Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 09:14 PM JST

PDB ID	:	7WRG
Title	:	Crystal structure of full-length kinesin-3 KLP-6
Authors	:	Wang, W.J.; Ren, J.Q.; Song, W.Y.; Feng, W.
Deposited on	:	2022-01-26
Resolution	:	3.16 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 (i) 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 (i)) were used in the production of this report:

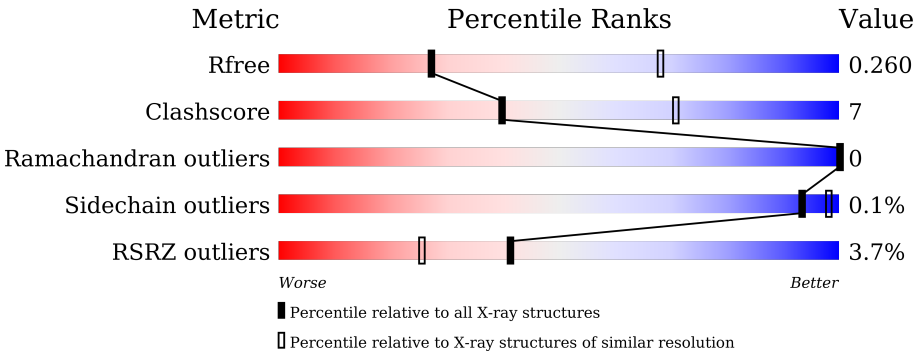
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

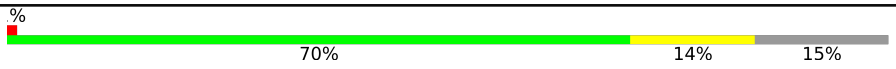
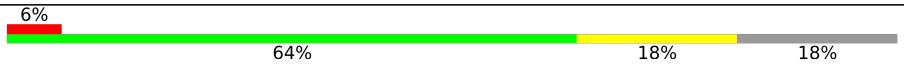
The reported resolution of this entry is 3.16 Å.

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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 <=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	960	
1	B	960	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12589 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 Kinesin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	0	0
			6376	4010	1101	1236	29			
1	B	783	Total	C	N	O	S	0	0	0
			6154	3872	1064	1190	28			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	929	GLY	-	expression tag	UNP G5EFQ4
A	930	THR	-	expression tag	UNP G5EFQ4
A	931	LYS	-	expression tag	UNP G5EFQ4
A	932	LEU	-	expression tag	UNP G5EFQ4
A	933	LEU	-	expression tag	UNP G5EFQ4
A	934	GLU	-	expression tag	UNP G5EFQ4
A	935	VAL	-	expression tag	UNP G5EFQ4
A	936	LEU	-	expression tag	UNP G5EFQ4
A	937	PHE	-	expression tag	UNP G5EFQ4
A	938	GLN	-	expression tag	UNP G5EFQ4
A	939	GLY	-	expression tag	UNP G5EFQ4
A	940	PRO	-	expression tag	UNP G5EFQ4
A	941	HIS	-	expression tag	UNP G5EFQ4
A	942	HIS	-	expression tag	UNP G5EFQ4
A	943	HIS	-	expression tag	UNP G5EFQ4
A	944	HIS	-	expression tag	UNP G5EFQ4
A	945	HIS	-	expression tag	UNP G5EFQ4
A	946	HIS	-	expression tag	UNP G5EFQ4
A	947	GLY	-	expression tag	UNP G5EFQ4
A	948	SER	-	expression tag	UNP G5EFQ4
A	949	GLY	-	expression tag	UNP G5EFQ4
A	950	SER	-	expression tag	UNP G5EFQ4
A	951	GLY	-	expression tag	UNP G5EFQ4
A	952	SER	-	expression tag	UNP G5EFQ4
A	953	TRP	-	expression tag	UNP G5EFQ4

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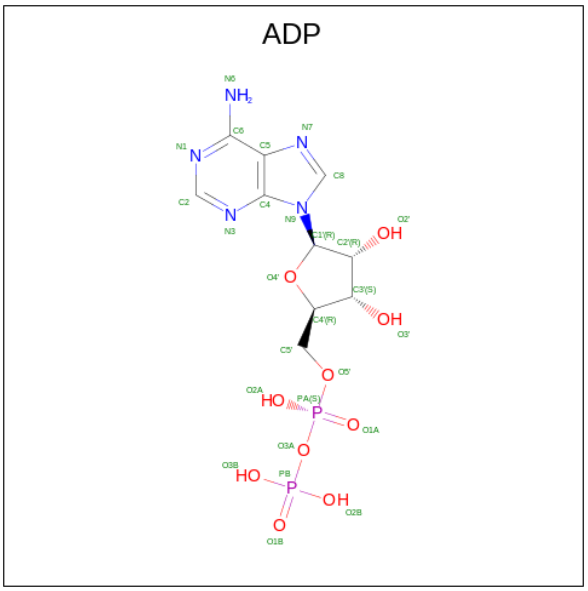
Chain	Residue	Modelled	Actual	Comment	Reference
A	954	SER	-	expression tag	UNP G5EFQ4
A	955	HIS	-	expression tag	UNP G5EFQ4
A	956	PRO	-	expression tag	UNP G5EFQ4
A	957	GLN	-	expression tag	UNP G5EFQ4
A	958	PHE	-	expression tag	UNP G5EFQ4
A	959	GLU	-	expression tag	UNP G5EFQ4
A	960	LYS	-	expression tag	UNP G5EFQ4
B	929	GLY	-	expression tag	UNP G5EFQ4
B	930	THR	-	expression tag	UNP G5EFQ4
B	931	LYS	-	expression tag	UNP G5EFQ4
B	932	LEU	-	expression tag	UNP G5EFQ4
B	933	LEU	-	expression tag	UNP G5EFQ4
B	934	GLU	-	expression tag	UNP G5EFQ4
B	935	VAL	-	expression tag	UNP G5EFQ4
B	936	LEU	-	expression tag	UNP G5EFQ4
B	937	PHE	-	expression tag	UNP G5EFQ4
B	938	GLN	-	expression tag	UNP G5EFQ4
B	939	GLY	-	expression tag	UNP G5EFQ4
B	940	PRO	-	expression tag	UNP G5EFQ4
B	941	HIS	-	expression tag	UNP G5EFQ4
B	942	HIS	-	expression tag	UNP G5EFQ4
B	943	HIS	-	expression tag	UNP G5EFQ4
B	944	HIS	-	expression tag	UNP G5EFQ4
B	945	HIS	-	expression tag	UNP G5EFQ4
B	946	HIS	-	expression tag	UNP G5EFQ4
B	947	GLY	-	expression tag	UNP G5EFQ4
B	948	SER	-	expression tag	UNP G5EFQ4
B	949	GLY	-	expression tag	UNP G5EFQ4
B	950	SER	-	expression tag	UNP G5EFQ4
B	951	GLY	-	expression tag	UNP G5EFQ4
B	952	SER	-	expression tag	UNP G5EFQ4
B	953	TRP	-	expression tag	UNP G5EFQ4
B	954	SER	-	expression tag	UNP G5EFQ4
B	955	HIS	-	expression tag	UNP G5EFQ4
B	956	PRO	-	expression tag	UNP G5EFQ4
B	957	GLN	-	expression tag	UNP G5EFQ4
B	958	PHE	-	expression tag	UNP G5EFQ4
B	959	GLU	-	expression tag	UNP G5EFQ4
B	960	LYS	-	expression tag	UNP G5EFQ4

