



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:14 PM UTC

PDB ID : 5O6B / pdb_00005o6b
Title : Structure of ScPif1 in complex with GGGTTTT and ADP-AlF₄
Authors : Lu, K.Y.; Chen, W.F.; Rety, S.; Liu, N.N.; Xu, X.G.
Deposited on : 2017-06-06
Resolution : 2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

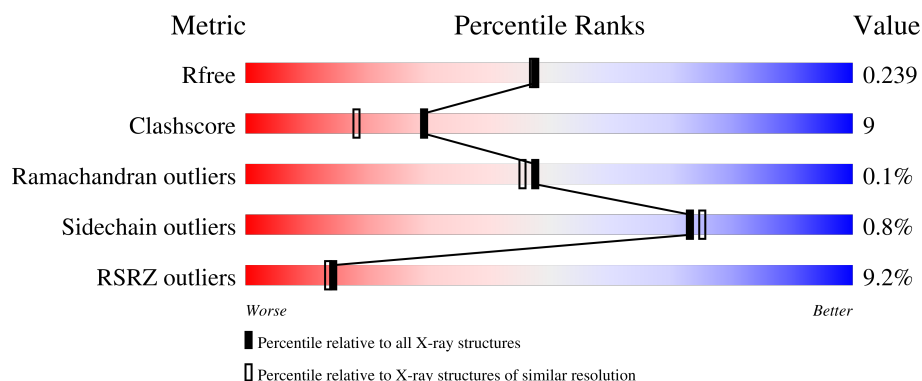
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	545	7% 82% 15% .
1	B	545	10% 75% 18% 7%
2	C	8	62% 12% 25%
2	D	8	50% 25% 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9104 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
1	A	528	Total	C	N	O	S	0	0	0
			4190	2654	740	776	20			
1	B	507	Total	C	N	O	S	0	0	0
			4040	2563	720	737	20			

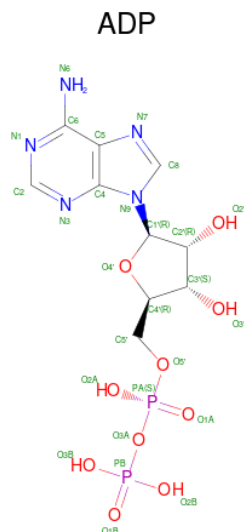
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLY	-	expression tag	UNP P07271
B	236	GLY	-	expression tag	UNP P07271

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*TP*TP*T)-3').

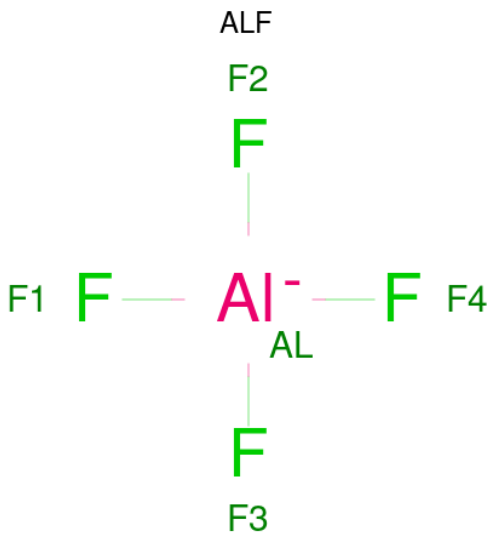
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			123	60	21	37	5			
2	D	6	Total	C	N	O	P	0	0	0
			123	60	21	37	5			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

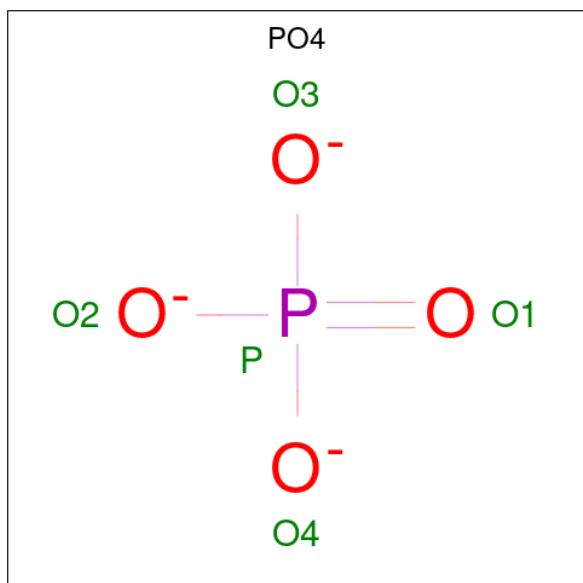


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	Al 1	F 4	0	0
4	B	1	Total 5	Al 1	F 4	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

