Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:36 AM EDT

PDB ID	:	6HPU
Title	:	Crystal structure of human Pif1 helicase in complex with ADP-AlF4
Authors	:	Levdikov, V.M.; Dehghani-Tafti, S.; Bax, B.D.; Sanders, C.M.; Antson, A.A.
Deposited on	:	2018-09-21
Resolution	:	3.96 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:

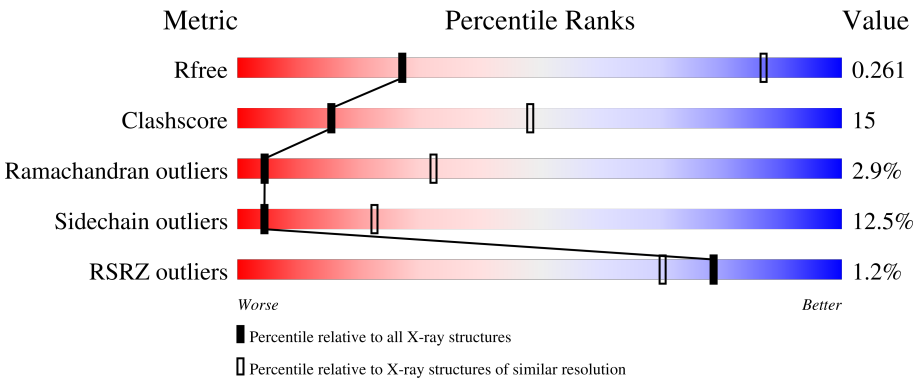
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.96 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	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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	418	% 63% 35% •
1	B	418	% 59% 34% 6% •

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	ALF	A	802	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6495 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.

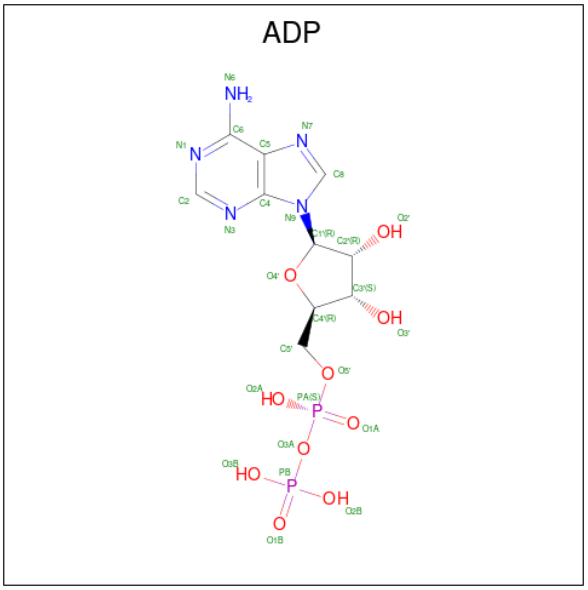
- Molecule 1 is a protein called ATP-dependent DNA helicase PIF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3219	2019	602	579	19	0	5	0
1	B	416	3210	2014	600	577	19	0	6	0

There are 6 discrepancies between the modelled and reference sequences:

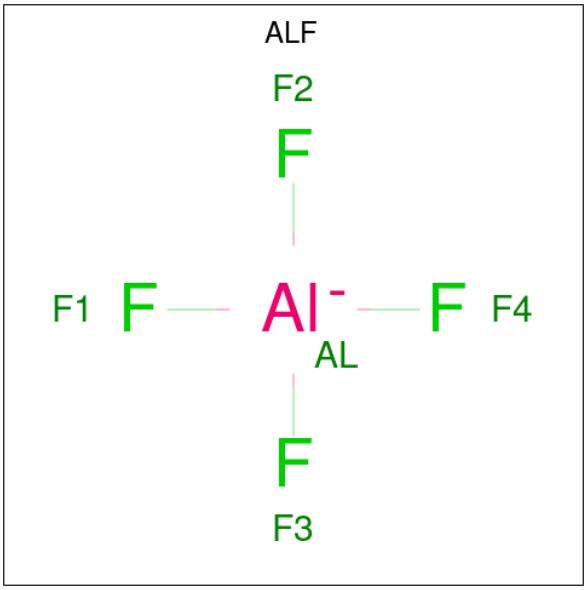
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	-	expression tag	UNP Q9H611
A	204	ARG	-	expression tag	UNP Q9H611
A	205	MET	-	expression tag	UNP Q9H611
B	203	SER	-	expression tag	UNP Q9H611
B	204	ARG	-	expression tag	UNP Q9H611
B	205	MET	-	expression tag	UNP Q9H611

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

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
3	A	1	5	1	4	0	0
3	B	1	5	1	4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

