



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:34 AM EDT

PDB ID : 6YCX / pdb_00006ycx
Title : Plasmodium falciparum Myosin A full-length, pre-powerstroke state
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Deposited on : 2020-03-19
Resolution : 3.99 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

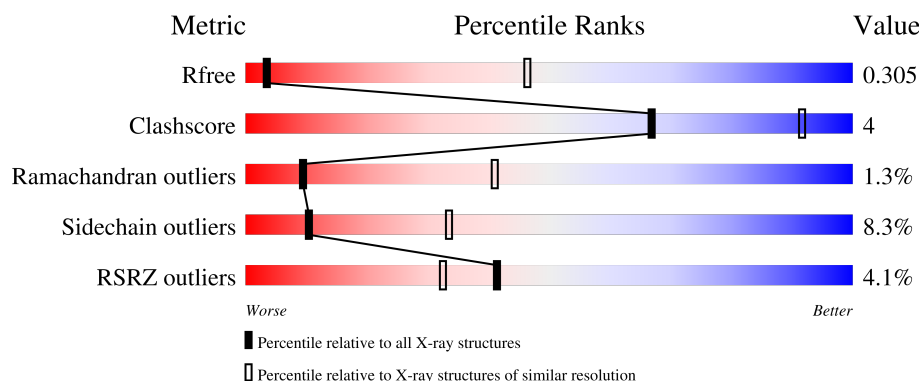
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	818	2% 81% 16% .
1	B	818	7% 82% 16% .
2	D	204	2% 56% 9% 35%
2	H	204	3% 52% 12% . 35%
3	F	134	5% 78% 17% . .

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Mol	Chain	Length	Quality of chain
4	G	134	% 66% 24% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	VO4	A	902	-	-	X	-
6	VO4	B	902	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17452 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-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	P	S	0	11	0
			6541	4157	1110	1236	1	37			
1	B	817	Total	C	N	O	P	S	0	11	0
			6561	4169	1113	1241	1	37			

- Molecule 2 is a protein called Myosin A tail domain interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	133	Total	C	N	O	S	0	0	0
			1066	670	169	222	5			
2	H	133	Total	C	N	O	S	0	1	0
			1077	676	173	223	5			

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	133	Total	C	N	O	S	0	1	0
			1102	701	180	215	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	119	THR	SER	conflict	UNP A0A2I0BQX1

- Molecule 4 is a protein called Uncharacterized protein.

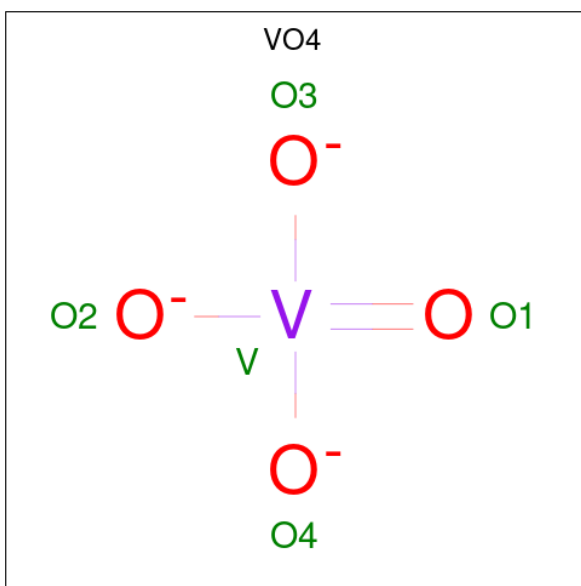
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	125	Total	C	N	O	S	0	1	0
			1039	665	167	201	6			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

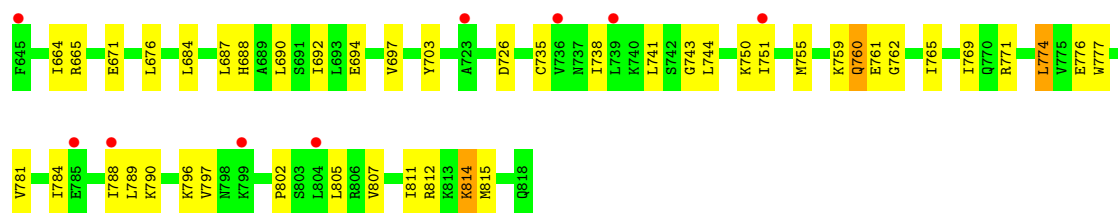
- Molecule 6 is VANADATE ION (CCD ID: VO4) (formula: O_4V).



