Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 08:31 PM BST

PDB ID	:	5O6E
Title	:	Structure of ScPif1 in complex with TTTGGGTT and ADP-AlF4
Authors	:	Lu, K.Y.; Chen, W.F.; Rety, S.; Liu, N.N.; Xu, X.G.
Deposited on	:	2017-06-06
Resolution	:	3.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

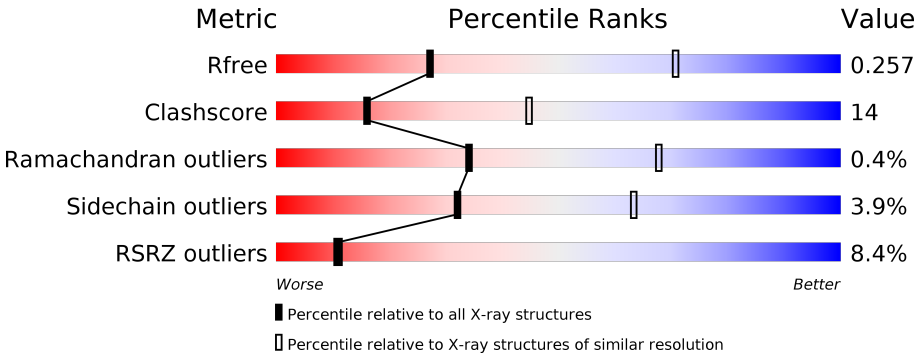
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 3.35 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6%, 64%, 29%, • 6%
1	B	545	10%, 61%, 29%, • 6%
2	C	7	57%, 29%, 14%
2	D	7	43%, 29%, 14%, 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8456 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	512	Total	C	N	O	S	0	0	0
			4081	2587	726	748	20			
1	B	513	Total	C	N	O	S	0	0	0
			4085	2592	724	749	20			

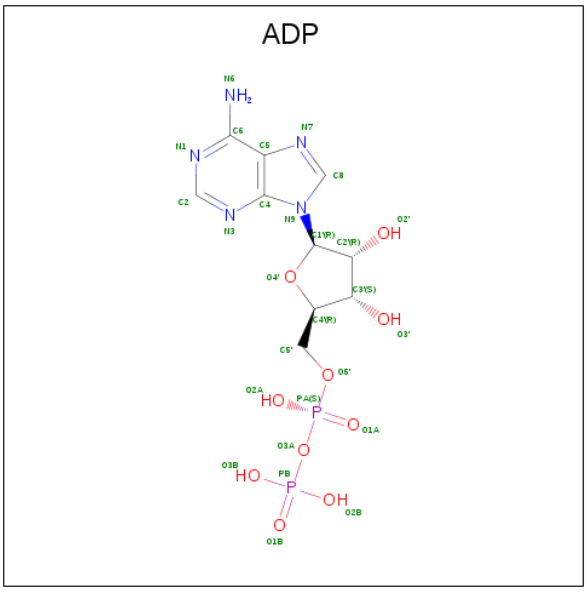
There are 2 discrepancies between the modelled and reference sequences:

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(*TP*TP*TP*GP*GP*T)-3').

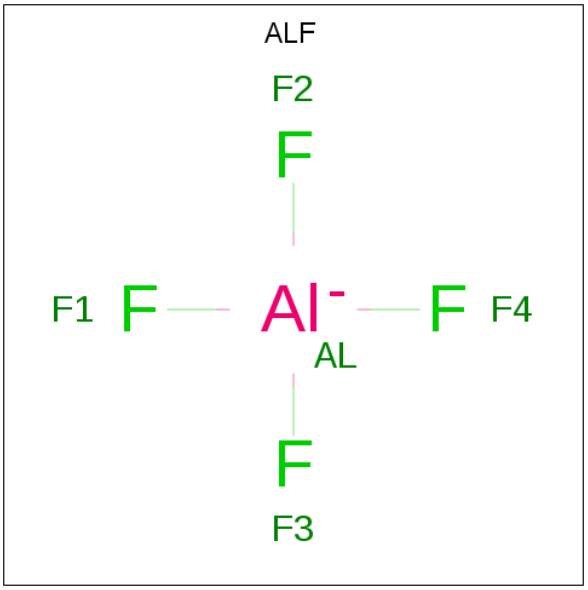
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			111	55	16	35	5			
2	D	6	Total	C	N	O	P	0	0	0
			112	55	16	36	5			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

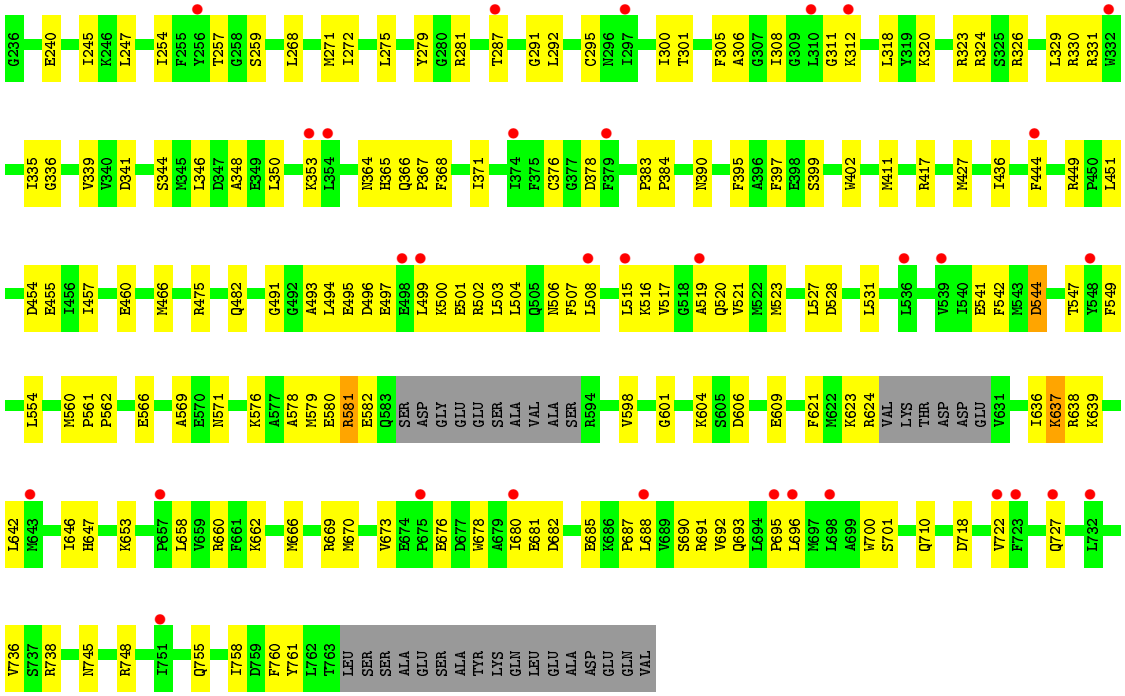
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

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.

