



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 PM UTC

PDB ID : 5X9W / pdb_00005x9w
Title : Mismatch Repair Protein
Authors : Nair, D.T.; Nirwal, S.
Deposited on : 2017-03-10
Resolution : 3.30 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

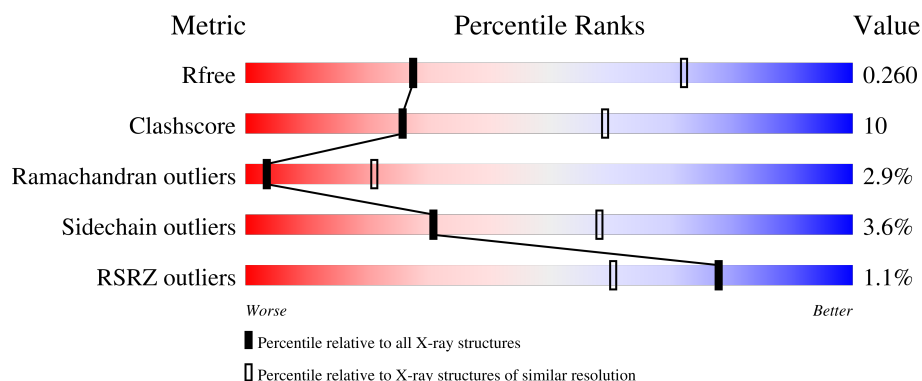
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	816	73%19%6%
1	B	816	72%20%6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11874 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.

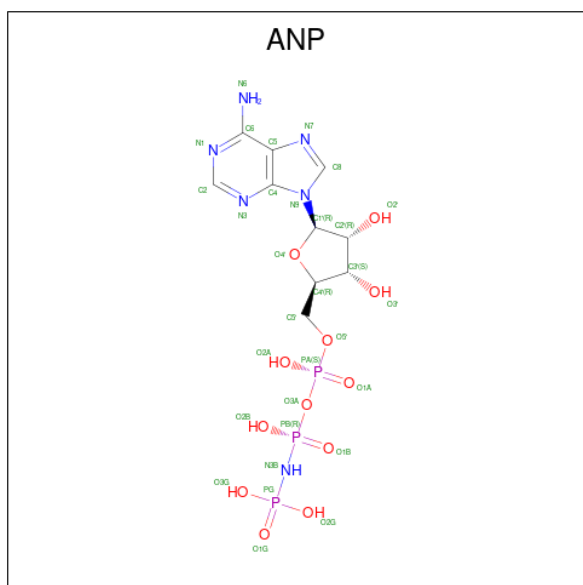
- Molecule 1 is a protein called DNA mismatch repair protein MutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total	C	N	O	S	0	0	0
			5906	3733	1046	1107	20			
1	B	771	Total	C	N	O	S	0	0	0
			5906	3733	1046	1107	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP Q5F5J4
A	0	SER	-	expression tag	UNP Q5F5J4
B	-1	GLN	-	expression tag	UNP Q5F5J4
B	0	SER	-	expression tag	UNP Q5F5J4