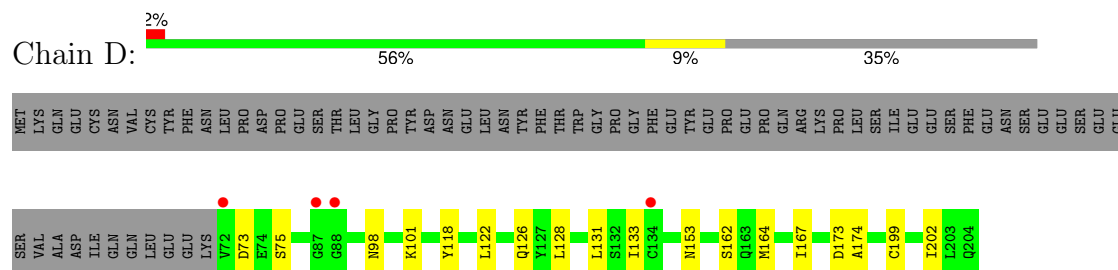
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	V 1	0	0
6	B	1	Total 5	O 4	V 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

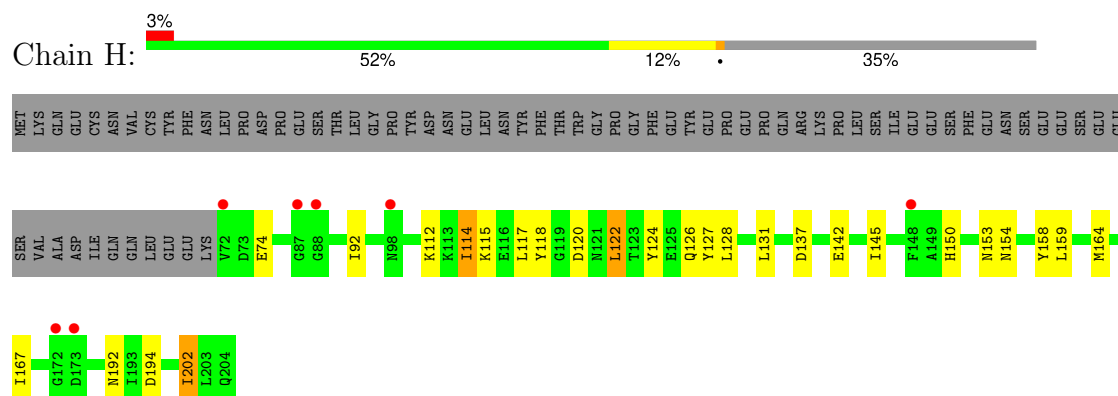
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Mg 1	0	0
7	B	1	Total 1	Mg 1	0	0



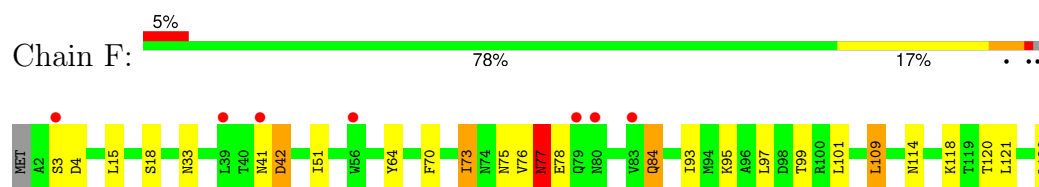
• Molecule 2: Myosin A tail domain interacting protein



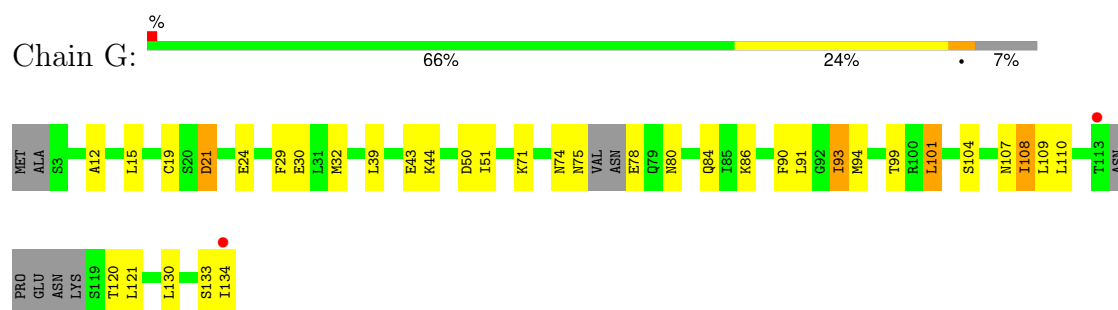
• Molecule 2: Myosin A tail domain interacting protein



• Molecule 3: Uncharacterized protein



• Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.24Å 287.43Å 78.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 3.99 48.40 – 3.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.40-3.99) 99.5 (48.40-3.99)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 4.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.237 , 0.273 0.269 , 0.305	Depositor DCC
R_{free} test set	1663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	154.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 154.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17452	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, ADP, SEP, MG

