1:A:159:ASN:HB2	1:A:163:TYR:CE2	2.44	0.52
1:A:194:ASN:OD1	1:A:291:TYR:HB3	2.10	0.52
1:A:324:PRO:HB2	1:A:357:PHE:CD1	2.45	0.52
1:A:358:GLU:HB3	1:A:359:PRO:HD3	1.92	0.52
1:A:439:GLY:C	1:A:441:ASP:H	2.11	0.52
1:A:136:TRP:HZ3	1:A:295:VAL:HG22	1.74	0.52
1:A:162:LYS:N	1:A:162:LYS:HE2	2.25	0.51
1:A:368:ASP:CG	1:A:369:THR:H	2.13	0.51
1:A:346:LEU:N	1:A:346:LEU:HD12	2.26	0.51
1:A:202:ARG:CB	1:A:202:ARG:NH1	2.74	0.51
1:A:224:ALA:HB2	1:A:405:VAL:HG22	1.92	0.51
1:A:202:ARG:HB3	1:A:203:PRO:HD2	1.93	0.51
1:A:270:LEU:HD21	1:A:327:LEU:CD2	2.41	0.51
1:A:148:GLN:HE21	1:A:148:GLN:HA	1.76	0.51
1:A:522:ILE:CG1	1:A:559:LEU:HD12	2.40	0.51
1:A:414:ASN:ND2	1:A:538:LEU:HA	2.25	0.51
1:A:162:LYS:CE	1:A:162:LYS:H	2.23	0.51
1:A:250:ALA:O	1:A:254:MET:HB2	2.11	0.51
1:A:285:GLU:HG3	1:A:289:PHE:CE2	2.46	0.51
1:A:328:VAL:O	1:A:332:GLU:HG3	2.11	0.51
1:A:478:ARG:NH1	1:A:478:ARG:HG2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:O	1:A:310:ILE:HG13	2.11	0.50
1:A:442:SER:OG	1:A:511:LYS:HD3	2.12	0.50
1:A:162:LYS:HA	1:A:165:ASP:OD2	2.12	0.50
1:A:202:ARG:CB	1:A:202:ARG:HH11	2.24	0.50
1:A:490:GLY:O	1:A:492:SER:N	2.45	0.50
1:A:480:ARG:NH1	1:A:505:LEU:HG	2.27	0.50
1:A:485:HIS:ND1	1:A:488:ARG:NH2	2.59	0.49
1:A:241:GLN:HA	1:A:241:GLN:NE2	2.28	0.49
1:A:139:PRO:HB3	1:A:190:ILE:HG12	1.94	0.48
1:A:146:LEU:C	1:A:146:LEU:HD23	2.34	0.48
1:A:550:ILE:HD12	1:A:553:THR:HG1	1.79	0.48
1:A:295:VAL:HG13	1:A:318:HIS:CB	2.45	0.47
1:A:354:VAL:C	1:A:356:GLY:H	2.17	0.47
1:A:482:GLU:O	1:A:485:HIS:HB2	2.15	0.47
1:A:469:THR:HG21	1:A:486:GLN:NE2	2.29	0.47
1:A:414:ASN:ND2	1:A:537:ASN:C	2.68	0.47
1:A:552:ILE:O	1:A:552:ILE:CG1	2.59	0.47
1:A:159:ASN:O	1:A:163:TYR:CD2	2.64	0.47
1:A:471:ILE:HD12	1:A:497:ALA:CB	2.45	0.47
1:A:214:ILE:HD13	1:A:379:MET:SD	2.55	0.46
1:A:168:VAL:HG22	1:A:405:VAL:CG1	2.44	0.46
1:A:351:ARG:NH2	1:A:534:ARG:NH2	2.60	0.46
1:A:480:ARG:CB	1:A:505:LEU:HD21	2.46	0.46
1:A:416:THR:HB	1:A:540:LEU:HD12	1.98	0.46
1:A:160:PHE:CE2	1:A:202:ARG:NH2	2.80	0.46
1:A:186:GLU:CD	1:A:186:GLU:H	2.18	0.46
1:A:531:ARG:HH11	1:A:531:ARG:CG	2.29	0.45
1:A:158:ILE:O	1:A:160:PHE:N	2.49	0.45
1:A:341:CYS:SG	1:A:370:MET:HE2	2.56	0.45
1:A:545:PHE:CD2	1:A:545:PHE:C	2.89	0.45
1:A:435:LEU:HA	1:A:438:THR:OG1	2.17	0.45
1:A:457:LEU:O	1:A:461:LEU:HD12	2.16	0.45
1:A:514:ILE:HA	1:A:542:THR:O	2.16	0.45
