



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:42 AM EDT

PDB ID : 5N6A / pdb_00005n6a
Title : Cardiac muscle myosin motor domain in the pre-powerstroke state
Authors : Planelles-Herrero, V.J.; Hartman, J.J.; Robert-Paganin, J.; Malik, F.I.; Houdusse, A.
Deposited on : 2017-02-14
Resolution : 3.10 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

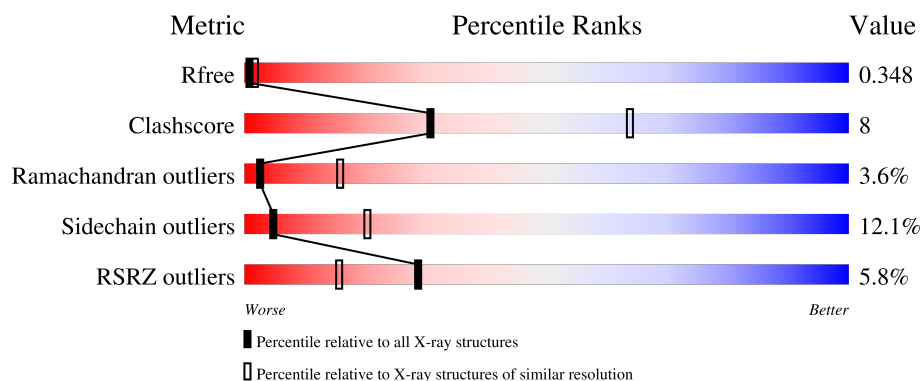
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	828	5% 59% 23% • 14%

2 Entry composition [i](#)

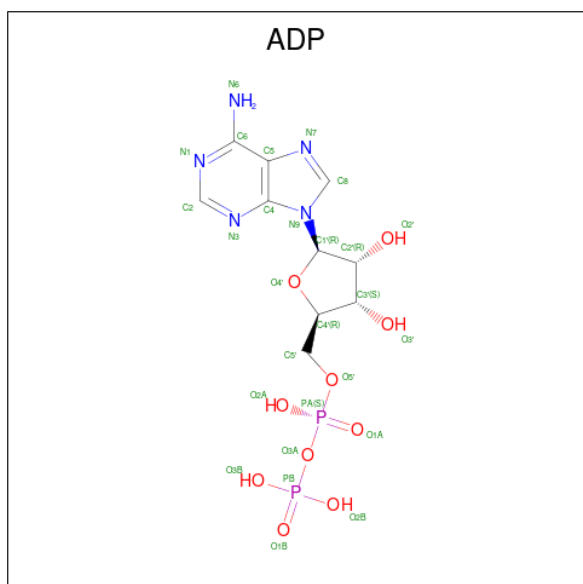
There are 6 unique types of molecules in this entry. The entry contains 5569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-7.

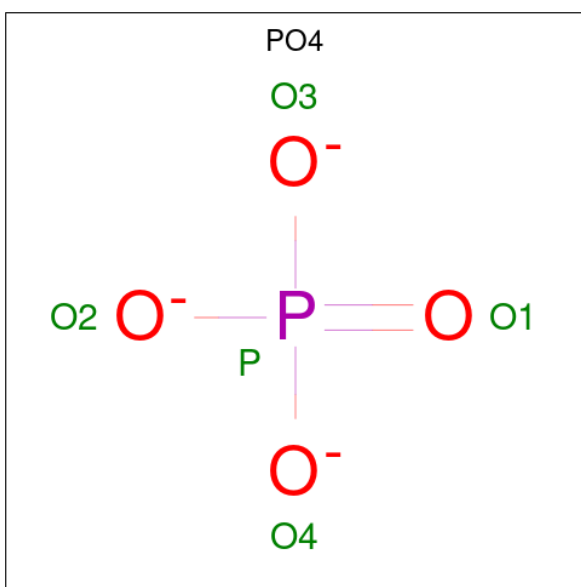
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	710	5494	3511	926	1035	22	0	1	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

