



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:46 AM UTC

PDB ID : 7WBT / pdb_00007wbt
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 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

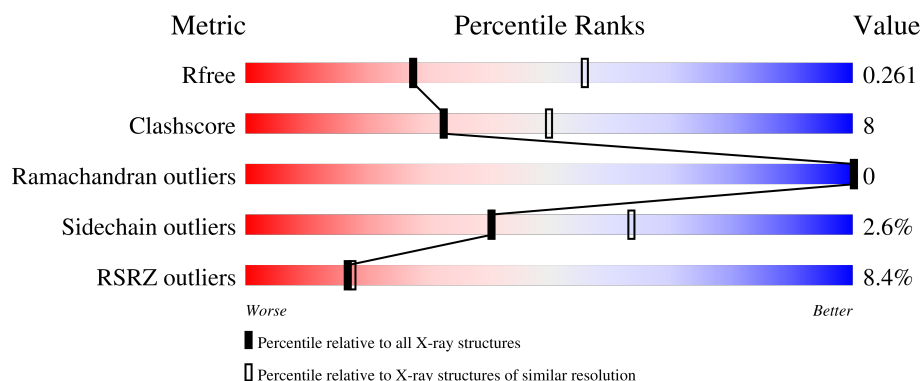
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	912	9% 79% 19% ..
1	B	912	8% 78% 20% ..

2 Entry composition

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.

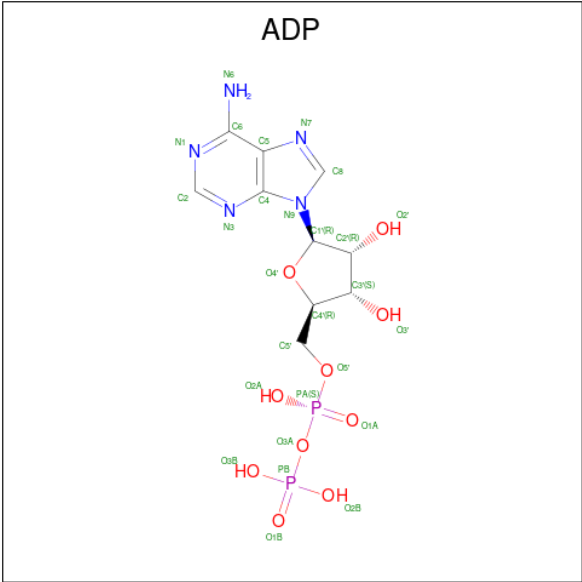
- Molecule 1 is a protein called NACHT, LRR and PYD domains-containing protein 9.

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 (CCD ID: 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		