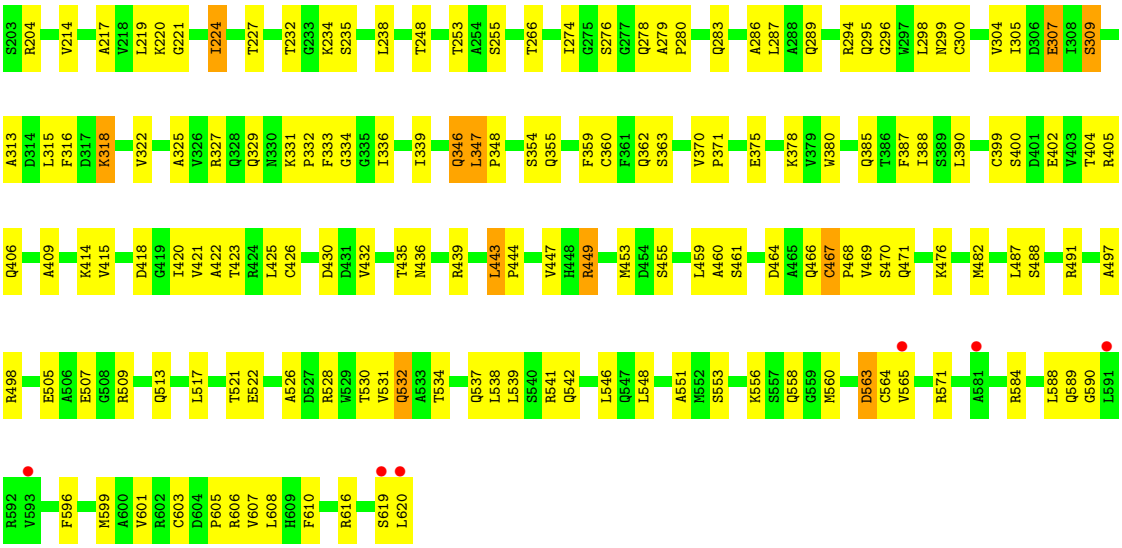
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

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.

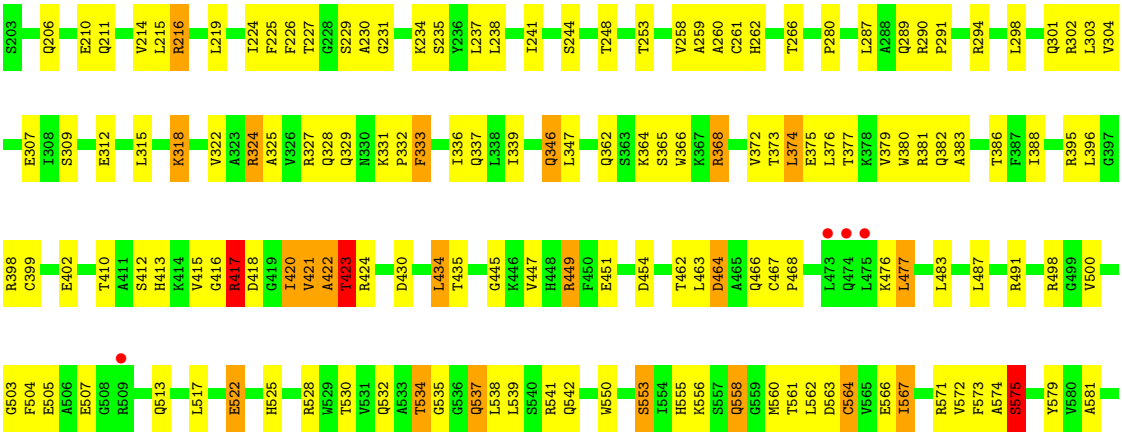
• Molecule 1: ATP-dependent DNA helicase PIF1

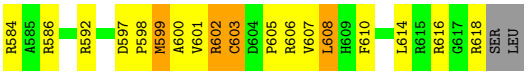
Chain A:



• Molecule 1: ATP-dependent DNA helicase PIF1

Chain B:




R584
A585
R586
R592
D597
P598
M599
A600
V601
R602
C603
D604
P605
R606
V607
L608
H609
F610
L614
R615
R616
G617
R618
SER
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.85Å 209.85Å 78.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.03 – 3.96 90.87 – 3.96	Depositor EDS
% Data completeness (in resolution range)	98.8 (91.03-3.96) 98.8 (90.87-3.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.175 , 0.253 0.186 , 0.261	Depositor DCC
R_{free} test set	794 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	142.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 132.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6495	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, 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	0.51	0/3286	0.76	0/4443
1	B	0.57	0/3280	0.84	1/4436 (0.0%)
All	All	0.54	0/6566	0.80	1/8879 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	8
All	All	0	14

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	398	ARG	NE-CZ-NH2	-6.08	117.26	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	SER	Peptide
1	A	405	ARG	Sidechain
1	A	449[A]	ARG	Sidechain
1	A	449[B]	ARG	Sidechain
1	A	467	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	563	ASP	Peptide
1	B	216	ARG	Sidechain
1	B	280	PRO	Peptide
1	B	324	ARG	Sidechain
1	B	328	GLN	Peptide
1	B	396	LEU	Peptide
1	B	417	ARG	Sidechain
1	B	422	ALA	Peptide
1	B	616	ARG	Peptide

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	3219	0	3321	89	0
1	B	3210	0	3311	115	0
2	A	27	0	12	2	0
2	B	27	0	12	3	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	6495	0	6656	194	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 15.