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

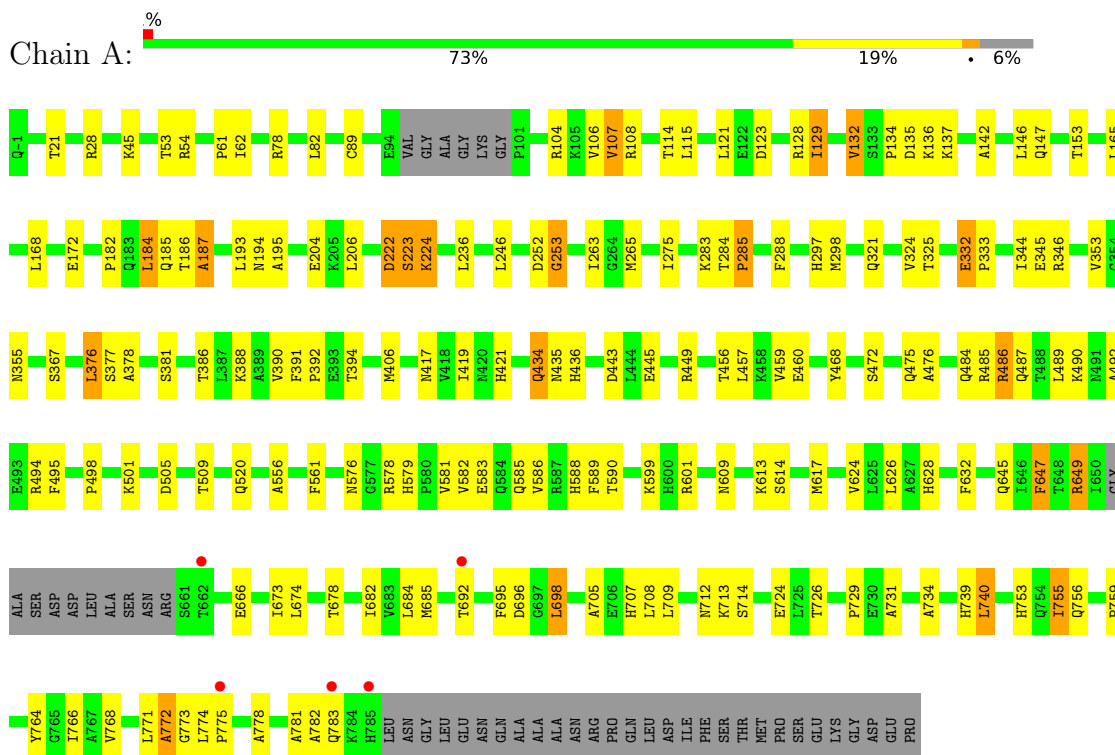


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

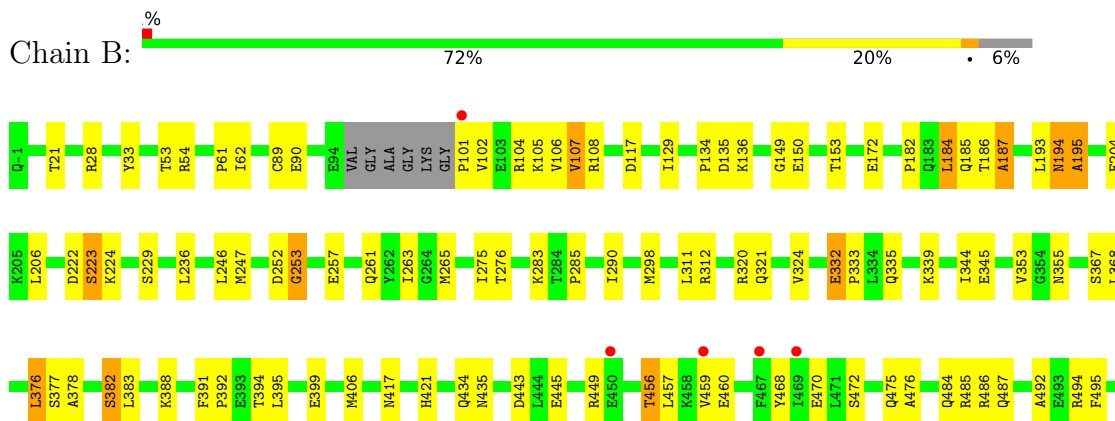
3 Residue-property plots

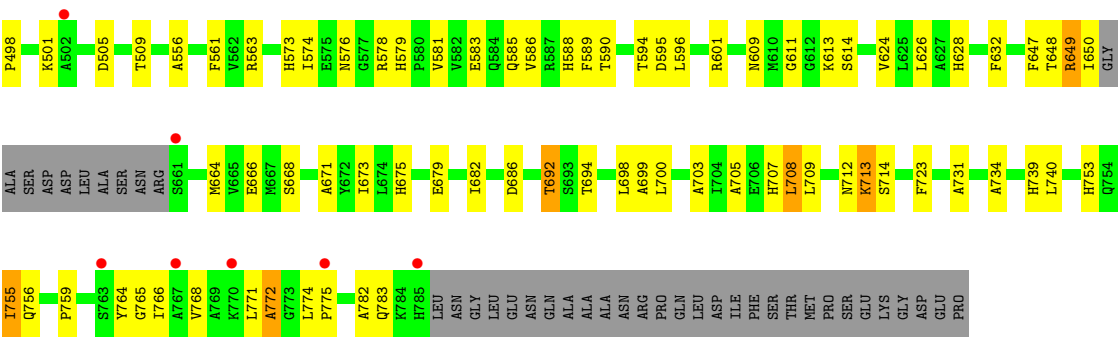
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: DNA mismatch repair protein MutS





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	89.51Å 102.07Å 235.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.30 49.93 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.93-3.30) 97.3 (49.93-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.221 , 0.273 (Not available) , 0.260	Depositor DCC
R_{free} test set	1646 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11874	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: ANP

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	0.87	1/6015 (0.0%)	0.92	4/8154 (0.0%)
1	B	0.65	0/6015	0.81	3/8154 (0.0%)
All	All	0.77	1/12030 (0.0%)	0.87	7/16308 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	773	GLY	CA-C	7.00	1.60	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	PRO	N-CA-CB	7.20	110.82	102.33
1	B	775	PRO	N-CA-CB	7.17	110.78	103.25
1	A	775	PRO	N-CA-C	-5.85	106.49	114.80
1	B	765	GLY	N-CA-C	-5.71	106.68	113.99
1	A	284	THR	CA-C-N	5.38	126.56	119.84
1	A	284	THR	C-N-CA	5.38	126.56	119.84
1	B	102	VAL	N-CA-C	5.29	115.89	108.17

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	5906	0	5861	121	0
1	B	5906	0	5861	120	0
2	A	31	0	13	4	0
2	B	31	0	13	8	0
All	All	11874	0	11748	225	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 10.