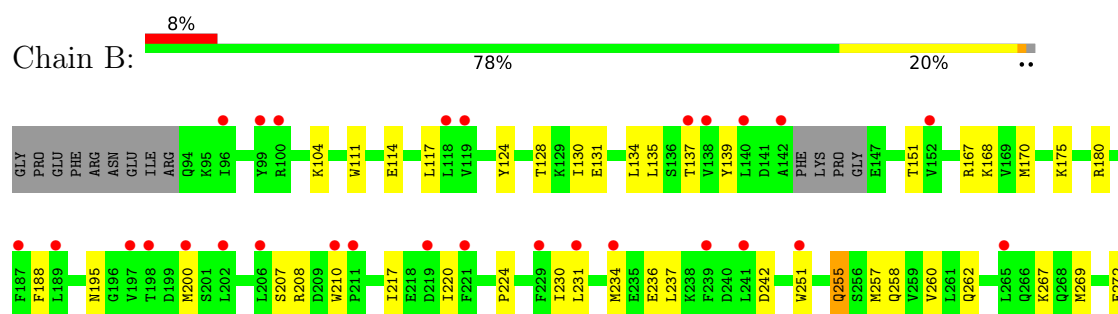
3 Residue-property plots

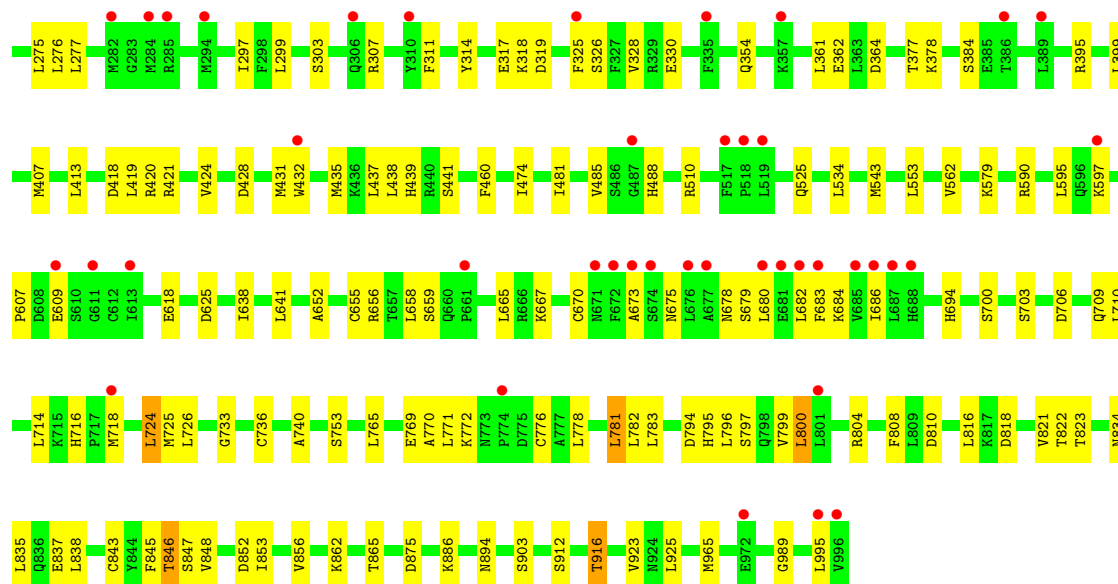
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.262 0.234 , 0.261	Depositor DCC
R_{free} test set	4529 reflections (5.14%)	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 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

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	0.23	0/7303	0.42	0/9870
1	B	0.21	0/7303	0.40	0/9870
All	All	0.22	0/14606	0.41	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	118	0
1	B	7156	0	7116	112	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
All	All	14366	0	14256	227	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 8.

All (227) 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:395:ARG:HD3	1:B:431:MET:HE1	1.65	0.78
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:B:170:MET:HE3	1:B:188:PHE:HB2	1.74	0.70
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:B:875:ASP:OD2	1:B:903:SER:OG	2.16	0.60
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:B:231:LEU:HB3	1:B:234:MET:HE3	1.84	0.60
1:A:231:LEU:HB3	1:A:234:MET:HE3	1.85	0.59
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:A:395:ARG:HD3	1:A:431:MET:HE1	1.84	0.58
1:A:251:TRP:HA	1:A:269:MET:HE2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLU:OE1	1:B:318:LYS:N	2.37	0.57
1:A:462:MET:HE3	1:A:502:PHE:HB3	1.86	0.57
1:B:251:TRP:HA	1:B:269:MET:HE2	1.86	0.56
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: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
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: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:288:TYR:HD1	1:A:294:MET:HE1	1.75	0.51
1:A:846:THR:OG1	1:A:847:SER:N	2.38	0.51
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:200:MET:HE1	1:B:208:ARG:HH21	1.78	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:291:LEU:HB2	1:A:294:MET:HE2	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:170:MET:HE2	1:B:230:ILE:HD12	1.95	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: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:B:311:PHE:CE2	1:B:328:VAL:HG11	2.50	0.46
1:A:170:MET:HE1	1:A:186:VAL:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:288:TYR:CD1	1:A:294:MET:HE1	2.51	0.45
1:B:886:LYS:HZ1	1:B:912:SER:HB3	1.81	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:CD	1:B:317:GLU:C	2.85	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: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:579:LYS:HZ1	1:B:618:GLU:CD	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.85	0.43
1:B:257:MET:HE3	1:B:260:VAL:HB	2.01	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
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:B:437:LEU:C	1:B:438:LEU:HD12	2.44	0.42
1:A:462:MET:HE3	1:A:502:PHE:CB	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ARG:HG3	1:A:738:ASP:OD2	2.20	0.41
1:A:875:ASP:HB3	1:A:879:LYS:NZ	2.36	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
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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	795 (97%)	26 (3%)	34	58
1	B	821/832 (99%)	804 (98%)	17 (2%)	47	67
All	All	1642/1664 (99%)	1599 (97%)	43 (3%)	40	63