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	0.75	1/6642 (0.0%)	1.38	26/8952 (0.3%)
1	B	0.73	0/6663	1.36	18/8981 (0.2%)
2	D	0.71	0/1083	1.43	7/1461 (0.5%)
2	H	0.72	0/1094	1.36	0/1475
3	F	0.77	0/1122	1.46	8/1514 (0.5%)
4	G	0.77	0/1056	1.45	3/1420 (0.2%)
All	All	0.74	1/17660 (0.0%)	1.39	62/23803 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	ILE	CA-CB	5.95	1.57	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	ASN	CA-C-N	7.43	127.57	120.43
1	A	800	ASN	C-N-CA	7.43	127.57	120.43
1	B	760	GLN	CA-C-N	6.46	129.23	120.38
1	B	760	GLN	C-N-CA	6.46	129.23	120.38
1	A	784	ILE	CA-C-N	6.24	128.97	120.54
1	A	784	ILE	C-N-CA	6.24	128.97	120.54
1	B	65	LYS	CA-C-N	6.07	130.36	121.31
1	B	65	LYS	C-N-CA	6.07	130.36	121.31
1	A	760	GLN	CA-C-N	6.00	128.24	120.44
1	A	760	GLN	C-N-CA	6.00	128.24	120.44
3	F	33	ASN	CA-CB-CG	5.97	118.57	112.60
3	F	77	ASN	CA-CB-CG	5.93	118.53	112.60
2	D	199	CYS	CA-C-N	5.87	128.47	120.54
2	D	199	CYS	C-N-CA	5.87	128.47	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	HIS	CA-C-N	5.57	127.75	120.28
1	A	160	HIS	C-N-CA	5.57	127.75	120.28
1	B	160	HIS	CA-C-N	5.53	127.69	120.28
1	B	160	HIS	C-N-CA	5.53	127.69	120.28
4	G	30	GLU	CA-C-N	5.48	127.56	120.44
4	G	30	GLU	C-N-CA	5.48	127.56	120.44
1	B	61	SER	CA-C-N	5.47	132.00	121.54
1	B	61	SER	C-N-CA	5.47	132.00	121.54
1	A	640	LEU	CA-C-N	5.44	127.61	120.60
1	A	640	LEU	C-N-CA	5.44	127.61	120.60
1	B	640	LEU	CA-C-N	5.42	127.59	120.60
1	B	640	LEU	C-N-CA	5.42	127.59	120.60
1	B	807	VAL	CA-C-N	5.39	127.51	120.28
1	B	807	VAL	C-N-CA	5.39	127.51	120.28
1	A	789	LEU	CA-C-N	5.37	127.74	120.44
1	A	789	LEU	C-N-CA	5.37	127.74	120.44
1	A	24	PHE	N-CA-C	5.36	115.46	108.07
1	A	812	ARG	CA-C-N	5.28	127.35	120.28
1	A	812	ARG	C-N-CA	5.28	127.35	120.28
1	B	169	THR	CA-C-N	5.27	127.61	120.44
1	B	169	THR	C-N-CA	5.27	127.61	120.44
4	G	21	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	788	ILE	N-CA-C	-5.18	107.36	111.81
1	A	169	THR	CA-C-N	5.18	127.48	120.44
1	A	169	THR	C-N-CA	5.18	127.48	120.44
3	F	73	ILE	N-CA-C	-5.17	106.10	111.58
3	F	76	VAL	CA-C-N	5.13	131.34	121.54
3	F	76	VAL	C-N-CA	5.13	131.34	121.54
1	A	223	ALA	CA-C-N	5.10	127.18	120.60
1	A	223	ALA	C-N-CA	5.10	127.18	120.60
1	B	789	LEU	CA-C-N	5.09	127.56	120.63
1	B	789	LEU	C-N-CA	5.09	127.56	120.63
3	F	42	ASP	CA-CB-CG	5.07	117.67	112.60
2	D	73	ASP	CA-C-N	5.07	127.33	120.38
2	D	73	ASP	C-N-CA	5.07	127.33	120.38
1	A	752	GLY	CA-C-N	5.07	127.38	120.54
1	A	752	GLY	C-N-CA	5.07	127.38	120.54
1	B	223	ALA	CA-C-N	5.04	127.10	120.60
1	B	223	ALA	C-N-CA	5.04	127.10	120.60
3	F	18	SER	CA-C-N	5.04	129.29	122.19
3	F	18	SER	C-N-CA	5.04	129.29	122.19
2	D	173	ASP	CA-CB-CG	5.03	117.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLU	CA-C-N	5.01	127.40	120.29
1	A	333	GLU	C-N-CA	5.01	127.40	120.29
1	A	734	LYS	CA-C-N	5.00	126.94	120.44
1	A	734	LYS	C-N-CA	5.00	126.94	120.44
2	D	126	GLN	CA-C-N	5.00	127.39	120.29
2	D	126	GLN	C-N-CA	5.00	127.39	120.29

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	6541	0	6628	47	0
1	B	6561	0	6654	46	0
2	D	1066	0	1018	4	0
2	H	1077	0	1030	10	0
3	F	1102	0	1080	11	0
4	G	1039	0	1021	17	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	5	0	0	4	0
6	B	5	0	0	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	17452	0	17455	129	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 4.