All (225) 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:A:614:SER:OG	2:A:901:ANP:O3G	1.81	0.98
1:A:186:THR:HA	1:A:187:ALA:CB	2.06	0.85
1:B:186:THR:HA	1:B:187:ALA:CB	2.07	0.84
1:A:376:LEU:O	1:A:378:ALA:N	2.11	0.83
1:A:772:ALA:CB	1:B:675:HIS:CE1	2.62	0.83
1:A:696:ASP:HB2	1:B:764:TYR:CB	2.11	0.81
1:B:376:LEU:O	1:B:378:ALA:N	2.14	0.80
1:A:764:TYR:CB	1:B:692:THR:HG21	2.13	0.78
1:B:134:PRO:HG3	1:B:182:PRO:HD3	1.67	0.76
1:B:186:THR:HA	1:B:187:ALA:HB2	1.68	0.76
1:A:186:THR:HA	1:A:187:ALA:HB2	1.65	0.75
1:A:332:GLU:HG2	1:A:333:PRO:HD3	1.69	0.74
1:A:772:ALA:HB1	1:B:675:HIS:ND1	2.02	0.74
1:A:647:PHE:HD2	1:A:673:ILE:HG12	1.52	0.74
1:B:106:VAL:O	1:B:108:ARG:N	2.21	0.71
1:B:611:GLY:O	2:B:901:ANP:O1B	2.07	0.71
1:B:332:GLU:HG2	1:B:333:PRO:HD3	1.72	0.71
1:A:772:ALA:HB2	1:B:675:HIS:CE1	2.27	0.69
1:A:486:ARG:HG2	1:A:487:GLN:H	1.57	0.69
1:A:28:ARG:O	1:A:104:ARG:NH2	2.26	0.69
1:B:486:ARG:HG2	1:B:487:GLN:H	1.58	0.68
1:B:609:ASN:O	2:B:901:ANP:O2B	2.10	0.68
1:A:468:TYR:CE1	1:A:494:ARG:HD3	2.29	0.67
1:B:753:HIS:ND1	2:B:901:ANP:N3	2.42	0.67
1:A:772:ALA:HB1	1:B:675:HIS:CE1	2.28	0.67
1:A:134:PRO:HG3	1:A:182:PRO:HD3	1.75	0.67
1:B:712:ASN:O	1:B:714:SER:N	2.28	0.66
1:B:614:SER:OG	2:B:901:ANP:PG	2.54	0.65
1:A:391:PHE:O	1:A:394:THR:HG22	1.97	0.64
1:A:298:MET:HE1	1:A:344:ILE:HG12	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:MET:HE1	1:B:344:ILE:HG12	1.81	0.63
1:A:252:ASP:O	1:A:253:GLY:O	2.17	0.63
1:A:434:GLN:HG3	1:A:435:ASN:N	2.13	0.62
1:B:193:LEU:O	1:B:194:ASN:C	2.43	0.62
1:B:186:THR:CA	1:B:187:ALA:HB2	2.30	0.61
1:B:186:THR:CA	1:B:187:ALA:CB	2.78	0.61
1:A:106:VAL:O	1:A:108:ARG:N	2.29	0.61
1:A:186:THR:CA	1:A:187:ALA:HB2	2.31	0.61
1:B:460:GLU:HB2	1:B:468:TYR:CE1	2.37	0.60
1:A:609:ASN:O	2:A:901:ANP:O1B	2.20	0.60
1:B:89:CYS:SG	1:B:104:ARG:HG3	2.41	0.60
1:B:265:MET:HE1	1:B:275:ILE:HD11	1.82	0.60
1:A:613:LYS:HB2	2:A:901:ANP:O2B	2.02	0.60
1:A:771:LEU:HA	1:B:671:ALA:HB2	1.83	0.59
1:A:186:THR:CA	1:A:187:ALA:CB	2.79	0.59
1:B:186:THR:HA	1:B:187:ALA:HB3	1.85	0.59
1:A:712:ASN:O	1:A:714:SER:N	2.37	0.58
1:A:647:PHE:CD2	1:A:673:ILE:HG12	2.36	0.58
1:B:185:GLN:HG2	1:B:187:ALA:HB2	1.86	0.57
1:A:724:GLU:OE1	1:B:694:THR:OG1	2.20	0.57
1:A:460:GLU:HB2	1:A:468:TYR:CE1	2.39	0.57
1:A:649:ARG:HE	1:A:666:GLU:HG2	1.70	0.57
1:A:498:PRO:HA	1:A:501:LYS:HB2	1.87	0.57
1:B:391:PHE:O	1:B:394:THR:HG22	2.04	0.57
1:B:434:GLN:HG3	1:B:435:ASN:N	2.20	0.57
1:A:617:MET:HB3	1:A:684:LEU:HD23	1.86	0.56
1:B:586:VAL:HG21	1:B:589:PHE:HB2	1.87	0.56
1:B:782:ALA:HA	1:B:783:GLN:C	2.30	0.56
1:A:434:GLN:HG3	1:A:435:ASN:H	1.70	0.56
1:B:614:SER:OG	2:B:901:ANP:O2G	2.24	0.56
1:A:78:ARG:O	1:A:82:LEU:HG	2.05	0.56
1:B:614:SER:OG	2:B:901:ANP:O1G	2.23	0.56
1:A:53:THR:HG21	1:A:61:PRO:HB3	1.87	0.56
1:A:457:LEU:HD12	1:A:457:LEU:O	2.06	0.56
1:A:472:SER:O	1:A:476:ALA:N	2.38	0.56
1:B:445:GLU:O	1:B:449:ARG:HG2	2.06	0.56
1:B:556:ALA:HA	1:B:561:PHE:HB2	1.86	0.55
1:A:186:THR:HA	1:A:187:ALA:HB3	1.88	0.55
1:B:353:VAL:HG23	1:B:355:ASN:HB2	1.87	0.55
1:A:472:SER:HA	1:A:492:ALA:HA	1.89	0.55
1:A:298:MET:HE3	1:A:345:GLU:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:MET:HE1	1:B:421:HIS:CE1	2.43	0.54
1:A:614:SER:CB	2:A:901:ANP:O3G	2.56	0.54
1:B:579:HIS:O	1:B:583:GLU:HB2	2.07	0.54
1:A:586:VAL:HG21	1:A:589:PHE:HB2	1.89	0.54
1:A:321:GLN:HA	1:A:324:VAL:HG12	1.89	0.53
1:A:556:ALA:HA	1:A:561:PHE:HB2	1.90	0.53
1:A:486:ARG:CG	1:A:487:GLN:H	2.21	0.53
1:A:696:ASP:CB	1:B:764:TYR:CB	2.86	0.53
1:A:185:GLN:HG2	1:A:187:ALA:HB2	1.91	0.53
1:A:89:CYS:SG	1:A:104:ARG:HG3	2.49	0.53
1:B:581:VAL:HG12	1:B:585:GLN:NE2	2.24	0.52
1:B:590:THR:OG1	1:B:753:HIS:O	2.27	0.52
1:A:445:GLU:O	1:A:449:ARG:HG2	2.11	0.51
1:B:601:ARG:HB2	1:B:734:ALA:HB1	1.93	0.51
1:A:298:MET:HE1	1:A:344:ILE:CG1	2.40	0.51
1:B:298:MET:HE1	1:B:344:ILE:CG1	2.40	0.51
1:A:578:ARG:NE	1:A:583:GLU:OE2	2.44	0.51
1:B:193:LEU:O	1:B:195:ALA:N	2.44	0.51
1:A:193:LEU:O	1:A:194:ASN:C	2.50	0.51
1:B:498:PRO:HA	1:B:501:LYS:HB2	1.92	0.51
1:B:28:ARG:O	1:B:104:ARG:NH2	2.42	0.51
1:B:624:VAL:HG11	1:B:682:ILE:HD12	1.93	0.50
1:A:586:VAL:O	1:A:588:HIS:N	2.44	0.50
1:B:129:ILE:HD12	1:B:172:GLU:HB3	1.93	0.50
1:B:298:MET:HE3	1:B:345:GLU:HB2	1.93	0.50
1:B:485:ARG:HA	1:B:495:PHE:HA	1.93	0.50
1:B:204:GLU:OE2	1:B:223:SER:OG	2.29	0.49
1:A:54:ARG:O	1:A:62:ILE:HB	2.12	0.49
1:B:368:LEU:HD22	1:B:394:THR:HG21	1.95	0.49
1:B:609:ASN:O	2:B:901:ANP:PB	2.70	0.49
1:A:194:ASN:O	1:A:194:ASN:CG	2.55	0.49
1:B:391:PHE:HB2	1:B:392:PRO:HD3	1.95	0.49
1:B:468:TYR:CE1	1:B:494:ARG:HD3	2.48	0.48
1:A:391:PHE:HB2	1:A:392:PRO:HD3	1.94	0.48
1:B:472:SER:HA	1:B:492:ALA:HA	1.95	0.48
1:B:573:HIS:ND1	1:B:595:ASP:OD1	2.45	0.48
1:A:581:VAL:HG12	1:A:585:GLN:NE2	2.28	0.48
1:B:434:GLN:HG3	1:B:435:ASN:H	1.77	0.48
1:A:456:THR:CG2	1:A:475:GLN:HE22	2.26	0.48
1:B:486:ARG:CG	1:B:487:GLN:H	2.24	0.48
1:A:265:MET:HE1	1:A:275:ILE:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ALA:HA	1:A:783:GLN:C	2.39	0.48
1:B:117:ASP:OD1	1:B:355:ASN:ND2	2.47	0.48