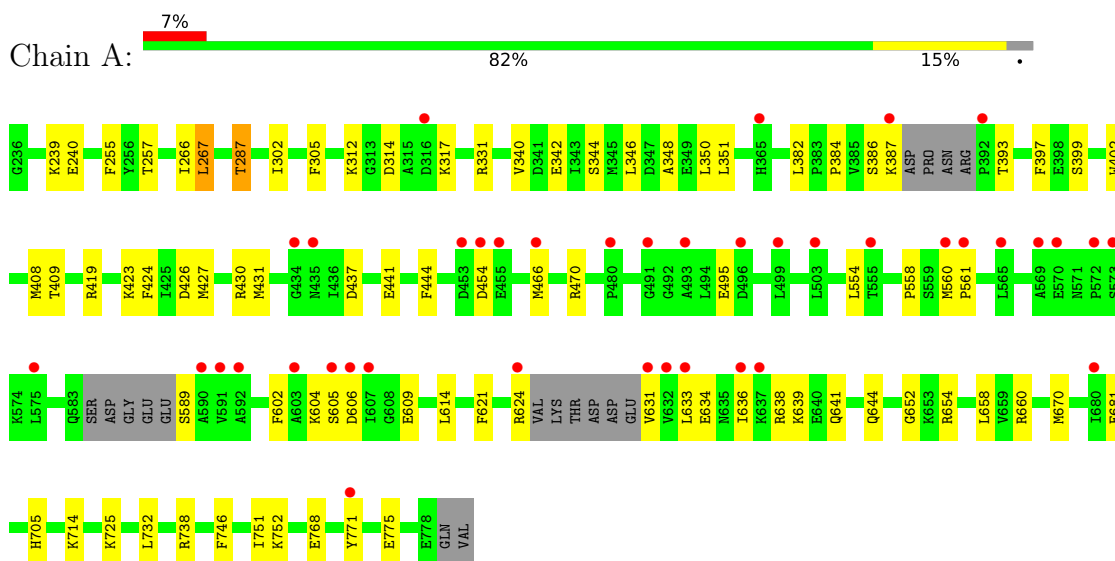
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	322	Total	O	0	0
			322	322		
7	B	205	Total	O	0	0
			205	205		
7	C	20	Total	O	0	0
			20	20		
7	D	10	Total	O	0	0
			10	10		

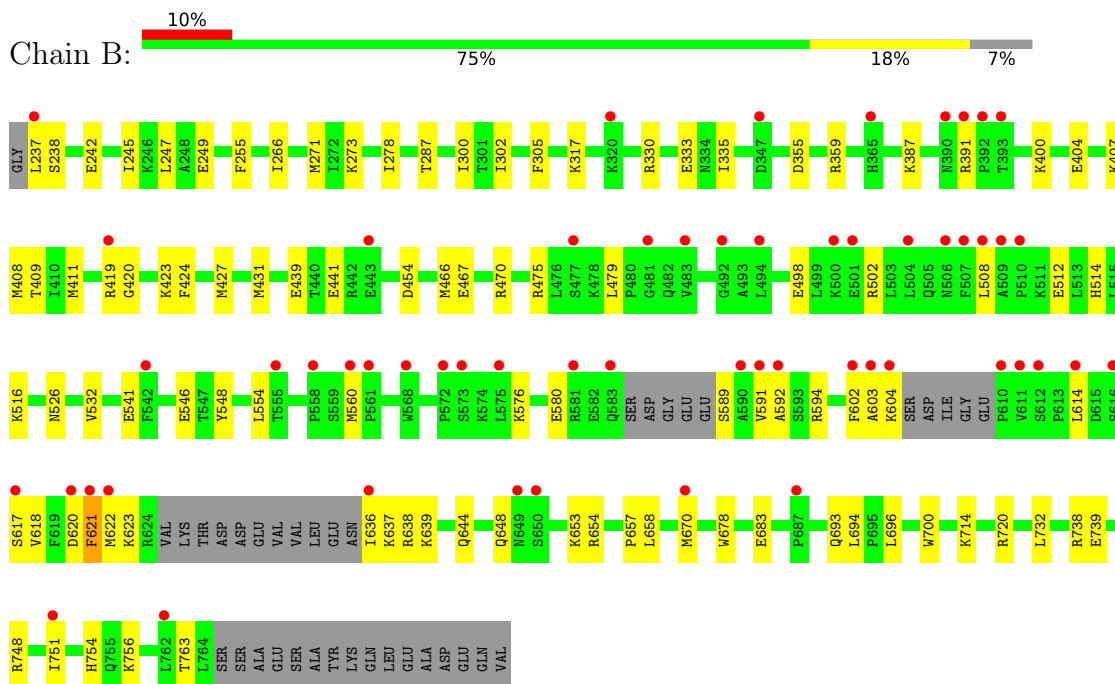
3 Residue-property plots [i](#)

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



• Molecule 1: ATP-dependent DNA helicase PIF1



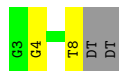
- Molecule 2: DNA (5'-D(*GP*GP*GP*TP*TP*T)-3')

Chain C:  62% 12% 25%



- Molecule 2: DNA (5'-D(*GP*GP*GP*TP*TP*T)-3')