All (129) 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)
4:G:39:LEU:HB2	4:G:44:LYS:HG3	1.74	0.68
1:A:93:GLN:HA	1:B:93:GLN:HA	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:LYS:HB3	2:H:150:HIS:HE1	1.60	0.65
1:B:788:ILE:HG21	4:G:108:ILE:HG22	1.78	0.65
6:B:902:VO4:O2	6:B:902:VO4:V	1.56	0.63
6:A:902:VO4:O1	6:A:902:VO4:V	1.56	0.61
6:A:902:VO4:V	6:A:902:VO4:O4	1.57	0.61
6:B:902:VO4:V	6:B:902:VO4:O4	1.56	0.61
6:A:902:VO4:V	6:A:902:VO4:O2	1.57	0.61
6:B:902:VO4:V	6:B:902:VO4:O3	1.56	0.61
3:F:114:ASN:HB2	3:F:121:LEU:HD13	1.83	0.61
6:B:902:VO4:V	6:B:902:VO4:O1	1.56	0.60
2:H:128:LEU:HA	2:H:131:LEU:HD12	1.83	0.60
1:A:41:SER:HB3	1:A:44:ILE:HD12	1.84	0.60
6:A:902:VO4:V	6:A:902:VO4:O3	1.58	0.57
4:G:75:ASN:HA	4:G:80:ASN:HB2	1.86	0.57
3:F:84[B]:GLN:HE21	3:F:120:THR:HG23	1.71	0.56
1:A:793:TYR:HB3	3:F:15:LEU:HD22	1.88	0.56
1:B:17:ARG:HH12	1:B:21:VAL:HG22	1.71	0.54
1:A:798:ASN:HA	1:A:801:ILE:HD12	1.90	0.53
2:D:164:MET:HA	2:D:167:ILE:HD12	1.90	0.53
1:A:777:TRP:HA	1:A:780:CYS:HB3	1.91	0.53
1:A:718:PHE:HE1	3:F:93:ILE:HG23	1.74	0.53
2:H:158:TYR:HB3	2:H:192:ASN:HB3	1.90	0.53
1:B:762:GLY:HA2	1:B:765:ILE:HD12	1.91	0.53
1:A:785:GLU:HA	3:F:101:LEU:HD11	1.91	0.52
1:B:372:GLU:HB2	1:B:378:ALA:HB3	1.92	0.52
1:A:508:LEU:HD21	1:A:755:MET:HE1	1.92	0.52
1:A:212:LYS:HE2	3:F:41:ASN:HD21	1.75	0.51
1:A:372:GLU:HB2	1:A:378:ALA:HB3	1.92	0.51
1:B:585:HIS:CD2	1:B:590:ILE:HD12	2.45	0.51
1:B:687:LEU:HA	1:B:692:ILE:HD12	1.92	0.51
1:A:585:HIS:CD2	1:A:590:ILE:HD12	2.45	0.51
4:G:91:LEU:HD21	4:G:109:LEU:HD11	1.93	0.51
4:G:90:PHE:HA	4:G:93:ILE:HD12	1.93	0.51
2:H:92:ILE:HD12	2:H:120:ASP:HA	1.93	0.51
4:G:101:LEU:HD23	4:G:104:SER:HB2	1.93	0.51
3:F:70:PHE:HB3	3:F:73:ILE:HD12	1.93	0.51
1:A:788:ILE:HG13	3:F:109:LEU:HB2	1.92	0.50
1:A:687:LEU:HA	1:A:692:ILE:HD12	1.93	0.50
1:B:133:LEU:HD23	1:B:665:ARG:HG3	1.94	0.50
1:B:777:TRP:HZ3	4:G:93:ILE:HG21	1.77	0.49
1:A:122:LEU:HA	1:A:676:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HA	1:B:676:LEU:HD22	1.94	0.49
2:H:164:MET:HA	2:H:167:ILE:HD12	1.95	0.49
2:H:124:TYR:HA	2:H:127:TYR:HB3	1.94	0.49
1:B:637:LYS:HA	1:B:640:LEU:HD12	1.95	0.49
1:A:751:ILE:HD12	1:A:756:VAL:HG22	1.94	0.49
4:G:107:ASN:HA	4:G:110:LEU:HD12	1.95	0.48
1:A:637:LYS:HA	1:A:640:LEU:HD12	1.95	0.48
1:B:252:MET:HG2	1:B:267:VAL:HG22	1.96	0.48
1:A:36:ILE:HD11	1:A:68:VAL:HG11	1.95	0.47
1:B:54:LYS:HB3	1:B:72:ASP:HB3	1.97	0.47
1:A:5:ASN:HA	1:A:8:ILE:HD12	1.96	0.47
1:A:684:LEU:HA	1:A:687:LEU:HD12	1.96	0.47
1:A:133:LEU:HD23	1:A:665:ARG:HG3	1.96	0.47
1:B:95:ASP:HB3	1:B:98:SER:HB2	1.96	0.47
1:B:684:LEU:HA	1:B:687:LEU:HD12	1.96	0.47
1:A:278:ILE:HG13	1:A:437:LYS:HE2	1.97	0.47
1:A:54:LYS:HB3	1:A:72:ASP:HB3	1.97	0.47
1:B:5:ASN:HA	1:B:8:ILE:HD12	1.95	0.47
4:G:12:ALA:HA	4:G:15:LEU:HD12	1.97	0.47
1:A:252:MET:HG2	1:A:267:VAL:HG22	1.97	0.46
1:B:178:LEU:HD13	1:B:465:MET:HE2	1.98	0.46
1:B:508:LEU:HD11	1:B:755:MET:HE2	1.97	0.46
1:A:373:ALA:HB2	1:A:422:ARG:HB2	1.97	0.46
2:H:112:LYS:HG2	2:H:115:LYS:HD2	1.96	0.46
1:B:788:ILE:HG13	4:G:108:ILE:HB	1.96	0.46