1:A:202:ARG:CZ	1:A:202:ARG:HB2	2.46	0.45
1:A:389:ILE:HA	1:A:389:ILE:HD13	1.84	0.45
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.82	0.45
1:A:146:LEU:O	1:A:146:LEU:HD23	2.17	0.45
1:A:247:PRO:HB2	1:A:251:LEU:HD12	1.98	0.44
1:A:269:SER:CB	1:A:319:LEU:HD12	2.42	0.44
1:A:415:ILE:HD11	1:A:532:THR:HG23	1.98	0.44
1:A:512:HIS:NE2	1:A:540:LEU:HD23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HB	1:A:184:ASP:HB2	1.98	0.44
1:A:407:ARG:HG2	1:A:413:GLU:OE1	2.18	0.44
1:A:274:PRO:HG3	1:A:348:GLU:OE1	2.17	0.44
1:A:480:ARG:HH11	1:A:505:LEU:HG	1.83	0.44
1:A:522:ILE:HG13	1:A:559:LEU:HD12	2.00	0.44
1:A:376:ARG:O	1:A:376:ARG:HG3	2.18	0.43
1:A:431:LEU:HD22	1:A:516:PHE:CE1	2.53	0.43
1:A:162:LYS:CE	1:A:162:LYS:N	2.81	0.43
1:A:454:ALA:O	1:A:458:GLU:HB2	2.18	0.43
1:A:442:SER:HB3	1:A:511:LYS:HB2	2.00	0.43
1:A:452:LYS:HB3	1:A:452:LYS:NZ	2.34	0.43
1:A:209:HIS:O	1:A:213:ILE:HG13	2.19	0.43
1:A:204:THR:O	1:A:208:LYS:HG3	2.19	0.43
1:A:414:ASN:ND2	1:A:537:ASN:O	2.51	0.43
1:A:204:THR:HB	1:A:205:PRO:CD	2.49	0.43
1:A:143:SER:O	1:A:147:GLU:HB2	2.18	0.42
1:A:324:PRO:O	1:A:328:VAL:HG23	2.20	0.42
1:A:140:LEU:HD21	1:A:294:ARG:HH21	1.84	0.42
1:A:151:PHE:CE1	1:A:197:LEU:HB2	2.55	0.42
1:A:178:HIS:HA	1:A:212:PRO:HG3	2.02	0.42
1:A:196:GLU:O	1:A:198:THR:N	2.53	0.42
1:A:385:PHE:CZ	1:A:390:GLN:HG2	2.54	0.42
1:A:158:ILE:HD12	2:A:601:ADP:C8	2.55	0.42
1:A:363:ARG:HD2	1:A:367:GLN:HB2	2.01	0.42
1:A:551:ASN:C	1:A:553:THR:H	2.23	0.42
1:A:136:TRP:CE2	1:A:247:PRO:HD3	2.55	0.42
1:A:291:TYR:CD2	1:A:292:ARG:HG3	2.55	0.42
1:A:471:ILE:HD12	1:A:497:ALA:HB2	2.00	0.42
1:A:434:LEU:HD21	1:A:542:THR:HG21	2.02	0.42
1:A:446:VAL:HB	1:A:496:VAL:HG22	2.00	0.41
1:A:162:LYS:HE3	1:A:162:LYS:H	1.84	0.41
1:A:457:LEU:HG	1:A:461:LEU:HD12	2.03	0.41
1:A:438:THR:O	1:A:439:GLY:C	2.57	0.41
1:A:176:PRO:HA	1:A:177:PRO:HD2	1.85	0.41
1:A:443:LEU:HD13	1:A:487:PHE:CE2	2.56	0.41
1:A:503:ARG:HH12	1:A:527:HIS:CD2	2.38	0.41
1:A:191:ILE:HA	1:A:191:ILE:HD13	1.85	0.41
1:A:136:TRP:CE3	1:A:294:ARG:HB2	2.56	0.41
1:A:412:SER:O	1:A:415:ILE:HG22	2.20	0.41
1:A:477:GLN:HA	1:A:480:ARG:HB2	2.04	0.41
1:A:241:GLN:NE2	1:A:241:GLN:CA	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:O	1:A:399:GLU:C	2.60	0.40
1:A:500:VAL:O	1:A:503:ARG:N	2.50	0.40
1:A:353:LEU:HD22	1:A:358:GLU:HB2	2.03	0.40