- 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 27 10 5 10 2	0	0
2	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

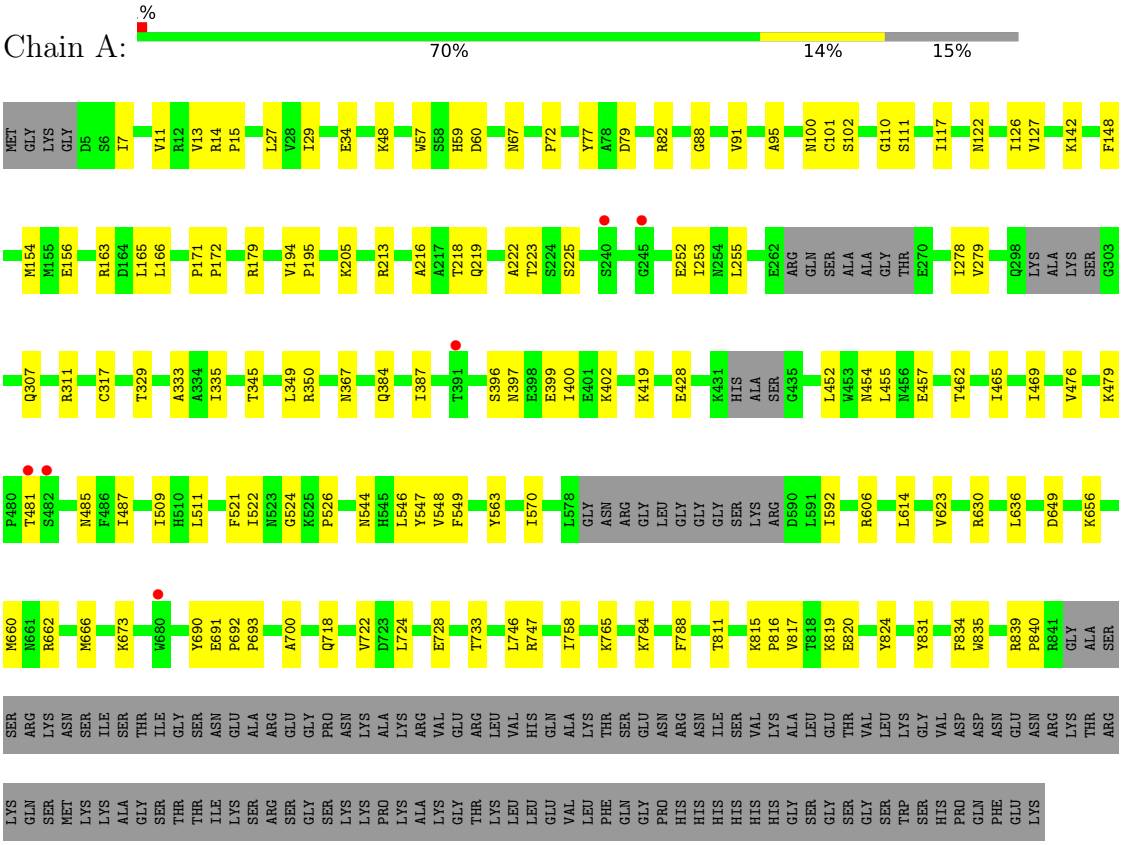
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0

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.