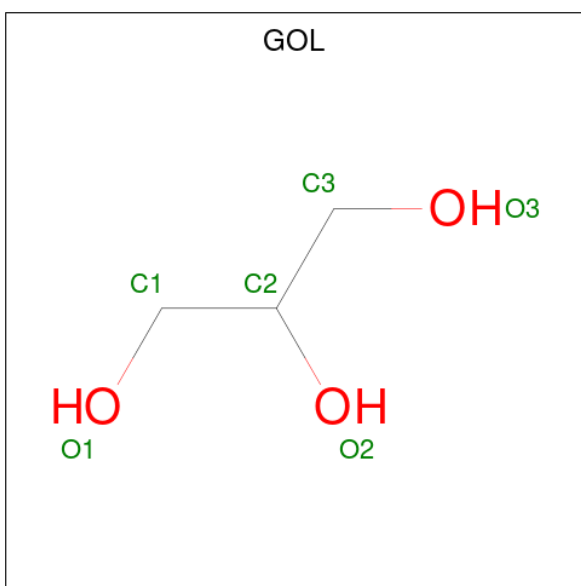


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

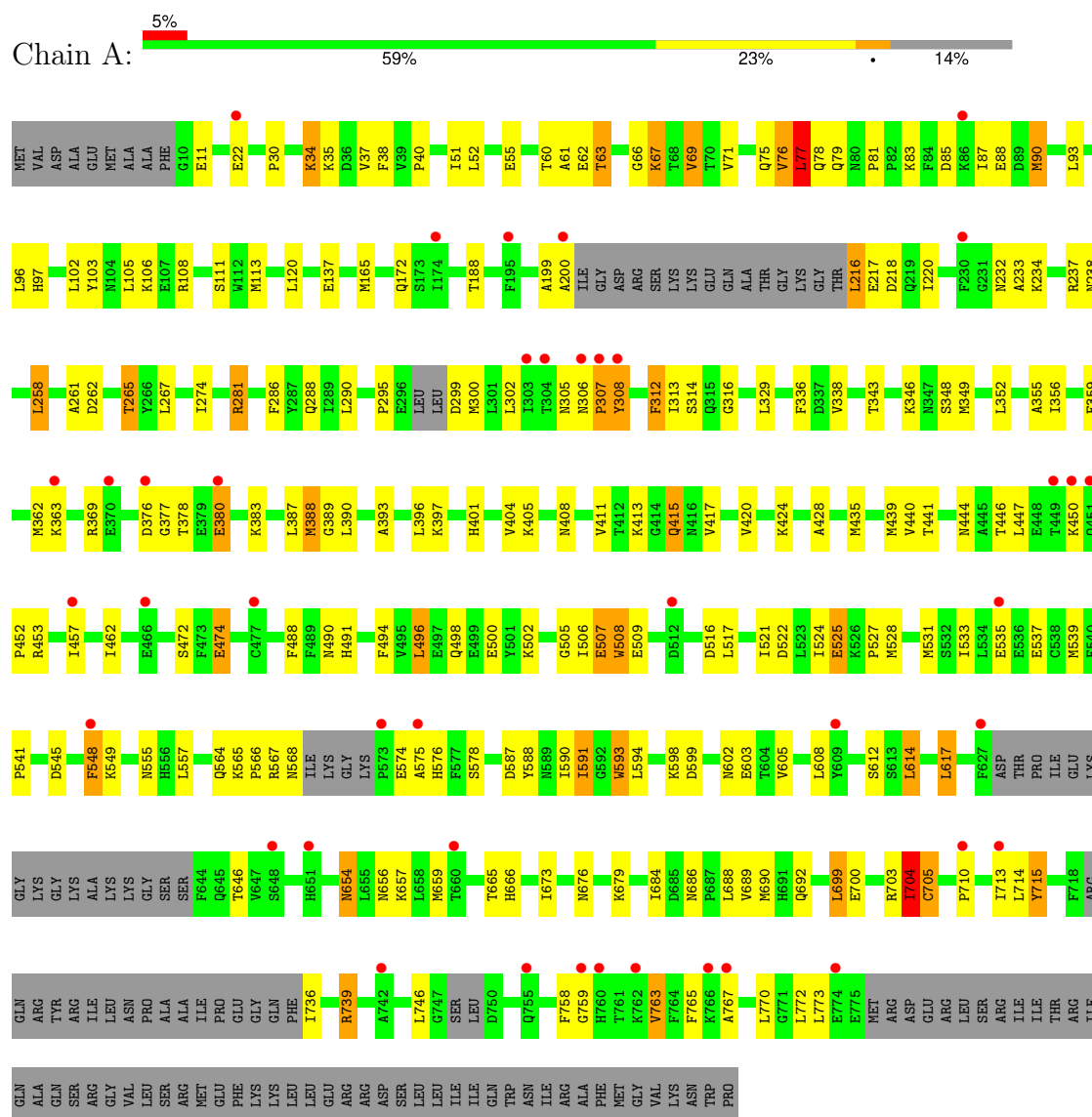
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		

