Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2022 – 02:14 PM JST

PDB ID	:	7WBT
Title	:	Crystal structure of bovine NLRP9
Authors	:	Kamitsukasa, Y.; Shimizu, T.; Ohto, U.
Deposited on	:	2021-12-17
Resolution	:	2.75 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:

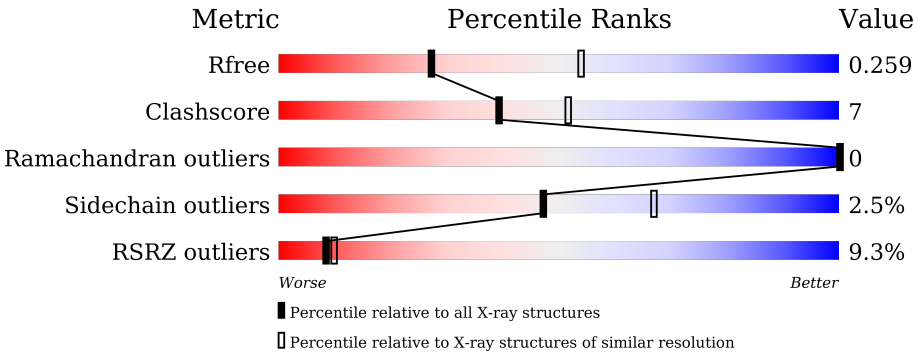
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	912	8% 80% 17% ••
1	B	912	10% 79% 18% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14366 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.

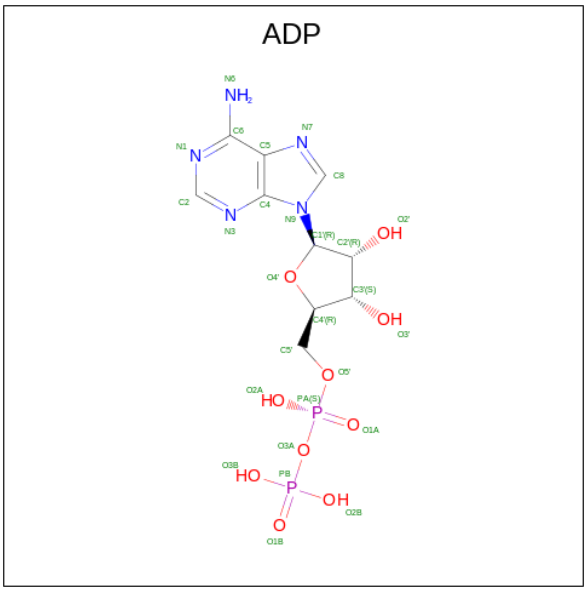
- Molecule 1 is a protein called NACHT, LRR and PYD domains-containing protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	0	0	0
			7156	4555	1185	1339	77			
1	B	899	Total	C	N	O	S	0	0	0
			7156	4555	1185	1339	77			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLY	-	expression tag	UNP Q288C4
A	86	PRO	-	expression tag	UNP Q288C4
A	87	GLU	-	expression tag	UNP Q288C4
A	88	PHE	-	expression tag	UNP Q288C4
B	85	GLY	-	expression tag	UNP Q288C4
B	86	PRO	-	expression tag	UNP Q288C4
B	87	GLU	-	expression tag	UNP Q288C4
B	88	PHE	-	expression tag	UNP Q288C4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