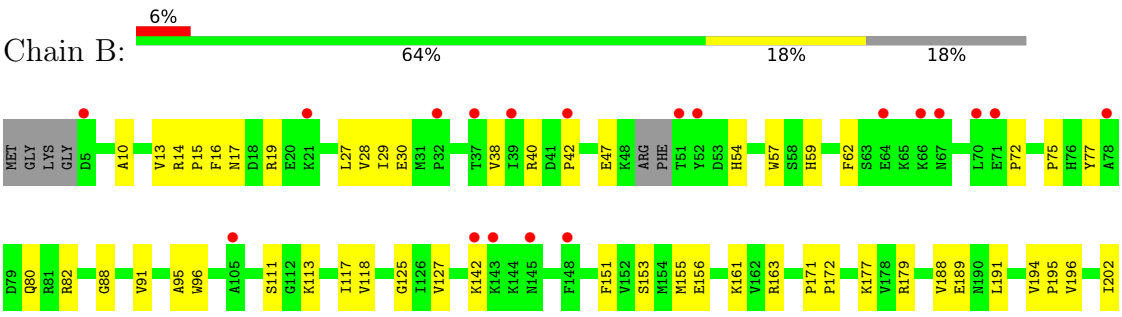
• Molecule 1: Kinesin-like protein

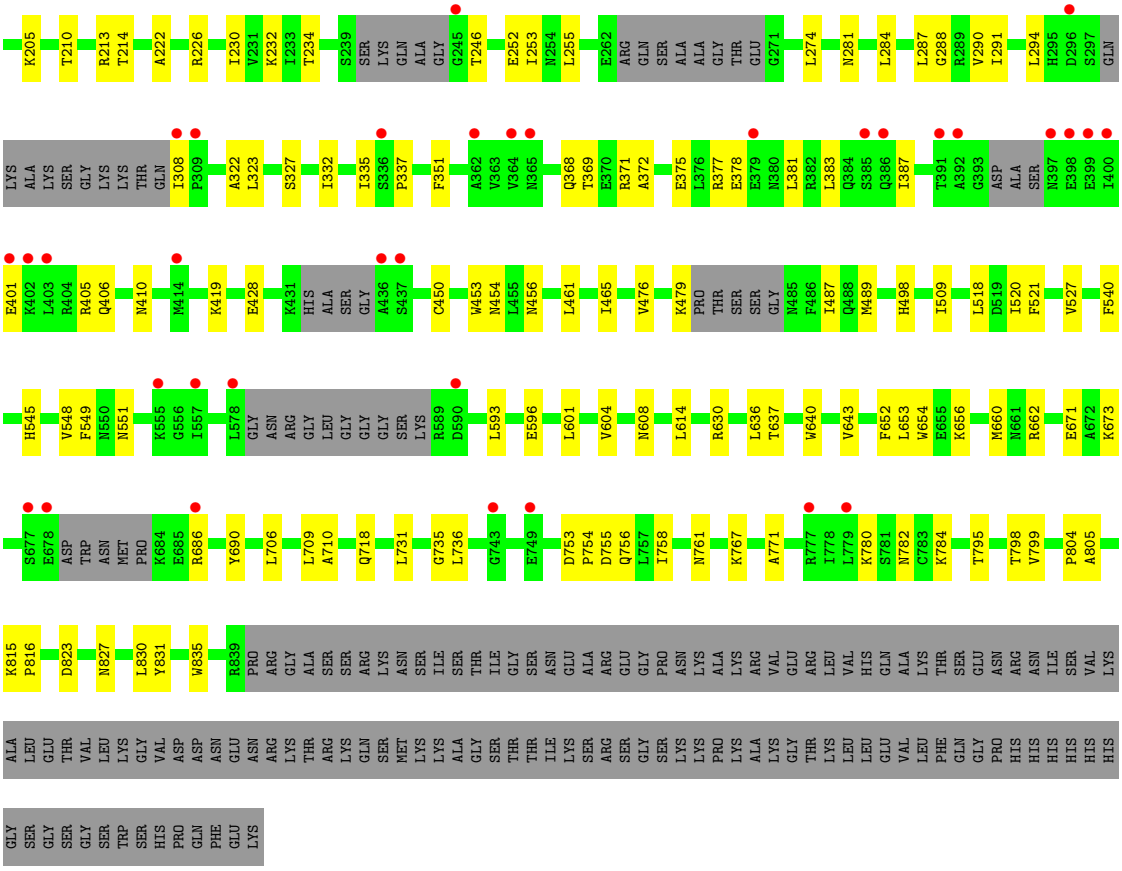
Chain A:



• Molecule 1: Kinesin-like protein

Chain B:




K205 T210 R213 T214 A222 R226 I230 V231 K232 I233 T234 S239 SER LYS GLN ALA GLY G245 T246 E252 I253 N254 L255 E262 ARG GLN SER ALA ALA GLY THR GLU G271 L274 N281 L284 L287 G288 R289 V290 I291 L294 H295 D296 S297 GLN
LYS ALA LYS SER GLY LYS LYS THR GLN I308 P309 A322 L323 S327 I332 I335 S336 P337 F351 A362 V363 V364 N365 Q368 T369 E370 R371 A372 E375 L376 R377 E378 E379 N380 L381 R382 L383 Q384 S385 Q386 I387 T391 A392 G393 ASP ALA SER N397 E398 E399 I400
E401 K402 L403 R404 R405 Q406 N410 M414 K419 E428 K431 HIS ALA SER GLY A436 S437 C450 W453 N454 L455 N456 L461 I465 V476 K479 PRO THR SER SER GLY N485 F486 I487 Q488 M489 H498 I509 L518 D519 I520 F521 V527 F540
H545 V548 F549 N550 N551 K555 G556 I557 L578 GLY ASN ARG GLY LEU GLY GLY SER LYS R589 D590 L593 E596 L601 V604 N608 L614 R630 L636 T637 W640 V643 F652 L653 W654 E655 K656 M660 N661 R662 E671 A672 K673
S677 E678 ASP TRP ASN MET PRO K684 E685 R686 Y690 L706 L709 A710 Q718 L731 G735 L736 G743 E749 D753 P754 D755 Q756 L757 I758 N761 K767 A771 R777 I778 L779 K780 S781 N782 C783 K784 T795 T798 V799 P804 A805
K815 P816 D823 N827 L830 Y831 W835 R839 PRO ARG GLY ALA SER SER ARG LYS ASN SER ILE SER THR ILE GLY SER ASN GLU ALA ARG GLU GLY PRO ASN LYS ALA LYS ARG VAL GLU ARG LEU VAL HIS GLN ALA LYS THR SER GLU ASN ARG ASN ILE SER VAL LYS
ALA LEU GLU THR VAL LEU LYS GLY VAL ASP ASN GLU ASN ARG LYS THR ARG LYS GLN SER MET LYS LYS ALA GLY SER THR THR ILE LYS SER ARG SER GLY SER LYS LYS PRO LYS ALA LYS GLY THR LYS LEU LEU GLU VAL LEU PHE GLN GLY PRO HIS HIS HIS HIS HIS HIS
GLY SER GLY SER GLY SER TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.14Å 68.82Å 253.22Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	33.20 – 3.16 33.20 – 3.16	Depositor EDS
% Data completeness (in resolution range)	97.7 (33.20-3.16) 97.7 (33.20-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.213 , 0.263 0.214 , 0.260	Depositor DCC
R_{free} test set	1622 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12589	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/6492	0.45	0/8767
1	B	0.24	0/6259	0.43	0/8443
All	All	0.25	0/12751	0.44	0/17210

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	6376	0	6296	83	0
1	B	6154	0	6069	101	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
All	All	12589	0	12389	183	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 7.