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: Myosin-7



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.66Å 149.83Å 154.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 3.10 43.83 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.83-3.10) 99.8 (43.83-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.247 , 0.320 0.263 , 0.348	Depositor DCC
R_{free} test set	940 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5569	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: GOL, PO4, MG, 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	0.88	0/5605	1.45	52/7576 (0.7%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	705	CYS	N-CA-C	-7.12	103.85	112.54
1	A	654	ASN	CA-C-N	7.03	130.27	120.29
1	A	654	ASN	C-N-CA	7.03	130.27	120.29
1	A	507	GLU	CA-C-N	6.30	133.57	121.54
1	A	507	GLU	C-N-CA	6.30	133.57	121.54
1	A	262	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	312	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	308	TYR	CA-C-N	6.14	128.79	120.38
1	A	308	TYR	C-N-CA	6.14	128.79	120.38
1	A	380	GLU	N-CA-C	-6.02	105.98	113.38
1	A	591	ILE	N-CA-C	-5.91	100.50	108.06
1	A	415	GLN	N-CA-C	5.88	118.29	110.53
1	A	692	GLN	N-CA-C	-5.79	104.57	111.69
1	A	67	LYS	CA-C-N	5.79	132.60	121.54
1	A	67	LYS	C-N-CA	5.79	132.60	121.54
1	A	549	LYS	N-CA-C	-5.63	104.76	111.69
1	A	383	LYS	N-CA-C	-5.62	105.24	111.36
1	A	396	LEU	N-CA-C	-5.62	105.06	111.07
1	A	567	ARG	CA-C-N	5.54	131.66	121.70
1	A	567	ARG	C-N-CA	5.54	131.66	121.70
1	A	765	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	75	GLN	CA-C-N	5.45	131.78	121.97
1	A	75	GLN	C-N-CA	5.45	131.78	121.97
1	A	218	ASP	N-CA-C	-5.44	105.38	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	ASN	CA-C-N	5.43	127.88	120.54
1	A	656	ASN	C-N-CA	5.43	127.88	120.54
1	A	408	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	111	SER	CA-C-N	5.40	129.85	122.34
1	A	111	SER	C-N-CA	5.40	129.85	122.34
1	A	704	ILE	N-CA-CB	5.35	120.05	111.23
1	A	490	ASN	CA-C-N	5.28	127.89	120.28
1	A	490	ASN	C-N-CA	5.28	127.89	120.28
1	A	120	LEU	CA-C-N	5.28	128.60	121.05
1	A	120	LEU	C-N-CA	5.28	128.60	121.05
1	A	232	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	356	ILE	N-CA-C	-5.26	105.41	110.72
1	A	78	GLN	N-CA-C	5.25	117.30	110.53
1	A	656	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	599	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	188	THR	CA-C-N	5.16	127.44	120.38
1	A	188	THR	C-N-CA	5.16	127.44	120.38
1	A	614	LEU	CA-C-N	5.11	127.13	120.28
1	A	614	LEU	C-N-CA	5.11	127.13	120.28
1	A	69	VAL	CA-C-N	5.10	127.12	120.28
1	A	69	VAL	C-N-CA	5.10	127.12	120.28
1	A	428	ALA	CA-C-N	5.06	127.06	120.28
1	A	428	ALA	C-N-CA	5.06	127.06	120.28
1	A	548	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	452	PRO	CA-C-N	5.02	131.12	121.54
1	A	452	PRO	C-N-CA	5.02	131.12	121.54
1	A	539	MET	CA-C-N	5.01	127.38	120.67
1	A	539	MET	C-N-CA	5.01	127.38	120.67