1:B:276:THR:O	1:B:283:LYS:NZ	2.47	0.47
1:A:624:VAL:HG11	1:A:682:ILE:HD12	1.95	0.47
1:B:649:ARG:HE	1:B:666:GLU:HG2	1.79	0.47
1:A:645:GLN:HB2	1:A:647:PHE:HE1	1.79	0.47
1:B:472:SER:O	1:B:476:ALA:N	2.48	0.47
1:B:563:ARG:HB2	1:B:632:PHE:CZ	2.49	0.47
1:A:685:MET:HE2	1:A:685:MET:HB3	1.87	0.47
1:B:470:GLU:HA	1:B:494:ARG:HA	1.97	0.47
1:B:263:ILE:HD11	1:B:628:HIS:CD2	2.50	0.47
1:A:485:ARG:HA	1:A:495:PHE:HA	1.97	0.47
1:B:586:VAL:O	1:B:588:HIS:N	2.45	0.46
1:B:311:LEU:HD11	1:B:320:ARG:CZ	2.46	0.46
1:A:129:ILE:HG23	1:A:236:LEU:HD11	1.97	0.46
1:A:486:ARG:HG2	1:A:487:GLN:N	2.27	0.46
1:A:778:ALA:O	1:B:699:ALA:HB1	2.15	0.46
1:A:674:LEU:O	1:A:712:ASN:ND2	2.49	0.46
1:B:505:ASP:O	1:B:509:THR:OG1	2.28	0.46
1:A:263:ILE:HD11	1:A:628:HIS:CD2	2.52	0.45
1:A:406:MET:HE1	1:A:421:HIS:CE1	2.52	0.45
1:A:705:ALA:O	1:A:709:LEU:HD12	2.16	0.45
1:A:698:LEU:HD22	1:A:698:LEU:O	2.16	0.45
1:A:252:ASP:O	1:A:253:GLY:C	2.58	0.45
1:B:53:THR:HG21	1:B:61:PRO:HB3	1.99	0.45
1:A:132:VAL:O	1:A:132:VAL:HG23	2.17	0.45
1:A:505:ASP:O	1:A:509:THR:OG1	2.19	0.45
1:B:153:THR:OG1	1:B:229:SER:HB2	2.16	0.45
1:A:114:THR:HB	1:A:146:LEU:HD12	1.99	0.45
1:A:435:ASN:OD1	1:A:436:HIS:N	2.50	0.45
1:B:574:ILE:HB	1:B:594:THR:HB	1.98	0.44
1:B:650:ILE:HA	1:B:686:ASP:HB3	1.99	0.44
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.85	0.44
1:B:335:GLN:O	1:B:339:LYS:HB2	2.18	0.44
1:B:755:ILE:HD12	1:B:755:ILE:O	2.17	0.44
1:A:726:THR:O	1:A:729:PRO:HD2	2.17	0.44
1:B:578:ARG:NE	1:B:583:GLU:OE2	2.51	0.44
1:A:129:ILE:HD12	1:A:172:GLU:HB3	1.98	0.44
1:B:252:ASP:O	1:B:253:GLY:O	2.36	0.44
1:A:579:HIS:O	1:A:583:GLU:HB2	2.18	0.44
1:A:696:ASP:CG	1:B:764:TYR:CB	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ILE:HD12	1:A:755:ILE:O	2.18	0.44
1:A:579:HIS:ND1	1:A:582:VAL:HG23	2.33	0.43
1:A:649:ARG:NE	1:A:666:GLU:HG2	2.32	0.43
1:A:781:ALA:HB3	1:B:699:ALA:HA	2.00	0.43
1:B:708:LEU:HA	1:B:712:ASN:OD1	2.18	0.43
1:A:386:THR:O	1:A:390:VAL:HG23	2.18	0.43
1:A:578:ARG:HE	1:A:583:GLU:CD	2.26	0.43
1:A:128:ARG:NH1	1:A:168:LEU:O	2.47	0.43
1:B:648:THR:HB	1:B:650:ILE:CD1	2.48	0.43
1:A:132:VAL:O	1:A:132:VAL:CG2	2.66	0.43
1:A:184:LEU:HD23	1:A:185:GLN:O	2.18	0.43
1:A:115:LEU:HB2	1:A:121:LEU:HD21	2.01	0.43
1:A:445:GLU:HG3	1:A:459:VAL:HG23	2.00	0.43
1:A:764:TYR:CA	1:B:692:THR:HG21	2.48	0.43
1:B:321:GLN:HA	1:B:324:VAL:HG12	2.01	0.43
1:B:486:ARG:NH2	1:B:494:ARG:HD2	2.34	0.43
1:A:778:ALA:CB	1:B:700:LEU:HD23	2.48	0.43
1:B:54:ARG:O	1:B:62:ILE:HB	2.18	0.43
1:B:382:SER:OG	1:B:383:LEU:N	2.50	0.43
1:B:129:ILE:HG23	1:B:236:LEU:HD11	2.00	0.43
1:A:147:GLN:OE1	1:A:346:ARG:NE	2.50	0.43
1:A:489:LEU:HB3	1:A:490:LYS:H	1.72	0.42
1:B:33:TYR:OH	1:B:90:GLU:OE2	2.27	0.42
1:B:614:SER:HB2	2:B:901:ANP:N3B	2.34	0.42
1:B:290:ILE:HD13	1:B:290:ILE:HA	1.89	0.42
1:B:766:ILE:C	1:B:768:VAL:H	2.26	0.42
1:A:484:GLN:O	1:A:485:ARG:HB3	2.19	0.42
1:B:679:GLU:HA	1:B:713:LYS:O	2.20	0.42
1:B:184:LEU:HD23	1:B:185:GLN:O	2.19	0.42
1:B:486:ARG:HG2	1:B:487:GLN:N	2.29	0.42
1:B:648:THR:HB	1:B:650:ILE:HD11	2.01	0.42
1:A:204:GLU:OE2	1:A:223:SER:OG	2.36	0.42
1:A:695:PHE:CD1	1:B:723:PHE:HB3	2.55	0.42
1:B:611:GLY:O	1:B:613:LYS:N	2.50	0.42
1:A:590:THR:OG1	1:A:753:HIS:O	2.38	0.42
1:A:647:PHE:CD1	1:A:647:PHE:N	2.87	0.42
1:B:457:LEU:HD12	1:B:457:LEU:O	2.20	0.42
1:B:149:GLY:O	1:B:150:GLU:C	2.62	0.42
1:B:456:THR:CG2	1:B:475:GLN:HE22	2.33	0.42
1:B:771:LEU:O	1:B:772:ALA:HB2	2.20	0.42
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:THR:HG23	1:A:632:PHE:HZ	1.85	0.41
1:B:445:GLU:HG3	1:B:459:VAL:HG23	2.01	0.41
1:A:222:ASP:O	1:A:224:LYS:N	2.52	0.41
1:B:664:MET:O	1:B:668:SER:N	2.48	0.41
1:A:137:LYS:HE2	1:A:137:LYS:HB2	1.93	0.41
1:A:599:LYS:O	1:A:734:ALA:HA	2.21	0.41
1:B:388:LYS:HA	1:B:388:LYS:HD3	1.95	0.41
1:A:766:ILE:C	1:A:768:VAL:H	2.28	0.41
1:B:484:GLN:O	1:B:485:ARG:HB3	2.21	0.41
1:A:283:LYS:HE3	1:A:288:PHE:HD2	1.86	0.41
1:A:678:THR:O	1:A:714:SER:OG	2.35	0.41
1:B:647:PHE:HB3	1:B:673:ILE:HG12	2.02	0.41
1:B:705:ALA:O	1:B:709:LEU:HD12	2.21	0.41
1:B:185:GLN:HG2	1:B:187:ALA:CB	2.50	0.41
1:B:246:LEU:HD13	1:B:247:MET:N	2.36	0.41
1:A:123:ASP:HB3	1:A:297:HIS:CE1	2.56	0.41
1:A:378:ALA:HB3	1:A:388:LYS:NZ	2.36	0.41
1:A:468:TYR:CZ	1:A:494:ARG:HD3	2.56	0.41
1:A:739:HIS:CE1	1:A:756:GLN:HB2	2.56	0.41
1:B:257:GLU:HA	1:B:261:GLN:OE1	2.21	0.41
1:B:739:HIS:CE1	1:B:756:GLN:HB2	2.56	0.40
1:A:142:ALA:HA	1:A:153:THR:HA	2.03	0.40
1:A:613:LYS:HG2	1:A:740:LEU:HD12	2.03	0.40
1:A:778:ALA:N	1:B:703:ALA:HB2	2.36	0.40
1:B:395:LEU:O	1:B:399:GLU:HG2	2.21	0.40
1:A:353:VAL:HG23	1:A:355:ASN:HB2	2.03	0.40
1:A:601:ARG:HB2	1:A:734:ALA:HB1	2.02	0.40
1:B:106:VAL:O	1:B:107:VAL:HG22	2.20	0.40
1:B:709:LEU:HD23	1:B:734:ALA:HB3	2.04	0.40
1:B:595:ASP:C	1:B:596:LEU:HD12	2.47	0.40
1:A:406:MET:HE2	1:A:419:ILE:O	2.22	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	765/816 (94%)	677 (88%)	65 (8%)	23 (3%)	3	20
1	B	765/816 (94%)	677 (88%)	66 (9%)	22 (3%)	3	21
All	All	1530/1632 (94%)	1354 (88%)	131 (9%)	45 (3%)	3	21