1:A:415:ILE:HD11	1:A:532:THR:CG2	2.51	0.40
1:A:547:GLU:HG2	1:A:548:ARG:N	2.36	0.40
1:A:426:ASP:O	1:A:430:PHE:HB2	2.21	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	440/467 (94%)	379 (86%)	41 (9%)	20 (4%)	2	18

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	LYS
1	A	491	LYS
1	A	159	ASN
1	A	178	HIS
1	A	258	GLY
1	A	501	ALA
1	A	535	VAL
1	A	197	LEU
1	A	263	ARG
1	A	155	ASN
1	A	174	ASN
1	A	355	MET
1	A	226	THR
1	A	509	ASN
1	A	324	PRO

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Mol	Chain	Res	Type
1	A	531	ARG
1	A	365	VAL
1	A	439	GLY
1	A	500	VAL
1	A	552	ILE

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	380/402 (94%)	351 (92%)	29 (8%)	13	45

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ILE
1	A	161	GLU
1	A	162	LYS
1	A	185	VAL
1	A	252	ARG
1	A	260	TYR
1	A	262	ARG
1	A	285	GLU
1	A	301	TYR
1	A	317	CYS
1	A	395	ASP
1	A	420	VAL
1	A	425	SER
1	A	429	SER
1	A	430	PHE
1	A	441	ASP
1	A	455	ASP
1	A	461	LEU
1	A	477	GLN
1	A	481	GLU
1	A	486	GLN

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Mol	Chain	Res	Type
1	A	495	LEU
1	A	510	VAL
1	A	523	GLU
1	A	537	ASN
1	A	545	PHE
1	A	549	ASN
1	A	552	ILE
1	A	559	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	241	GLN
1	A	414	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 carbohydrates 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	PO4	A	606	-	4,4,4	1.80	2 (50%)	6,6,6	0.42	0
3	PO4	A	605	-	4,4,4	1.74	0	6,6,6	0.44	0
3	PO4	A	602	-	4,4,4	1.64	0	6,6,6	0.42	0
3	PO4	A	603	-	4,4,4	1.77	1 (25%)	6,6,6	0.44	0
3	PO4	A	604	-	4,4,4	1.79	2 (50%)	6,6,6	0.43	0
2	ADP	A	601	-	24,29,29	1.19	2 (8%)	29,45,45	1.98	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	601	-	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	O4'-C1'	3.37	1.45	1.41
2	A	601	ADP	C8-N7	-2.35	1.30	1.34
3	A	606	PO4	P-O3	-2.09	1.48	1.54
3	A	606	PO4	P-O4	-2.03	1.48	1.54
3	A	603	PO4	P-O2	-2.03	1.48	1.54
3	A	604	PO4	P-O3	-2.02	1.48	1.54
3	A	604	PO4	P-O4	-2.00	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	PA-O3A-PB	-6.78	109.54	132.83
2	A	601	ADP	N3-C2-N1	-4.58	121.52	128.68
2	A	601	ADP	C3'-C2'-C1'	3.39	106.08	100.98
2	A	601	ADP	PA-O5'-C5'	-2.84	105.03	121.68
2	A	601	ADP	O4'-C4'-C3'	2.43	109.91	105.11
2	A	601	ADP	C4-C5-N7	-2.04	107.27	109.40

There are no chirality outliers.