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	5494	0	5216	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	12	2	0
3	A	5	0	0	1	0
4	A	1	0	0	0	0
5	A	6	0	8	1	0
6	A	36	0	0	6	0
All	All	5569	0	5236	89	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 (89) 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:77:LEU:HB2	1:A:97:HIS:CD2	2.00	0.96
1:A:593:TRP:HB2	6:A:1018:HOH:O	1.74	0.88
1:A:90:MET:HE1	1:A:105:LEU:HG	1.63	0.80
1:A:238:ASN:HA	1:A:679:LYS:HE3	1.69	0.74
1:A:77:LEU:CB	1:A:97:HIS:CD2	2.74	0.69
1:A:305:ASN:HD22	1:A:307:PRO:HD2	1.59	0.66
1:A:703:ARG:O	1:A:704:ILE:HG13	1.95	0.66
1:A:77:LEU:HB2	1:A:97:HIS:NE2	2.10	0.65
1:A:388:MET:CB	1:A:612:SER:HB2	2.29	0.63
1:A:498:GLN:HE21	1:A:508:TRP:HE1	1.48	0.61
1:A:491:HIS:O	1:A:496:LEU:HB2	2.02	0.60
1:A:524:ILE:O	1:A:531:MET:HG2	2.00	0.60
1:A:349:MET:HA	1:A:352:LEU:HD12	1.84	0.58
1:A:37:VAL:HG11	1:A:60:THR:HG21	1.85	0.58
1:A:531:MET:O	1:A:535:GLU:HG2	2.03	0.57
1:A:363:LYS:HG2	1:A:376:ASP:H	1.69	0.56
1:A:234:LYS:HB3	1:A:281:ARG:HB2	1.88	0.55
1:A:265:THR:HG21	1:A:440:VAL:HG21	1.89	0.55
1:A:710:PRO:HG2	1:A:767:ALA:HB2	1.88	0.55
1:A:295:PRO:HB2	1:A:300:MET:H	1.73	0.54
1:A:564:GLN:HB3	1:A:578:SER:HB2	1.89	0.54
1:A:199:ALA:HB3	1:A:258:LEU:HD12	1.90	0.54
1:A:594:LEU:O	1:A:598:LYS:HG2	2.08	0.54
1:A:288:GLN:HB3	1:A:329:LEU:HB2	1.91	0.53
1:A:38:PHE:CE1	1:A:79:GLN:HG2	2.43	0.53
1:A:404:VAL:HG12	1:A:405:LYS:N	2.24	0.53
1:A:35:LYS:HG2	1:A:51:ILE:HD12	1.91	0.52
2:A:901:ADP:O1B	3:A:902:PO4:P	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:HIS:HB2	1:A:588:TYR:O	2.09	0.52
1:A:575:ALA:HB3	5:A:904:GOL:H31	1.92	0.52
1:A:290:LEU:HD13	1:A:306:ASN:HA	1.90	0.52
1:A:352:LEU:HD21	1:A:617:LEU:HB3	1.90	0.52
1:A:265:THR:CG2	1:A:440:VAL:HG21	2.39	0.51
1:A:474:GLU:CD	1:A:474:GLU:H	2.18	0.51
1:A:217:GLU:HB3	1:A:220:ILE:HD12	1.93	0.51
1:A:537:GLU:HG3	1:A:548:PHE:CB	2.41	0.50
1:A:81:PRO:C	1:A:83:LYS:H	2.19	0.50
1:A:76:VAL:HG13	1:A:77:LEU:H	1.78	0.49
1:A:281:ARG:NH1	6:A:1001:HOH:O	2.46	0.49
1:A:488:PHE:HB2	1:A:659:MET:HE1	1.94	0.48
1:A:316:GLY:HA3	6:A:1005:HOH:O	2.13	0.48
1:A:527:PRO:HA	1:A:528:MET:HA	1.55	0.48