All (194) 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:B:261:CYS:SG	1:B:468:PRO:HG2	2.09	0.92
1:B:454:ASP:OD1	1:B:541:ARG:HA	1.76	0.85
1:B:603:CYS:SG	1:B:608:LEU:HD11	2.19	0.82
1:B:224:ILE:HD12	1:B:374:LEU:CD1	2.14	0.77
1:B:261:CYS:SG	1:B:468:PRO:CG	2.76	0.73
1:A:455:SER:HA	1:B:537:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:HD23	1:A:348:PRO:HD2	1.71	0.72
1:A:387:PHE:HB2	1:A:588:LEU:HD22	1.70	0.71
1:A:346:GLN:HB3	1:A:558:GLN:HE21	1.57	0.69
1:B:380:TRP:CD2	2:B:801:ADP:C2	2.80	0.69
1:A:532:GLN:CD	1:B:528:ARG:HH12	1.95	0.69
1:A:313:ALA:HB1	1:A:363:SER:HB2	1.74	0.69
1:B:395:ARG:HD2	1:B:579:TYR:CE2	2.29	0.67
1:B:368:ARG:HG2	1:B:368:ARG:HH11	1.59	0.67
1:A:526:ALA:HB3	1:B:291:PRO:HG3	1.75	0.67
1:A:526:ALA:HB3	1:B:291:PRO:CG	2.24	0.67
1:B:603:CYS:SG	1:B:608:LEU:CD1	2.84	0.66
1:B:449[A]:ARG:CZ	1:B:451[A]:GLU:OE2	2.44	0.66
1:B:210:GLU:OE2	1:B:377:THR:HG23	1.96	0.65
1:A:538:LEU:HD12	1:B:528:ARG:HD3	1.77	0.65
1:B:318:LYS:O	1:B:322:VAL:HG23	1.98	0.64
1:A:309:SER:HB2	1:A:347:LEU:O	1.97	0.64
1:A:509:ARG:HH22	1:A:542[B]:GLN:HE21	1.46	0.64
1:A:307:GLU:OE2	3:A:802:ALF:F3	2.05	0.64
1:B:528:ARG:HA	1:B:541:ARG:O	1.98	0.64
1:B:294:ARG:HG2	1:B:298:LEU:HD11	1.80	0.63
1:A:406:GLN:O	1:A:409:ALA:HB3	1.99	0.62
1:B:416:GLY:HA2	1:B:421:VAL:HG13	1.80	0.62
1:A:304:VAL:HA	1:A:339:ILE:O	2.00	0.61
1:B:302:ARG:HG2	1:B:337:GLN:HB3	1.81	0.61
1:B:347:LEU:HB2	1:B:558:GLN:NE2	2.15	0.61
1:A:530[B]:THR:HA	1:A:539:LEU:O	2.01	0.61
1:A:455:SER:HA	1:B:537:GLN:NE2	2.16	0.60
1:A:530[A]:THR:HA	1:A:539:LEU:O	2.01	0.60
1:B:327:ARG:HD2	1:B:336:ILE:HD11	1.83	0.60
1:A:283:GLN:O	1:A:286:ALA:HB3	2.02	0.59
1:B:227:THR:O	1:B:375:GLU:HA	2.03	0.59
1:B:324:ARG:HD3	1:B:331:LYS:O	2.03	0.59
1:B:368:ARG:HH11	1:B:368:ARG:CG	2.16	0.58
1:B:226:PHE:HA	1:B:374:LEU:O	2.04	0.58
1:B:561:THR:O	1:B:562:LEU:HG	2.04	0.57
1:A:482:MET:HA	1:A:497:ALA:O	2.04	0.57
1:A:553:SER:OG	1:A:556:LYS:HG2	2.04	0.57
1:A:532:GLN:NE2	1:B:528:ARG:HH12	2.01	0.57
1:A:443:LEU:HD12	1:A:444:PRO:HD2	1.87	0.57
1:B:225:PHE:CD2	1:B:373:THR:HG23	2.40	0.57
1:B:289:GLN:HA	1:B:289:GLN:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:MET:O	1:A:584:ARG:NH2	2.38	0.56
1:B:449[A]:ARG:NE	1:B:451[A]:GLU:OE2	2.39	0.56
1:A:279:ALA:HB1	1:A:280:PRO:CD	2.37	0.55
1:B:420:ILE:HG23	1:B:500:VAL:HB	1.88	0.55
1:B:415:VAL:HG21	1:B:592:ARG:HB2	1.90	0.54
1:A:390:LEU:HD13	1:A:406:GLN:OE1	2.07	0.54
1:B:381:ARG:HE	1:B:561:THR:HG23	1.72	0.53
1:B:463:LEU:O	1:B:467:CYS:HB2	2.07	0.53
1:B:331:LYS:HB3	1:B:332:PRO:CD	2.38	0.53
1:A:362:GLN:HE22	1:A:606:ARG:HD2	1.72	0.53
1:A:387:PHE:CB	1:A:588:LEU:HD22	2.39	0.53
1:B:567:ILE:HD12	1:B:581:ALA:HB1	1.90	0.53
1:B:421:VAL:HB	1:B:423:THR:HG23	1.91	0.53
1:B:234:LYS:HG2	1:B:376:LEU:HD12	1.90	0.53
1:B:230:ALA:HB2	1:B:579:TYR:CE2	2.44	0.53
1:B:420:ILE:CD1	1:B:517:LEU:HD22	2.38	0.53
1:B:307:GLU:OE2	3:B:802:ALF:F3	2.17	0.52
1:B:530[B]:THR:HG22	1:B:538:LEU:HD22	1.90	0.52
1:A:385:GLN:HA	1:A:388:ILE:HD12	1.92	0.52
1:A:422:ALA:O	1:A:565:VAL:HA	2.09	0.52