All (43) 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	346	LEU
1	A	363	LEU
1	A	377	THR
1	A	439	HIS
1	A	525	GLN
1	A	526	GLU
1	A	547	GLN
1	A	620	LEU
1	A	676	LEU
1	A	715	LYS
1	A	781	LEU
1	A	811	LEU
1	A	840	LEU
1	A	846	THR
1	A	868	LEU
1	A	879	LYS
1	A	882	CYS
1	A	897	LEU
1	A	916	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	965	MET
1	B	134	LEU
1	B	139	TYR
1	B	180	ARG
1	B	255	GLN
1	B	361	LEU
1	B	377	THR
1	B	407	MET
1	B	525	GLN
1	B	595	LEU
1	B	641	LEU
1	B	724	LEU
1	B	725	MET
1	B	781	LEU
1	B	800	LEU
1	B	846	THR
1	B	916	THR
1	B	965	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	262	GLN
1	A	266	GLN
1	A	536	GLN
1	A	541	ASN
1	A	671	ASN
1	A	675	ASN
1	A	678	ASN
1	A	689	ASN
1	A	691	HIS
1	A	716	HIS
1	A	746	ASN
1	A	795	HIS
1	A	836	GLN
1	B	305	HIS
1	B	541	ASN
1	B	675	ASN
1	B	691	HIS
1	B	836	GLN

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 oligosaccharides 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	B	1001	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	8 (18%)
2	ADP	A	1001	-	28,29,29	1.42	4 (14%)	43,45,45	1.88	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	1001	-	-	3/16/32/32	0/3/3/3
2	ADP	A	1001	-	-	1/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	4.92	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ADP	C5-C4	4.70	1.47	1.39
2	B	1001	ADP	C5-C6	2.58	1.48	1.41
2	A	1001	ADP	C5-N7	-2.55	1.34	1.39
2	B	1001	ADP	C8-N7	2.36	1.36	1.31
2	A	1001	ADP	C5-C6	2.35	1.47	1.41
2	B	1001	ADP	C5-N7	-2.33	1.34	1.39
2	A	1001	ADP	C8-N7	2.27	1.36	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ADP	C5-C4-N3	-5.86	118.65	126.72
2	A	1001	ADP	C5-C4-N3	-5.74	118.81	126.72
2	A	1001	ADP	N3-C4-N9	4.81	135.35	127.17
2	B	1001	ADP	N3-C4-N9	4.69	135.14	127.17
2	B	1001	ADP	C2-N3-C4	3.63	120.69	111.83
2	A	1001	ADP	C2-N3-C4	3.37	120.06	111.83
2	B	1001	ADP	N3-C2-N1	-3.05	123.96	128.58
2	B	1001	ADP	C4-C5-N7	-3.05	107.09	110.58
2	A	1001	ADP	N3-C2-N1	-3.03	124.00	128.58
2	A	1001	ADP	C4-C5-N7	-2.96	107.20	110.58
2	A	1001	ADP	C3'-C2'-C1'	2.69	106.56	101.46
2	B	1001	ADP	C3'-C2'-C1'	2.54	106.27	101.46
2	A	1001	ADP	O2A-PA-O1A	2.48	123.99	112.44
2	B	1001	ADP	C4-N9-C8	2.43	108.29	105.74
2	A	1001	ADP	C4-N9-C8	2.42	108.27	105.74
2	B	1001	ADP	C5-N7-C8	2.22	106.94	103.45
2	A	1001	ADP	C5-N7-C8	2.21	106.92	103.45
2	A	1001	ADP	O3B-PB-O2B	2.21	116.08	107.80
2	A	1001	ADP	N6-C6-N1	2.04	122.93	118.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