1:B:802:PRO:HA	1:B:805:LEU:HD12	1.98	0.46
1:A:66:LEU:O	1:A:81:ASP:HA	2.16	0.46
1:B:278:ILE:HG13	1:B:437:LYS:HE2	1.98	0.46
1:B:510:LYS:HG2	1:B:516:THR:HA	1.98	0.46
1:B:771:ARG:HA	1:B:774:LEU:HB3	1.99	0.45
1:A:510:LYS:HG2	1:A:516:THR:HA	1.98	0.45
1:B:373:ALA:HB2	1:B:422:ARG:HB2	1.97	0.45
1:B:777:TRP:CZ3	4:G:93:ILE:HG21	2.52	0.45
1:A:55:CYS:HB3	1:A:68:VAL:HB	1.98	0.45
1:A:178:LEU:HD13	1:A:465:MET:HE2	1.98	0.45
1:B:58:GLN:C	1:B:60:GLY:H	2.26	0.45
3:F:114:ASN:HD21	3:F:118:LYS:H	1.66	0.44
4:G:39:LEU:HB3	4:G:43:GLU:HB3	1.99	0.44
1:B:784:ILE:HG23	4:G:130:LEU:HD11	1.99	0.43
2:H:114:ILE:HA	2:H:117:LEU:HD12	1.99	0.43
1:A:181:VAL:HG21	1:A:707:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:HG2	1:B:291:TYR:CZ	2.53	0.43
1:B:358:GLY:HA3	1:B:396:MET:HG3	2.01	0.43
2:D:128:LEU:HA	2:D:131:LEU:HD12	1.99	0.43
1:A:232:GLU:O	1:A:236:ASN:HB2	2.19	0.43
1:A:358:GLY:HA3	1:A:396:MET:HG3	2.01	0.43
1:B:703:TYR:HA	1:B:759:LYS:HA	2.00	0.43
4:G:39:LEU:H	4:G:44:LYS:HE3	1.83	0.43
1:A:285:ARG:HG2	1:A:291:TYR:CZ	2.54	0.43
1:A:706:ARG:HB2	1:A:757:PHE:CD2	2.54	0.43
1:A:774:LEU:O	1:A:778:GLU:HB2	2.18	0.43
1:B:232:GLU:O	1:B:236:ASN:HB2	2.19	0.43
1:B:64:GLU:H	1:B:64:GLU:CD	2.27	0.42
1:B:814:LYS:HD2	2:H:202:ILE:HA	2.01	0.42
4:G:84:GLN:HB3	4:G:120:THR:HB	2.00	0.42
1:A:97:MET:HE2	1:A:120:ARG:HG2	2.01	0.42
1:B:399:ASP:HB3	1:B:402:LEU:HB2	2.00	0.42
1:A:286:SER:HB3	1:A:291:TYR:HE2	1.84	0.42
1:A:399:ASP:HB3	1:A:402:LEU:HB2	2.00	0.42
1:A:762:GLY:HA2	1:A:765:ILE:HD12	2.00	0.42
1:B:234:PHE:HB3	1:B:444:PHE:CD1	2.55	0.42
1:B:665:ARG:HE	1:B:690:LEU:HB3	1.85	0.42
1:A:369:GLU:HG3	1:A:425:LYS:HB2	2.02	0.41
1:A:234:PHE:HB3	1:A:444:PHE:CD1	2.55	0.41
4:G:29:PHE:HA	4:G:32:MET:HG2	2.01	0.41
1:A:56:VAL:O	1:A:68:VAL:HA	2.20	0.41
1:B:286:SER:HB3	1:B:291:TYR:HE2	1.85	0.41
1:B:694:GLU:O	1:B:697:VAL:HG22	2.19	0.41
1:B:735:CYS:HA	1:B:738:ILE:HD12	2.02	0.41
2:H:122:LEU:HB2	2:H:126:GLN:HB2	2.01	0.41
1:A:336:ILE:HA	1:A:339:LEU:HD12	2.02	0.41
1:A:665:ARG:HE	1:A:690:LEU:HB3	1.85	0.41
1:B:369:GLU:HG3	1:B:425:LYS:HB2	2.03	0.41
1:B:336:ILE:HA	1:B:339:LEU:HD12	2.02	0.41
1:A:545[A]:GLN:HB3	1:A:598:LEU:HD21	2.03	0.41
1:B:531:LEU:C	1:B:537:SER:HB2	2.46	0.41
2:D:98:ASN:HA	2:D:101:LYS:HD3	2.03	0.41
1:B:811:ILE:O	1:B:815:MET:HG2	2.21	0.41
3:F:95:LYS:HA	3:F:99:THR:HG22	2.03	0.41
3:F:130:LEU:HA	3:F:133:SER:HB3	2.03	0.40
4:G:104:SER:HA	4:G:107:ASN:HD22	1.85	0.40
1:A:21:VAL:HA	1:A:89:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LYS:HD2	2:D:202:ILE:HA	2.02	0.40
1:A:315:LEU:HD12	1:A:360:LEU:HA	2.03	0.40
1:B:257:SER:HB3	1:B:260:GLY:O	2.22	0.40
1:B:315:LEU:HD12	1:B:360:LEU:HA	2.03	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	820/818 (100%)	757 (92%)	56 (7%)	7 (1%)	14	48
1	B	825/818 (101%)	759 (92%)	52 (6%)	14 (2%)	7	36
2	D	131/204 (64%)	122 (93%)	8 (6%)	1 (1%)	16	52
2	H	132/204 (65%)	120 (91%)	12 (9%)	0	100	100
3	F	132/134 (98%)	116 (88%)	13 (10%)	3 (2%)	5	31
4	G	120/134 (90%)	109 (91%)	9 (8%)	2 (2%)	7	36
All	All	2160/2312 (93%)	1983 (92%)	150 (7%)	27 (1%)	9	41