1:B:597:ASP:OD1	1:B:599:MET:HG2	2.09	0.52
1:A:279:ALA:HB1	1:A:283:GLN:OE1	2.10	0.52
1:A:399:CYS:SG	1:A:601:VAL:HG21	2.50	0.52
1:B:447:VAL:HG22	1:B:476:LYS:HE2	1.91	0.52
1:A:318:LYS:O	1:A:322:VAL:HG23	2.09	0.52
1:B:530[B]:THR:HA	1:B:539:LEU:O	2.09	0.51
1:A:404:THR:HG23	1:A:596:PHE:CE2	2.46	0.51
1:A:214:VAL:HG13	1:A:224:ILE:HD11	1.91	0.51
1:A:460:ALA:CB	1:A:471:GLN:HE22	2.24	0.51
1:A:355:GLN:N	1:A:355:GLN:OE1	2.44	0.51
1:A:331:LYS:HB3	1:A:332:PRO:CD	2.41	0.51
1:A:235:SER:O	1:A:238:LEU:HB2	2.11	0.50
1:A:274:ILE:HA	1:A:287:LEU:HD12	1.94	0.50
1:A:430:ASP:OD1	1:A:430:ASP:N	2.45	0.50
1:A:532:GLN:HG2	1:B:528:ARG:NH1	2.26	0.50
1:A:422:ALA:HB3	1:A:564:CYS:HB3	1.93	0.50
1:B:420:ILE:HD11	1:B:517:LEU:HB2	1.94	0.50
1:B:421:VAL:HB	1:B:423:THR:CG2	2.41	0.50
1:B:304:VAL:HG22	1:B:339:ILE:HB	1.94	0.50
1:B:530[A]:THR:HA	1:B:539:LEU:O	2.11	0.50
1:A:387:PHE:CD2	1:A:588:LEU:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:THR:HA	1:B:266:THR:O	2.12	0.50
1:A:234:LYS:NZ	3:A:802:ALF:F2	2.25	0.49
1:B:365:SER:O	1:B:366:TRP:C	2.50	0.49
1:B:215:LEU:HD11	1:B:219:LEU:HD11	1.94	0.49
1:B:395:ARG:HD2	1:B:579:TYR:CZ	2.47	0.49
1:B:416:GLY:HA2	1:B:421:VAL:CG1	2.42	0.49
1:B:303:LEU:HD12	1:B:304:VAL:N	2.27	0.49
1:A:327:ARG:HD2	1:A:336:ILE:HD11	1.94	0.49
1:B:225:PHE:HD2	1:B:373:THR:HG23	1.75	0.49
1:B:605:PRO:HA	1:B:608:LEU:HB2	1.95	0.49
1:A:299:ASN:O	1:A:300:CYS:C	2.51	0.49
1:B:346:GLN:HB3	1:B:558:GLN:NE2	2.27	0.49
1:A:603:CYS:HB3	1:A:608:LEU:HD11	1.95	0.49
1:A:443:LEU:CD1	1:A:444:PRO:HD2	2.43	0.48
1:A:217:ALA:HA	1:A:220:LYS:HD3	1.96	0.48
1:B:553:SER:OG	1:B:556:LYS:HG2	2.13	0.48
1:B:287:LEU:N	1:B:287:LEU:HD23	2.27	0.48
1:B:304:VAL:HA	1:B:339:ILE:O	2.14	0.48
1:B:379:VAL:HG21	1:B:388:ILE:HG23	1.96	0.48
1:B:483:LEU:HD11	1:B:487:LEU:HD12	1.96	0.47
1:B:410:THR:HG22	1:B:413:HIS:CE1	2.49	0.47
1:B:435:THR:HG22	1:B:435:THR:O	2.14	0.47
1:B:504:PHE:O	1:B:513:GLN:NE2	2.48	0.47
1:A:253:THR:HA	1:A:266:THR:O	2.15	0.46
1:B:381:ARG:HG2	1:B:382:GLN:NE2	2.30	0.46
1:B:571:ARG:NH2	1:B:573:PHE:CE2	2.83	0.46
1:B:463:LEU:O	1:B:464:ASP:C	2.54	0.46
1:B:434:LEU:HD23	1:B:435:THR:OG1	2.16	0.46
1:B:312:GLU:O	1:B:315:LEU:HB3	2.16	0.46
1:A:467:CYS:HB3	1:A:469:VAL:H	1.81	0.46
1:B:607:VAL:O	1:B:610:PHE:N	2.49	0.46
1:A:466:GLN:HG2	1:A:531:VAL:HG11	1.98	0.45
1:A:460:ALA:HB1	1:A:471:GLN:HE22	1.80	0.45
1:A:362:GLN:NE2	1:A:606:ARG:HD2	2.31	0.45
1:A:219:LEU:O	1:A:220:LYS:C	2.54	0.45
1:B:422:ALA:CB	1:B:562:LEU:HD22	2.46	0.45
1:A:415:VAL:HG13	1:A:590:GLY:C	2.37	0.45
1:B:241:ILE:O	1:B:244:SER:N	2.47	0.45
1:B:449[A]:ARG:NH2	1:B:451[A]:GLU:OE2	2.50	0.45
1:A:447:VAL:HG22	1:A:476:LYS:HE3	1.99	0.44
1:A:616:ARG:HE	1:A:616:ARG:HB3	1.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TRP:CG	2:B:801:ADP:C2	3.06	0.44
1:A:278:GLN:OE1	1:A:278:GLN:HA	2.17	0.44
1:A:420:ILE:O	1:A:420:ILE:HD12	2.18	0.44
1:A:436:ASN:HD22	1:A:548:LEU:HB2	1.82	0.44
1:B:224:ILE:HD12	1:B:374:LEU:HD11	1.99	0.44
1:B:260:ALA:C	1:B:262:HIS:N	2.70	0.44
1:B:420:ILE:CD1	1:B:517:LEU:HB2	2.47	0.44