1:A:537:GLU:HG3	1:A:548:PHE:HB2	1.94	0.48
1:A:305:ASN:ND2	1:A:307:PRO:HD2	2.27	0.47
1:A:590:ILE:HG23	6:A:1018:HOH:O	2.14	0.47
1:A:686:ASN:O	1:A:690:MET:HB2	2.15	0.47
1:A:343:THR:HA	1:A:346:LYS:HE3	1.97	0.47
1:A:88:GLU:HG2	1:A:108:ARG:HH12	1.80	0.46
1:A:85:ASP:CG	1:A:103:TYR:HE2	2.23	0.46
1:A:401:HIS:HA	1:A:413:LYS:O	2.15	0.46
1:A:770:LEU:HA	1:A:773:LEU:HB2	1.98	0.45
1:A:216:LEU:HB3	1:A:217:GLU:H	1.57	0.45
1:A:172:GLN:OE1	1:A:666:HIS:HB3	2.17	0.45
1:A:703:ARG:C	1:A:705:CYS:H	2.24	0.45
1:A:336:PHE:HD2	1:A:346:LYS:HG2	1.82	0.45
1:A:673:ILE:HG21	1:A:689:VAL:HG13	1.99	0.45
1:A:359:PHE:HA	1:A:362:MET:HE2	1.97	0.45
1:A:545:ASP:HA	1:A:548:PHE:CE2	2.51	0.45
1:A:61:ALA:O	1:A:67:LYS:HA	2.17	0.44
1:A:286:PHE:HB3	1:A:313:ILE:HD11	1.98	0.44
1:A:713:ILE:HG13	1:A:714:LEU:H	1.81	0.44
1:A:758:PHE:HB3	1:A:763:VAL:HG13	2.00	0.44
1:A:387:LEU:HD23	1:A:617:LEU:HD22	2.00	0.44
1:A:545:ASP:HA	1:A:548:PHE:HE2	1.83	0.44
1:A:81:PRO:C	1:A:83:LYS:N	2.75	0.43
1:A:172:GLN:HB2	1:A:457:ILE:HD13	2.00	0.43
1:A:97:HIS:HA	1:A:699:LEU:HD21	2.00	0.43
1:A:34:LYS:HE3	1:A:34:LYS:HB3	1.36	0.43
1:A:261:ALA:HB3	1:A:447:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD22	1:A:216:LEU:HA	1.63	0.43
1:A:233:ALA:HA	6:A:1001:HOH:O	2.19	0.43
1:A:404:VAL:HG12	1:A:405:LYS:H	1.83	0.43
1:A:238:ASN:ND2	2:A:901:ADP:H5'2	2.34	0.42
1:A:274:ILE:HG22	1:A:312:PHE:CZ	2.54	0.42
1:A:355:ALA:CB	1:A:387:LEU:HG	2.50	0.41
1:A:420:VAL:HG12	6:A:1032:HOH:O	2.19	0.41
1:A:435:MET:O	1:A:439:MET:HG2	2.20	0.41
1:A:715:TYR:HB3	1:A:739:ARG:HA	2.01	0.41
1:A:525:GLU:H	1:A:525:GLU:HG3	1.72	0.41
1:A:63:THR:HA	1:A:66:GLY:O	2.20	0.41
1:A:614:LEU:HD23	1:A:617:LEU:HD23	2.03	0.41
1:A:200:ALA:HB2	1:A:258:LEU:HD13	2.03	0.41
1:A:444:ASN:C	1:A:446:THR:H	2.27	0.41
1:A:566:PRO:HD2	1:A:576:HIS:O	2.20	0.40
1:A:348:SER:HA	1:A:614:LEU:HD21	2.02	0.40
1:A:393:ALA:O	1:A:397:LYS:HG2	2.21	0.40
1:A:676:ASN:HA	1:A:688:LEU:CD2	2.50	0.40
1:A:557:LEU:HD13	1:A:565:LYS:HB3	2.03	0.40
1:A:505:GLY:C	1:A:507:GLU:H	2.30	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	697/828 (84%)	595 (85%)	77 (11%)	25 (4%)	2 16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	VAL