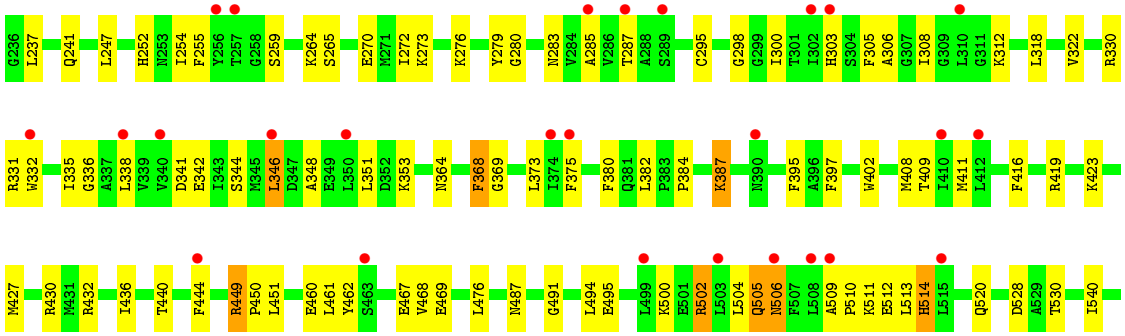
- Molecule 1: ATP-dependent DNA helicase PIF1

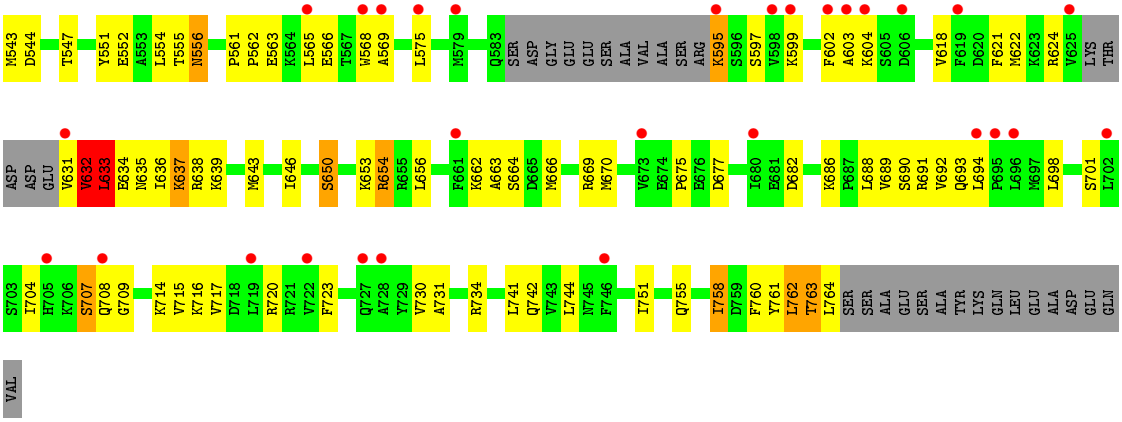
Chain A:



- Molecule 1: ATP-dependent DNA helicase PIF1

Chain B:





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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.60Å 150.60Å 136.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.21 – 3.35 130.43 – 3.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (65.21-3.35) 95.6 (130.43-3.34)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.178 , 0.257 0.182 , 0.257	Depositor DCC
R_{free} test set	1257 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	91.6	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 83.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: ALF, MG, ADP, CL

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	0.48	1/4150 (0.0%)	0.69	2/5573 (0.0%)
1	B	0.46	0/4154	0.72	3/5580 (0.1%)
2	C	1.46	0/123	1.44	4/188 (2.1%)
2	D	1.38	0/124	1.31	1/190 (0.5%)
All	All	0.53	1/8551 (0.0%)	0.74	10/11531 (0.1%)

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	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	CYS	CB-SG	-5.52	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	556	ASN	CB-CG-ND2	-13.68	83.88	116.70
1	B	556	ASN	CB-CG-OD1	8.69	138.98	121.60
2	C	3	DT	O5'-P-OP2	-6.89	99.50	105.70
2	C	3	DT	O4'-C1'-N1	5.94	112.16	108.00
1	A	508	LEU	CA-CB-CG	5.73	128.49	115.30
2	D	3	DT	O4'-C1'-N1	5.28	111.69	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	515	LEU	CA-CB-CG	5.25	127.38	115.30
2	C	3	DT	OP1-P-OP2	5.24	127.46	119.60
2	C	3	DT	C1'-O4'-C4'	-5.17	104.93	110.10
1	B	624	ARG	C-N-CA	-5.06	109.06	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	637	LYS	Peptide
1	B	505	GLN	Peptide
1	B	556	ASN	Sidechain

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	4081	0	4190	119	0
1	B	4085	0	4197	134	0
2	C	111	0	66	1	0
2	D	112	0	66	6	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
All	All	8456	0	8543	246	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 14.