1:B:567:ILE:HD12	1:B:581:ALA:CB	2.46	0.44
1:A:331:LYS:HB3	1:A:332:PRO:HD2	2.00	0.44
1:B:224:ILE:HD12	1:B:374:LEU:HD12	1.96	0.44
1:B:598:PRO:C	1:B:600:ALA:H	2.21	0.44
1:A:232:THR:HG22	1:A:378:LYS:O	2.17	0.44
1:B:477:LEU:HD23	1:B:503:GLY:HA2	2.00	0.44
1:B:530[B]:THR:CG2	1:B:538:LEU:HD22	2.47	0.44
1:A:532:GLN:CG	1:B:528:ARG:NH1	2.81	0.44
1:B:266:THR:HG21	1:B:532:GLN:HE22	1.83	0.44
1:B:303:LEU:HD12	1:B:304:VAL:H	1.83	0.43
1:A:420:ILE:HD11	1:A:517:LEU:HD13	1.99	0.43
1:A:432:VAL:HG13	1:A:551:ALA:O	2.18	0.43
1:B:362:GLN:HE22	1:B:606:ARG:HD2	1.84	0.43
1:A:289:GLN:OE1	1:A:289:GLN:HA	2.17	0.43
1:B:423:THR:HG22	1:B:566:GLU:HB2	2.00	0.43
1:B:417:ARG:NH2	1:B:418:ASP:HB2	2.34	0.43
1:A:528:ARG:HA	1:A:541:ARG:O	2.19	0.43
1:B:211:GLN:HA	1:B:237:LEU:HD22	2.00	0.43
1:B:362:GLN:HE22	1:B:606:ARG:CD	2.32	0.43
1:A:327:ARG:NH2	1:A:334:GLY:O	2.45	0.43
1:B:601:VAL:O	1:B:601:VAL:HG12	2.17	0.43
1:A:505:GLU:HG3	1:A:513:GLN:NE2	2.34	0.42
1:B:416:GLY:CA	1:B:421:VAL:HG13	2.46	0.42
1:A:380:TRP:HB3	2:A:801:ADP:N3	2.34	0.42
1:B:598:PRO:C	1:B:600:ALA:N	2.73	0.42
1:A:294:ARG:CZ	1:A:298:LEU:HD11	2.50	0.42
1:A:605:PRO:HA	1:A:608:LEU:HB2	2.01	0.42
1:B:381:ARG:O	1:B:586:ARG:HG3	2.19	0.42
1:A:227:THR:O	1:A:375:GLU:HA	2.20	0.42
1:B:253:THR:OG1	1:B:304:VAL:O	2.32	0.42
1:B:574:ALA:O	1:B:575:SER:C	2.59	0.42
1:B:598:PRO:O	1:B:600:ALA:N	2.53	0.42
1:A:295:GLN:O	1:A:296:GLY:C	2.59	0.41
1:A:359:PHE:CE2	1:A:607:VAL:CG2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ARG:HB3	1:B:573:PHE:CE1	2.56	0.41
1:A:380:TRP:CE3	2:A:801:ADP:C2	3.08	0.41
1:A:459:LEU:O	1:A:461:SER:N	2.54	0.41
1:B:491[A]:ARG:HH21	1:B:522[A]:GLU:HG3	1.86	0.41
1:A:279:ALA:HB1	1:A:280:PRO:HD2	2.02	0.41
1:A:295:GLN:O	1:A:299:ASN:ND2	2.54	0.41
1:B:381:ARG:NE	1:B:561:THR:HG23	2.34	0.41
1:A:422:ALA:O	1:A:564:CYS:O	2.38	0.41
1:A:460:ALA:HB1	1:A:471:GLN:NE2	2.36	0.41
1:A:488:SER:OG	1:A:491[A]:ARG:NH1	2.54	0.41
1:B:258:VAL:CG2	1:B:259:ALA:N	2.84	0.41
1:A:435:THR:O	1:A:439:ARG:HG2	2.20	0.41
1:B:560:MET:O	1:B:584:ARG:NH2	2.54	0.41
1:A:316:PHE:CD2	1:A:360:CYS:SG	3.14	0.40
1:B:235:SER:O	1:B:238:LEU:HB2	2.21	0.40
1:B:380:TRP:CE2	2:B:801:ADP:N1	2.89	0.40
1:B:410:THR:O	1:B:592:ARG:HA	2.21	0.40
1:B:572:VAL:CG1	1:B:602:ARG:NH2	2.85	0.40
1:A:532:GLN:CG	1:B:528:ARG:HH12	2.34	0.40
1:B:417:ARG:HH21	1:B:418:ASP:HB2	1.85	0.40
1:A:415:VAL:HG13	1:A:590:GLY:O	2.21	0.40
1:A:482:MET:O	1:A:546:LEU:HA	2.21	0.40
1:A:607:VAL:O	1:A:610:PHE:N	2.54	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	421/418 (101%)	353 (84%)	58 (14%)	10 (2%)	6 36
1	B	420/418 (100%)	354 (84%)	52 (12%)	14 (3%)	4 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	841/836 (101%)	707 (84%)	110 (13%)	24 (3%)	4 32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	346	GLN
1	A	534	THR
1	B	214	VAL
1	B	231	GLY
1	B	325	ALA
1	B	346	GLN
1	B	424	ARG
1	B	445	GLY
1	B	477	LEU
1	B	534	THR
1	B	423	THR
1	B	575	SER
1	A	307	GLU
1	A	571	ARG
1	A	619	SER
1	B	333	PHE
1	B	564	CYS
1	A	325	ALA
1	A	453	MET
1	A	468	PRO
1	B	383	ALA
1	B	535	GLY
1	A	221	GLY