Chain D:  50% 25% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.25Å 88.37Å 187.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.71 – 2.03 58.71 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.1 (58.71-2.03) 98.1 (58.71-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.193 , 0.238 0.196 , 0.239	Depositor DCC
R_{free} test set	4425 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9104	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6537e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, ADP, PO4, ALF

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	0.34	0/4258	0.54	1/5716 (0.0%)
1	B	0.33	0/4108	0.53	0/5514
2	C	0.54	0/137	0.84	0/211
2	D	0.47	0/137	0.62	0/211
All	All	0.34	0/8640	0.54	1/11652 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	CA-CB-CG	5.75	136.43	116.30

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	4190	0	4293	65	0
1	B	4040	0	4157	84	0
2	C	123	0	71	1	0
2	D	123	0	71	2	0
3	A	27	0	12	1	0
3	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	5	0	0	0	0
7	A	322	0	0	13	0
7	B	205	0	0	19	0
7	C	20	0	0	0	0
7	D	10	0	0	1	0
All	All	9104	0	8616	148	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 9.

All (148) 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:589:SER:N	7:B:1102:HOH:O	1.84	1.09
1:B:431:MET:HG3	1:B:751:ILE:CD1	1.83	1.06
1:B:431:MET:HE1	1:B:732:LEU:HD12	1.35	1.03
1:A:725:LYS:NZ	7:A:1102:HOH:O	1.90	1.01
1:B:763:THR:OG1	7:B:1101:HOH:O	1.80	0.99
1:A:681:GLU:OE2	7:A:1101:HOH:O	1.84	0.95
1:B:431:MET:HG3	1:B:751:ILE:HD11	1.51	0.92
1:A:752:LYS:NZ	7:A:1104:HOH:O	2.02	0.92
1:B:237:LEU:HB2	3:B:1001:ADP:HN62	1.38	0.89
1:A:554:LEU:HD22	1:A:621:PHE:CZ	2.12	0.84
1:A:554:LEU:HD22	1:A:621:PHE:HZ	1.41	0.81
1:A:314:ASP:OD1	7:A:1103:HOH:O	1.98	0.81
1:B:720:ARG:NH1	7:B:1105:HOH:O	2.15	0.80
1:A:604:LYS:H	1:A:604:LYS:HD2	1.46	0.79
2:D:8:DT:OP1	7:D:101:HOH:O	2.00	0.78
1:B:614:LEU:H	1:B:644:GLN:HE22	1.34	0.75
1:B:548:TYR:OH	7:B:1103:HOH:O	2.03	0.75
1:A:424:PHE:HA	1:A:427:MET:HE3	1.69	0.75
1:A:387:LYS:N	7:A:1110:HOH:O	2.19	0.74
1:B:237:LEU:N	7:B:1106:HOH:O	2.21	0.73
1:A:641:GLN:OE1	7:A:1106:HOH:O	2.08	0.71
1:B:424:PHE:HA	1:B:427:MET:HE3	1.71	0.71
1:B:554:LEU:HD21	1:B:621:PHE:CZ	2.25	0.71
1:A:644:GLN:OE1	7:A:1107:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:MET:CG	1:B:751:ILE:HD11	2.21	0.70
1:B:431:MET:HE1	1:B:732:LEU:CD1	2.20	0.69
1:B:512:GLU:OE2	1:B:514:HIS:NE2	2.25	0.69
1:A:454:ASP:OD1	1:A:714:LYS:NZ	2.22	0.69
1:A:266:ILE:HG13	3:A:1001:ADP:H2'	1.76	0.68
1:B:560:MET:O	1:B:639:LYS:NZ	2.27	0.68
1:A:638:ARG:NH2	7:A:1111:HOH:O	2.21	0.67
1:A:423:LYS:HG3	1:A:427:MET:HE2	1.77	0.66