All (246) 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:631:VAL:HG12	1:B:631:VAL:O	1.76	0.85
1:B:502:ARG:O	1:B:505:GLN:NE2	2.16	0.79
1:B:599:LYS:O	1:B:654:ARG:NH2	2.17	0.77
1:A:346:LEU:HD21	1:A:350:LEU:HD23	1.66	0.77
1:A:312:LYS:HE3	2:C:4:DG:H22	1.50	0.75
1:A:755:GLN:HA	1:A:758:ILE:HD12	1.67	0.74
1:A:494:LEU:HG	1:A:495:GLU:H	1.52	0.74
1:B:312:LYS:HE2	2:D:4:DG:H22	1.54	0.73
1:B:364:ASN:HB3	1:B:369:GLY:HA2	1.70	0.72
1:A:499:LEU:O	1:A:503:LEU:N	2.22	0.71
1:A:491:GLY:O	1:A:690:SER:N	2.24	0.71
1:A:502:ARG:HH21	1:B:502:ARG:HH22	1.38	0.71
1:A:578:ALA:O	1:A:581:ARG:NH2	2.23	0.70
1:A:499:LEU:HD23	1:A:502:ARG:NE	2.07	0.70
1:B:298:GLY:HA2	1:B:664:SER:HB3	1.73	0.69
1:A:364:ASN:OD1	1:A:365:HIS:N	2.27	0.68
1:B:561:PRO:HB2	1:B:563:GLU:HG2	1.75	0.68
1:B:312:LYS:HE2	2:D:4:DG:N2	2.09	0.68
1:B:436:ILE:HD13	1:B:751:ILE:HD13	1.75	0.67
1:B:704:ILE:HD13	1:B:731:ALA:HB2	1.76	0.67
1:A:722:VAL:HG12	1:A:727:GLN:HG2	1.78	0.66
1:A:311:GLY:HA2	1:A:318:LEU:HD21	1.78	0.65
1:A:760:PHE:HD2	1:A:761:TYR:HD1	1.44	0.65
1:B:682:ASP:HB3	1:B:688:LEU:HD11	1.80	0.64
1:B:704:ILE:HA	1:B:707:SER:HB3	1.79	0.64
1:B:544:ASP:OD1	1:B:547:THR:OG1	2.10	0.63
1:B:650:SER:HA	1:B:653:LYS:HD3	1.81	0.63
1:B:528:ASP:OD2	1:B:669:ARG:NH2	2.31	0.63
1:B:506:ASN:ND2	2:D:5:DG:O6	2.32	0.63
1:B:416:PHE:O	1:B:419:ARG:HB3	1.99	0.62
1:B:761:TYR:C	1:B:762:LEU:HG	2.19	0.62
1:B:279:TYR:CD1	1:B:336:GLY:HA3	2.35	0.62
1:B:633:LEU:O	1:B:633:LEU:HD12	2.00	0.62
1:A:718:ASP:OD1	1:A:745:ASN:ND2	2.34	0.61
1:B:562:PRO:HD3	1:B:636:ILE:HG13	1.83	0.61
1:A:427:MET:HE3	1:A:738:ARG:HD3	1.81	0.60
1:B:758:ILE:O	1:B:762:LEU:HD12	2.02	0.60
1:B:287:THR:HA	1:B:300:ILE:O	2.01	0.60
1:A:502:ARG:O	1:A:506:ASN:HB3	2.01	0.60
1:B:637:LYS:HD2	1:B:637:LYS:N	2.15	0.59
1:A:682:ASP:HB3	1:A:688:LEU:HD11	1.85	0.59
1:A:305:PHE:CE1	1:A:331:ARG:HG2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HA	1:A:329:LEU:HD13	1.85	0.59
1:B:397:PHE:HA	1:B:402:TRP:CG	2.37	0.59
1:A:501:GLU:HA	1:A:504:LEU:HB2	1.85	0.59
1:A:326:ARG:O	1:A:330:ARG:HG2	2.03	0.58
1:A:606:ASP:HB2	1:A:609:GLU:HG2	1.84	0.58
1:A:499:LEU:HD21	1:A:502:ARG:NH2	2.19	0.58
1:B:387:LYS:HZ3	2:D:4:DG:H22	1.52	0.58
1:B:487:ASN:HB2	1:B:604:LYS:HE3	1.85	0.57
1:B:494:LEU:HB2	1:B:688:LEU:O	2.04	0.57
1:B:569:ALA:HA	1:B:646:ILE:HG12	1.86	0.57
1:A:240:GLU:OE1	1:A:240:GLU:N	2.36	0.57
1:B:423:LYS:O	1:B:427:MET:HG3	2.04	0.57
1:A:306:ALA:HB3	1:A:308:ILE:HG12	1.87	0.56
1:B:512:GLU:HG2	1:B:514:HIS:HE1	1.70	0.56
1:B:368:PHE:CD1	1:B:373:LEU:HD11	2.40	0.56
1:B:631:VAL:CG1	1:B:631:VAL:O	2.49	0.56
1:A:566:GLU:HA	1:A:569:ALA:HB3	1.88	0.56
1:B:342:GLU:OE2	4:B:1002:ALF:F2	2.14	0.55
1:B:462:TYR:HB3	1:B:467:GLU:HB2	1.89	0.55
1:A:500:LYS:O	1:A:503:LEU:HB2	2.06	0.55
1:B:552:GLU:O	1:B:555:THR:OG1	2.21	0.55
1:B:603:ALA:HB3	1:B:654:ARG:HB2	1.88	0.55
1:A:502:ARG:NH1	1:B:312:LYS:NZ	2.56	0.54
1:B:491:GLY:O	1:B:690:SER:N	2.39	0.54
1:B:476:LEU:HD22	1:B:698:LEU:HD11	1.89	0.54
1:B:566:GLU:OE1	1:B:638:ARG:NH2	2.38	0.54
1:B:468:VAL:HG12	1:B:701:SER:HB3	1.88	0.54
1:A:502:ARG:HH11	1:B:312:LYS:NZ	2.06	0.54
1:B:259:SER:O	1:B:264:LYS:NZ	2.40	0.54
1:B:682:ASP:OD1	1:B:686:LYS:HB3	2.07	0.54
1:A:279:TYR:CD2	1:A:336:GLY:HA3	2.43	0.54
1:B:255:PHE:O	1:B:409:THR:HA	2.07	0.54
1:B:252:HIS:CE1	1:B:254:ILE:HG22	2.42	0.54
1:A:245:ILE:HD13	1:A:271:MET:HB2	1.89	0.53
1:A:519:ALA:HA	1:A:700:TRP:CZ2	2.43	0.53
1:A:581:ARG:HH22	1:A:582:GLU:HG2	1.74	0.53
1:B:636:ILE:O	1:B:639:LYS:HE2	2.09	0.53
1:A:320:LYS:O	1:A:324:ARG:HG3	2.09	0.53
1:A:308:ILE:HB	1:A:318:LEU:HD22	1.90	0.52
1:B:430:ARG:HD2	1:B:440:THR:OG1	2.09	0.52
1:B:751:ILE:HD12	1:B:751:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:MET:O	1:B:656:LEU:N	2.42	0.52
1:A:541:GLU:HG3	1:A:542:PHE:N	2.23	0.52
1:B:540:ILE:HG13	1:B:670:MET:SD	2.48	0.52
1:B:500:LYS:HG3	1:B:689:VAL:HG22	1.92	0.52
1:A:247:LEU:HD22	1:A:254:ILE:HG22	1.91	0.52
1:A:344:SER:O	1:A:384:PRO:HD3	2.10	0.52
1:A:517:VAL:HG22	1:A:541:GLU:HA	1.92	0.52
1:A:287:THR:HA	1:A:300:ILE:O	2.10	0.51
1:A:504:LEU:HA	1:A:507:PHE:HD2	1.74	0.51
1:B:494:LEU:HB3	1:B:500:LYS:HD3	1.92	0.51
1:B:322:VAL:HG11	1:B:332:TRP:CD1	2.46	0.51
1:B:555:THR:HA	1:B:621:PHE:CE1	2.44	0.51
1:A:549:PHE:CZ	1:A:579:MET:HA	2.45	0.51
1:B:380:PHE:HB3	1:B:432:ARG:HG3	1.92	0.51
1:B:568:TRP:CD1	1:B:575:LEU:HA	2.45	0.51
1:A:495:GLU:HG3	1:A:497:GLU:OE2	2.10	0.51
1:A:247:LEU:HD22	1:A:254:ILE:CG2	2.40	0.50
1:A:528:ASP:OD2	1:A:669:ARG:NH2	2.41	0.50
1:B:461:LEU:HD22	1:B:715:VAL:HG21	1.93	0.50
1:B:730:VAL:O	1:B:734:ARG:HG2	2.11	0.50
1:A:366:GLN:HB3	1:A:367:PRO:HD2	1.93	0.50
1:B:512:GLU:HG2	1:B:514:HIS:CE1	2.46	0.50
1:B:461:LEU:HB2	1:B:717:VAL:HG22	1.94	0.49
1:A:291:GLY:HA2	1:A:301:THR:HG22	1.93	0.49
1:A:681:GLU:HB2	1:A:685:GLU:HA	1.95	0.49
1:B:265:SER:OG	1:B:341:ASP:OD2	2.31	0.49
1:B:662:LYS:HD2	1:B:666:MET:SD	2.51	0.49
1:A:383:PRO:HB3	1:A:395:PHE:CE2	2.47	0.49
1:B:551:TYR:CE1	1:B:618:VAL:HG22	2.46	0.49
1:A:259:SER:HA	1:A:378:ASP:OD2	2.12	0.49
1:B:305:PHE:HA	1:B:331:ARG:NH1	2.28	0.49
1:A:390:ASN:ND2	1:B:469:GLU:OE2	2.44	0.49
1:A:499:LEU:CD2	1:A:502:ARG:NE	2.75	0.49
1:B:373:LEU:HD13	1:B:375:PHE:CZ	2.47	0.48
1:B:510:PRO:HG2	1:B:513:LEU:HB2	1.94	0.48
1:B:595:LYS:HD3	1:B:677:ASP:HB2	1.94	0.48
1:B:758:ILE:O	1:B:762:LEU:CD1	2.60	0.48
1:A:527:LEU:HD21	1:A:676:GLU:HG3	1.95	0.48
1:B:506:ASN:ND2	1:B:506:ASN:O	2.47	0.48
1:B:427:MET:HB3	1:B:440:THR:HG23	1.96	0.48
2:D:3:DT:H2'	2:D:4:DG:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PHE:HE1	1:A:331:ARG:HG2	1.79	0.47
1:A:581:ARG:NH2	1:A:582:GLU:HG2	2.29	0.47
1:A:662:LYS:HD3	1:A:666:MET:HE2	1.97	0.47