All (183) 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:718:GLN:HG2	1:A:733:THR:HG22	1.65	0.78
1:B:195:PRO:HD2	1:B:428:GLU:HG3	1.70	0.73
1:B:710:ALA:HB1	1:B:754:PRO:HB3	1.70	0.73
1:A:454:ASN:HB2	1:A:465:ILE:HG12	1.71	0.72
1:A:57:TRP:HE1	1:A:60:ASP:HB2	1.55	0.72
1:B:761:ASN:ND2	1:B:815:LYS:O	2.22	0.72
1:B:188:VAL:HB	1:B:191:LEU:HD12	1.72	0.71
1:B:823:ASP:OD1	1:B:827:ASN:ND2	2.23	0.70
1:B:13:VAL:HG21	1:B:29:ILE:HG21	1.72	0.70
1:A:630:ARG:NH2	1:A:636:LEU:O	2.22	0.68
1:A:765:LYS:HB3	1:A:811:THR:HG22	1.75	0.68
1:A:195:PRO:HD2	1:A:428:GLU:HG3	1.76	0.67
1:A:213:ARG:NH2	1:A:222:ALA:O	2.28	0.65
1:A:11:VAL:HG22	1:A:333:ALA:HB3	1.80	0.63
1:B:614:LEU:HD23	1:B:673:LYS:HD2	1.80	0.63
1:B:476:VAL:HG22	1:B:487:ILE:HB	1.80	0.63
1:A:485:ASN:OD1	1:B:756:GLN:NE2	2.32	0.62
1:B:709:LEU:HD11	1:B:736:LEU:HB3	1.82	0.62
1:B:450:CYS:SG	1:B:551:ASN:ND2	2.64	0.62
1:A:662:ARG:NH2	1:A:690:TYR:O	2.33	0.62
1:B:604:VAL:O	1:B:608:ASN:ND2	2.32	0.62
1:B:784:LYS:HG2	1:B:795:THR:HG22	1.81	0.61
1:A:154:MET:HG2	1:A:165:LEU:HD12	1.82	0.60
1:A:839:ARG:HB3	1:A:840:PRO:HD2	1.83	0.60
1:B:226:ARG:NH1	1:B:281:ASN:OD1	2.34	0.60
1:A:34:GLU:OE1	1:A:82:ARG:NH2	2.35	0.59
1:B:14:ARG:HE	1:B:111:SER:HA	1.68	0.59
1:B:454:ASN:HB2	1:B:465:ILE:HG12	1.85	0.59
1:A:592:ILE:HG21	1:A:636:LEU:HD11	1.85	0.59
1:A:693:PRO:HB2	1:A:839:ARG:HB2	1.85	0.58
1:A:142:LYS:HG2	1:A:148:PHE:HZ	1.69	0.58
1:B:274:LEU:HB3	1:B:686:ARG:HG3	1.87	0.57
1:B:40:ARG:HG2	1:B:47:GLU:HG2	1.85	0.57
1:B:368:GLN:O	1:B:372:ALA:N	2.33	0.57
1:A:67:ASN:O	1:A:122:ASN:ND2	2.37	0.57
1:A:307:GLN:N	1:A:307:GLN:OE1	2.38	0.57
1:A:524:GLY:HA2	1:A:570:ILE:HG12	1.86	0.57
1:B:156:GLU:HG2	1:B:163:ARG:HB3	1.87	0.57
1:A:397:ASN:HA	1:A:400:ILE:HG12	1.87	0.56
1:A:384:GLN:O	1:A:387:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LYS:O	1:A:481:THR:N	2.38	0.56
1:B:815:LYS:HB2	1:B:816:PRO:HD3	1.87	0.56
1:B:177:LYS:HB2	1:B:189:GLU:HG2	1.87	0.56
1:B:214:THR:HG22	1:B:461:LEU:HB3	1.88	0.56
1:A:72:PRO:HD3	1:A:79:ASP:HB3	1.88	0.55
1:B:210:THR:O	1:B:214:THR:HG23	2.07	0.55
1:B:520:ILE:HG13	1:B:527:VAL:HB	1.89	0.55
1:B:799:VAL:HB	1:B:804:PRO:HB3	1.89	0.54
1:B:15:PRO:HA	1:B:59:HIS:ND1	2.23	0.54
1:B:75:PRO:O	1:B:82:ARG:NH2	2.40	0.54
1:B:799:VAL:HG11	1:B:805:ALA:H	1.73	0.54
1:B:284:LEU:O	1:B:287:LEU:HB3	2.08	0.54
1:B:456:ASN:HD22	1:B:461:LEU:HB2	1.72	0.54
1:A:662:ARG:NH1	1:A:691:GLU:OE1	2.30	0.53
1:A:335:ILE:HB	1:A:345:THR:HG23	1.90	0.53
1:A:656:LYS:O	1:A:660:MET:HG2	2.08	0.53
1:A:27:LEU:HD21	1:A:57:TRP:HH2	1.74	0.53
1:A:662:ARG:O	1:A:666:MET:HG3	2.09	0.53
1:A:48:LYS:HE2	1:A:350:ARG:HH21	1.72	0.53
1:B:454:ASN:ND2	1:B:461:LEU:O	2.42	0.52
1:B:72:PRO:HB3	1:B:77:TYR:HB3	1.91	0.52
1:B:601:LEU:HA	1:B:604:VAL:HG12	1.92	0.52
1:A:815:LYS:HB3	1:A:816:PRO:HD3	1.91	0.52
1:B:290:VAL:HG11	1:B:323:LEU:HD23	1.93	0.51
1:B:155:MET:HG2	1:B:230:ILE:HB	1.93	0.51
1:A:14:ARG:NH1	1:A:110:GLY:O	2.43	0.51
1:A:455:LEU:HD23	1:A:546:LEU:HG	1.92	0.51
1:B:735:GLY:N	1:B:767:LYS:O	2.42	0.51
1:B:234:THR:HG22	1:B:252:GLU:HG3	1.92	0.51
1:A:154:MET:HB3	1:A:166:LEU:HD13	1.93	0.50
1:A:88:GLY:HA2	1:A:91:VAL:HG22	1.94	0.50
1:A:110:GLY:N	2:A:1001:ADP:O2B	2.39	0.50
1:B:521:PHE:HB2	1:B:540:PHE:HB3	1.93	0.50
1:A:614:LEU:HD23	1:A:673:LYS:HD2	1.93	0.50
1:A:278:ILE:HG13	1:A:279:VAL:HG23	1.94	0.50
1:B:153:SER:HB2	1:B:232:LYS:HB3	1.94	0.50
1:A:7:ILE:HG13	1:A:329:THR:HB	1.94	0.49
1:B:95:ALA:HB2	1:B:253:ILE:HD11	1.94	0.49
1:A:117:ILE:O	1:A:126:ILE:N	2.45	0.49
1:A:758:ILE:HA	1:A:817:VAL:O	2.12	0.49
1:A:311:ARG:HA	1:A:317:CYS:SG	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:HG	1:B:308:ILE:HG12	1.94	0.49
1:A:156:GLU:HG2	1:A:163:ARG:HB3	1.94	0.49
1:B:80:GLN:HE22	1:B:125:GLY:HA2	1.78	0.49
1:B:246:THR:O	1:B:369:THR:N	2.43	0.49
1:B:596:GLU:HG2	1:B:656:LYS:HE3	1.94	0.49
1:B:213:ARG:NH2	1:B:222:ALA:O	2.46	0.49
1:B:322:ALA:HA	1:B:327:SER:HB3	1.95	0.49
1:B:27:LEU:HD21	1:B:57:TRP:HH2	1.78	0.48
1:B:630:ARG:HG2	1:B:831:TYR:CZ	2.48	0.48
1:A:179:ARG:NH1	1:A:402:LYS:HE3	2.28	0.48
1:A:15:PRO:HA	1:A:59:HIS:ND1	2.29	0.48
1:B:662:ARG:NH2	1:B:690:TYR:O	2.46	0.48
1:A:758:ILE:HD11	1:A:819:LYS:HD3	1.94	0.48
1:B:755:ASP:O	1:B:758:ILE:HG12	2.13	0.48
1:B:383:LEU:O	1:B:387:ILE:HG23	2.14	0.48