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	751	ILE
3	F	3	SER
1	A	32	LYS
1	A	271	LEU
1	A	321	THR
1	A	603	ASP
1	B	62	LYS
1	B	271	LEU

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Mol	Chain	Res	Type
1	B	321	THR
1	B	603	ASP
1	B	726	ASP
3	F	64	TYR
3	F	77	ASN
1	A	594	ALA
1	A	722	ALA
1	B	28	GLY
1	B	61	SER
1	B	594	ALA
2	D	174	ALA
4	G	101	LEU
1	B	373	ALA
4	G	74	ASN
1	B	60	GLY
1	A	131	VAL
1	B	131	VAL
1	B	743	GLY
1	B	415	GLY

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	732/725 (101%)	674 (92%)	58 (8%)	11	35
1	B	735/725 (101%)	677 (92%)	58 (8%)	11	35
2	D	119/186 (64%)	113 (95%)	6 (5%)	22	45
2	H	120/186 (64%)	108 (90%)	12 (10%)	7	26
3	F	126/126 (100%)	114 (90%)	12 (10%)	8	28
4	G	119/126 (94%)	103 (87%)	16 (13%)	4	18
All	All	1951/2074 (94%)	1789 (92%)	162 (8%)	10	33

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	26	LYS
1	A	36	ILE
1	A	64	GLU
1	A	66	LEU
1	A	69	VAL
1	A	91	ASN
1	A	92	SER
1	A	93	GLN
1	A	137	ILE
1	A	169	THR
1	A	172	ARG
1	A	173	GLU
1	A	178	LEU
1	A	187	ILE
1	A	190	SER
1	A	205	MET
1	A	221	GLN
1	A	254	LEU
1	A	274	LYS
1	A	298	ASN
1	A	324	SER
1	A	334	GLU
1	A	362	LEU
1	A	371	GLN
1	A	402	LEU
1	A	431	LEU
1	A	448	ILE
1	A	462	LYS
1	A	470	ILE
1	A	471	PHE
1	A	493	LEU
1	A	518	GLU
1	A	519	LEU
1	A	566	GLU
1	A	582	ILE
1	A	637	LYS
1	A	664	ILE
1	A	671	GLU
1	A	688	HIS
1	A	706	ARG
1	A	717	LYS
1	A	720	ASP

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Mol	Chain	Res	Type
1	A	738	ILE
1	A	741	LEU
1	A	748	MET
1	A	761	GLU
1	A	767	THR
1	A	768	LYS
1	A	769	ILE
1	A	771	ARG
1	A	774	LEU
1	A	784	ILE
1	A	789	LEU
1	A	797	VAL
1	A	804	LEU
1	A	805	LEU
1	A	814	LYS
1	B	6	GLU
1	B	21	VAL
1	B	24	PHE
1	B	25	ASP
1	B	26	LYS
1	B	32	LYS
1	B	35	GLN
1	B	41	SER
1	B	58	GLN
1	B	63	LYS
1	B	66	LEU
1	B	91	ASN
1	B	92	SER
1	B	93	GLN
1	B	137	ILE
1	B	169	THR
1	B	172	ARG
1	B	173	GLU
1	B	178	LEU
1	B	187	ILE
1	B	190	SER
1	B	205	MET
1	B	221	GLN
1	B	254	LEU
1	B	274	LYS
1	B	298	ASN
1	B	324	SER