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	346/341 (102%)	308 (89%)	38 (11%)	6 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	345/341 (101%)	294 (85%)	51 (15%)	3 18
All	All	691/682 (101%)	602 (87%)	89 (13%)	4 22

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ARG
1	A	224	ILE
1	A	248	THR
1	A	276	SER
1	A	305	ILE
1	A	309	SER
1	A	315	LEU
1	A	318	LYS
1	A	329	GLN
1	A	333	PHE
1	A	347	LEU
1	A	354	SER
1	A	370	VAL
1	A	371	PRO
1	A	402	GLU
1	A	414	LYS
1	A	418	ASP
1	A	421	VAL
1	A	423	THR
1	A	425	LEU
1	A	426	CYS
1	A	443	LEU
1	A	449[A]	ARG
1	A	449[B]	ARG
1	A	464	ASP
1	A	470	SER
1	A	487	LEU
1	A	498	ARG
1	A	507	GLU
1	A	521	THR
1	A	522[A]	GLU
1	A	522[B]	GLU
1	A	532	GLN
1	A	537	GLN
1	A	563	ASP
1	A	589	GLN

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Mol	Chain	Res	Type
1	A	599	MET
1	A	620	LEU
1	B	206	GLN
1	B	216	ARG
1	B	229	SER
1	B	248	THR
1	B	290	ARG
1	B	301	GLN
1	B	309	SER
1	B	318	LYS
1	B	329	GLN
1	B	333	PHE
1	B	364	LYS
1	B	368	ARG
1	B	372	VAL
1	B	374	LEU
1	B	386	THR
1	B	399	CYS
1	B	402	GLU
1	B	412	SER
1	B	417	ARG
1	B	420	ILE
1	B	421	VAL
1	B	423	THR
1	B	430	ASP
1	B	434	LEU
1	B	449[A]	ARG
1	B	449[B]	ARG
1	B	462	THR
1	B	464	ASP
1	B	466	GLN
1	B	498	ARG
1	B	505	GLU
1	B	507	GLU
1	B	522[A]	GLU
1	B	522[B]	GLU
1	B	525	HIS
1	B	534	THR
1	B	537	GLN
1	B	550	TRP
1	B	553	SER
1	B	555	HIS

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Mol	Chain	Res	Type
1	B	558	GLN
1	B	563	ASP
1	B	564	CYS
1	B	567	ILE
1	B	575	SER
1	B	599	MET
1	B	602	ARG
1	B	603	CYS
1	B	608	LEU
1	B	614	LEU
1	B	618	ARG

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	299	ASN
1	A	329	GLN
1	A	346	GLN
1	A	429	GLN
1	A	456	ASN
1	A	466	GLN
1	A	471	GLN
1	A	525	HIS
1	A	537	GLN
1	A	558	GLN
1	B	206	GLN
1	B	346	GLN
1	B	382	GLN
1	B	392	GLN
1	B	413	HIS
1	B	537	GLN
1	B	558	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	801	4	24,29,29	1.13	3 (12%)	29,45,45	1.49	4 (13%)
2	ADP	A	801	4	24,29,29	0.99	1 (4%)	29,45,45	1.96	8 (27%)
3	ALF	A	802	-	4,4,4	1.46	0	-		
3	ALF	B	802	-	4,4,4	1.45	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	B	801	4	-	3/12/32/32	0/3/3/3
2	ADP	A	801	4	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	C4-N3	-2.78	1.31	1.35
2	A	801	ADP	PA-O3A	2.17	1.61	1.59
2	B	801	ADP	C2-N3	2.11	1.35	1.32
2	B	801	ADP	C5-N7	-2.05	1.32	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	ADP	N3-C2-N1	-6.39	120.00	128.67
2	A	801	ADP	C1'-N9-C4	-3.75	120.06	126.64
2	A	801	ADP	N6-C6-N1	3.06	124.88	118.33
2	B	801	ADP	C4'-O4'-C1'	3.01	112.68	109.92
2	A	801	ADP	O4'-C1'-N9	-2.72	105.13	108.75
2	B	801	ADP	O3'-C3'-C4'	-2.69	103.36	111.08
2	A	801	ADP	O3B-PB-O2B	2.58	117.48	107.80
2	B	801	ADP	O3A-PB-O1B	-2.52	97.80	111.04
2	A	801	ADP	C5-C6-N6	-2.24	116.89	120.31
2	B	801	ADP	C4-C5-N7	-2.21	107.00	109.34
2	A	801	ADP	O3'-C3'-C2'	-2.08	105.14	111.82
2	A	801	ADP	C2'-C3'-C4'	2.05	106.58	102.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ADP	O4'-C4'-C5'-O5'
2	B	801	ADP	C3'-C4'-C5'-O5'
2	B	801	ADP	C5'-O5'-PA-O1A