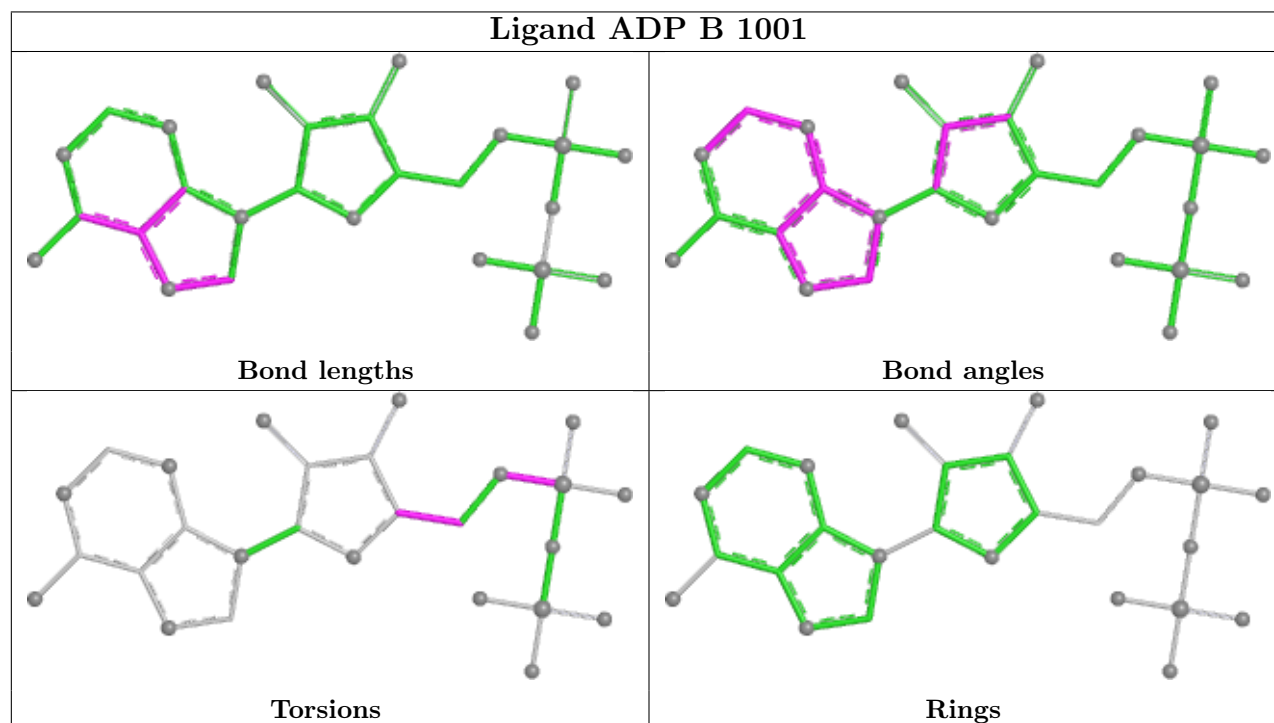
Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	PB-O3A-PA-O1A
2	B	1001	ADP	C5'-O5'-PA-O1A
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	B	1001	ADP	C3'-C4'-C5'-O5'