1:A:544:ASN:OD1	1:A:606:ARG:NE	2.47	0.47
1:A:95:ALA:HB2	1:A:253:ILE:HD11	1.96	0.47
1:A:788:PHE:HB2	1:A:824:TYR:CE2	2.49	0.47
1:A:72:PRO:HB3	1:A:77:TYR:HB3	1.96	0.46
1:B:406:GLN:O	1:B:410:ASN:ND2	2.40	0.46
1:A:127:VAL:HG22	1:A:255:LEU:HD13	1.98	0.46
1:B:88:GLY:HA2	1:B:91:VAL:HG22	1.98	0.46
1:B:377:ARG:O	1:B:381:LEU:HG	2.15	0.46
1:A:693:PRO:CB	1:A:839:ARG:HB2	2.46	0.46
1:A:630:ARG:HG2	1:A:831:TYR:CZ	2.51	0.46
1:B:127:VAL:HG22	1:B:255:LEU:HD13	1.98	0.45
1:A:14:ARG:HH11	1:A:111:SER:HA	1.82	0.45
1:B:30:GLU:HB3	1:B:38:VAL:HB	1.99	0.45
1:A:511:LEU:HD22	1:A:522:ILE:HD11	1.99	0.45
1:B:28:VAL:HG11	1:B:42:PRO:HG3	1.98	0.45
1:A:101:CYS:SG	1:A:102:SER:N	2.90	0.45
1:A:765:LYS:HA	1:A:811:THR:HA	1.98	0.45
1:A:784:LYS:HD2	1:A:835:TRP:NE1	2.32	0.45
1:A:509:ILE:HD13	1:A:549:PHE:HZ	1.81	0.45
1:B:782:ASN:OD1	1:B:835:TRP:HB2	2.16	0.45
1:A:163:ARG:HH22	1:A:216:ALA:HB2	1.82	0.44
1:B:368:GLN:HB3	1:B:371:ARG:HB3	1.99	0.44
1:B:753:ASP:OD2	1:B:755:ASP:HB2	2.16	0.44
1:B:10:ALA:HB3	1:B:332:ILE:HD13	1.99	0.44
1:A:476:VAL:HA	1:A:487:ILE:O	2.17	0.44
1:A:469:ILE:HA	1:A:487:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HG22	1:B:335:ILE:HG13	1.99	0.44
1:B:630:ARG:NH2	1:B:636:LEU:O	2.49	0.44
1:A:700:ALA:HB3	1:A:834:PHE:HB2	1.99	0.44
1:B:62:PHE:HB3	1:B:77:TYR:CE2	2.53	0.44
1:B:656:LYS:O	1:B:660:MET:HG3	2.17	0.44
1:A:722:VAL:HG12	1:A:728:GLU:HA	1.99	0.44
1:B:287:LEU:O	1:B:291:ILE:HG12	2.17	0.44
1:B:780:LYS:HB3	1:B:798:THR:HG22	1.99	0.44
1:B:161:LYS:HZ2	1:B:671:GLU:HG3	1.82	0.44
1:A:100:ASN:HB3	1:A:252:GLU:H	1.83	0.43
1:B:72:PRO:HG3	1:B:77:TYR:HD1	1.83	0.43
1:A:13:VAL:HG21	1:A:29:ILE:HG21	1.99	0.43
1:A:452:LEU:HB3	1:A:547:TYR:HB3	2.00	0.43
1:B:10:ALA:HA	1:B:54:HIS:O	2.19	0.43
1:B:194:VAL:HG21	1:B:205:LYS:HE3	2.00	0.43
1:B:401:GLU:O	1:B:405:ARG:HG3	2.17	0.43
1:B:706:LEU:HD21	1:B:830:LEU:HB2	2.00	0.43
1:A:820:GLU:OE1	1:A:820:GLU:N	2.52	0.43
1:B:113:LYS:HG2	2:B:1001:ADP:O3B	2.18	0.43
1:A:396:SER:HB2	1:A:399:GLU:HB3	2.01	0.43
1:B:17:ASN:HD21	1:B:19:ARG:HG2	1.82	0.43
1:B:643:VAL:HB	1:B:652:PHE:HB2	2.01	0.43
1:A:457:GLU:HA	1:A:563:TYR:CD2	2.54	0.43
1:B:246:THR:OG1	1:B:369:THR:HB	2.19	0.43
1:B:16:PHE:CD1	1:B:337:PRO:HG2	2.53	0.42
1:B:171:PRO:HA	1:B:172:PRO:HD3	1.91	0.42
1:B:375:GLU:O	1:B:378:GLU:HG2	2.18	0.42
1:B:453:TRP:CE2	1:B:548:VAL:HB	2.54	0.42
1:B:718:GLN:HB3	1:B:731:LEU:HB3	2.00	0.42
1:A:746:LEU:HG	1:A:747:ARG:H	1.84	0.42
1:B:509:ILE:HD13	1:B:549:PHE:HZ	1.85	0.42
1:B:489:MET:HB3	1:B:545:HIS:CD2	2.54	0.42
1:A:223:THR:HG22	1:A:225:SER:H	1.85	0.42
1:B:177:LYS:HB3	1:B:179:ARG:NH1	2.34	0.42
1:A:455:LEU:HD22	1:A:548:VAL:HG23	2.02	0.42
1:B:17:ASN:ND2	1:B:19:ARG:HG2	2.34	0.42
1:B:151:PHE:HB2	1:B:234:THR:OG1	2.20	0.42
1:B:479:LYS:HE3	1:B:479:LYS:HB2	1.95	0.42
1:B:498:HIS:CD2	1:B:518:LEU:HD21	2.55	0.42
1:B:640:TRP:HE3	1:B:653:LEU:HG	1.85	0.42
1:B:654:TRP:CZ3	1:B:662:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLY:HA2	1:B:351:PHE:HE2	1.84	0.42
1:A:419:LYS:HE3	1:A:419:LYS:HB2	1.78	0.41
1:A:335:ILE:HD13	1:A:349:LEU:HD21	2.01	0.41
1:A:163:ARG:HH22	1:A:216:ALA:CB	2.34	0.41
1:A:218:THR:HG23	1:A:219:GLN:HG3	2.03	0.41
1:A:692:PRO:HA	1:A:693:PRO:HD3	1.91	0.41
1:A:171:PRO:HA	1:A:172:PRO:HD3	1.98	0.41
1:A:194:VAL:HG21	1:A:205:LYS:HE3	2.03	0.41
1:A:649:ASP:O	1:A:839:ARG:NH2	2.54	0.41
1:B:196:VAL:HG21	1:B:202:ILE:HB	2.01	0.41
1:A:455:LEU:HA	1:A:462:THR:HG23	2.02	0.41
1:B:96:TRP:CZ3	1:B:142:LYS:HG3	2.55	0.41
1:B:291:ILE:HG13	1:B:351:PHE:CZ	2.55	0.41
1:B:287:LEU:HG	1:B:351:PHE:HZ	1.86	0.40
1:B:419:LYS:HE3	1:B:419:LYS:HB2	1.95	0.40
1:B:593:LEU:HD13	1:B:637:THR:HB	2.04	0.40
1:B:771:ALA:HB3	1:B:804:PRO:HD2	2.04	0.40
1:A:521:PHE:HD1	1:A:526:PRO:HA	1.87	0.40
1:A:623:VAL:HG11	1:A:724:LEU:HB3	2.02	0.40
1:B:117:ILE:HG22	1:B:118:VAL:HG23	2.02	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	802/960 (84%)	754 (94%)	48 (6%)	0	100	100
1	B	763/960 (80%)	719 (94%)	44 (6%)	0	100	100
All	All	1565/1920 (82%)	1473 (94%)	92 (6%)	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	698/827 (84%)	697 (100%)	1 (0%)	93 98
1	B	672/827 (81%)	672 (100%)	0	100 100
All	All	1370/1654 (83%)	1369 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN