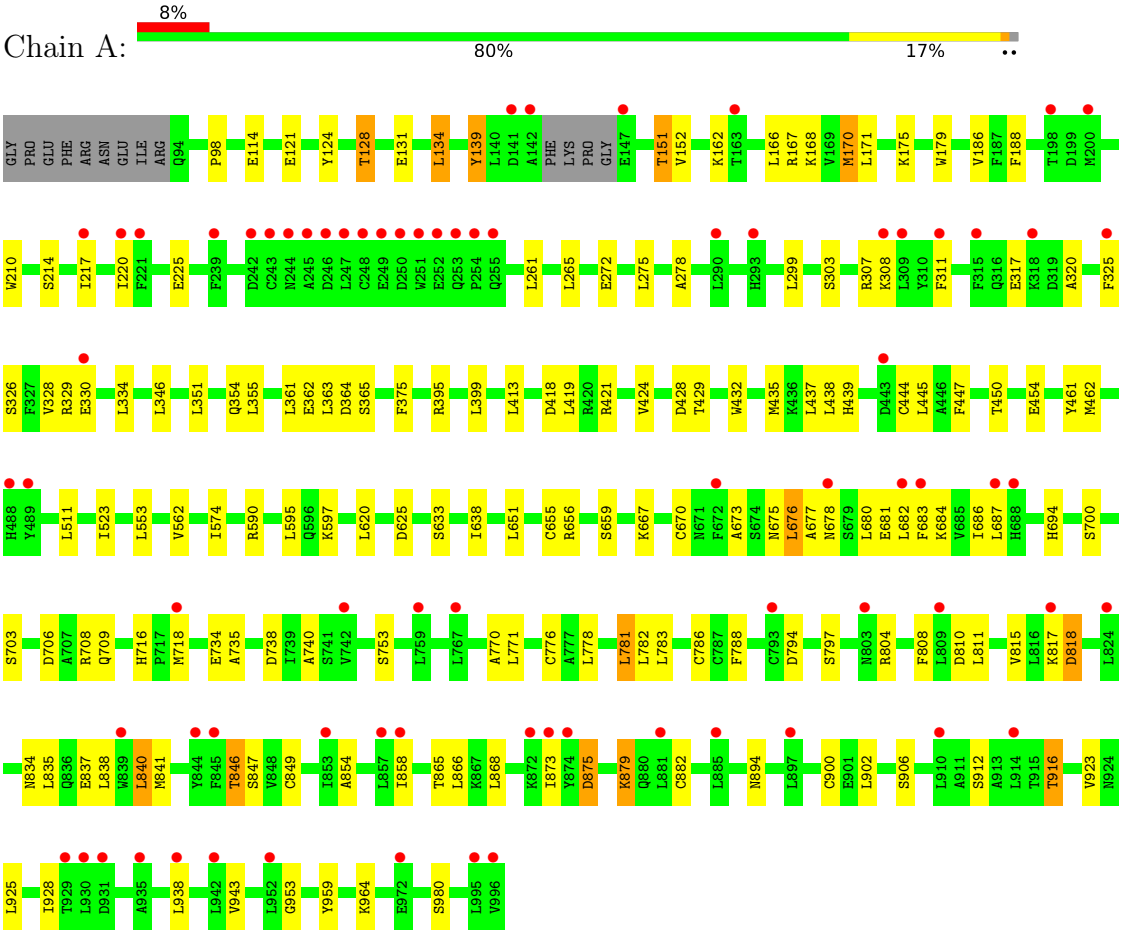


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

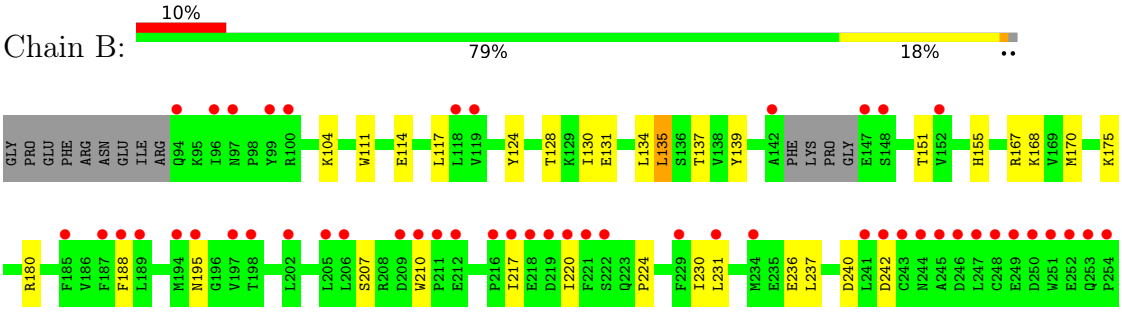
3 Residue-property plots (i)

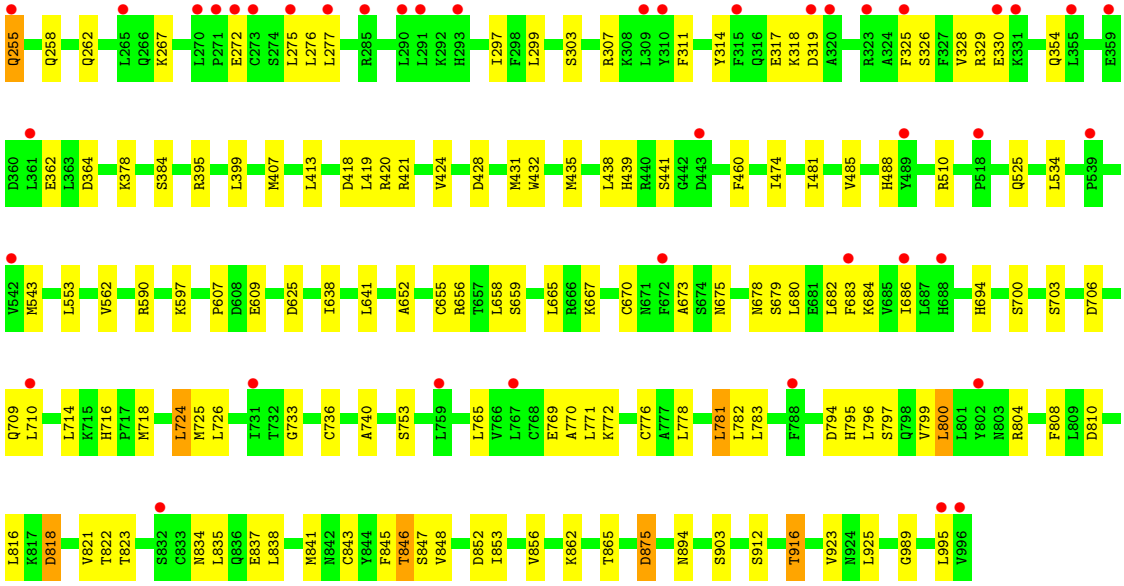
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NACHT, LRR and PYD domains-containing protein 9



• Molecule 1: NACHT, LRR and PYD domains-containing protein 9




Q255 Q258 Q262 L265 Q266 K267 L270 P271 E272 C273 S274 L275 L276 L277 R285 L290 L291 K292 H293 I297 F298 L299 S303 R307 K308 L309 Y310 F311 Y314 F315 Q316 E317 K318 D319 A320 R323 A324 F325 S326 F327 V328 R329 E330 K331 Q354 L355 E359
D360 L361 E362 L363 D364 K378 S384 R395 L399 M407 L413 D418 L419 R420 R421 V424 D428 M431 W432 M435 L438 H439 R440 S441 G442 D443 F460 I474 I481 V485 H488 Y489 R510 P518 Q525 L534 P539
V542 M543 L553 V562 R590 K597 P607 D608 E609 D625 I638 L641 A652 C655 R656 T657 L658 S659 L665 R666 K667 C670 N671 F672 A673 S674 N675 N678 S679 L680 E681 L682 F683 K684 V685 I686 L687 H688 H694 S700 S703 D706
Q709 L710 L714 K715 H716 P717 M718 L724 M725 L726 I731 T732 G733 C736 A740 S753 L759 L765 V766 L767 C768 E769 A770 L771 K772 C776 A777 L778 L781 L782 L783 F788 D794 H795 L796 S797 Q798 V799 L800 L801 Y802 N803 R804 F808 L809 D810
L816 K817 D818 V821 T822 T823 S832 C833 N834 L835 Q836 E837 L838 M841 N842 C843 Y844 F845 T846 S847 V848 D852 I853 V856 K862 T865 D875 N894 S903 S912 T916 V923 N924 L925 G989 L995 V996