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Mol	Chain	Res	Type
1	A	308	TYR
1	A	453	ARG
1	A	508	TRP
1	A	509	GLU
1	A	593	TRP
1	A	71	VAL
1	A	77	LEU
1	A	267	LEU
1	A	377	GLY
1	A	388	MET
1	A	506	ILE
1	A	704	ILE
1	A	55	GLU
1	A	307	PRO
1	A	369	ARG
1	A	450	LYS
1	A	314	SER
1	A	389	GLY
1	A	11	GLU
1	A	30	PRO
1	A	502	LYS
1	A	541	PRO
1	A	759	GLY
1	A	40	PRO

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	555/716 (78%)	487 (88%)	68 (12%)	4 20

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	GLU
1	A	22[B]	GLU

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Mol	Chain	Res	Type
1	A	34	LYS
1	A	52	LEU
1	A	62	GLU
1	A	63	THR
1	A	69	VAL
1	A	77	LEU
1	A	87	ILE
1	A	90	MET
1	A	93	LEU
1	A	96	LEU
1	A	102	LEU
1	A	106	LYS
1	A	113	MET
1	A	137	GLU
1	A	165	MET
1	A	216	LEU
1	A	237	ARG
1	A	258	LEU
1	A	265	THR
1	A	281	ARG
1	A	299	ASP
1	A	302	LEU
1	A	338	VAL
1	A	378	THR
1	A	380	GLU
1	A	390	LEU
1	A	411	VAL
1	A	415	GLN
1	A	417	VAL
1	A	424	LYS
1	A	441	THR
1	A	462	ILE
1	A	472	SER
1	A	474	GLU
1	A	494	PHE
1	A	496	LEU
1	A	500	GLU
1	A	516	ASP
1	A	517	LEU
1	A	521	ILE
1	A	522	ASP
1	A	525	GLU

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Mol	Chain	Res	Type
1	A	533	ILE
1	A	555	ASN
1	A	568	ASN
1	A	574	GLU
1	A	587	ASP
1	A	591	ILE
1	A	602	ASN
1	A	603	GLU
1	A	605	VAL
1	A	608	LEU
1	A	617	LEU
1	A	646	THR
1	A	654	ASN
1	A	657	LYS
1	A	665	THR
1	A	684	ILE
1	A	699	LEU
1	A	700	GLU
1	A	715	TYR
1	A	736	ILE
1	A	739	ARG
1	A	746	LEU
1	A	763	VAL
1	A	772	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	97	HIS
1	A	135	ASN
1	A	187	ASN
1	A	224	ASN
1	A	232	ASN
1	A	238	ASN
1	A	240	ASN
1	A	288	GLN
1	A	292	ASN
1	A	305	ASN
1	A	306	ASN
1	A	347	ASN
1	A	415	GLN

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Mol	Chain	Res	Type
1	A	416	ASN
1	A	419	GLN
1	A	479	ASN
1	A	486	GLN
1	A	490	ASN
1	A	491	HIS
1	A	498	GLN
1	A	562	ASN
1	A	696	ASN
1	A	711	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	901	4	28,29,29	0.70	1 (3%)	43,45,45	0.79	1 (2%)
5	GOL	A	904	-	5,5,5	0.06	0	5,5,5	0.43	0
3	PO4	A	902	4	4,4,4	2.50	2 (50%)	6,6,6	1.06	1 (16%)

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	901	4	-	1/16/32/32	0/3/3/3
5	GOL	A	904	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	PO4	P-O1	4.15	1.60	1.50
2	A	901	ADP	PB-O2B	-2.94	1.43	1.54
3	A	902	PO4	P-O2	2.03	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ADP	O2B-PB-O3A	2.63	113.44	104.64
3	A	902	PO4	O3-P-O2	2.07	114.34	107.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ADP	PB-O3A-PA-O2A