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

Mol	Chain	Res	Type
1	A	367	ASN
1	A	485	ASN
1	B	756	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ADP	B	1001	3	24,29,29	0.97	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	A	1001	3	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)

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	B	1001	3	-	4/12/32/32	0/3/3/3
2	ADP	A	1001	3	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	2.52	1.47	1.40
2	B	1001	ADP	C5-C4	2.49	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	ADP	PA-O3A-PB	-3.49	120.84	132.83
2	B	1001	ADP	PA-O3A-PB	-3.37	121.26	132.83
2	A	1001	ADP	C3'-C2'-C1'	3.37	106.05	100.98
2	B	1001	ADP	C3'-C2'-C1'	3.35	106.02	100.98
2	B	1001	ADP	N3-C2-N1	-3.20	123.67	128.68
2	A	1001	ADP	N3-C2-N1	-3.20	123.68	128.68
2	B	1001	ADP	C4-C5-N7	-2.65	106.64	109.40
2	A	1001	ADP	C4-C5-N7	-2.56	106.73	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O2A
2	B	1001	ADP	C5'-O5'-PA-O1A
2	B	1001	ADP	C5'-O5'-PA-O2A
2	A	1001	ADP	C5'-O5'-PA-O3A
2	B	1001	ADP	C5'-O5'-PA-O3A
2	B	1001	ADP	PB-O3A-PA-O1A

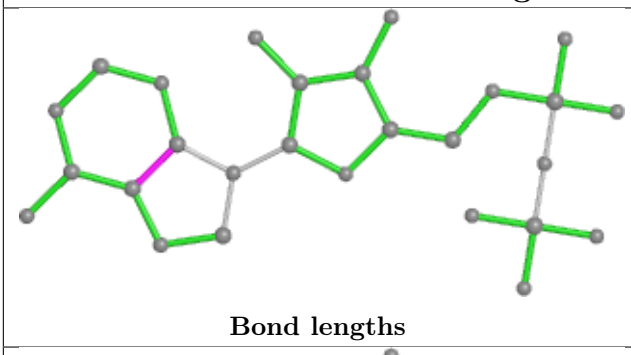
There are no ring outliers.

2 monomers are involved in 2 short contacts:

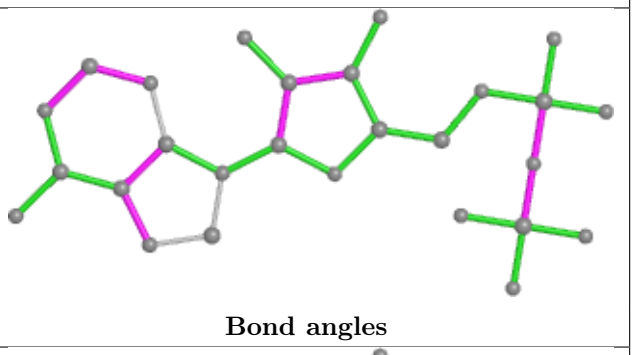
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	ADP	1	0
2	A	1001	ADP	1	0

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 then 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.