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	253	GLY
1	A	285	PRO
1	A	377	SER
1	A	713	LYS
1	A	774	LEU
1	B	187	ALA
1	B	195	ALA
1	B	285	PRO
1	B	377	SER
1	B	713	LYS
1	A	136	LYS
1	A	195	ALA
1	A	222	ASP
1	A	224	LYS
1	A	576	ASN
1	A	692	THR
1	B	136	LYS
1	B	224	LYS
1	B	253	GLY
1	B	576	ASN
1	B	692	THR
1	B	772	ALA
1	B	774	LEU
1	A	135	ASP
1	A	223	SER
1	A	376	LEU
1	A	731	ALA
1	A	759	PRO
1	B	222	ASP
1	B	376	LEU
1	B	731	ALA
1	B	759	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	434	GLN
1	A	707	HIS
1	A	772	ALA
1	B	107	VAL
1	B	194	ASN
1	B	382	SER
1	B	707	HIS
1	A	107	VAL
1	A	381	SER
1	B	135	ASP
1	A	486	ARG
1	B	223	SER

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	564/668 (84%)	542 (96%)	22 (4%)	28	56
1	B	529/668 (79%)	512 (97%)	17 (3%)	34	60
All	All	1093/1336 (82%)	1054 (96%)	39 (4%)	31	58

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	45	LYS
1	A	107	VAL
1	A	129	ILE
1	A	132	VAL
1	A	165	LEU
1	A	184	LEU
1	A	206	LEU
1	A	246	LEU
1	A	285	PRO
1	A	332	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	367	SER
1	A	417	ASN
1	A	443	ASP
1	A	520	GLN
1	A	626	LEU
1	A	647	PHE
1	A	649	ARG
1	A	698	LEU
1	A	708	LEU
1	A	740	LEU
1	A	755	ILE
1	B	21	THR
1	B	101	PRO
1	B	105	LYS
1	B	184	LEU
1	B	206	LEU
1	B	312	ARG
1	B	332	GLU
1	B	367	SER
1	B	417	ASN
1	B	443	ASP
1	B	456	THR
1	B	626	LEU
1	B	649	ARG
1	B	698	LEU
1	B	708	LEU
1	B	740	LEU
1	B	755	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	214	GLN
1	A	249	GLN
1	A	421	HIS
1	A	475	GLN
1	A	537	GLN
1	A	585	GLN
1	A	592	ASN
1	A	754	GLN
1	B	249	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	ASN
1	B	373	GLN
1	B	421	HIS
1	B	475	GLN
1	B	584	GLN
1	B	585	GLN
1	B	592	ASN
1	B	754	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ANP	B	901	-	33,33,33	2.74	13 (39%)	45,52,52	2.56	17 (37%)
2	ANP	A	901	-	33,33,33	2.30	11 (33%)	45,52,52	2.17	13 (28%)

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	ANP	B	901	-	-	9/18/38/38	0/3/3/3
2	ANP	A	901	-	-	1/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ANP	C2-N1	-6.52	1.22	1.33
2	B	901	ANP	PB-N3B	6.09	1.79	1.63
2	A	901	ANP	PB-N3B	6.03	1.79	1.63
2	B	901	ANP	PG-N3B	5.82	1.78	1.63
2	A	901	ANP	PG-N3B	5.31	1.77	1.63
2	A	901	ANP	C5-C4	5.19	1.48	1.39
2	B	901	ANP	PG-O1G	4.57	1.53	1.46
2	B	901	ANP	C5-N7	-4.49	1.30	1.39
2	B	901	ANP	PA-O3A	3.65	1.63	1.59
2	A	901	ANP	PG-O1G	3.42	1.51	1.46
2	B	901	ANP	PB-O1B	3.40	1.51	1.46
2	A	901	ANP	PA-O3A	3.19	1.62	1.59
2	B	901	ANP	C4-N3	-3.17	1.28	1.34
2	A	901	ANP	C8-N7	3.03	1.37	1.31
2	B	901	ANP	C8-N9	-3.00	1.32	1.37
2	A	901	ANP	PB-O2B	-2.99	1.48	1.56
2	B	901	ANP	C6-N6	-2.96	1.26	1.34
2	B	901	ANP	C4-N9	-2.84	1.31	1.37
2	A	901	ANP	C5-N7	-2.61	1.34	1.39
2	A	901	ANP	PB-O3A	2.27	1.61	1.59
2	A	901	ANP	PG-O3G	-2.19	1.51	1.56
2	A	901	ANP	C5-C6	2.16	1.47	1.41
2	B	901	ANP	PB-O3A	2.13	1.61	1.59
2	B	901	ANP	PB-O2B	-2.08	1.51	1.56