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.26Å 169.12Å 177.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.75 49.14 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.14-2.75) 96.0 (49.14-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.262 0.230 , 0.259	Depositor DCC
R_{free} test set	4021 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	88.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14366	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.31	0/7303	0.52	0/9870
1	B	0.30	0/7303	0.51	0/9870
All	All	0.31	0/14606	0.52	0/19740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7156	0	7116	112	0
1	B	7156	0	7116	103	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
All	All	14366	0	14256	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (212) 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:837:GLU:HG3	1:B:865:THR:HB	1.56	0.87
1:A:114:GLU:HG2	1:A:167:ARG:HH12	1.45	0.81
1:B:590:ARG:NH1	1:B:625:ASP:OD2	2.12	0.80
1:B:912:SER:O	1:B:916:THR:OG1	2.02	0.76
1:A:651:LEU:HD22	1:A:678:ASN:HD22	1.56	0.71
1:A:837:GLU:HG3	1:A:865:THR:HB	1.73	0.70
1:B:117:LEU:HD22	1:B:314:TYR:HD1	1.57	0.69
1:B:675:ASN:H	1:B:678:ASN:HB2	1.57	0.69
1:B:242:ASP:O	1:B:262:GLN:NE2	2.26	0.68
1:A:334:LEU:HD13	1:A:365:SER:HB3	1.75	0.67
1:B:597:LYS:HG3	1:B:638:ILE:HB	1.76	0.66
1:A:121:GLU:OE2	1:A:168:LYS:NZ	2.29	0.66
1:B:418:ASP:OD1	1:B:421:ARG:NH2	2.28	0.66
1:B:432:TRP:HB3	1:B:438:LEU:HD13	1.77	0.66
1:A:651:LEU:CD2	1:A:678:ASN:HD22	2.08	0.66
1:A:912:SER:O	1:A:916:THR:OG1	2.13	0.66
1:B:740:ALA:HB1	1:B:770:ALA:HB2	1.79	0.65
1:A:835:LEU:HD21	1:A:838:LEU:HD13	1.79	0.65
1:A:114:GLU:HG2	1:A:167:ARG:NH1	2.12	0.64
1:B:804:ARG:HA	1:B:834:ASN:HD22	1.62	0.63
1:A:597:LYS:HG3	1:A:638:ILE:HB	1.79	0.63
1:A:675:ASN:H	1:A:678:ASN:HB2	1.64	0.63
1:A:590:ARG:NH1	1:A:625:ASP:OD2	2.32	0.62
1:A:778:LEU:HD21	1:A:781:LEU:HG	1.82	0.62
1:B:364:ASP:OD2	1:B:510:ARG:NH2	2.33	0.61
1:A:354:GLN:NE2	1:A:362:GLU:O	2.29	0.60
1:A:217:ILE:O	1:A:220:ILE:HG13	2.02	0.60
1:A:418:ASP:OD1	1:A:421:ARG:NH2	2.36	0.59
1:B:317:GLU:OE1	1:B:319:ASP:N	2.35	0.59
1:B:655:CYS:O	1:B:659:SER:OG	2.18	0.59
1:B:846:THR:OG1	1:B:847:SER:N	2.36	0.59
1:B:835:LEU:HD21	1:B:838:LEU:HD13	1.84	0.58
1:A:435:MET:HG3	1:A:437:LEU:HD23	1.86	0.58
1:B:683:PHE:HE2	1:B:709:GLN:HB3	1.67	0.58
1:A:419:LEU:HB3	1:A:424:VAL:HB	1.86	0.58
1:B:317:GLU:OE1	1:B:318:LYS:N	2.37	0.57
1:A:651:LEU:HD22	1:A:678:ASN:ND2	2.19	0.56
1:B:778:LEU:HD21	1:B:781:LEU:HG	1.87	0.56
1:A:846:THR:OG1	1:A:847:SER:N	2.38	0.56
1:B:131:GLU:HG2	1:B:299:LEU:HD23	1.88	0.56
1:B:771:LEU:HD11	1:B:781:LEU:HD12	1.86	0.56
1:A:740:ALA:HB1	1:A:770:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:VAL:HG13	1:B:432:TRP:HZ3	1.71	0.55
1:A:673:ALA:H	1:A:700:SER:HB3	1.72	0.55
1:A:676:LEU:HD12	1:A:677:ALA:H	1.72	0.54
1:B:231:LEU:HB2	1:B:277:LEU:HD23	1.88	0.54
1:A:162:LYS:NZ	2:A:1001:ADP:O2B	2.37	0.54
1:B:311:PHE:HE2	1:B:328:VAL:HG11	1.73	0.54
1:B:675:ASN:O	1:B:679:SER:OG	2.16	0.54
1:A:210:TRP:HH2	1:A:220:ILE:HG21	1.72	0.54
1:A:225:GLU:HG3	1:A:272:GLU:HB3	1.89	0.53
1:B:384:SER:OG	1:B:431:MET:SD	2.67	0.53
1:A:782:LEU:HG	1:A:808:PHE:HE2	1.74	0.53
1:B:875:ASP:OD2	1:B:903:SER:OG	2.16	0.52
1:B:170:MET:HE2	1:B:188:PHE:HD2	1.74	0.52
1:A:716:HIS:CD2	1:A:718:MET:HB2	2.44	0.52
1:A:225:GLU:CG	1:A:272:GLU:HB3	2.40	0.52
1:A:953:GLY:HA2	1:A:980:SER:O	2.10	0.52
1:B:135:LEU:HG	1:B:297:ILE:HD12	1.92	0.52
1:B:207:SER:HA	1:B:210:TRP:HB3	1.91	0.52
1:A:326:SER:O	1:A:330:GLU:HG3	2.11	0.51
1:A:667:LYS:HG3	1:A:694:HIS:CD2	2.45	0.51
1:B:796:LEU:O	1:B:800:LEU:HD22	2.10	0.51
1:B:667:LYS:HG3	1:B:694:HIS:CD2	2.46	0.51
1:A:873:ILE:HG12	1:A:900:CYS:HB3	1.92	0.50
1:B:217:ILE:O	1:B:220:ILE:HG13	2.12	0.50
1:A:128:THR:O	1:A:128:THR:OG1	2.27	0.50
1:B:865:THR:HG23	1:B:894:ASN:HB2	1.93	0.50
1:A:655:CYS:O	1:A:659:SER:OG	2.25	0.49
1:A:716:HIS:HD2	1:A:718:MET:HB2	1.77	0.49
1:A:781:LEU:HD13	1:A:783:LEU:HD21	1.94	0.49
1:B:420:ARG:NH1	1:B:424:VAL:O	2.45	0.49
1:B:354:GLN:NE2	1:B:378:LYS:HE3	2.27	0.49
1:B:765:LEU:HG	1:B:795:HIS:CD2	2.47	0.49
1:A:131:GLU:HG2	1:A:299:LEU:HD23	1.94	0.49
1:A:134:LEU:HD11	1:B:652:ALA:HB1	1.95	0.49
1:B:432:TRP:HA	1:B:435:MET:HG2	1.94	0.49
1:A:687:LEU:HG	1:A:716:HIS:CD2	2.48	0.49
1:B:428:ASP:HB3	1:B:432:TRP:CZ3	2.48	0.49
1:B:771:LEU:HD23	1:B:776:CYS:SG	2.52	0.49
1:B:781:LEU:HD13	1:B:783:LEU:HD21	1.95	0.49
1:B:989:GLY:HA3	1:B:995:LEU:HD13	1.94	0.49
1:A:656:ARG:NH2	1:B:137:THR:OG1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:ALA:H	1:B:700:SER:HB3	1.77	0.49
1:B:797:SER:OG	1:B:823:THR:HG22	2.13	0.48
1:A:438:LEU:HD23	1:A:447:PHE:HA	1.96	0.48
1:B:853:ILE:O	1:B:856:VAL:HG22	2.13	0.48
1:B:395:ARG:NE	1:B:428:ASP:OD1	2.47	0.48
1:B:419:LEU:HB3	1:B:424:VAL:HB	1.95	0.48
1:A:395:ARG:NE	1:A:428:ASP:OD1	2.47	0.48
1:A:124:TYR:O	1:A:128:THR:HG23	2.14	0.48
1:A:670:CYS:SG	1:A:673:ALA:HB3	2.54	0.48
1:A:873:ILE:HD11	1:A:902:LEU:HD21	1.96	0.48
1:A:838:LEU:HG	1:A:840:LEU:HD22	1.95	0.47
1:B:195:ASN:ND2	1:B:236:GLU:O	2.45	0.47
1:B:399:LEU:HD11	1:B:438:LEU:HD11	1.96	0.47
1:A:683:PHE:HE2	1:A:709:GLN:HB3	1.79	0.47
1:A:838:LEU:HB3	1:A:866:LEU:HD23	1.96	0.47
1:B:303:SER:O	1:B:307:ARG:HG3	2.14	0.47
1:B:680:LEU:O	1:B:684:LYS:HG2	2.14	0.47
1:A:171:LEU:HD13	1:A:175:LYS:HE2	1.96	0.47
1:B:354:GLN:NE2	1:B:362:GLU:O	2.46	0.47