1:A:431:MET:HE2	1:A:751:ILE:HD13	1.79	0.64
1:B:546:GLU:OE2	7:B:1104:HOH:O	2.15	0.64
1:B:604:LYS:HB3	7:B:1127:HOH:O	1.96	0.64
1:A:441:GLU:OE2	7:A:1108:HOH:O	2.16	0.63
1:A:589:SER:N	7:A:1105:HOH:O	2.31	0.62
1:B:238:SER:O	1:B:242:GLU:HG3	2.01	0.61
1:B:330:ARG:NH1	1:B:333:GLU:OE2	2.34	0.61
1:B:423:LYS:HG3	1:B:427:MET:HE2	1.84	0.60
1:B:589:SER:HB2	1:B:592:ALA:HB3	1.84	0.59
1:B:454:ASP:OD1	1:B:714:LYS:NZ	2.35	0.59
1:B:602:PHE:HE2	1:B:694:LEU:HD12	1.68	0.59
1:A:287:THR:HG21	1:A:302:ILE:HD13	1.85	0.58
1:B:266:ILE:HG13	3:B:1001:ADP:H2'	1.85	0.57
1:B:237:LEU:HB2	3:B:1001:ADP:N6	2.15	0.57
1:B:603:ALA:HB3	1:B:654:ARG:HA	1.88	0.56
1:B:604:LYS:HE3	7:B:1127:HOH:O	2.06	0.56
1:A:466:MET:SD	1:A:470:ARG:NH1	2.79	0.56
1:A:240:GLU:HG3	1:A:771:TYR:OH	2.06	0.55
2:C:8:DT:O2	2:C:8:DT:H2'	2.07	0.55
1:B:431:MET:CG	1:B:751:ILE:CD1	2.73	0.55
1:B:427:MET:HE1	1:B:738:ARG:HD3	1.88	0.55
1:A:558:PRO:O	1:A:639:LYS:NZ	2.37	0.55
1:B:400:LYS:HG2	7:B:1160:HOH:O	2.05	0.55
1:B:317:LYS:NZ	7:B:1110:HOH:O	2.33	0.54
1:B:637:LYS:N	7:B:1114:HOH:O	2.40	0.54
1:A:317:LYS:HE3	1:B:498:GLU:HG3	1.89	0.53
1:B:387:LYS:HG2	2:D:4:DG:O6	2.09	0.53
1:A:658:LEU:HD11	1:A:670:MET:HE3	1.91	0.52
1:B:508:LEU:HB3	7:B:1119:HOH:O	2.09	0.52
1:A:636:ILE:C	1:A:638:ARG:H	2.18	0.51
1:B:638:ARG:N	7:B:1114:HOH:O	2.43	0.51
1:B:441:GLU:OE2	1:B:748:ARG:NH1	2.44	0.51
1:B:479:LEU:O	1:B:516:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:TRP:NE1	7:B:1119:HOH:O	2.43	0.51
1:A:495:GLU:OE2	1:B:683:GLU:HA	2.11	0.50
1:A:589:SER:OG	7:A:1105:HOH:O	2.06	0.50
1:A:386:SER:HB3	1:A:393:THR:OG1	2.11	0.50
1:B:526:ASN:HA	1:B:532:VAL:HA	1.94	0.50
1:B:554:LEU:HD21	1:B:621:PHE:HZ	1.74	0.50
1:A:636:ILE:O	1:A:636:ILE:HG13	2.11	0.50
1:B:404:GLU:O	1:B:407:LYS:HE2	2.12	0.50
1:B:636:ILE:N	7:B:1114:HOH:O	2.45	0.49
1:B:305:PHE:HZ	1:B:335:ILE:HD13	1.77	0.49
1:B:693:GLN:HG3	1:B:694:LEU:N	2.27	0.49
1:B:694:LEU:HD23	1:B:696:LEU:HD12	1.94	0.49
1:A:312:LYS:HE3	1:B:502:ARG:HG3	1.94	0.48
1:A:240:GLU:HG3	1:A:771:TYR:HH	1.78	0.48
1:A:287:THR:HG22	1:A:340:VAL:HA	1.95	0.48
1:A:305:PHE:CE1	1:A:331:ARG:HG2	2.48	0.48
1:A:426:ASP:CG	1:A:430:ARG:HD2	2.39	0.48
1:B:591:VAL:O	1:B:594:ARG:HB3	2.14	0.48
1:A:631:VAL:CG1	1:A:633:LEU:HG	2.43	0.47
1:B:644:GLN:O	1:B:648:GLN:OE1	2.32	0.47
1:A:419:ARG:NE	7:A:1125:HOH:O	2.48	0.47
1:B:273:LYS:HE2	7:B:1181:HOH:O	2.14	0.47
1:B:602:PHE:CE2	1:B:694:LEU:HD12	2.49	0.46
1:A:768:GLU:OE1	1:A:768:GLU:N	2.43	0.46
1:B:411:MET:HE3	1:B:411:MET:HB2	1.68	0.46
1:B:658:LEU:HD11	1:B:670:MET:CG	2.46	0.46
1:A:431:MET:HE1	1:A:746:PHE:HE2	1.80	0.46
1:A:602:PHE:O	1:A:654:ARG:HD3	2.15	0.45
1:B:470:ARG:NH1	7:B:1116:HOH:O	2.40	0.45