1:B:635:ASN:O	1:B:638:ARG:HB3	2.15	0.47
1:B:397:PHE:HA	1:B:402:TRP:CD2	2.50	0.47
1:A:681:GLU:O	1:B:495:GLU:HB2	2.14	0.47
1:B:308:ILE:HB	1:B:318:LEU:HD22	1.95	0.47
1:A:569:ALA:HA	1:A:646:ILE:HG12	1.97	0.47
1:A:517:VAL:CG2	1:A:541:GLU:HA	2.45	0.47
1:A:547:THR:HG21	1:A:647:HIS:CD2	2.50	0.46
1:B:348:ALA:HB2	1:B:395:PHE:O	2.15	0.46
1:A:601:GLY:HA2	1:A:604:LYS:HG3	1.97	0.46
1:B:716:LYS:HE3	1:B:744:LEU:HD11	1.97	0.46
1:A:305:PHE:HZ	1:A:335:ILE:HD13	1.80	0.46
1:B:530:THR:HB	1:B:663:ALA:HB1	1.98	0.46
1:A:436:ILE:HB	1:A:748:ARG:HD3	1.98	0.46
1:B:331:ARG:O	1:B:335:ILE:HG23	2.16	0.46
1:B:599:LYS:HB3	1:B:692:VAL:HG11	1.97	0.46
1:A:523:MET:HE3	1:A:531:LEU:HD11	1.98	0.45
1:A:500:LYS:O	1:A:500:LYS:HG2	2.15	0.45
1:A:678:TRP:HZ3	1:A:693:GLN:HB3	1.81	0.45
1:B:504:LEU:HD22	1:B:691:ARG:HB2	1.98	0.45
1:A:335:ILE:HD11	1:A:371:ILE:HD13	1.98	0.45
1:A:541:GLU:HG3	1:A:542:PHE:H	1.80	0.45
1:A:562:PRO:HG3	1:A:636:ILE:HG13	1.98	0.45
1:B:449:ARG:HB2	1:B:450:PRO:HD2	1.98	0.45
1:B:693:GLN:OE1	1:B:694:LEU:N	2.41	0.45
1:A:300:ILE:HD11	1:A:305:PHE:HB2	1.97	0.45
1:B:602:PHE:CE2	1:B:675:PRO:HB3	2.52	0.45
1:B:427:MET:HE2	1:B:427:MET:HB2	1.76	0.45
1:B:634:GLU:HB3	1:B:636:ILE:HG22	1.99	0.45
1:A:504:LEU:O	1:A:691:ARG:NH1	2.49	0.45
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.79	0.45
1:A:257:THR:HG23	1:A:411:MET:HG2	1.99	0.44
1:A:499:LEU:HD23	1:A:502:ARG:HE	1.80	0.44
1:A:500:LYS:O	1:A:504:LEU:HD12	2.17	0.44
1:B:504:LEU:HD21	1:B:689:VAL:HG12	1.98	0.44
1:A:554:LEU:HD22	1:A:621:PHE:CZ	2.52	0.44
1:B:270:GLU:HA	1:B:273:LYS:HD2	1.98	0.44
1:A:454:ASP:HB2	1:A:455:GLU:OE1	2.17	0.44
1:A:397:PHE:HA	1:A:402:TRP:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:PHE:HD2	1:A:761:TYR:CD1	2.31	0.44
1:B:387:LYS:NZ	2:D:4:DG:H22	2.14	0.44
1:A:502:ARG:HH11	1:B:312:LYS:HZ2	1.64	0.44
1:B:451:LEU:HD13	1:B:714:LYS:HG3	2.00	0.44
1:A:623:LYS:HE2	1:A:623:LYS:HB2	1.72	0.44
1:A:364:ASN:O	1:A:365:HIS:ND1	2.51	0.44
1:A:544:ASP:OD2	1:A:653:LYS:HD2	2.18	0.44
1:B:382:LEU:HB2	1:B:708:GLN:OE1	2.18	0.44
1:A:547:THR:HG21	1:A:647:HIS:HD2	1.83	0.43
1:B:638:ARG:HH11	1:B:638:ARG:HG3	1.82	0.43
1:B:509:ALA:O	1:B:691:ARG:NH1	2.50	0.43
1:A:624:ARG:HA	1:A:624:ARG:HD3	1.83	0.43
1:A:427:MET:HB3	1:A:444:PHE:CE2	2.53	0.43
1:B:709:GLY:H	1:B:734:ARG:NH1	2.15	0.43
1:A:460:GLU:O	1:A:701:SER:HA	2.19	0.43
1:A:673:VAL:HG12	1:A:695:PRO:HD2	1.99	0.43
1:B:636:ILE:HG12	1:B:639:LYS:HE2	2.00	0.43
1:A:348:ALA:HB1	1:A:399:SER:HB3	2.00	0.43
1:B:427:MET:HE3	1:B:444:PHE:CZ	2.53	0.43
1:B:554:LEU:HD22	1:B:621:PHE:CZ	2.54	0.43
1:B:500:LYS:HG3	1:B:689:VAL:HG13	2.00	0.43
1:A:493:ALA:HB2	1:A:688:LEU:HA	2.01	0.43
1:A:502:ARG:NH1	1:B:312:LYS:HZ1	2.17	0.43
1:A:560:MET:HG3	1:A:561:PRO:HD2	2.01	0.43
1:B:427:MET:HA	1:B:430:ARG:HG2	2.01	0.43
1:A:275:LEU:O	1:A:279:TYR:HD1	2.02	0.42
1:A:502:ARG:NH1	1:B:312:LYS:HZ2	2.16	0.42
1:B:723:PHE:CD1	1:B:723:PHE:N	2.86	0.42
1:A:341:ASP:HA	1:A:376:CYS:HB3	2.01	0.42
1:B:272:ILE:HG22	1:B:276:LYS:HE3	2.00	0.42
1:B:285:ALA:HB3	1:B:338:LEU:HD12	2.02	0.42
1:B:449:ARG:O	1:B:742:GLN:HG3	2.19	0.42
1:A:676:GLU:HG2	1:A:695:PRO:HG3	2.01	0.42
1:B:451:LEU:HD23	1:B:451:LEU:HA	1.70	0.42
1:B:462:TYR:HB2	1:B:468:VAL:HG13	2.01	0.42
1:B:528:ASP:CG	1:B:669:ARG:HH22	2.22	0.42
1:A:554:LEU:HD22	1:A:621:PHE:HZ	1.85	0.42
1:A:680:ILE:HG13	1:A:680:ILE:H	1.72	0.42
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.74	0.42
1:B:318:LEU:HD12	1:B:353:LYS:HD3	2.01	0.42
1:A:254:ILE:HG21	1:A:254:ILE:HD13	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD12	1:A:353:LYS:HD3	2.00	0.42
1:A:417:ARG:O	1:A:736:VAL:HG13	2.20	0.42
1:A:576:LYS:O	1:A:580:GLU:HG2	2.19	0.42
1:A:658:LEU:HD11	1:A:670:MET:HE3	2.02	0.42
1:B:280:GLY:HA3	1:B:283:ASN:HD22	1.85	0.41
1:B:638:ARG:HG3	1:B:638:ARG:NH1	2.34	0.41
1:B:254:ILE:HD13	1:B:254:ILE:HG21	1.71	0.41
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.81	0.41
1:A:542:PHE:N	1:A:542:PHE:CD1	2.88	0.41
1:B:715:VAL:O	1:B:741:LEU:HD12	2.19	0.41
1:B:662:LYS:HB3	1:B:662:LYS:HE2	1.92	0.41
1:B:755:GLN:HA	1:B:758:ILE:HD12	2.03	0.41
1:A:482:GLN:O	1:A:516:LYS:HG2	2.20	0.41
1:B:306:ALA:HB3	1:B:308:ILE:HG12	2.02	0.41
1:B:427:MET:HE3	1:B:444:PHE:CE2	2.55	0.41
1:B:554:LEU:HD21	1:B:622:MET:SD	2.60	0.41
1:A:499:LEU:HA	1:A:502:ARG:HB2	2.03	0.41
1:A:292:LEU:HG	1:A:710:GLN:OE1	2.21	0.41
1:B:760:PHE:O	1:B:763:THR:HA	2.20	0.41
1:A:521:VAL:HG21	1:A:696:LEU:HD22	2.03	0.41
1:A:673:VAL:HG11	1:A:696:LEU:HD11	2.02	0.41
1:B:237:LEU:HD22	1:B:241:GLN:HB2	2.03	0.41
1:A:581:ARG:O	1:A:581:ARG:HG2	2.21	0.41
1:B:460:GLU:HB3	1:B:462:TYR:CE2	2.56	0.41
1:A:499:LEU:HD21	1:A:502:ARG:HH21	1.83	0.40
1:B:632:VAL:HG12	1:B:633:LEU:HD23	2.02	0.40
1:A:457:ILE:HD11	1:A:475:ARG:HG2	2.04	0.40
1:A:493:ALA:HB2	1:A:687:PRO:O	2.21	0.40
1:B:344:SER:O	1:B:384:PRO:HD3	2.20	0.40
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.82	0.40
1:A:272:ILE:HD11	1:A:339:VAL:HG11	2.02	0.40
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.77	0.40
1:A:501:GLU:OE2	1:A:501:GLU:N	2.54	0.40
1:B:247:LEU:HD21	1:B:408:MET:SD	2.62	0.40
1:B:551:TYR:HB2	1:B:643:MET:HE1	2.01	0.40
1:A:598:VAL:HG12	1:A:692:VAL:HG21	2.03	0.40
1:B:565:LEU:HD12	1:B:639:LYS:HG2	2.03	0.40
1:A:638:ARG:HE	1:A:638:ARG:HB3	1.70	0.40
1:A:639:LYS:HA	1:A:642:LEU:HD12	2.04	0.40
1:B:554:LEU:HD22	1:B:621:PHE:HZ	1.86	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	506/545 (93%)	484 (96%)	22 (4%)	0	100 100
1	B	507/545 (93%)	483 (95%)	20 (4%)	4 (1%)	19 53
All	All	1013/1090 (93%)	967 (96%)	42 (4%)	4 (0%)	34 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	633	LEU
1	B	763	THR
1	B	758	ILE
1	B	632	VAL