1:B:656:ARG:HA	1:B:656:ARG:HD3	1.65	0.47
1:A:462:MET:HE1	1:A:523:ILE:HD12	1.96	0.47
1:B:808:PHE:CD1	1:B:837:GLU:HB3	2.49	0.47
1:B:808:PHE:HD1	1:B:837:GLU:HB3	1.78	0.47
1:A:928:ILE:O	1:A:959:TYR:OH	2.27	0.47
1:A:771:LEU:HD23	1:A:776:CYS:SG	2.54	0.47
1:A:804:ARG:HA	1:A:834:ASN:HD22	1.80	0.47
1:B:710:LEU:O	1:B:714:LEU:HG	2.15	0.47
1:B:683:PHE:CE2	1:B:709:GLN:HB3	2.49	0.46
1:A:680:LEU:O	1:A:684:LYS:HG2	2.14	0.46
1:A:875:ASP:HB3	1:A:879:LYS:HZ3	1.79	0.46
1:B:311:PHE:CE2	1:B:328:VAL:HG11	2.50	0.46
1:A:428:ASP:HB3	1:A:432:TRP:CZ3	2.50	0.46
1:B:104:LYS:HE2	1:B:175:LYS:HD2	1.98	0.46
1:B:111:TRP:CZ3	1:B:168:LYS:HB2	2.51	0.46
1:B:670:CYS:SG	1:B:673:ALA:HB3	2.55	0.46
1:B:395:ARG:HD3	1:B:431:MET:HE1	1.98	0.46
1:B:753:SER:HB2	1:B:782:LEU:HD13	1.98	0.46
1:B:834:ASN:OD1	1:B:862:LYS:NZ	2.34	0.46
1:A:656:ARG:HB3	1:B:130:ILE:HD12	1.98	0.45
1:A:435:MET:HG3	1:A:437:LEU:CD2	2.47	0.45
1:A:923:VAL:HG12	1:A:925:LEU:HG	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TYR:HD2	1:A:179:TRP:CZ2	2.35	0.45
1:B:923:VAL:HG12	1:B:925:LEU:HG	1.99	0.45
1:A:334:LEU:HD12	1:A:334:LEU:HA	1.87	0.45
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.79	0.45
1:A:363:LEU:HD13	1:A:364:ASP:N	2.32	0.45
1:A:317:GLU:OE2	1:A:320:ALA:HB3	2.18	0.44
1:A:432:TRP:HA	1:A:435:MET:HG2	1.99	0.44
1:A:818:ASP:HB3	1:A:849:CYS:HB3	1.98	0.44
1:B:317:GLU:H	1:B:317:GLU:HG3	1.65	0.44
1:B:326:SER:O	1:B:330:GLU:HG3	2.17	0.44
1:B:816:LEU:HD22	1:B:843:CYS:SG	2.58	0.44
1:A:703:SER:H	1:A:706:ASP:HB2	1.83	0.44
1:B:195:ASN:HD21	1:B:237:LEU:HA	1.83	0.44
1:B:553:LEU:HB3	1:B:562:VAL:HG22	2.00	0.44
1:B:733:GLY:O	1:B:736:CYS:HB2	2.18	0.44
1:B:821:VAL:HG21	1:B:845:PHE:CD2	2.53	0.44
1:A:450:THR:O	1:A:454:GLU:HG3	2.16	0.44
1:A:462:MET:HE1	1:A:523:ILE:CD1	2.48	0.44
1:B:124:TYR:O	1:B:128:THR:HG22	2.17	0.44
1:B:794:ASP:O	1:B:797:SER:HB2	2.18	0.44
1:B:822:THR:HG22	1:B:852:ASP:OD2	2.18	0.44
1:A:265:LEU:HD23	1:A:275:LEU:HD13	2.00	0.43
1:A:753:SER:HB2	1:A:782:LEU:HD13	2.00	0.43
1:A:943:VAL:HG12	1:A:943:VAL:O	2.17	0.43
1:A:413:LEU:HD22	1:A:444:CYS:HB2	1.99	0.43
1:B:796:LEU:O	1:B:799:VAL:HB	2.19	0.43
1:A:682:LEU:O	1:A:686:ILE:HG13	2.18	0.43
1:A:794:ASP:O	1:A:797:SER:HB2	2.18	0.43
1:B:682:LEU:O	1:B:686:ILE:HG13	2.19	0.43
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.85	0.43
1:A:399:LEU:HB2	1:A:432:TRP:CH2	2.54	0.43
1:A:308:LYS:HG3	1:A:325:PHE:CZ	2.53	0.43
1:A:461:TYR:O	1:A:523:ILE:HD11	2.19	0.43
1:B:224:PRO:HB2	1:B:272:GLU:HB2	2.00	0.43
1:A:151:THR:HB	1:A:275:LEU:HB2	2.01	0.43
1:A:311:PHE:CE2	1:A:328:VAL:HG11	2.53	0.43
1:A:655:CYS:SG	1:A:681:GLU:HB3	2.58	0.43
1:B:325:PHE:HA	1:B:328:VAL:HG12	2.00	0.42
1:B:658:LEU:HD22	1:B:665:LEU:HD22	2.00	0.42
1:A:595:LEU:N	1:A:633:SER:OG	2.52	0.42
1:B:488:HIS:NE2	1:B:543:MET:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:GLU:OE2	1:B:772:LYS:NZ	2.50	0.42
1:A:166:LEU:HD11	1:A:278:ALA:HB2	2.02	0.42
1:A:865:THR:HG23	1:A:894:ASN:HB2	2.00	0.42
1:B:818:ASP:OD2	1:B:848:VAL:HB	2.19	0.42
1:A:346:LEU:HD22	1:A:375:PHE:CD1	2.54	0.42
1:A:429:THR:HG23	1:A:445:LEU:HD11	2.02	0.42
1:B:114:GLU:HG2	1:B:167:ARG:HH12	1.84	0.42
1:B:413:LEU:HD21	1:B:441:SER:HB3	2.00	0.42
1:A:782:LEU:HA	1:A:810:ASP:HB3	2.02	0.42
1:A:854:ALA:O	1:A:858:ILE:HG13	2.20	0.42
1:B:724:LEU:HD13	1:B:726:LEU:HD21	2.02	0.42
1:A:651:LEU:HD21	1:A:678:ASN:HA	2.01	0.42
1:B:258:GLN:O	1:B:262:GLN:HG2	2.19	0.42
1:B:267:LYS:HA	1:B:267:LYS:HD2	1.90	0.42
1:B:460:PHE:CE2	1:B:474:ILE:HG21	2.55	0.42
1:B:716:HIS:ND1	1:B:718:MET:HB2	2.33	0.42
1:A:303:SER:O	1:A:307:ARG:HG3	2.20	0.42
1:A:553:LEU:HB3	1:A:562:VAL:HG22	2.02	0.42
1:A:131:GLU:OE1	1:A:131:GLU:N	2.41	0.41
1:B:114:GLU:OE2	1:B:439:HIS:NE2	2.48	0.41
1:A:346:LEU:HD22	1:A:375:PHE:CG	2.54	0.41
1:A:786:CYS:HB2	1:A:788:PHE:CE1	2.55	0.41
1:A:170:MET:SD	1:A:188:PHE:HB2	2.59	0.41
1:A:959:TYR:O	1:A:964:LYS:NZ	2.52	0.41
1:B:255:GLN:HE21	1:B:255:GLN:HB2	1.53	0.41
1:B:607:PRO:HB2	1:B:609:GLU:HG2	2.02	0.41
1:A:708:ARG:HG3	1:A:738:ASP:OD2	2.20	0.41
1:A:170:MET:HE1	1:A:186:VAL:O	2.20	0.41
1:B:782:LEU:HA	1:B:810:ASP:HB3	2.03	0.41
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.91	0.41
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.90	0.41
1:A:574:ILE:HD12	1:A:574:ILE:HA	1.91	0.41
1:A:675:ASN:ND2	1:A:678:ASN:OD1	2.54	0.41
1:A:938:LEU:HD12	1:A:938:LEU:HA	1.94	0.41
1:B:151:THR:HG23	1:B:275:LEU:HB2	2.02	0.41
1:B:534:LEU:HA	1:B:534:LEU:HD23	1.81	0.41
1:B:703:SER:H	1:B:706:ASP:HB2	1.86	0.41
1:A:815:VAL:HG13	1:A:817:LYS:HE2	2.03	0.41
1:A:351:LEU:HD12	1:A:361:LEU:HD22	2.02	0.40
1:A:734:GLU:HG2	1:A:735:ALA:N	2.36	0.40
1:A:98:PRO:HG2	1:A:214:SER:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PHE:HA	1:A:328:VAL:HG12	2.04	0.40
1:A:424:VAL:HG13	1:A:432:TRP:HZ3	1.86	0.40
1:B:114:GLU:HG2	1:B:167:ARG:NH1	2.37	0.40
1:B:230:ILE:HG12	1:B:276:LEU:HD23	2.02	0.40
1:A:879:LYS:HE3	1:A:906:SER:HA	2.03	0.40
1:B:481:ILE:O	1:B:485:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	895/912 (98%)	866 (97%)	29 (3%)	0	100	100
1	B	895/912 (98%)	866 (97%)	29 (3%)	0	100	100
All	All	1790/1824 (98%)	1732 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	821/832 (99%)	800 (97%)	21 (3%)	46	66
1	B	821/832 (99%)	801 (98%)	20 (2%)	49	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1642/1664 (99%)	1601 (98%)	41 (2%)	47 67