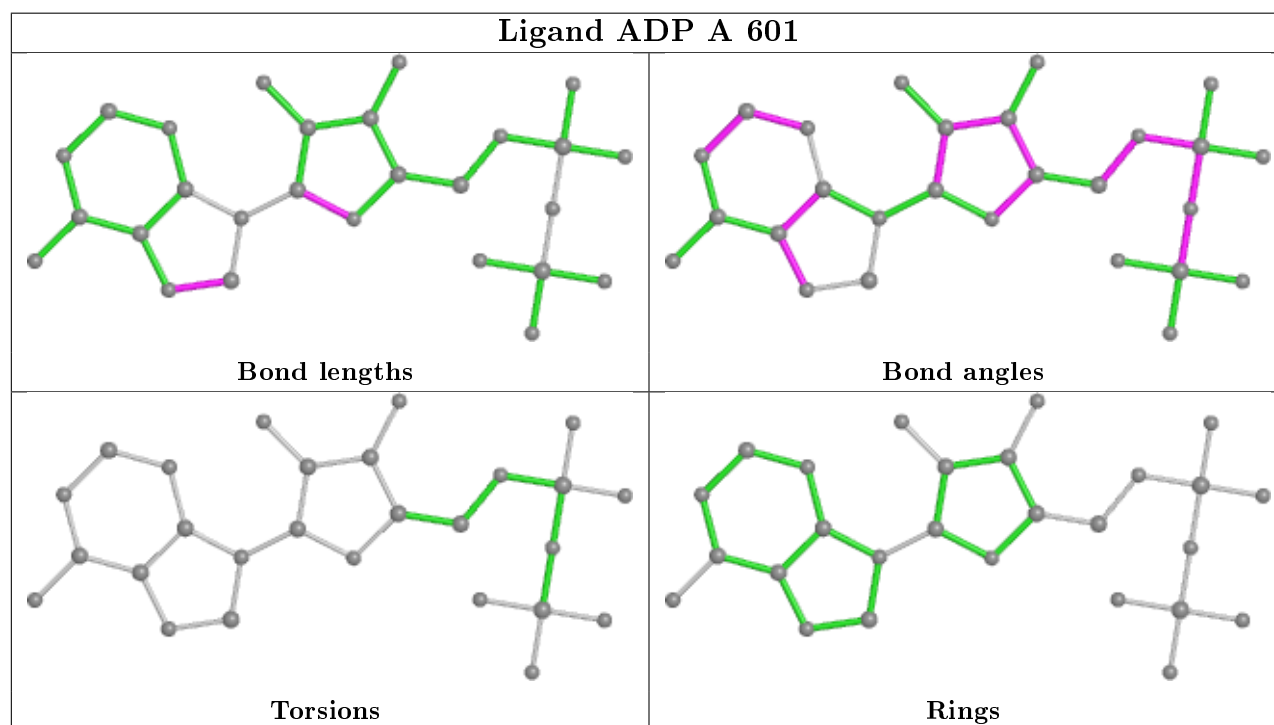
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ADP	3	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	442/467 (94%)	0.02	10 (2%) 60 47	43, 86, 169, 297	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ASN	5.8
1	A	489	SER	5.2
1	A	159	ASN	4.6
1	A	258	GLY	3.8
1	A	486	GLN	2.8
1	A	469	THR	2.7
1	A	158	ILE	2.7
1	A	165	ASP	2.3
1	A	440	LYS	2.0
1	A	166	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](#)