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	446/473 (94%)	435 (98%)	11 (2%)	47 74
1	B	447/473 (94%)	423 (95%)	24 (5%)	22 55
All	All	893/946 (94%)	858 (96%)	35 (4%)	32 63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	A	368	PHE

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Mol	Chain	Res	Type
1	A	449	ARG
1	A	466	MET
1	A	496	ASP
1	A	520	GLN
1	A	544	ASP
1	A	571	ASN
1	A	581	ARG
1	A	637	LYS
1	A	660	ARG
1	B	295	CYS
1	B	303	HIS
1	B	330	ARG
1	B	346	LEU
1	B	368	PHE
1	B	387	LYS
1	B	411	MET
1	B	449	ARG
1	B	502	ARG
1	B	506	ASN
1	B	511	LYS
1	B	514	HIS
1	B	520	GLN
1	B	595	LYS
1	B	597	SER
1	B	632	VAL
1	B	633	LEU
1	B	637	LYS
1	B	650	SER
1	B	654	ARG
1	B	707	SER
1	B	720	ARG
1	B	762	LEU
1	B	764	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	745	ASN
1	B	506	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
3	ADP	B	1001	5	24,29,29	0.99	1 (4%)	29,45,45	1.60	4 (13%)
4	ALF	A	1002	-	0,4,4	0.00	-	-		
3	ADP	A	1001	5	24,29,29	1.04	1 (4%)	29,45,45	1.86	9 (31%)
4	ALF	B	1002	-	0,4,4	0.00	-	-		