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	THR
1	A	134	LEU
1	A	139	TYR
1	A	151	THR
1	A	152	VAL
1	A	170	MET
1	A	329	ARG
1	A	439	HIS
1	A	620	LEU
1	A	676	LEU
1	A	781	LEU
1	A	811	LEU
1	A	818	ASP
1	A	840	LEU
1	A	841	MET
1	A	846	THR
1	A	868	LEU
1	A	875	ASP
1	A	879	LYS
1	A	882	CYS
1	A	916	THR
1	B	134	LEU
1	B	135	LEU
1	B	139	TYR
1	B	155	HIS
1	B	180	ARG
1	B	240	ASP
1	B	255	GLN
1	B	329	ARG
1	B	407	MET
1	B	525	GLN
1	B	641	LEU
1	B	724	LEU
1	B	725	MET
1	B	781	LEU
1	B	800	LEU
1	B	818	ASP

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Mol	Chain	Res	Type
1	B	841	MET
1	B	846	THR
1	B	875	ASP
1	B	916	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	262	GLN
1	A	675	ASN
1	A	678	ASN
1	A	716	HIS
1	A	836	GLN
1	B	675	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	A	1001	-	24,29,29	0.99	1 (4%)	29,45,45	1.56	7 (24%)
2	ADP	B	1001	-	24,29,29	0.98	1 (4%)	29,45,45	1.54	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	B	1001	-	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	2.62	1.47	1.40
2	B	1001	ADP	C5-C4	2.47	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	ADP	PA-O3A-PB	-4.35	117.89	132.83
2	A	1001	ADP	C3'-C2'-C1'	3.71	106.56	100.98
2	B	1001	ADP	C3'-C2'-C1'	3.52	106.27	100.98
2	B	1001	ADP	N3-C2-N1	-3.02	123.96	128.68
2	A	1001	ADP	N3-C2-N1	-2.99	124.00	128.68
2	A	1001	ADP	PA-O3A-PB	-2.53	124.15	132.83
2	A	1001	ADP	O2A-PA-O1A	2.38	123.99	112.24
2	B	1001	ADP	C4-C5-N7	-2.21	107.09	109.40
2	A	1001	ADP	O3B-PB-O2B	2.21	116.08	107.64
2	A	1001	ADP	C4-C5-N7	-2.11	107.20	109.40
2	A	1001	ADP	N6-C6-N1	2.10	122.93	118.57