1:B:431:MET:CE	1:B:732:LEU:HD12	2.26	0.45
1:A:606:ASP:HB2	1:A:609:GLU:HB2	1.99	0.45
1:A:560:MET:HG2	1:A:561:PRO:HD2	1.99	0.45
1:A:771:TYR:O	1:A:775:GLU:HG2	2.17	0.44
1:B:305:PHE:CZ	1:B:335:ILE:HD13	2.52	0.44
1:B:255:PHE:O	1:B:409:THR:HA	2.18	0.44
1:A:605:SER:HB2	1:A:652:GLY:C	2.42	0.44
1:B:247:LEU:HD22	1:B:408:MET:SD	2.58	0.44
1:B:754:HIS:CE1	1:B:756:LYS:HB2	2.52	0.44
1:A:427:MET:HE1	1:A:738:ARG:CZ	2.47	0.44
1:A:431:MET:SD	1:A:732:LEU:HD12	2.58	0.44
1:B:541:GLU:HB2	1:B:618:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:MET:HE3	1:B:470:ARG:HH22	1.83	0.44
1:A:444:PHE:CE1	1:A:732:LEU:HD13	2.53	0.43
1:B:431:MET:HG3	1:B:751:ILE:HD12	1.86	0.43
1:A:305:PHE:HE1	1:A:331:ARG:HG2	1.83	0.43
1:B:245:ILE:HG12	1:B:271:MET:HB2	1.99	0.43
1:B:423:LYS:NZ	1:B:439:GLU:OE1	2.45	0.43
1:B:431:MET:O	1:B:751:ILE:HD11	2.18	0.43
1:A:255:PHE:O	1:A:409:THR:HA	2.19	0.43
1:A:342:GLU:HA	1:A:342:GLU:OE1	2.19	0.43
1:B:617:SER:HA	7:B:1144:HOH:O	2.19	0.43
1:A:255:PHE:CZ	1:A:257:THR:HB	2.54	0.43
1:A:344:SER:O	1:A:384:PRO:HD3	2.19	0.43
1:A:427:MET:HE1	1:A:738:ARG:NH1	2.34	0.43
1:B:475:ARG:HG2	1:B:700:TRP:CD2	2.54	0.43
1:B:653:LYS:HD3	1:B:654:ARG:H	1.83	0.42
1:A:431:MET:HB2	1:A:431:MET:HE3	1.52	0.42
1:A:408:MET:HE3	1:A:408:MET:HB2	1.74	0.42
1:B:355:ASP:OD1	1:B:359:ARG:NE	2.39	0.42
1:A:426:ASP:OD1	1:A:430:ARG:HD2	2.19	0.42
1:B:287:THR:HA	1:B:300:ILE:O	2.20	0.42
1:B:576:LYS:O	1:B:580:GLU:HG3	2.18	0.42
1:A:631:VAL:HG12	1:A:634:GLU:H	1.85	0.42
1:B:249:GLU:HG3	1:B:278:ILE:HD11	2.00	0.42
1:A:348:ALA:HB1	1:A:399:SER:HB3	2.02	0.42
1:B:391:ARG:HD3	1:B:391:ARG:HA	1.76	0.42
1:A:346:LEU:HD22	1:A:350:LEU:HD23	2.02	0.42
1:B:330:ARG:HA	1:B:330:ARG:HD3	1.83	0.42
1:A:397:PHE:HA	1:A:402:TRP:CG	2.55	0.42
1:B:554:LEU:HD11	1:B:639:LYS:HD3	2.02	0.42
1:A:660:ARG:HD2	7:A:1377:HOH:O	2.20	0.41
1:A:430:ARG:HH22	1:A:437:ASP:CG	2.28	0.41
1:A:239:LYS:HG2	1:A:771:TYR:OH	2.20	0.41
1:A:351:LEU:HD12	1:A:351:LEU:HA	1.89	0.41
1:B:419:ARG:HG3	1:B:420:GLY:H	1.86	0.41
1:B:466:MET:HE2	1:B:467:GLU:HG3	2.03	0.41
1:B:636:ILE:HG23	1:B:637:LYS:HG2	2.03	0.41
1:B:614:LEU:HB2	1:B:644:GLN:NE2	2.36	0.41
1:B:302:ILE:HG22	7:B:1113:HOH:O	2.20	0.40
1:B:657:PRO:HG2	1:B:694:LEU:HD21	2.03	0.40
1:A:382:LEU:CD1	1:A:705:HIS:HA	2.52	0.40
1:A:554:LEU:HD22	1:A:621:PHE:CE2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:GLU:H	1:B:739:GLU:CD	2.29	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	520/545 (95%)	512 (98%)	8 (2%)	0	100	100
1	B	499/545 (92%)	493 (99%)	5 (1%)	1 (0%)	43	40
All	All	1019/1090 (94%)	1005 (99%)	13 (1%)	1 (0%)	48	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	621	PHE