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Mol	Chain	Res	Type
1	B	334	GLU
1	B	362	LEU
1	B	371	GLN
1	B	402	LEU
1	B	431	LEU
1	B	448	ILE
1	B	462	LYS
1	B	470	ILE
1	B	471	PHE
1	B	493	LEU
1	B	518	GLU
1	B	519	LEU
1	B	566	GLU
1	B	582	ILE
1	B	637	LYS
1	B	664	ILE
1	B	671	GLU
1	B	688	HIS
1	B	741	LEU
1	B	744	LEU
1	B	750	LYS
1	B	760	GLN
1	B	761	GLU
1	B	769	ILE
1	B	774	LEU
1	B	776	GLU
1	B	781	VAL
1	B	790	LYS
1	B	797	VAL
1	B	812	ARG
1	B	814	LYS
2	D	75	SER
2	D	118	TYR
2	D	122	LEU
2	D	133	ILE
2	D	153	ASN
2	D	162	SER
3	F	4	ASP
3	F	42	ASP
3	F	51	ILE
3	F	75	ASN
3	F	77	ASN

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Mol	Chain	Res	Type
3	F	78	GLU
3	F	84[A]	GLN
3	F	84[B]	GLN
3	F	97	LEU
3	F	109	LEU
3	F	133	SER
3	F	134	ILE
4	G	19	CYS
4	G	21	ASP
4	G	24	GLU
4	G	50	ASP
4	G	51[A]	ILE
4	G	51[B]	ILE
4	G	71	LYS
4	G	78	GLU
4	G	86	LYS
4	G	93	ILE
4	G	94	MET
4	G	99	THR
4	G	108	ILE
4	G	121	LEU
4	G	133	SER
4	G	134	ILE
2	H	74	GLU
2	H	114	ILE
2	H	118	TYR
2	H	122	LEU
2	H	137	ASP
2	H	142	GLU
2	H	145	ILE
2	H	153	ASN
2	H	154	ASN
2	H	159	LEU
2	H	194	ASP
2	H	202	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	49	ASN
1	A	107	HIS

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Mol	Chain	Res	Type
1	A	182	ASN
1	A	258	HIS
1	A	317	ASN
1	A	591	GLN
1	A	628	GLN
1	A	644	GLN
1	A	648	GLN
1	A	672	ASN
1	A	715	GLN
1	A	731	ASN
1	A	733	ASN
1	A	791	HIS
1	A	808	GLN
1	A	818	GLN
1	B	35	GLN
1	B	49	ASN
1	B	58	GLN
1	B	107	HIS
1	B	182	ASN
1	B	317	ASN
1	B	591	GLN
1	B	628	GLN
1	B	644	GLN
1	B	648	GLN
1	B	672	ASN
1	B	800	ASN
1	B	818	GLN
2	D	153	ASN
2	D	166	ASN
3	F	33	ASN
3	F	72	HIS
3	F	75	ASN
3	F	77	ASN
3	F	89	ASN
3	F	111	GLN
3	F	114	ASN
4	G	79	GLN
4	G	107	ASN
4	G	111	GLN
2	H	94	ASN
2	H	126	GLN
2	H	150	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	B	19	1	8,9,10	0.94	0	7,12,14	3.19	2 (28%)
1	SEP	A	19	1	8,9,10	0.97	0	7,12,14	1.90	3 (42%)

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
1	SEP	B	19	1	-	5/6/8/10	-
1	SEP	A	19	1	-	1/6/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	SEP	OG-CB-CA	7.84	115.77	108.14
1	A	19	SEP	O2P-P-OG	3.20	115.01	106.67
1	A	19	SEP	OG-CB-CA	3.04	111.10	108.14
1	B	19	SEP	O3P-P-OG	2.65	113.57	106.67
1	A	19	SEP	OG-P-O1P	2.01	111.88	106.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	SEP	N-CA-CB-OG
1	B	19	SEP	N-CA-CB-OG
1	B	19	SEP	C-CA-CB-OG
1	B	19	SEP	CB-OG-P-O1P
1	B	19	SEP	CA-CB-OG-P
1	B	19	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	VO4	B	902	-	0,4,4	-	-	-		
5	ADP	A	901	7	28,29,29	0.27	0	43,45,45	0.43	0
6	VO4	A	902	7	0,4,4	-	-	-		
5	ADP	B	901	7	28,29,29	0.48	0	43,45,45	0.63	1 (2%)

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
5	ADP	A	901	7	-	0/16/32/32	0/3/3/3
5	ADP	B	901	7	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	901	ADP	O3B-PB-O3A	2.19	111.97	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