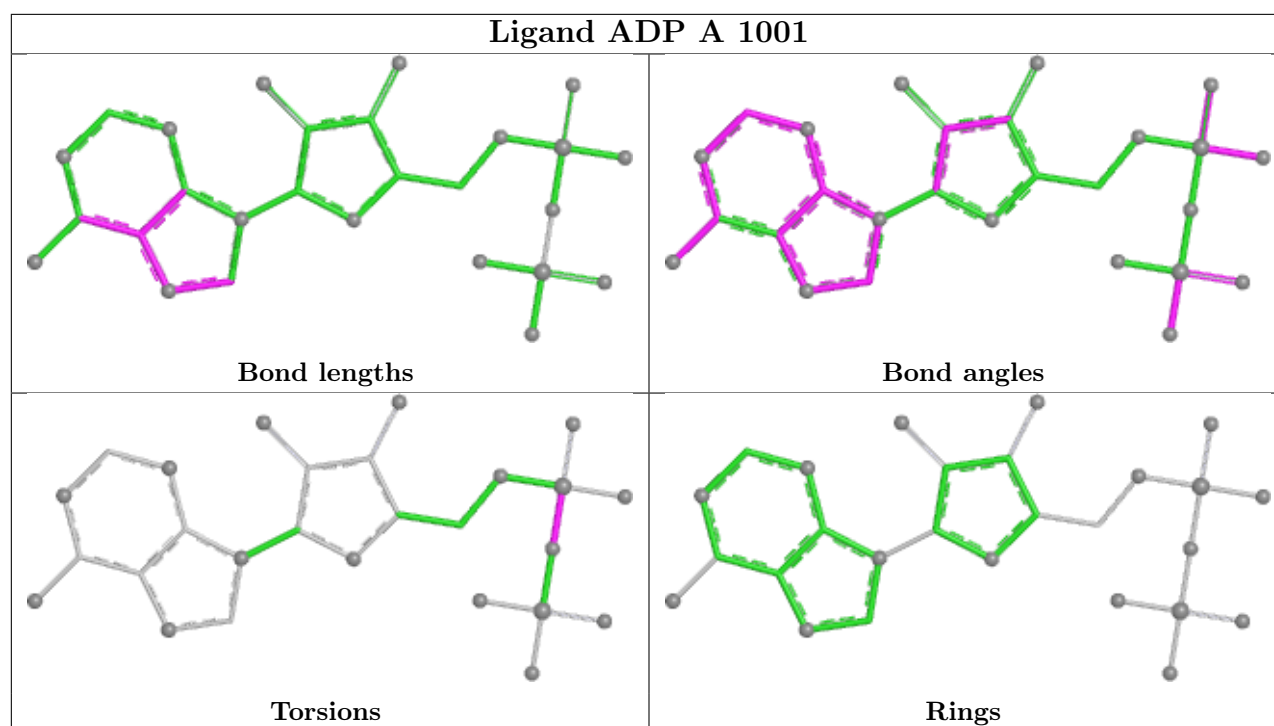
There are no ring outliers.