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	-	1/12/32/32	0/3/3/3
3	ADP	A	1001	5	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ADP	C5-C4	2.38	1.47	1.40
3	B	1001	ADP	C5-C4	2.15	1.46	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	ADP	C3'-C2'-C1'	4.42	107.63	100.98
3	A	1001	ADP	C4-C5-N7	-3.93	105.30	109.40
3	B	1001	ADP	C4-C5-N7	-3.91	105.33	109.40
3	B	1001	ADP	C3'-C2'-C1'	3.56	106.33	100.98
3	B	1001	ADP	O3B-PB-O3A	-3.35	93.41	104.64
3	A	1001	ADP	O3A-PB-O1B	-3.00	94.56	111.19
3	B	1001	ADP	N3-C2-N1	-2.82	124.28	128.68
3	A	1001	ADP	N3-C2-N1	-2.80	124.30	128.68
3	A	1001	ADP	C5-C6-N6	2.52	124.17	120.35
3	A	1001	ADP	PA-O3A-PB	-2.44	124.44	132.83
3	A	1001	ADP	O3B-PB-O3A	2.31	112.39	104.64
3	A	1001	ADP	O2'-C2'-C3'	-2.30	104.38	111.82
3	A	1001	ADP	C5'-C4'-C3'	-2.19	106.96	115.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	ADP	PA-O3A-PB-O2B
3	A	1001	ADP	PA-O3A-PB-O2B
3	A	1001	ADP	PA-O3A-PB-O3B
3	A	1001	ADP	C5'-O5'-PA-O3A
3	A	1001	ADP	PA-O3A-PB-O1B

There are no ring outliers.

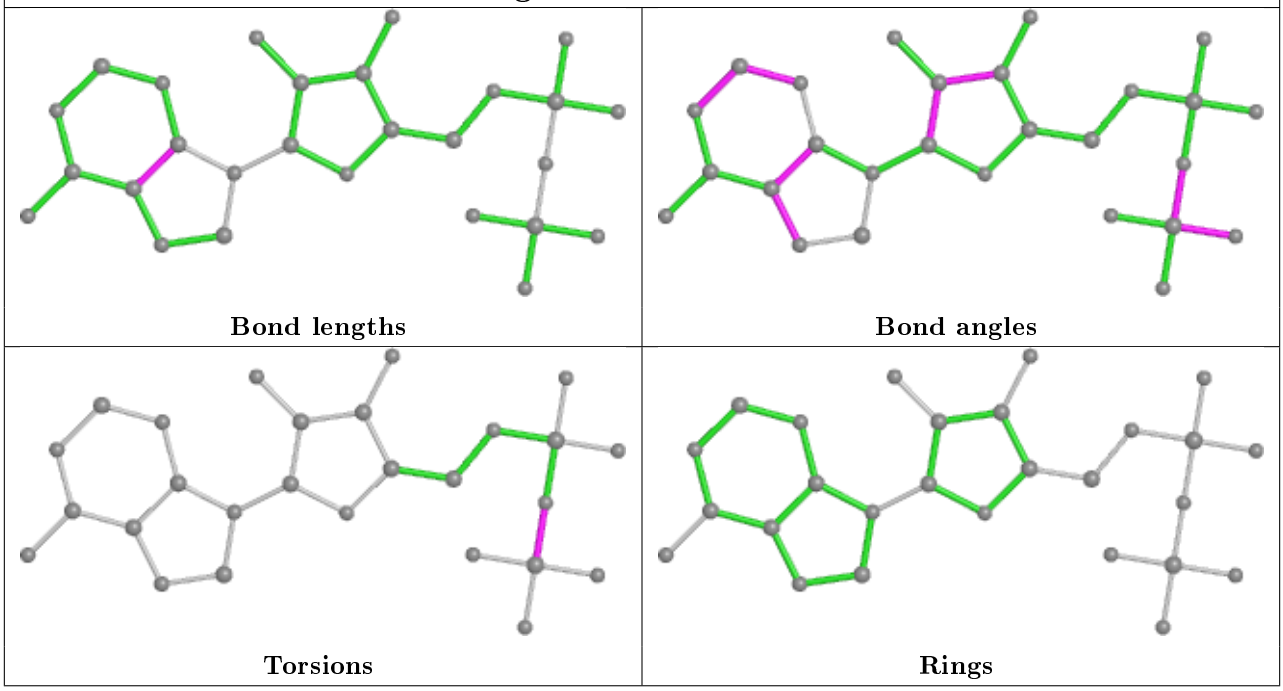
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	ALF	1	0