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	PB-O3A-PA-O1A
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	B	1001	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	O4'-C4'-C5'-O5'
2	B	1001	ADP	C5'-O5'-PA-O1A

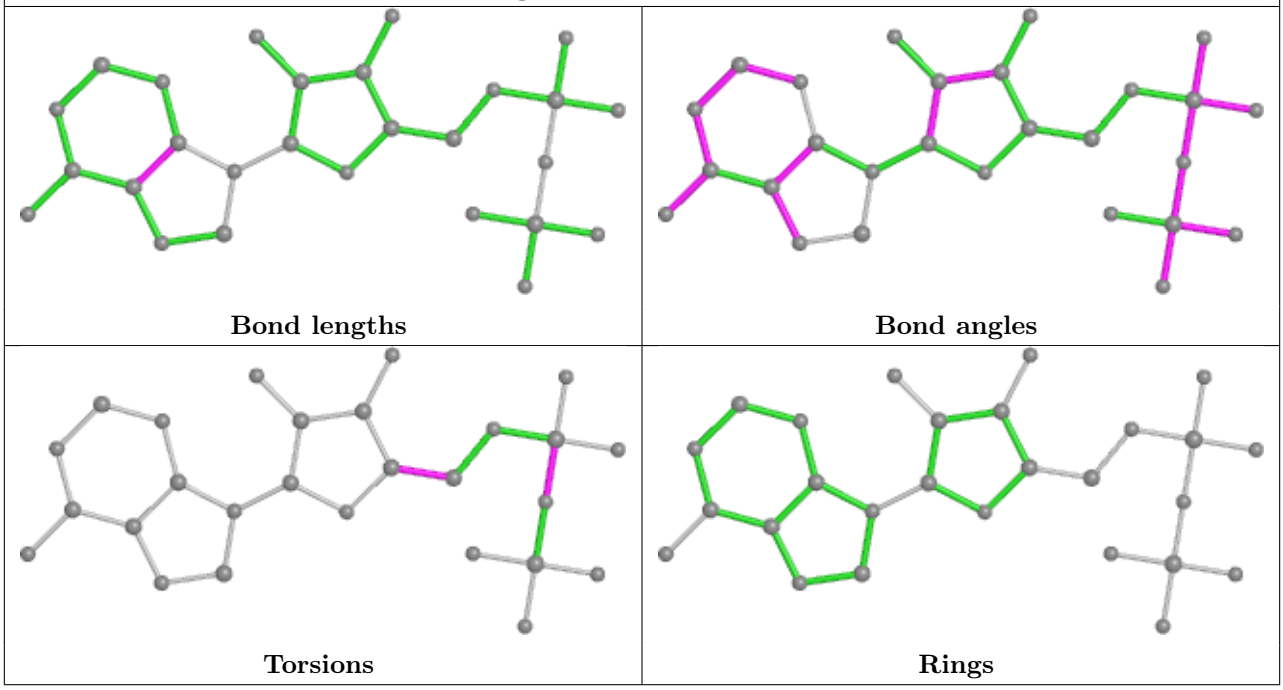
There are no ring outliers.

1 monomer is involved in 1 short contact:

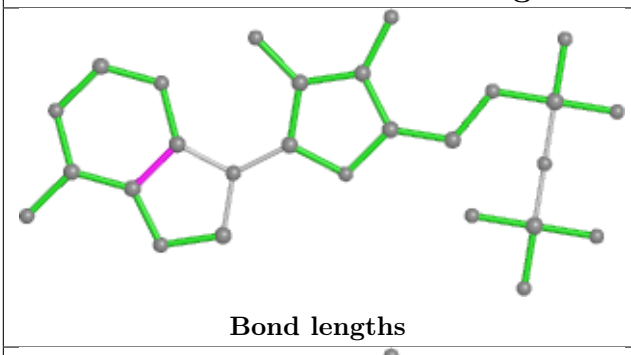
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