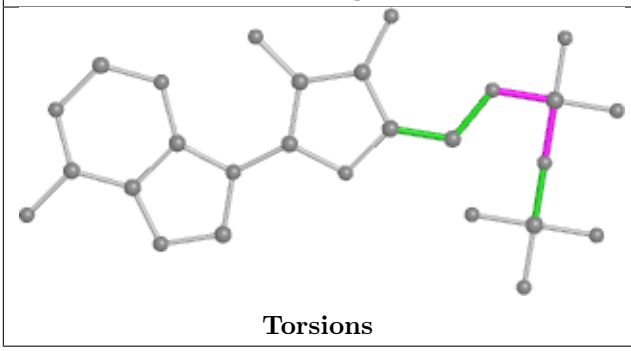
Ligand ADP B 1001



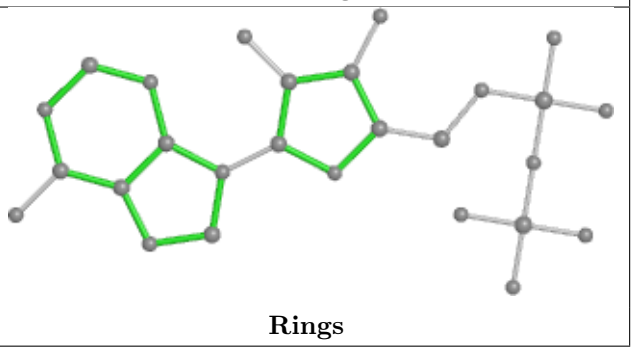
Bond lengths



Bond angles

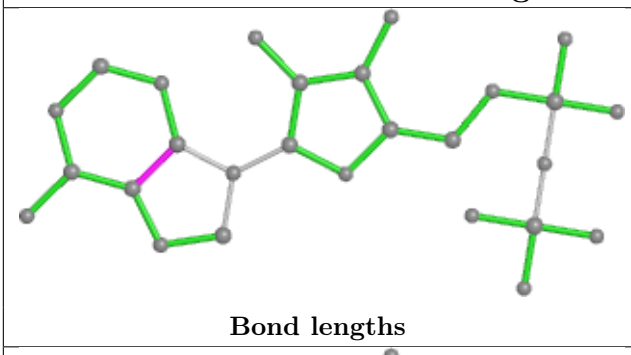


Torsions

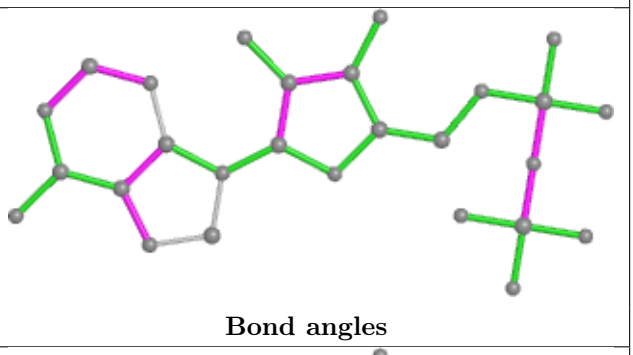


Rings

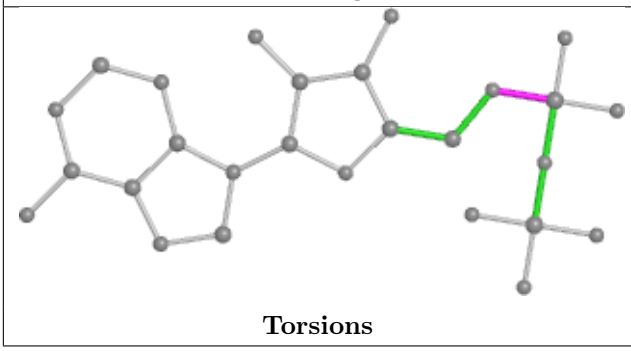
Ligand ADP A 1001



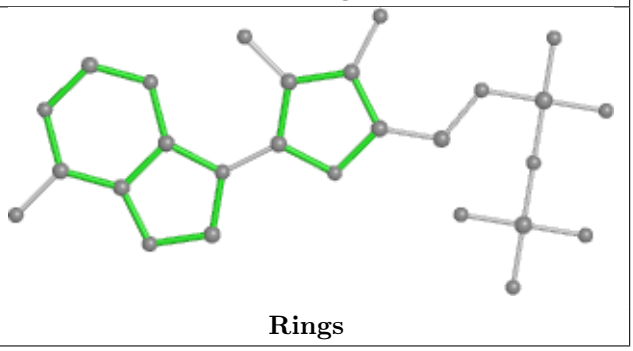
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	812/960 (84%)	-0.50	6 (0%) 87 81	9, 36, 87, 147	0
1	B	783/960 (81%)	0.29	53 (6%) 17 9	44, 96, 157, 198	0
All	All	1595/1920 (83%)	-0.11	59 (3%) 41 25	9, 65, 147, 198	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	4.9
1	B	397	ASN	4.5
1	B	39	ILE	4.2
1	B	32	PRO	4.0
1	B	245	GLY	3.9
1	B	37	THR	3.7
1	B	678	GLU	3.7
1	B	399	GLU	3.7
1	B	51	THR	3.6
1	B	437	SER	3.5
1	B	555	LYS	3.5
1	B	398	GLU	3.3
1	B	400	ILE	3.3
1	B	21	LYS	3.2
1	B	142	LYS	3.2
1	B	71	GLU	3.1
1	B	66	LYS	3.1
1	B	677	SER	3.1
1	B	590	ASP	3.0
1	B	5	ASP	2.9
1	A	482	SER	2.9
1	B	385	SER	2.9
1	B	308	ILE	2.9
1	B	743	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	391	THR	2.9
1	A	680	TRP	2.8
1	B	779	LEU	2.8
1	B	557	ILE	2.7
1	A	240	SER	2.7
1	B	386	GLN	2.7
1	B	145	ASN	2.7
1	B	392	ALA	2.6
1	B	42	PRO	2.6
1	A	245	GLY	2.5
1	B	401	GLU	2.5
1	B	52	TYR	2.5
1	B	78	ALA	2.5
1	B	336	SER	2.5
1	B	379	GLU	2.4
1	B	143	LYS	2.3
1	B	402	LYS	2.3
1	A	391	THR	2.3
1	B	414	MET	2.3
1	B	309	PRO	2.2
1	B	578	LEU	2.2
1	B	365	ASN	2.2
1	B	67	ASN	2.2
1	B	148	PHE	2.2
1	A	481	THR	2.2
1	B	296	ASP	2.2
1	B	686	ARG	2.2
1	B	403	LEU	2.2
1	B	777	ARG	2.2
1	B	64	GLU	2.1
1	B	364	VAL	2.1
1	B	749	GLU	2.1
1	B	105	ALA	2.1
1	B	362	ALA	2.0
1	B	436	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