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ANP	O1G-PG-N3B	-7.93	100.10	111.77
2	B	901	ANP	C5-C4-N3	-6.98	117.10	126.72
2	B	901	ANP	N3-C4-N9	5.69	136.84	127.17
2	B	901	ANP	N9-C8-N7	-5.43	106.24	113.94
2	B	901	ANP	C2-N3-C4	5.02	124.09	111.83
2	A	901	ANP	C5-C4-N3	-4.99	119.84	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ANP	C5-N7-C8	4.89	111.14	103.45
2	B	901	ANP	O2B-PB-O1B	4.68	119.91	109.87
2	A	901	ANP	N3-C4-N9	4.13	134.19	127.17
2	B	901	ANP	C4-N9-C8	4.05	109.99	105.74
2	B	901	ANP	C4-C5-N7	-3.68	106.38	110.58
2	B	901	ANP	C6-C5-N7	3.60	139.03	132.09
2	A	901	ANP	C4-C5-N7	-3.15	106.98	110.58
2	A	901	ANP	N3-C2-N1	-3.12	123.86	128.58
2	A	901	ANP	C4-N9-C8	3.00	108.89	105.74
2	B	901	ANP	N3-C2-N1	-3.00	124.05	128.58
2	A	901	ANP	O1B-PB-N3B	-2.98	107.39	111.77
2	A	901	ANP	C2-N3-C4	2.93	118.98	111.83
2	B	901	ANP	C3'-C2'-C1'	2.91	106.98	101.46
2	B	901	ANP	C5-C6-N6	-2.61	116.82	123.29
2	A	901	ANP	C5-N7-C8	2.48	107.35	103.45
2	B	901	ANP	C5-C6-N1	2.47	123.79	117.51
2	A	901	ANP	C3'-C2'-C1'	2.36	105.94	101.46
2	B	901	ANP	O2B-PB-O3A	2.36	112.51	104.64
2	B	901	ANP	O2G-PG-O3G	2.29	113.76	107.59
2	A	901	ANP	N9-C8-N7	-2.22	110.79	113.94
2	A	901	ANP	O2A-PA-O1A	2.12	122.31	112.44
2	B	901	ANP	C1'-N9-C8	-2.10	122.44	127.09
2	A	901	ANP	C2-N1-C6	2.08	122.15	118.73
2	B	901	ANP	O1G-PG-N3B	-2.06	108.74	111.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

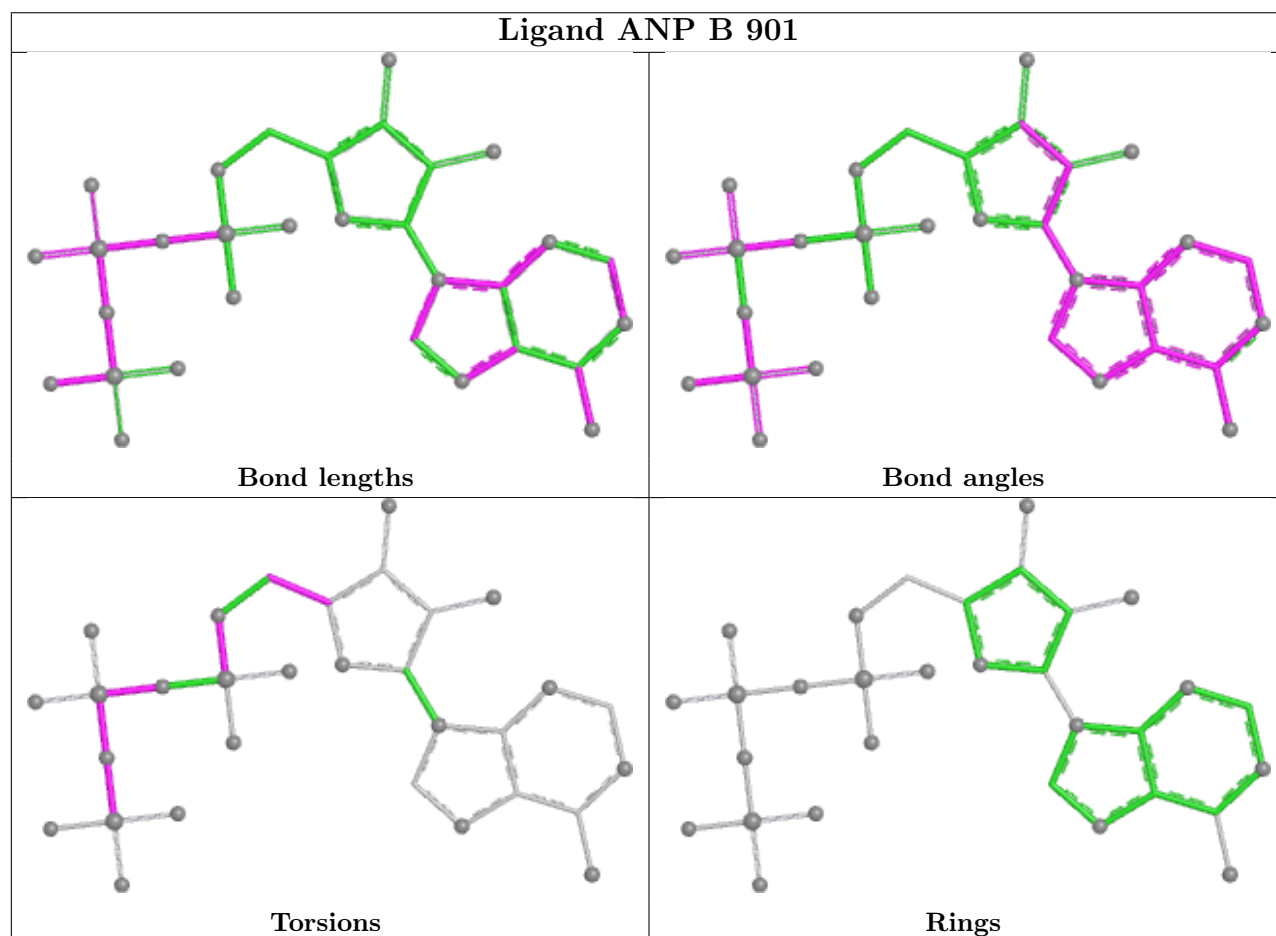
Mol	Chain	Res	Type	Atoms
2	A	901	ANP	PG-N3B-PB-O1B
2	B	901	ANP	PB-N3B-PG-O1G
2	B	901	ANP	PG-N3B-PB-O1B
2	B	901	ANP	PA-O3A-PB-O2B
2	B	901	ANP	C5'-O5'-PA-O1A
2	B	901	ANP	C5'-O5'-PA-O2A
2	B	901	ANP	C5'-O5'-PA-O3A
2	B	901	ANP	O4'-C4'-C5'-O5'
2	B	901	ANP	C3'-C4'-C5'-O5'
2	B	901	ANP	PG-N3B-PB-O3A