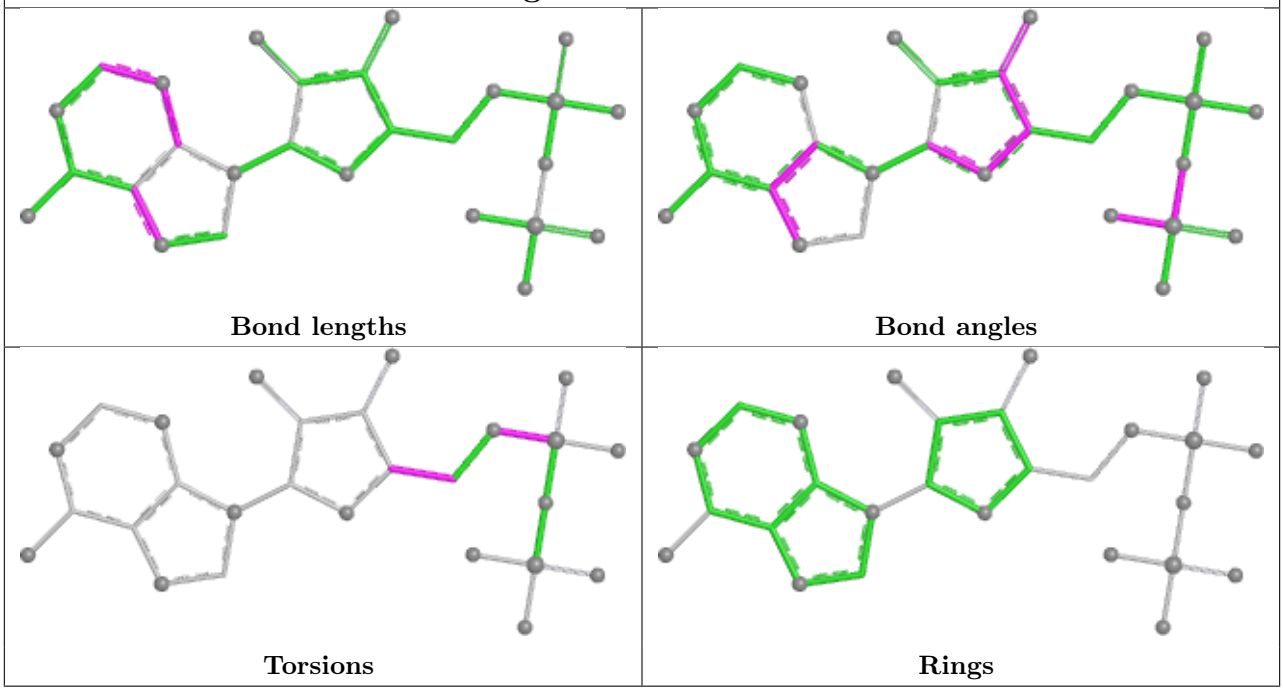
There are no ring outliers.

4 monomers are involved in 8 short contacts:

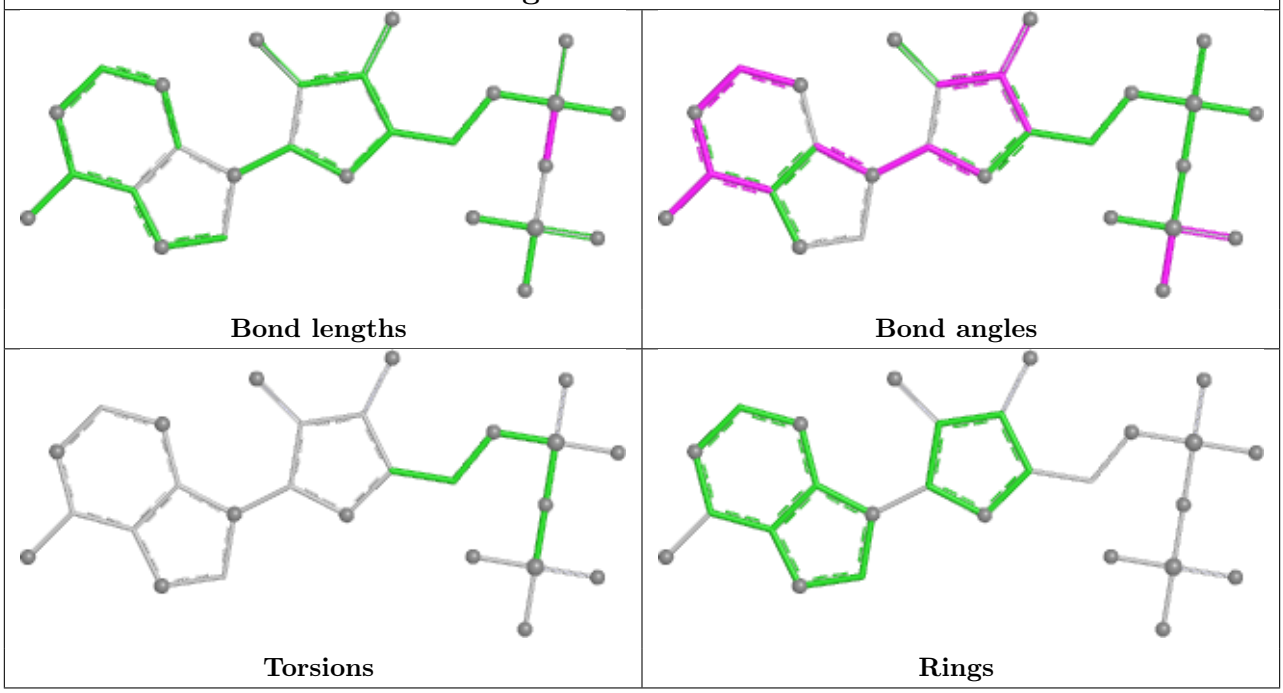
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ADP	3	0
2	A	801	ADP	2	0
3	A	802	ALF	2	0
3	B	802	ALF	1	0