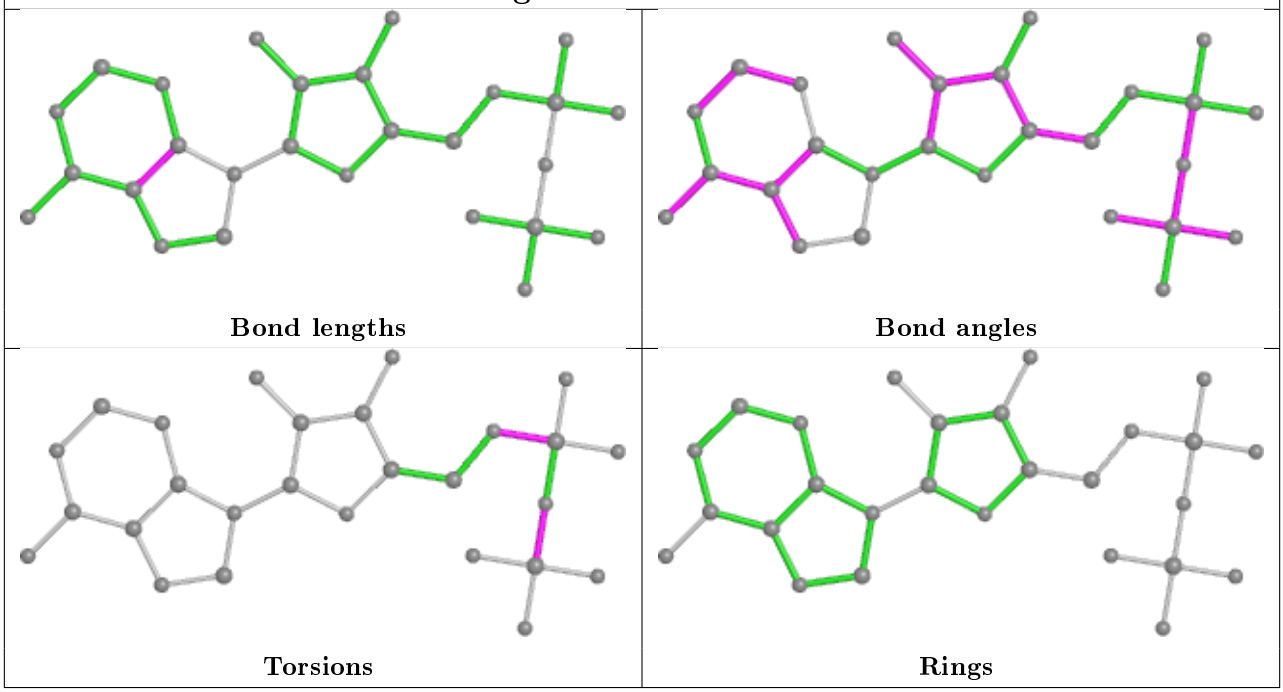
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1001



Ligand ADP A 1001



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, 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	512/545 (93%)	0.59	32 (6%) 20 21	61, 102, 175, 207	0
1	B	513/545 (94%)	0.72	55 (10%) 6 6	30, 108, 192, 223	0
2	C	6/7 (85%)	0.57	0 100 100	98, 111, 126, 129	0
2	D	6/7 (85%)	0.59	0 100 100	104, 118, 171, 179	0
All	All	1037/1104 (93%)	0.65	87 (8%) 11 11	30, 106, 184, 223	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	598	VAL	7.7
1	B	565	LEU	6.3
1	B	599	LYS	6.2
1	B	595	LYS	6.1
1	B	602	PHE	6.0
1	A	498	GLU	5.1
1	B	631	VAL	4.1
1	A	680	ILE	4.1
1	B	506	ASN	4.0
1	B	575	LEU	3.9
1	A	727	GLN	3.8
1	A	499	LEU	3.6
1	B	603	ALA	3.3
1	B	289	SER	3.2
1	B	568	TRP	3.2
1	B	680	ILE	3.2
1	A	310	LEU	3.2
1	A	643	MET	3.1
1	B	661	PHE	3.0
1	B	508	LEU	3.0
1	B	515	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	285	ALA	2.7
1	A	732	LEU	2.7
1	B	625	VAL	2.7
1	B	310	LEU	2.7
1	B	604	LYS	2.7
1	B	374	ILE	2.7
1	B	390	ASN	2.6
1	A	379	PHE	2.6
1	B	503	LEU	2.6
1	A	751	ILE	2.5
1	A	519	ALA	2.5
1	A	722	VAL	2.5
1	B	673	VAL	2.5
1	B	338	LEU	2.5
1	B	332	TRP	2.5
1	A	696	LEU	2.5
1	B	705	HIS	2.5
1	B	444	PHE	2.5
1	B	606	ASP	2.5
1	B	350	LEU	2.4
1	A	312	LYS	2.4
1	B	256	TYR	2.4
1	A	675	PRO	2.4
1	B	509	ALA	2.4
1	B	340	VAL	2.4
1	B	694	LEU	2.4
1	B	719	LEU	2.4
1	B	410	ILE	2.4
1	B	412	LEU	2.4
1	B	579	MET	2.3
1	B	303	HIS	2.3
1	A	354	LEU	2.3
1	B	746	PHE	2.3
1	B	708	GLN	2.3
1	B	619	PHE	2.3
1	A	297	ILE	2.3
1	B	463	SER	2.3
1	A	287	THR	2.2
1	B	695	PRO	2.2
1	A	688	LEU	2.2
1	A	695	PRO	2.2
1	B	346	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	332	TRP	2.2
1	A	256	TYR	2.2
1	B	499	LEU	2.2
1	A	515	LEU	2.2
1	A	508	LEU	2.2
1	A	548	TYR	2.2
1	A	723	PHE	2.2
1	B	287	THR	2.2
1	B	727	GLN	2.2
1	A	657	PRO	2.2
1	B	728	ALA	2.1
1	B	257	THR	2.1
1	A	536	LEU	2.1
1	A	698	LEU	2.1
1	B	696	LEU	2.1
1	A	444	PHE	2.0
1	B	569	ALA	2.0
1	B	722	VAL	2.0
1	B	375	PHE	2.0
1	A	539	VAL	2.0
1	A	374	ILE	2.0
1	B	302	ILE	2.0
1	B	702	LEU	2.0
1	A	353	LYS	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)