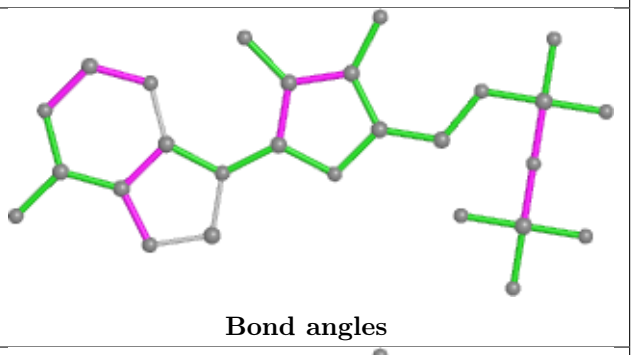
Ligand ADP A 1001



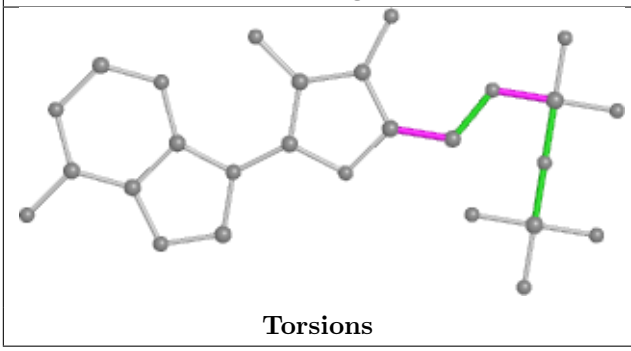
Ligand ADP B 1001



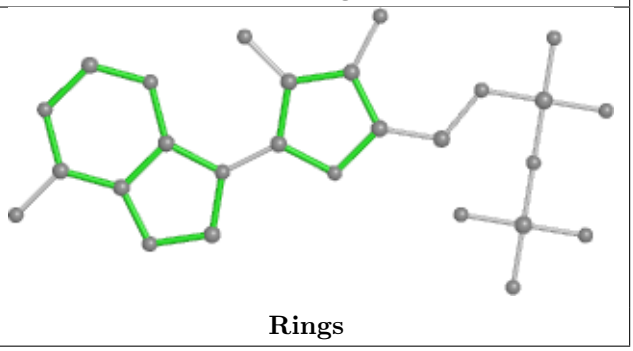
Bond lengths



Bond angles



Torsions



Rings

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	899/912 (98%)	0.58	75 (8%) 11 13	54, 111, 166, 258	0
1	B	899/912 (98%)	0.68	92 (10%) 6 7	61, 110, 205, 276	0
All	All	1798/1824 (98%)	0.63	167 (9%) 8 10	54, 111, 189, 276	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	9.9
1	B	247	LEU	9.5
1	A	996	VAL	9.0
1	A	246	ASP	8.9
1	B	217	ILE	7.8
1	B	244	ASN	7.4
1	B	683	PHE	7.4
1	B	241	LEU	7.1
1	A	245	ALA	7.0
1	A	683	PHE	6.8
1	B	100	ARG	6.8
1	B	210	TRP	6.7
1	A	489	TYR	6.6
1	B	248	CYS	6.4
1	A	688	HIS	6.4
1	B	252	GLU	6.3
1	B	246	ASP	6.3
1	A	248	CYS	6.0
1	B	293	HIS	6.0
1	B	219	ASP	5.9
1	B	229	PHE	5.9
1	B	221	PHE	5.8
1	A	243	CYS	5.6
1	B	251	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	935	ALA	5.3
1	A	251	TRP	5.3
1	B	189	LEU	5.2
1	B	249	GLU	5.2
1	B	443	ASP	5.1
1	B	96	ILE	5.1
1	A	910	LEU	5.1
1	B	218	GLU	5.0
1	A	931	ASP	5.0
1	A	247	LEU	4.9
1	B	206	LEU	4.9
1	B	996	VAL	4.8
1	A	914	LEU	4.8
1	B	99	TYR	4.8
1	B	202	LEU	4.8
1	A	250	ASP	4.4
1	B	489	TYR	4.3
1	A	938	LEU	4.3
1	B	209	ASP	4.3
1	B	220	ILE	4.3
1	A	930	LEU	4.2
1	A	244	ASN	4.2
1	B	291	LEU	4.2
1	B	94	GLN	4.2
1	A	249	GLU	4.1
1	B	187	PHE	4.0
1	B	148	SER	4.0
1	A	767	LEU	4.0
1	B	265	LEU	4.0
1	B	250	ASP	4.0
1	B	253	GLN	3.9
1	A	252	GLU	3.8
1	A	253	GLN	3.8
1	B	234	MET	3.8
1	B	243	CYS	3.8
1	A	885	LEU	3.8
1	B	197	VAL	3.8
1	B	212	GLU	3.8
1	A	759	LEU	3.8
1	A	254	PRO	3.7
1	B	273	CYS	3.7
1	B	142	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	315	PHE	3.6
1	A	147	GLU	3.6
1	A	325	PHE	3.6
1	B	254	PRO	3.5
1	B	290	LEU	3.5
1	A	718	MET	3.5
1	A	217	ILE	3.4
1	B	355	LEU	3.4
1	A	817	LYS	3.4
1	B	330	GLU	3.4
1	B	185	PHE	3.4
1	A	742	VAL	3.4
1	A	857	LEU	3.4
1	B	361	LEU	3.4
1	A	255	GLN	3.4
1	B	688	HIS	3.3
1	B	285	ARG	3.3
1	B	242	ASP	3.3
1	B	731	ILE	3.3
1	B	788	PHE	3.3
1	B	995	LEU	3.3
1	B	309	LEU	3.2
1	A	929	THR	3.2
1	A	488	HIS	3.1
1	A	897	LEU	3.1
1	B	310	TYR	3.1
1	A	443	ASP	3.1
1	A	872	LYS	3.0
1	A	315	PHE	3.0
1	B	255	GLN	3.0
1	B	320	ALA	3.0
1	A	220	ILE	3.0
1	B	118	LEU	2.9
1	A	839	TRP	2.9
1	B	672	PHE	2.9
1	A	142	ALA	2.9
1	B	211	PRO	2.9
1	A	672	PHE	2.8
1	A	845	PHE	2.8
1	B	686	ILE	2.8
1	B	231	LEU	2.8
1	B	222	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	802	TYR	2.8
1	B	518	PRO	2.7
1	A	308	LYS	2.7
1	A	318	LYS	2.7
1	A	311	PHE	2.7
1	A	309	LEU	2.7
1	A	881	LEU	2.7
1	B	195	ASN	2.7
1	B	198	THR	2.7
1	B	275	LEU	2.6
1	A	330	GLU	2.6
1	B	205	LEU	2.6
1	B	272	GLU	2.6
1	A	844	TYR	2.6
1	A	682	LEU	2.6
1	B	194	MET	2.5
1	B	188	PHE	2.5
1	B	97	ASN	2.5
1	B	277	LEU	2.5
1	B	119	VAL	2.5
1	B	767	LEU	2.5
1	A	803	ASN	2.4
1	A	824	LEU	2.4
1	A	242	ASP	2.4
1	B	759	LEU	2.4
1	A	972	GLU	2.4
1	B	271	PRO	2.4
1	B	270	LEU	2.4
1	A	853	ILE	2.4
1	A	141	ASP	2.3
1	A	221	PHE	2.3
1	A	942	LEU	2.3
1	B	147	GLU	2.3
1	A	687	LEU	2.3
1	B	832	SER	2.3
1	A	858	ILE	2.3
1	B	539	PRO	2.3
1	A	809	LEU	2.2
1	A	793	CYS	2.2
1	A	200	MET	2.2
1	B	710	LEU	2.2
1	A	239	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	163	THR	2.2
1	B	325	PHE	2.2
1	A	873	ILE	2.2
1	B	152	VAL	2.2
1	A	198	THR	2.1
1	A	678	ASN	2.1
1	B	542	VAL	2.1
1	A	995	LEU	2.1
1	B	323	ARG	2.1
1	A	293	HIS	2.1
1	A	952	LEU	2.1
1	B	331	LYS	2.0
1	B	319	ASP	2.0
1	A	290	LEU	2.0
1	B	359	GLU	2.0
1	A	874	TYR	2.0
1	B	216	PRO	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)