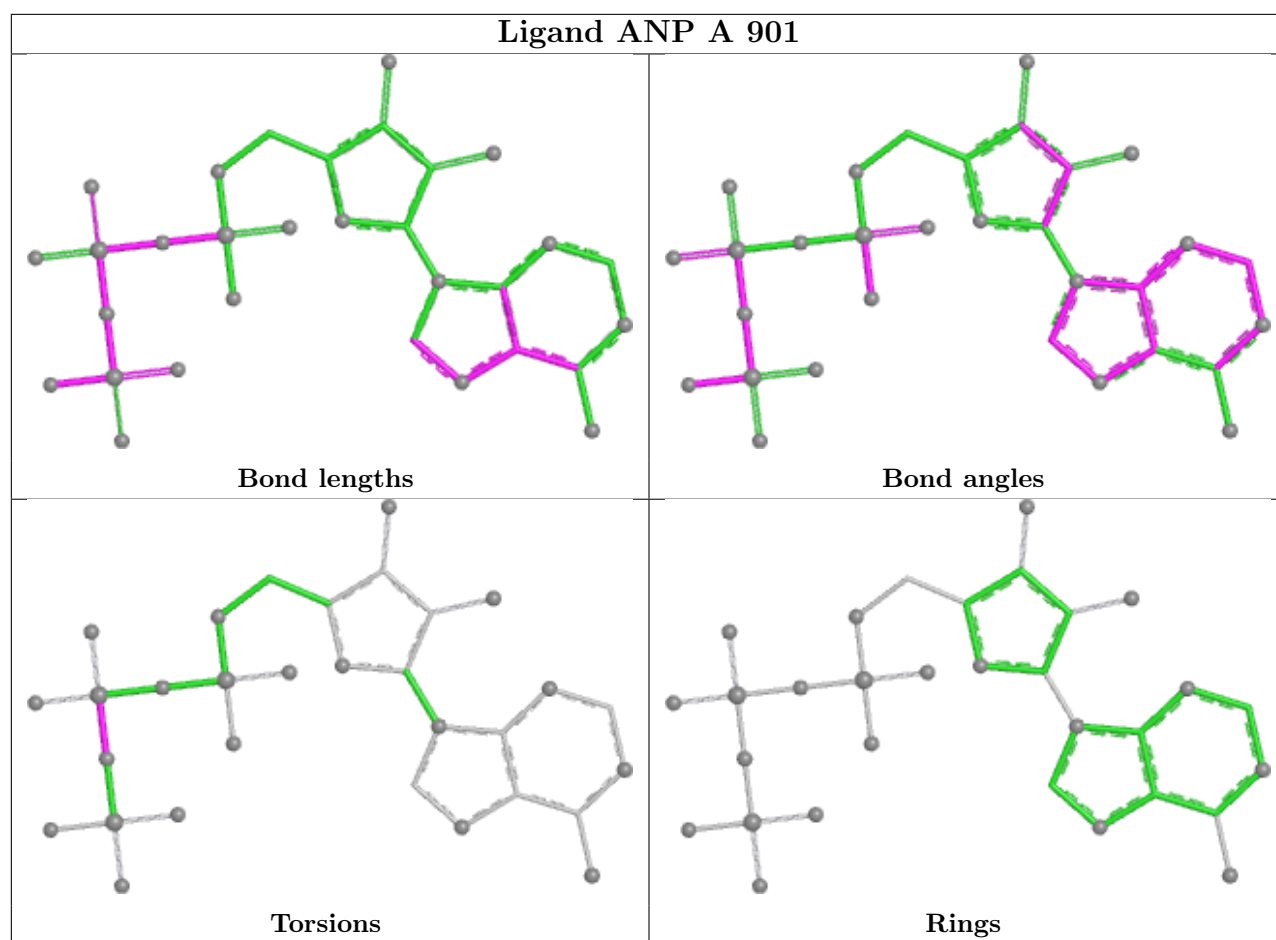
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ANP	8	0
2	A	901	ANP	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	771/816 (94%)	-0.26	5 (0%) 85 73	50, 84, 147, 212	0
1	B	771/816 (94%)	0.06	12 (1%) 70 52	75, 121, 210, 281	0
All	All	1542/1632 (94%)	-0.10	17 (1%) 78 60	50, 103, 182, 281	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	VAL	4.7
1	A	785	HIS	3.9
1	B	767	ALA	3.6
1	B	785	HIS	3.4
1	B	775	PRO	3.1
1	B	770	LYS	3.0
1	A	662	THR	2.6
1	B	661	SER	2.6
1	B	101	PRO	2.5
1	A	783	GLN	2.5
1	B	469	ILE	2.4
1	B	502	ALA	2.3
1	B	763	SER	2.3
1	A	692	THR	2.2
1	A	775	PRO	2.2
1	B	467	PHE	2.1
1	B	450	GLU	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](#)