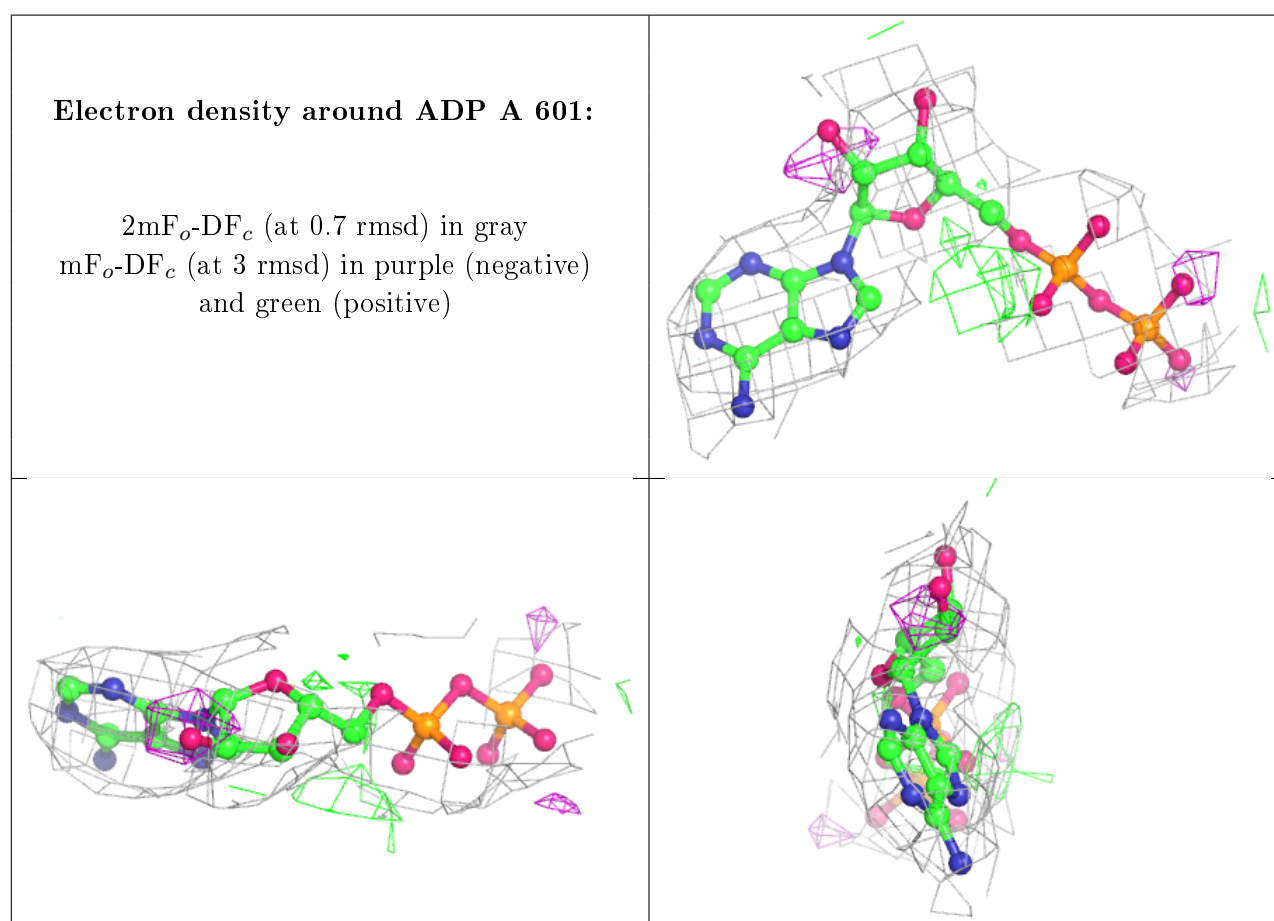
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
3	PO4	A	605	5/5	0.68	0.35	180,180,180,180	0
3	PO4	A	606	5/5	0.70	0.35	173,173,173,173	0
3	PO4	A	604	5/5	0.77	0.34	179,179,179,179	0
2	ADP	A	601	27/27	0.89	0.22	107,107,107,107	0
3	PO4	A	602	5/5	0.95	0.18	108,108,108,108	0
3	PO4	A	603	5/5	0.98	0.17	91,91,91,91	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.