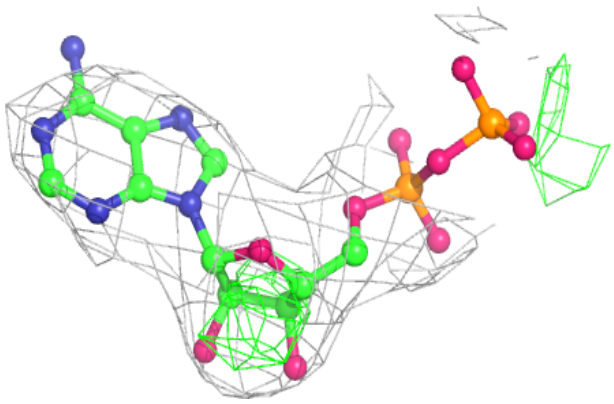
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

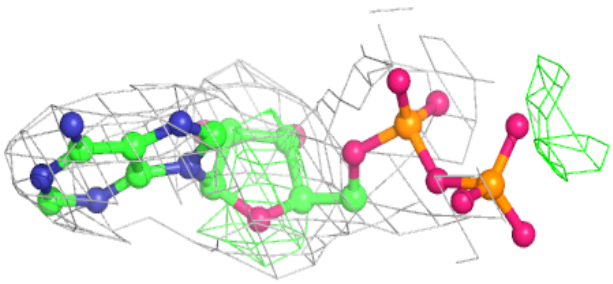
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	B	1001	27/27	0.96	0.27	69,96,111,121	0
5	MG	A	1003	1/1	0.97	0.29	74,74,74,74	0
6	CL	A	1004	1/1	0.97	0.31	49,49,49,49	1
5	MG	B	1003	1/1	0.97	0.21	68,68,68,68	0
4	ALF	B	1002	5/5	0.98	0.22	57,66,67,80	0
3	ADP	A	1001	27/27	0.98	0.28	69,98,114,117	0
4	ALF	A	1002	5/5	0.99	0.26	66,78,82,91	0

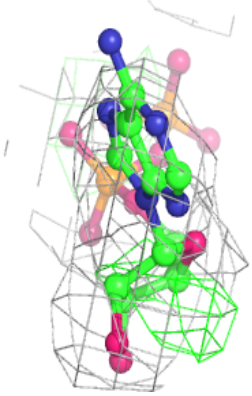
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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)

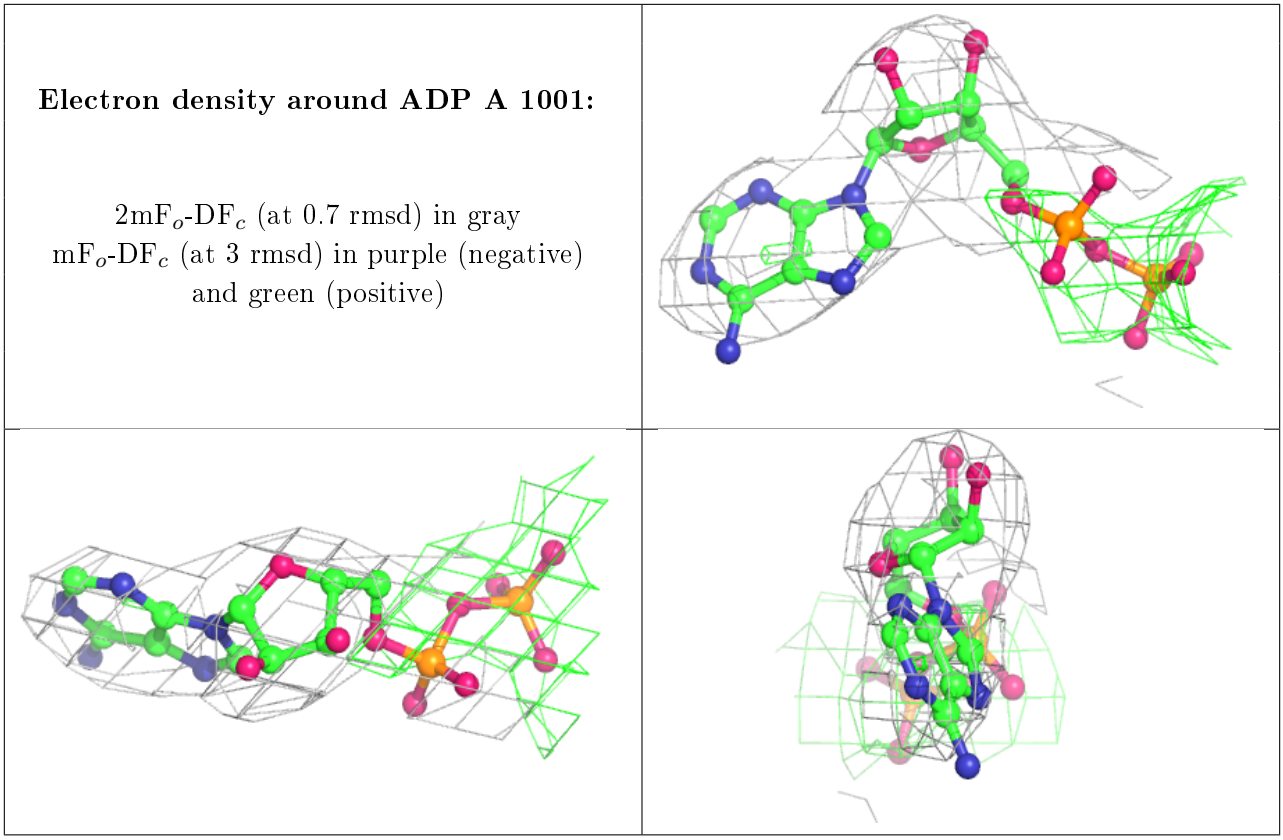






Electron density around ADP A 1001:

$2mF_o$-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

There are no such residues in this entry.