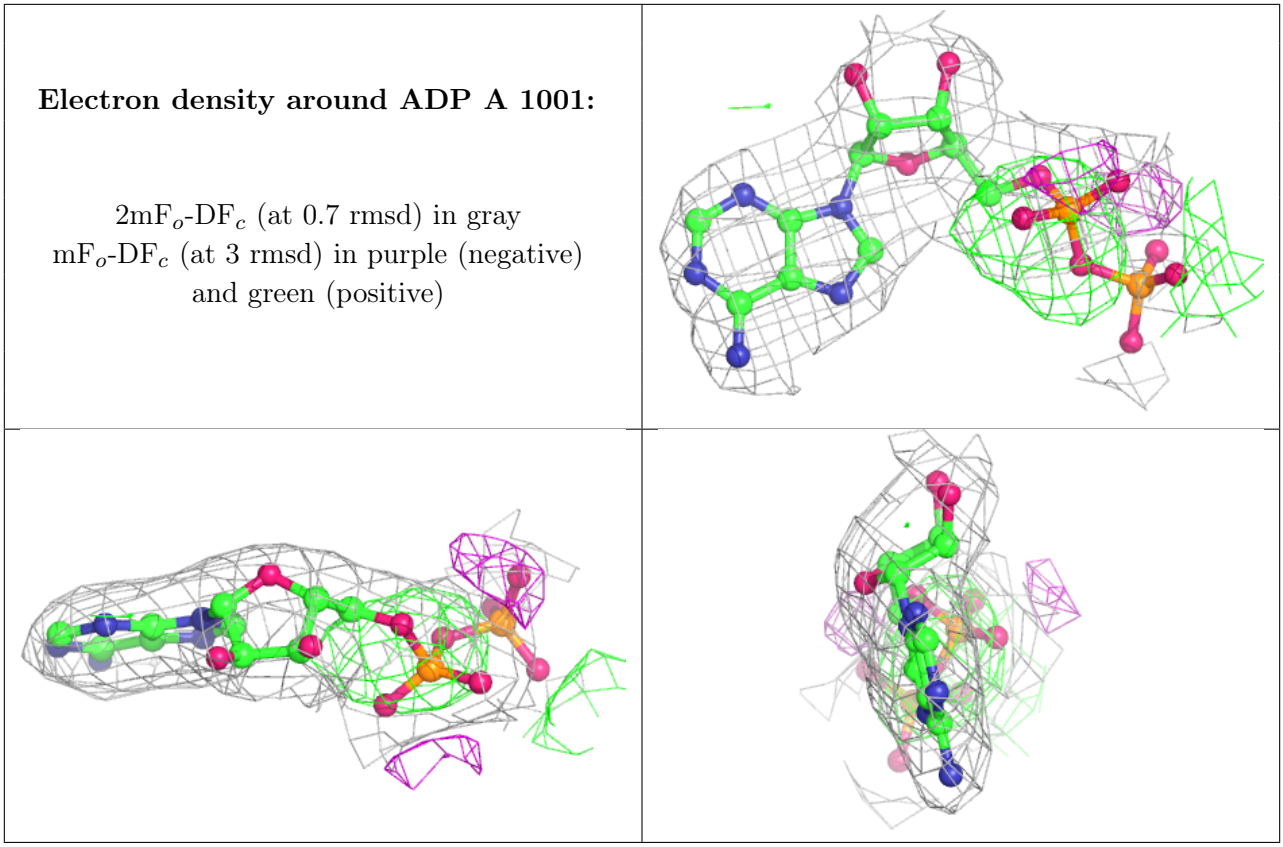
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ADP	A	1001	27/27	0.88	0.27	59,73,89,150	0
2	ADP	B	1001	27/27	0.92	0.26	74,99,107,116	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.

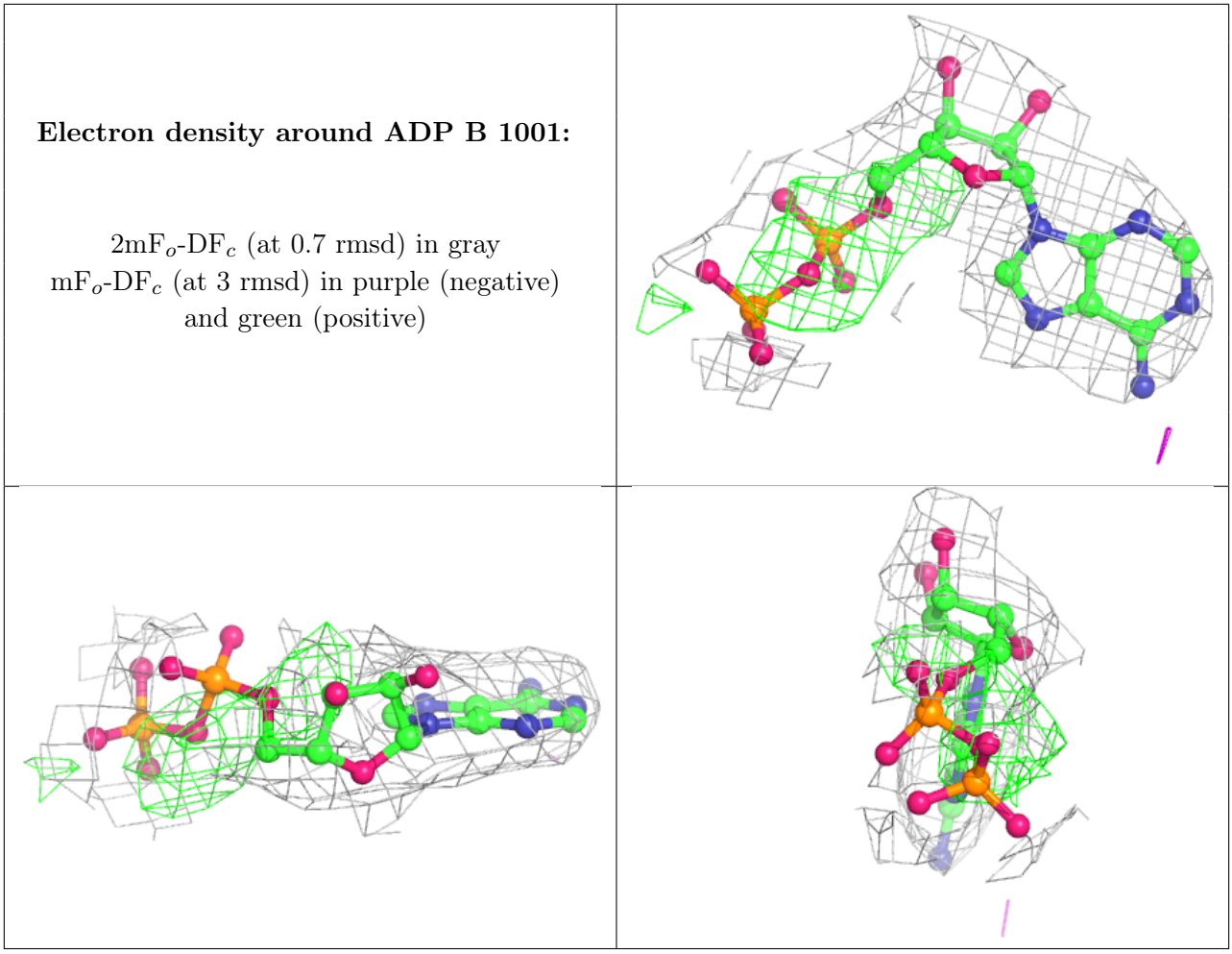
Electron density around ADP A 1001:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.