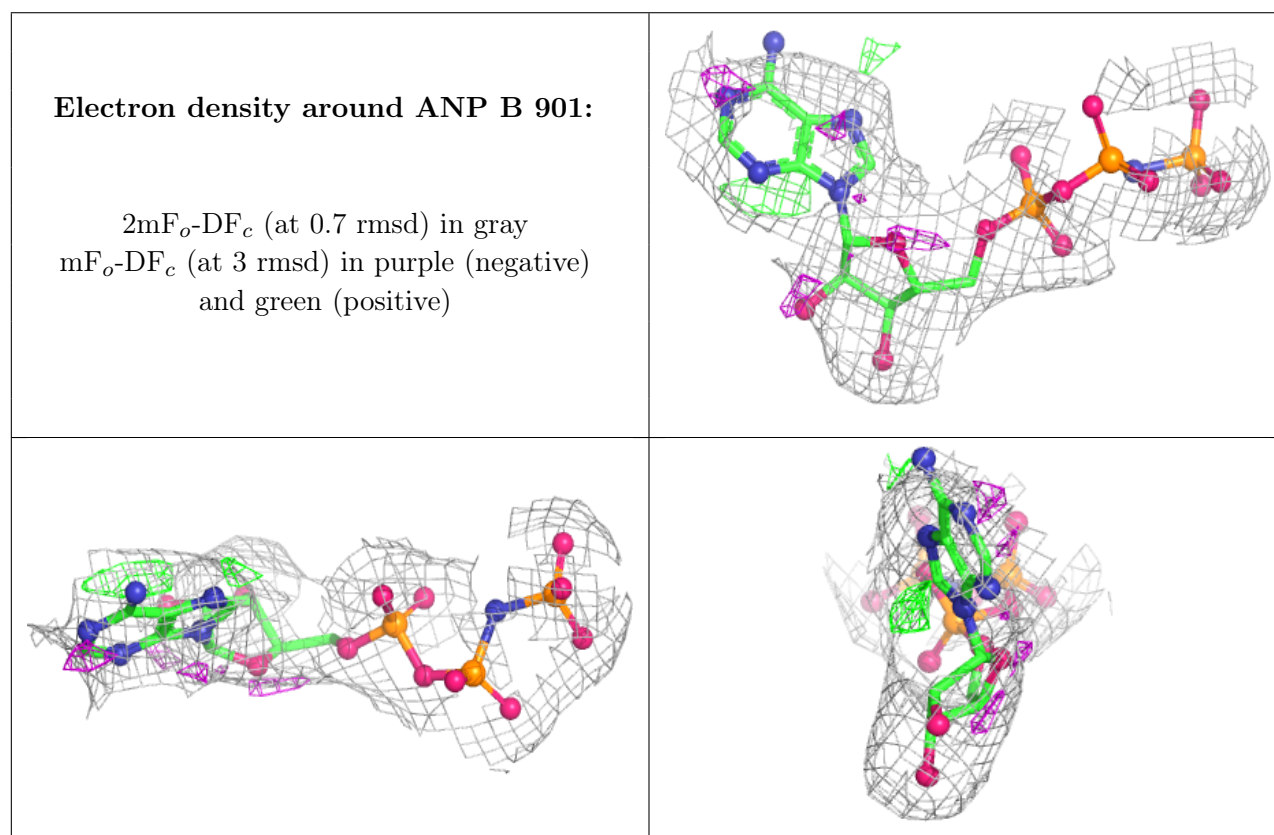
There are no oligosaccharides in this entry.

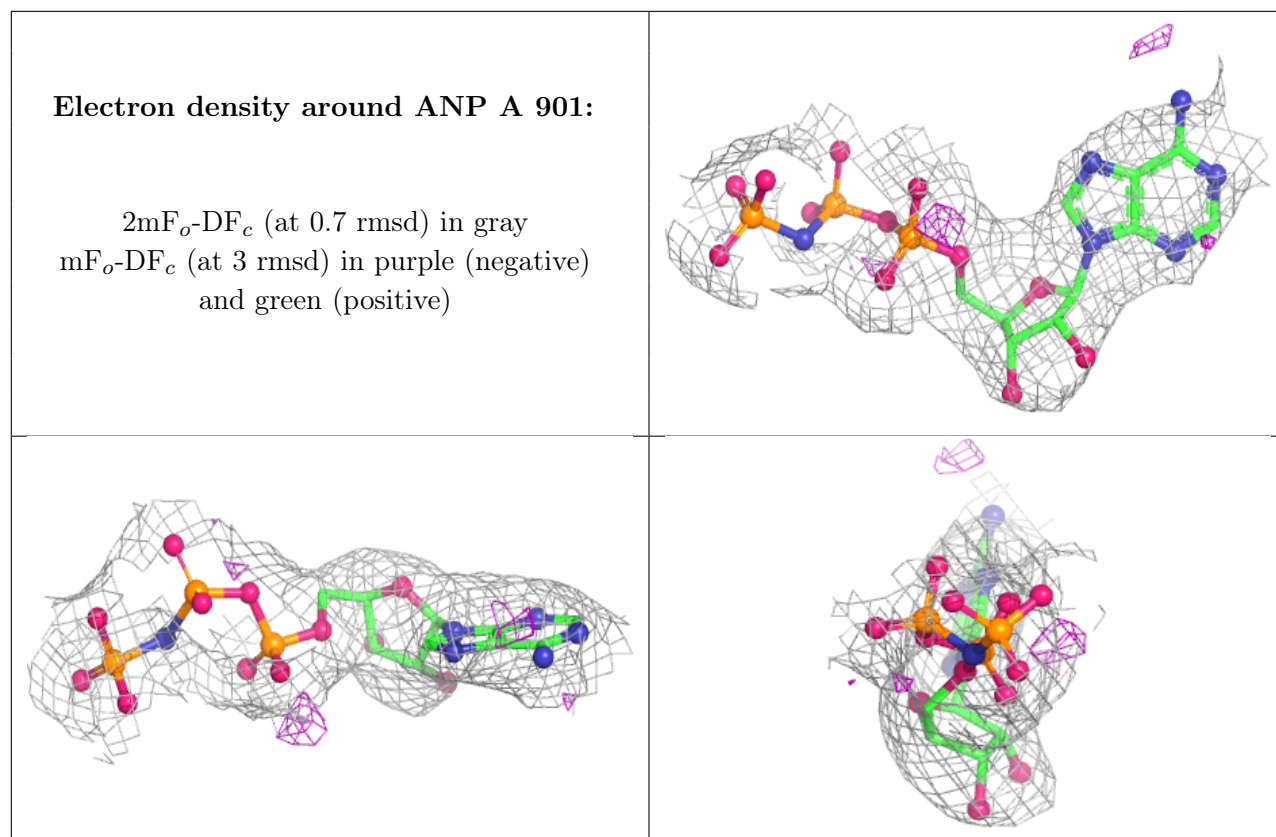
6.4 Ligands [i](#)

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	ANP	B	901	31/31	0.93	0.09	73,96,131,139	0
2	ANP	A	901	31/31	0.97	0.05	63,77,98,107	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.