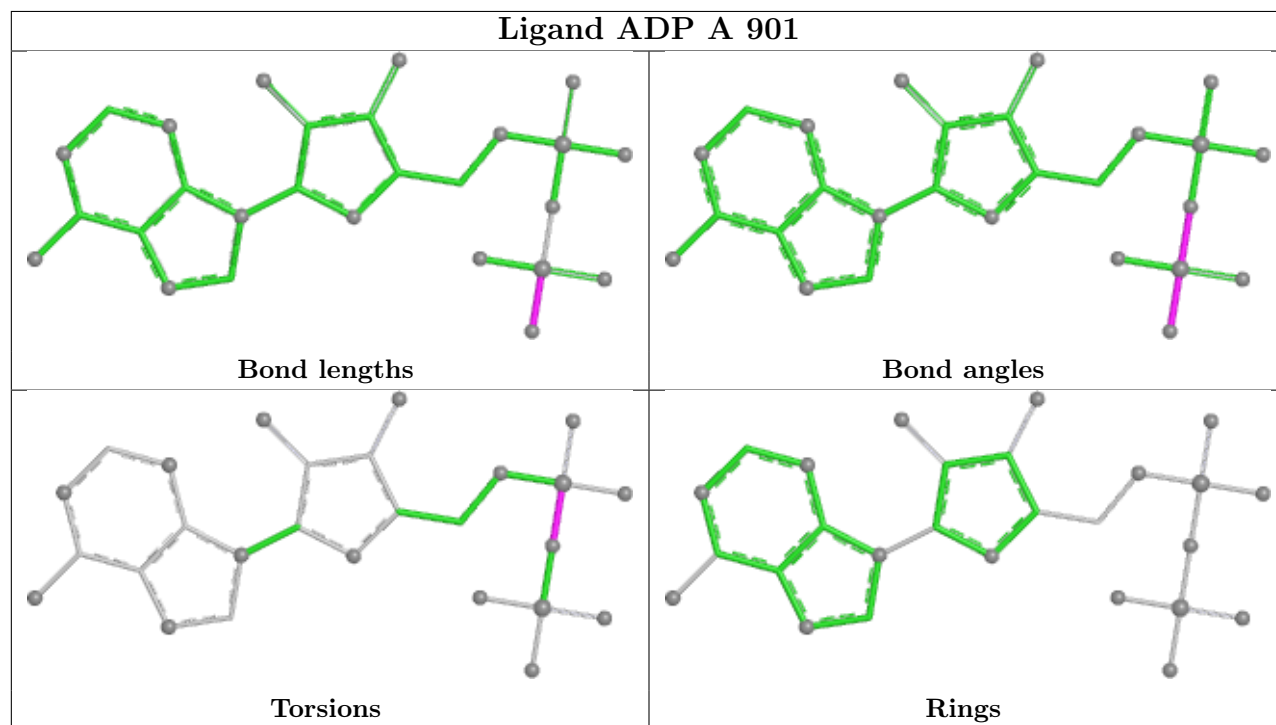
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ADP	2	0
5	A	904	GOL	1	0
3	A	902	PO4	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	710/828 (85%)	0.59	41 (5%) 29 16	39, 80, 160, 209	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ASN	4.2
1	A	195	PHE	3.7
1	A	86	LYS	3.6
1	A	575	ALA	3.6
1	A	512	ASP	3.1
1	A	380	GLU	3.0
1	A	307	PRO	3.0
1	A	573	PRO	2.9
1	A	308	TYR	2.9
1	A	363	LYS	2.9
1	A	759	GLY	2.8
1	A	200	ALA	2.8
1	A	660	THR	2.8
1	A	230	PHE	2.7
1	A	451	GLN	2.7
1	A	766	LYS	2.7
1	A	376	ASP	2.7
1	A	774	GLU	2.6
1	A	466	GLU	2.6
1	A	450	LYS	2.6
1	A	609	TYR	2.5
1	A	742	ALA	2.5
1	A	303	ILE	2.4
1	A	627	PHE	2.4
1	A	477	CYS	2.4
1	A	648	SER	2.3
1	A	755	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	535	GLU	2.3
1	A	457	ILE	2.3
1	A	710	PRO	2.3
1	A	762	LYS	2.3
1	A	713	ILE	2.2
1	A	304	THR	2.2
1	A	22[A]	GLU	2.2
1	A	370	GLU	2.2
1	A	548	PHE	2.2
1	A	651	HIS	2.2
1	A	760	HIS	2.1
1	A	449	THR	2.0
1	A	767	ALA	2.0
1	A	174	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](#)