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	457/473 (97%)	453 (99%)	4 (1%)	70	73
1	B	441/473 (93%)	438 (99%)	3 (1%)	76	77
All	All	898/946 (95%)	891 (99%)	7 (1%)	73	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	A	287	THR
1	A	614	LEU
1	A	624	ARG
1	B	620	ASP
1	B	622	MET
1	B	623	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	HIS
1	A	520	GLN
1	B	390	ASN
1	B	482	GLN
1	B	644	GLN
1	B	755	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
4	ALF	A	1002	-	4,4,4	1.41	0	-		
3	ADP	B	1001	5	28,29,29	1.41	4 (14%)	43,45,45	1.81	10 (23%)
3	ADP	A	1001	5	28,29,29	1.55	6 (21%)	43,45,45	1.70	9 (20%)
6	PO4	B	1004	-	4,4,4	0.92	0	6,6,6	0.54	0
4	ALF	B	1002	-	4,4,4	1.32	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
3	ADP	B	1001	5	-	1/16/32/32	0/3/3/3
3	ADP	A	1001	5	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ADP	C5-C4	4.88	1.47	1.39
3	B	1001	ADP	C5-C4	4.67	1.47	1.39
3	A	1001	ADP	PA-O3A	2.96	1.62	1.59
3	B	1001	ADP	C8-N7	2.63	1.36	1.31
3	A	1001	ADP	C5-C6	2.56	1.48	1.41
3	B	1001	ADP	C5-C6	2.54	1.48	1.41
3	A	1001	ADP	C4-N9	-2.41	1.32	1.37
3	A	1001	ADP	C5-N7	-2.40	1.34	1.39
3	A	1001	ADP	C8-N7	2.26	1.36	1.31
3	B	1001	ADP	C5-N7	-2.16	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	ADP	C5-C4-N3	-5.10	119.69	126.72
3	A	1001	ADP	C5-C4-N3	-5.00	119.83	126.72
3	A	1001	ADP	N3-C4-N9	4.39	134.63	127.17
3	B	1001	ADP	N3-C4-N9	4.19	134.29	127.17
3	B	1001	ADP	N3-C2-N1	-3.47	123.33	128.58
3	B	1001	ADP	C2-N3-C4	3.37	120.07	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ADP	C4-N9-C8	3.28	109.19	105.74
3	A	1001	ADP	C2-N3-C4	3.17	119.57	111.83
3	A	1001	ADP	N3-C2-N1	-3.16	123.81	128.58
3	B	1001	ADP	C4-C5-N7	-2.92	107.25	110.58
3	B	1001	ADP	C4-N9-C8	2.84	108.72	105.74
3	A	1001	ADP	C4-C5-N7	-2.82	107.36	110.58
3	A	1001	ADP	C2'-C1'-N9	-2.28	107.63	113.30
3	A	1001	ADP	C2-N1-C6	2.21	122.35	118.73
3	B	1001	ADP	C2-N1-C6	2.20	122.34	118.73
3	B	1001	ADP	C5-N7-C8	2.19	106.89	103.45
3	B	1001	ADP	O2B-PB-O1B	2.17	119.28	110.83
3	A	1001	ADP	C5-N7-C8	2.04	106.66	103.45
3	B	1001	ADP	O2A-PA-O1A	2.03	121.89	112.44