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 801



Ligand ADP A 801



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	418/418 (100%)	-0.11	6 (1%)	75	66	80, 169, 217, 276	15 (3%)
1	B	416/418 (99%)	-0.07	4 (0%)	82	74	72, 143, 204, 253	14 (3%)
All	All	834/836 (99%)	-0.09	10 (1%)	79	70	72, 158, 213, 276	29 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	LEU	2.9
1	A	619	SER	2.7
1	A	620	LEU	2.7
1	B	474	GLN	2.4
1	A	565	VAL	2.3
1	B	473	LEU	2.3
1	A	593	VAL	2.1
1	A	581	ALA	2.1
1	A	591	LEU	2.1
1	B	509	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

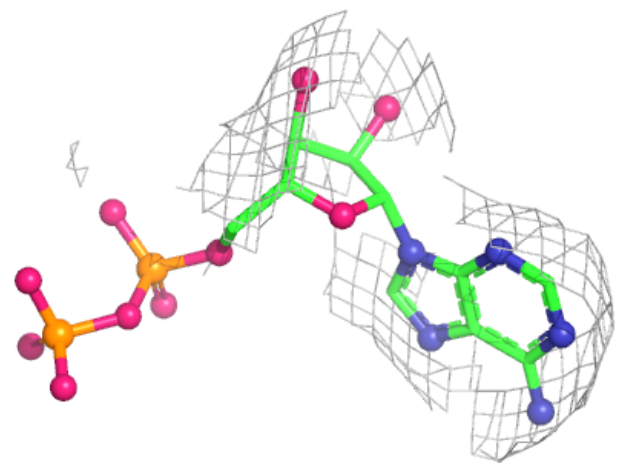
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

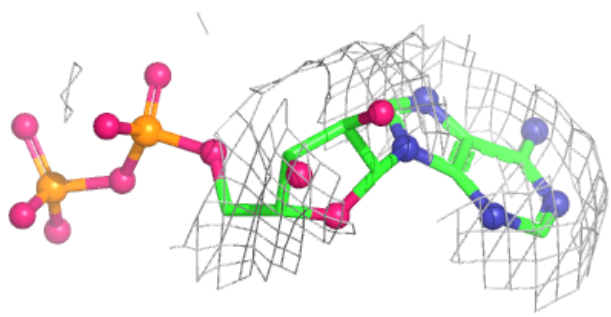
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	801	27/27	0.93	0.19	137,146,171,190	0
2	ADP	B	801	27/27	0.96	0.25	89,114,129,139	0
4	MG	B	803	1/1	0.98	0.21	58,58,58,58	0
3	ALF	B	802	5/5	0.99	0.20	79,80,120,123	0
4	MG	A	803	1/1	0.99	0.15	117,117,117,117	0
3	ALF	A	802	5/5	0.99	0.15	129,138,146,182	0

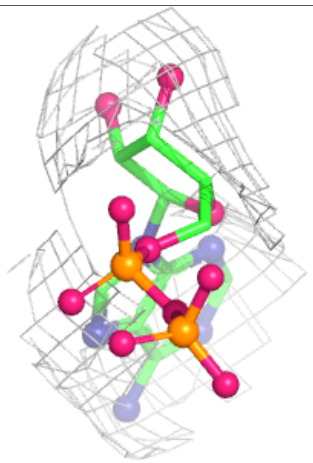
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

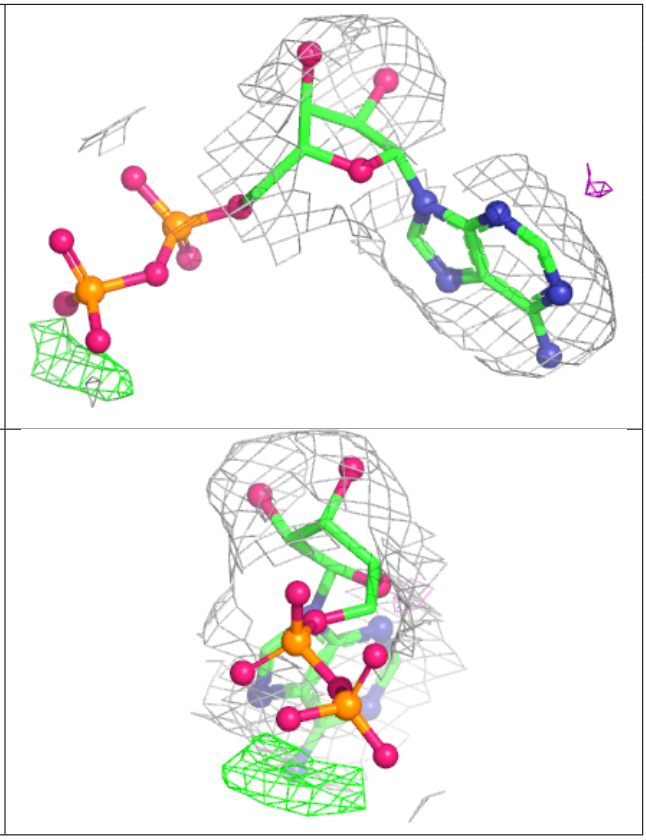






Electron density around ADP B 801:

$2mF_o$-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.