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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	899/912 (98%)	0.63	82 (9%)	15 14	54, 111, 166, 258	0
1	B	899/912 (98%)	0.59	69 (7%)	19 19	61, 110, 205, 276	0
All	All	1798/1824 (98%)	0.61	151 (8%)	17 17	54, 111, 189, 276	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	996	VAL	9.1
1	B	996	VAL	7.6
1	B	683	PHE	7.6
1	A	683	PHE	7.1
1	A	676	LEU	5.3
1	A	677	ALA	4.8
1	A	680	LEU	4.8
1	B	680	LEU	4.6
1	B	96	ILE	4.5
1	B	687	LEU	4.4
1	B	681	GLU	4.4
1	B	206	LEU	4.4
1	A	935	ALA	4.3
1	B	995	LEU	4.3
1	A	767	LEU	4.2
1	B	685	VAL	4.1
1	B	673	ALA	4.1
1	B	189	LEU	3.9
1	A	678	ASN	3.8
1	B	234	MET	3.8
1	A	687	LEU	3.7
1	A	824	LEU	3.7
1	A	857	LEU	3.6
1	A	245	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	HIS	3.4
1	B	142	ALA	3.4
1	A	688	HIS	3.3
1	A	611	GLY	3.3
1	A	885	LEU	3.3
1	A	910	LEU	3.3
1	B	310	TYR	3.3
1	B	676	LEU	3.2
1	A	139	TYR	3.2
1	B	229	PHE	3.1
1	B	210	TRP	3.1
1	A	673	ALA	3.0
1	A	140	LEU	2.9
1	B	202	LEU	2.9
1	A	198	THR	2.9
1	A	142	ALA	2.9
1	B	187	PHE	2.9
1	B	325	PHE	2.9
1	A	443	ASP	2.9
1	B	99	TYR	2.9
1	B	487	GLY	2.9
1	A	682	LEU	2.9
1	A	914	LEU	2.9
1	A	217	ILE	2.8
1	A	816	LEU	2.8
1	B	611	GLY	2.8
1	B	518	PRO	2.8
1	B	118	LEU	2.8
1	A	858	ILE	2.7
1	A	681	GLU	2.7
1	A	325	PHE	2.7
1	A	938	LEU	2.7
1	A	689	ASN	2.7
1	B	432	TRP	2.7
1	A	799	VAL	2.7
1	A	936	ALA	2.7
1	B	231	LEU	2.7
1	A	675	ASN	2.7
1	B	198	THR	2.7
1	B	677	ALA	2.7
1	B	219	ASP	2.7
1	A	809	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	828	LEU	2.6
1	B	285	ARG	2.6
1	A	672	PHE	2.6
1	B	386	THR	2.6
1	A	288	TYR	2.6
1	A	686	ILE	2.6
1	B	613	ILE	2.6
1	A	897	LEU	2.6
1	B	686	ILE	2.6
1	A	138	VAL	2.6
1	B	674	SER	2.5
1	B	282	MET	2.5
1	B	197	VAL	2.5
1	B	211	PRO	2.5
1	B	200	MET	2.5
1	A	853	ILE	2.5
1	A	873	ILE	2.5
1	A	798	GLN	2.5
1	A	942	LEU	2.5
1	A	844	TYR	2.5
1	B	140	LEU	2.4
1	B	672	PHE	2.4
1	B	294	MET	2.4
1	A	489	TYR	2.4
1	B	152	VAL	2.4
1	B	137	THR	2.4
1	B	251	TRP	2.4
1	B	718	MET	2.4
1	B	661	PRO	2.4
1	B	389	LEU	2.4
1	A	848	VAL	2.4
1	B	221	PHE	2.4
1	A	759	LEU	2.3
1	A	803	ASN	2.3
1	A	674	SER	2.3
1	B	774	PRO	2.3
1	A	850	CYS	2.3
1	A	881	LEU	2.3
1	A	895	LEU	2.3
1	B	357	LYS	2.3
1	A	856	VAL	2.3
1	B	688	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	932	TYR	2.3
1	A	774	PRO	2.3
1	A	847	SER	2.3
1	A	494	TRP	2.3
1	B	265	LEU	2.3
1	A	845	PHE	2.3
1	A	817	LYS	2.2
1	A	225	GLU	2.2
1	A	671	ASN	2.2
1	A	416	PRO	2.2
1	A	413	LEU	2.2
1	A	95	LYS	2.2
1	A	972	GLU	2.2
1	B	609	GLU	2.2
1	B	100	ARG	2.2
1	B	119	VAL	2.2
1	A	547	GLN	2.2
1	B	306	GLN	2.2
1	A	829	LYS	2.2
1	A	685	VAL	2.2
1	B	517	PHE	2.2
1	A	777	ALA	2.1
1	A	526	GLU	2.1
1	A	648	GLU	2.1
1	B	241	LEU	2.1
1	B	138	VAL	2.1
1	B	239	PHE	2.1
1	A	711	CYS	2.1
1	B	519	LEU	2.1
1	B	682	LEU	2.1
1	A	96	ILE	2.1
1	B	671	ASN	2.1
1	B	335	PHE	2.1
1	B	597	LYS	2.1
1	B	801	LEU	2.1
1	A	802	TYR	2.1
1	B	284	MET	2.0
1	A	801	LEU	2.0
1	B	972	GLU	2.0
1	A	790	SER	2.0
1	A	839	TRP	2.0
1	A	638	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	963	ILE	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 [i](#)