There are no chirality outliers.

All (3) torsion outliers are listed below:

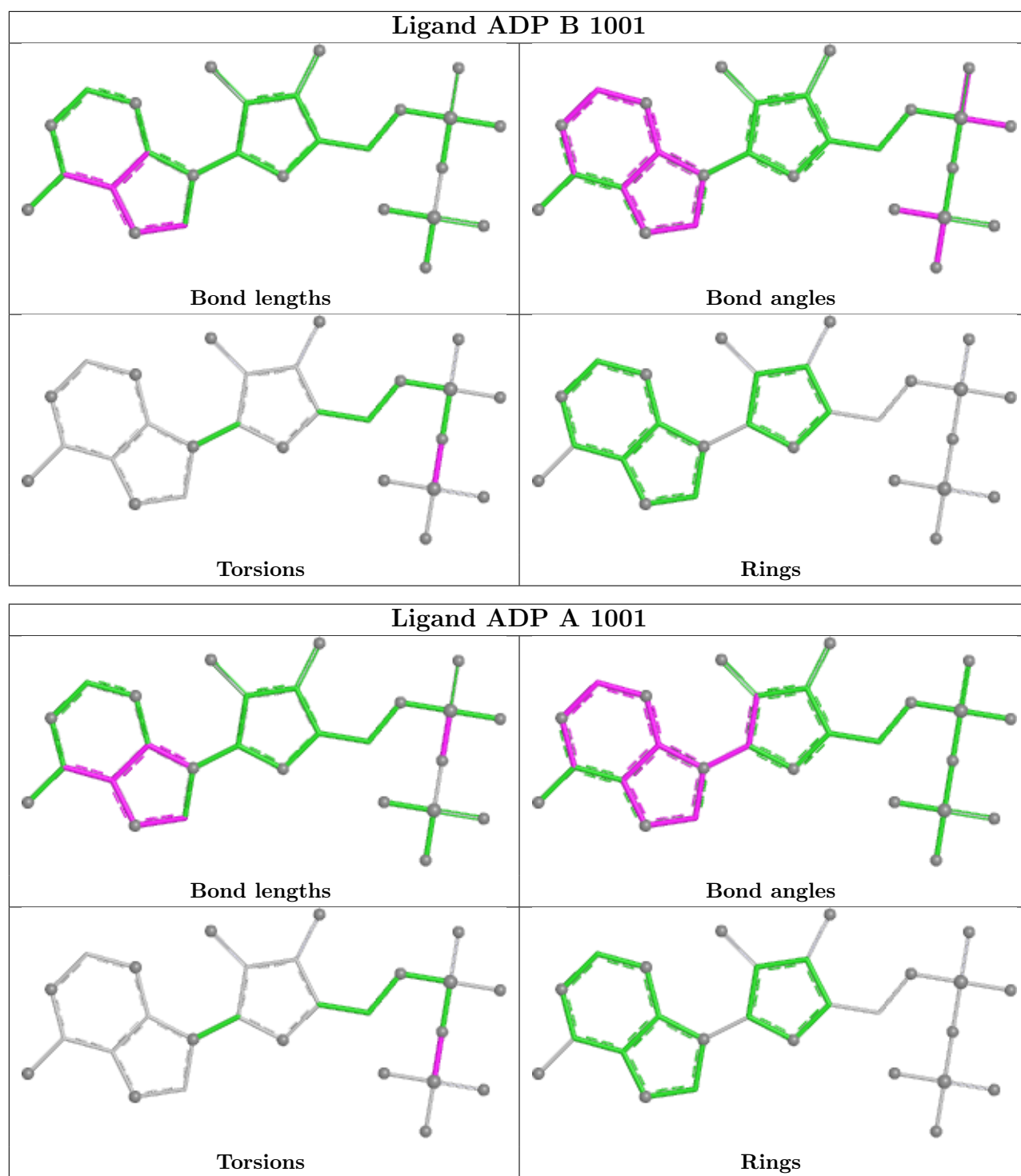
Mol	Chain	Res	Type	Atoms
3	B	1001	ADP	PA-O3A-PB-O3B
3	A	1001	ADP	PA-O3A-PB-O1B
3	A	1001	ADP	PA-O3A-PB-O3B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	ADP	3	0
3	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	528/545 (96%)	0.31	40 (7%) 20 19	23, 47, 94, 127	0
1	B	507/545 (93%)	0.54	56 (11%) 10 9	23, 54, 97, 143	0
2	C	6/8 (75%)	-0.17	0 100 100	36, 40, 52, 91	0
2	D	6/8 (75%)	-0.10	0 100 100	32, 37, 50, 94	0
All	All	1047/1106 (94%)	0.41	96 (9%) 14 13	23, 51, 97, 143	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	610	PRO	6.9
1	B	611	VAL	6.1
1	B	636	ILE	5.7
1	A	636	ILE	5.2
1	B	621	PHE	4.0
1	B	592	ALA	3.5
1	B	393	THR	3.5
1	B	558	PRO	3.4
1	B	237	LEU	3.3
1	B	477	SER	3.3
1	A	632	VAL	3.3
1	B	575	LEU	3.2
1	B	507	PHE	3.2
1	B	560	MET	3.1
1	B	392	PRO	3.1
1	B	510	PRO	3.0
1	B	670	MET	3.0
1	B	622	MET	3.0
1	B	583	GLN	3.0
1	B	391	ARG	3.0
1	A	453	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	591	VAL	3.0
1	B	501	GLU	2.9
1	A	605	SER	2.9
1	B	649	ASN	2.9
1	B	620	ASP	2.9
1	A	503	LEU	2.8
1	B	390	ASN	2.8
1	A	771	TYR	2.8
1	B	614	LEU	2.8
1	A	565	LEU	2.8
1	B	504	LEU	2.8
1	B	508	LEU	2.8
1	B	483	VAL	2.8
1	A	607	ILE	2.7
1	A	603	ALA	2.7
1	B	612	SER	2.7
1	A	624	ARG	2.6
1	A	555	THR	2.6
1	B	506	ASN	2.6
1	A	392	PRO	2.6
1	A	631	VAL	2.6
1	B	751	ILE	2.6
1	A	499	LEU	2.6
1	B	494	LEU	2.6
1	A	491	GLY	2.6
1	B	492	GLY	2.5
1	A	365	HIS	2.5
1	A	493	ALA	2.5
1	A	633	LEU	2.5
1	A	560	MET	2.5
1	A	680	ILE	2.5
1	A	466	MET	2.4
1	B	500	LYS	2.4
1	B	604	LYS	2.4
1	A	561	PRO	2.4
1	A	572	PRO	2.4
1	A	387	LYS	2.4
1	A	590	ALA	2.4
1	A	575	LEU	2.4
1	B	602	PHE	2.4
1	A	637	LYS	2.4
1	B	561	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	590	ALA	2.3
1	B	573	SER	2.3
1	A	570	GLU	2.3
1	B	509	ALA	2.3
1	A	480	PRO	2.3
1	B	347	ASP	2.3
1	A	434	GLY	2.3
1	B	481	GLY	2.3
1	B	762	LEU	2.3
1	B	568	TRP	2.3
1	B	419	ARG	2.2
1	A	569	ALA	2.2
1	A	435	ASN	2.2
1	B	591	VAL	2.2
1	B	616	SER	2.2
1	A	454	ASP	2.2
1	A	606	ASP	2.2
1	B	572	PRO	2.1
1	A	455	GLU	2.1
1	A	573	SER	2.1
1	B	320	LYS	2.1
1	B	603	ALA	2.1
1	B	650	SER	2.1
1	B	687	PRO	2.1
1	A	592	ALA	2.1
1	A	316	ASP	2.0
1	A	496	ASP	2.0
1	B	365	HIS	2.0
1	B	443	GLU	2.0
1	B	542	PHE	2.0
1	B	617	SER	2.0
1	B	581	ARG	2.0
1	B	555	THR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