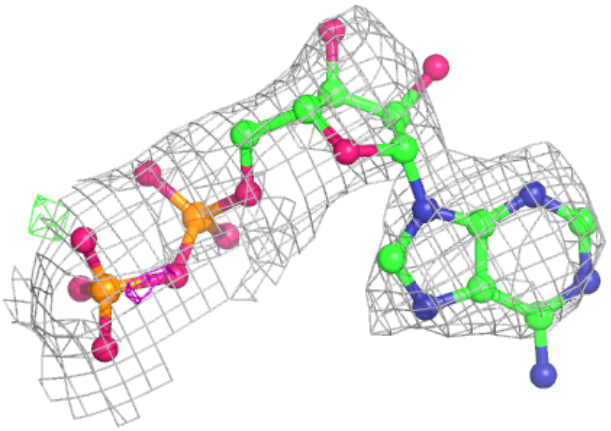
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

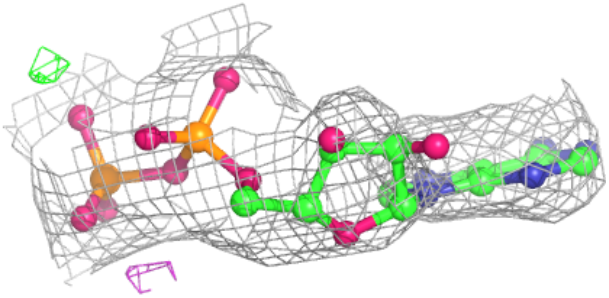
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	1002	1/1	0.86	0.64	80,80,80,80	0
2	ADP	B	1001	27/27	0.87	0.23	66,108,122,127	0
3	MG	A	1002	1/1	0.92	0.40	28,28,28,28	0
2	ADP	A	1001	27/27	0.97	0.19	11,32,43,53	0

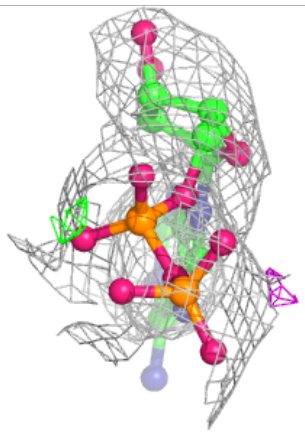
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 1001:

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

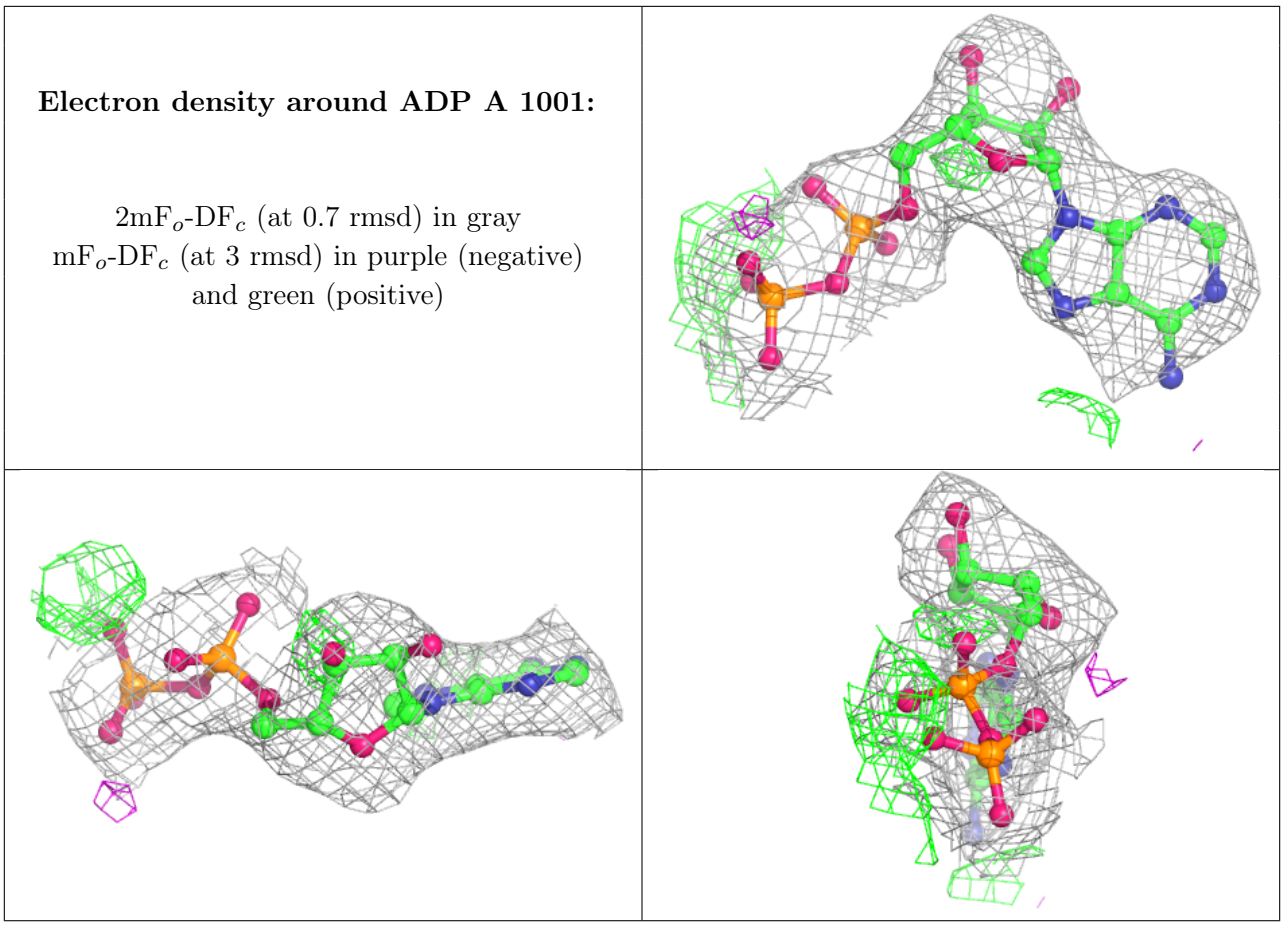






Electron density around ADP A 1001:

$2mF_o$-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.