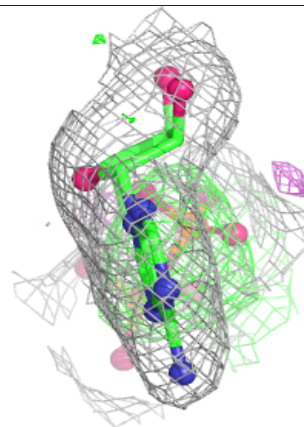
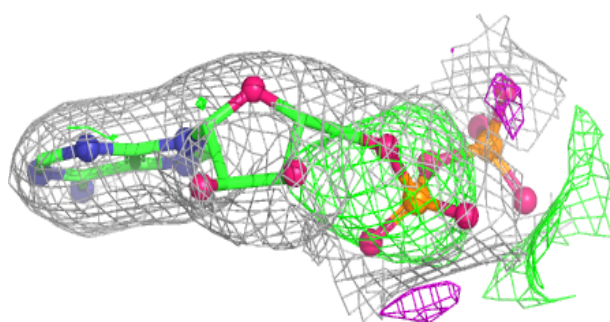
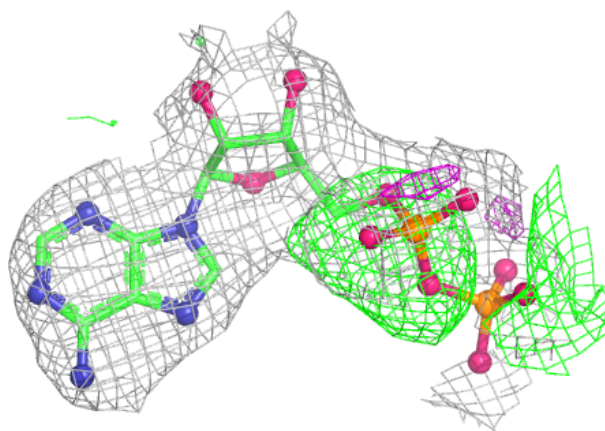
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1001	27/27	0.92	0.13	59,73,89,150	0
2	ADP	B	1001	27/27	0.94	0.13	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.

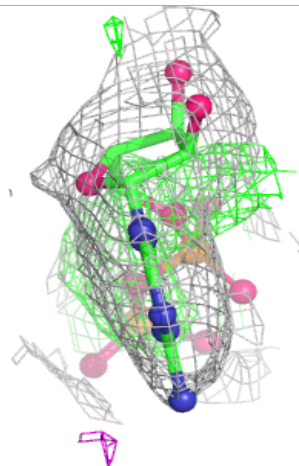
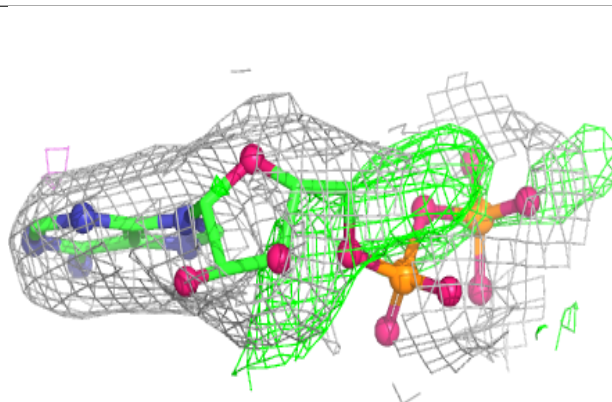
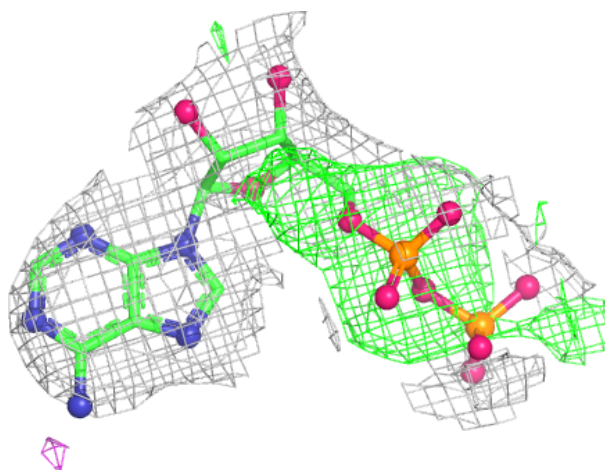
Electron density around ADP A 1001:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.