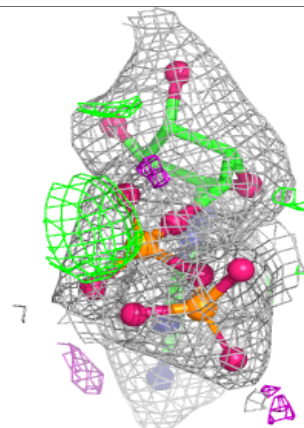
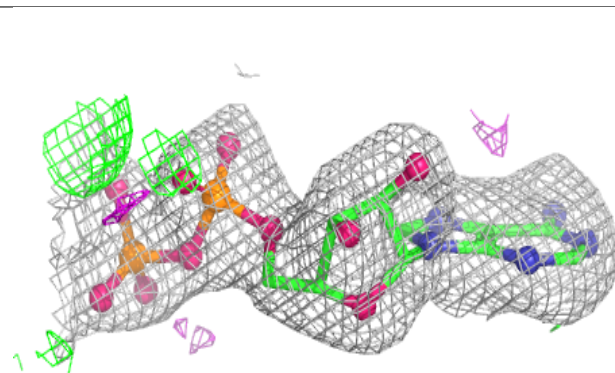
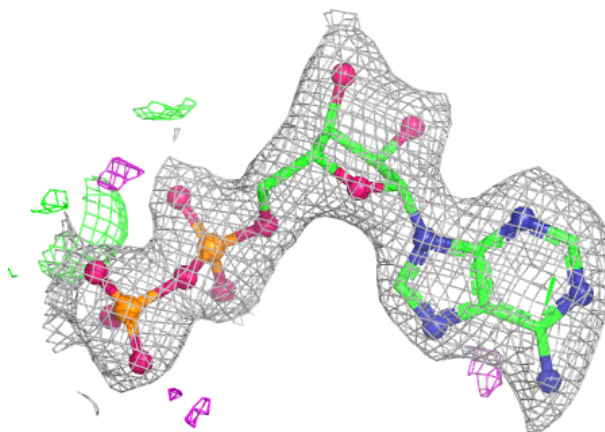
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	B	1004	5/5	0.91	0.12	65,66,69,72	0
5	MG	B	1003	1/1	0.95	0.05	30,30,30,30	0
3	ADP	B	1001	27/27	0.97	0.07	31,41,54,56	0
4	ALF	B	1002	5/5	0.97	0.07	29,29,32,32	0
3	ADP	A	1001	27/27	0.98	0.06	26,34,46,53	0
4	ALF	A	1002	5/5	0.99	0.04	27,29,31,31	0
5	MG	A	1003	1/1	0.99	0.02	26,26,26,26	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.

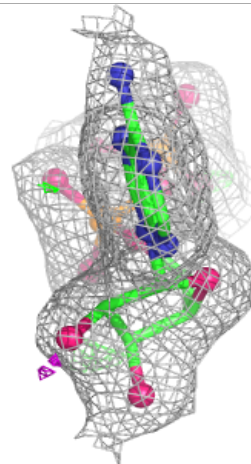
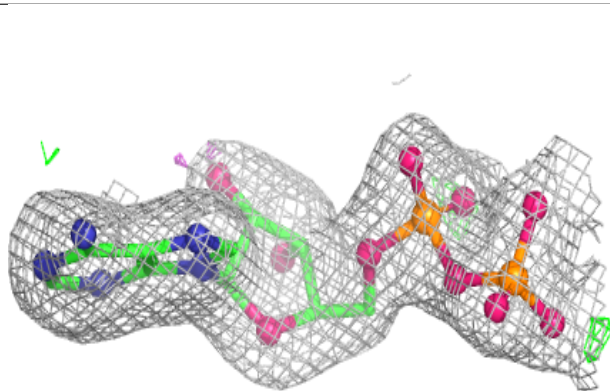
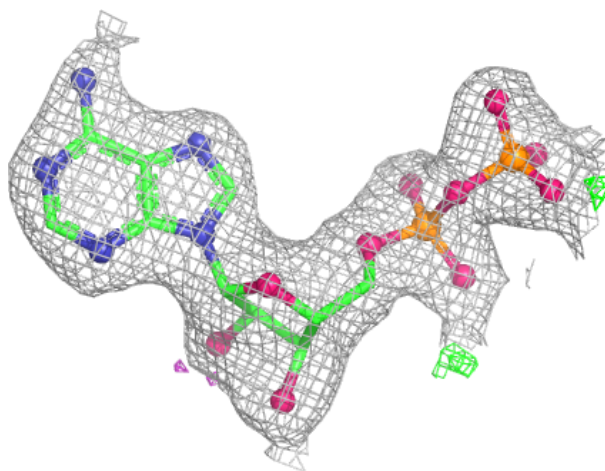
Electron density around ADP B 1001:

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.