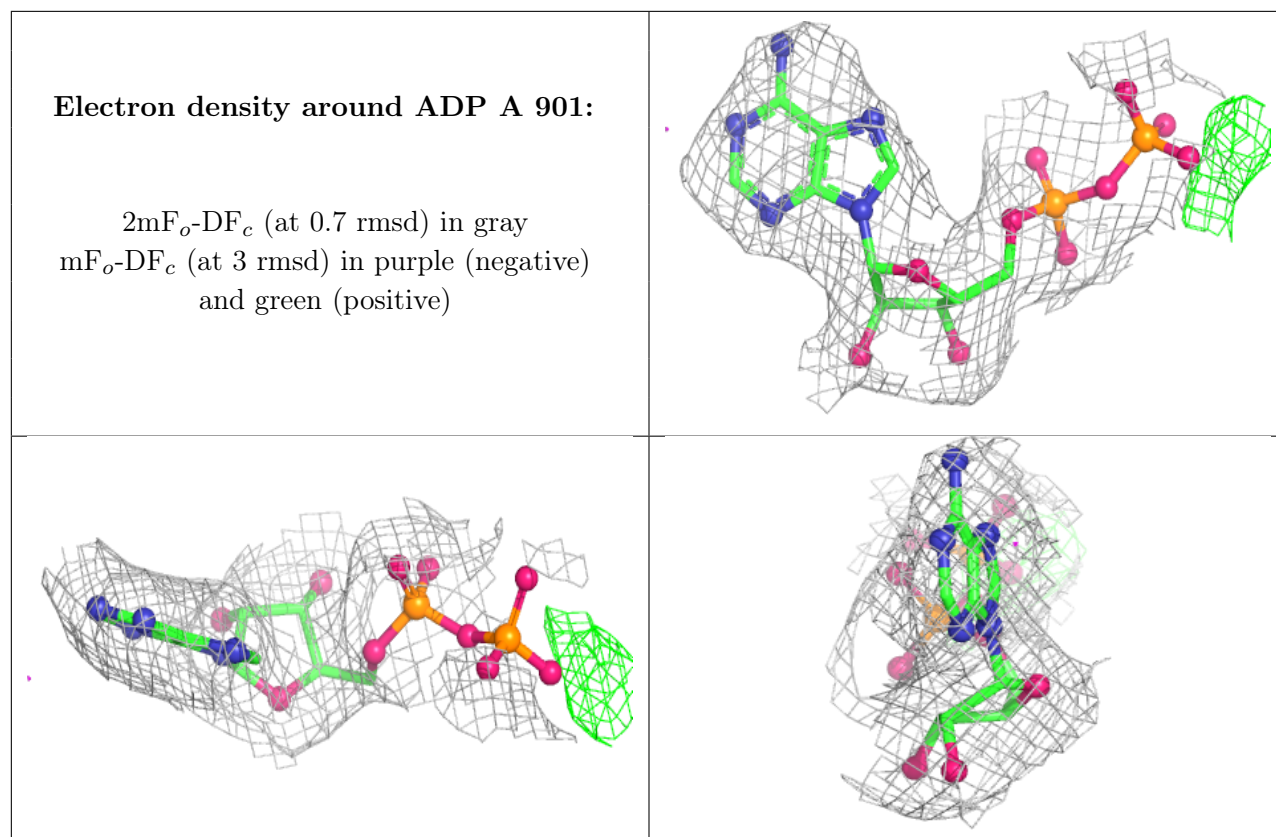
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
5	GOL	A	904	6/6	0.72	0.22	72,77,77,78	0
2	ADP	A	901	27/27	0.93	0.10	52,54,61,62	0
3	PO4	A	902	5/5	0.95	0.10	25,31,35,35	0
4	MG	A	903	1/1	0.98	0.08	70,70,70,70	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.