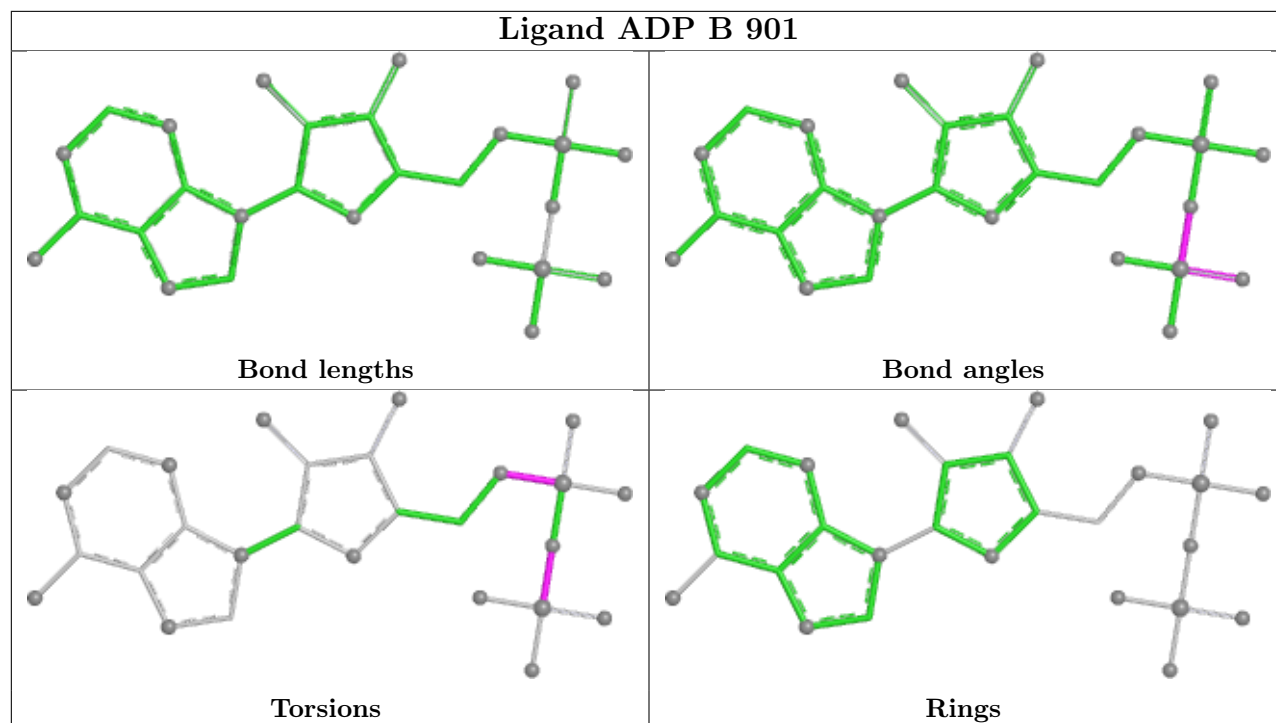
Mol	Chain	Res	Type	Atoms
5	B	901	ADP	PA-O3A-PB-O1B
5	B	901	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	902	VO4	4	0
6	A	902	VO4	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

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	813/818 (99%)	0.01	14 (1%)	69 51	3, 34, 119, 194	11 (1%)
1	B	816/818 (99%)	0.37	55 (6%)	24 22	13, 69, 210, 291	11 (1%)
2	D	133/204 (65%)	0.09	4 (3%)	52 38	46, 78, 130, 209	0
2	H	133/204 (65%)	0.15	7 (5%)	32 27	32, 92, 159, 208	1 (0%)
3	F	133/134 (99%)	0.33	7 (5%)	32 27	17, 72, 122, 176	1 (0%)
4	G	125/134 (93%)	0.29	2 (1%)	70 52	40, 102, 145, 170	1 (0%)
All	All	2153/2312 (93%)	0.20	89 (4%)	41 32	3, 61, 166, 291	25 (1%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ILE	5.4
3	F	80	ASN	5.1
1	B	267	VAL	5.0
1	B	739	LEU	4.6
1	B	234	PHE	4.6
1	B	444	PHE	4.4
2	D	134	CYS	4.4
1	A	547	LEU	4.3
1	B	37	TRP	4.1
2	H	72	VAL	4.1
1	B	788	ILE	4.1
1	B	736	VAL	4.0
1	B	437	LYS	4.0
1	B	15	VAL	4.0
1	B	613	ILE	3.8
2	H	87	GLY	3.7
1	B	502	PHE	3.6
2	D	72	VAL	3.6
1	B	36	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	3.5
1	B	785	GLU	3.4
1	B	38	THR	3.4
4	G	113	THR	3.4
2	H	172	GLY	3.3
1	B	473	PHE	3.3
4	G	134	ILE	3.3
1	B	415	GLY	3.2
1	B	265	GLY	3.2
2	H	148	PHE	3.1
1	B	403	ILE	3.0
1	B	501	VAL	3.0
1	B	342[A]	MET	3.0
1	A	683	ILE	2.9
1	B	441	GLU	2.9
1	B	290	PHE	2.9
1	B	799	LYS	2.9
1	B	277	ILE	2.8
1	B	14	ILE	2.7
1	B	7	GLU	2.7
1	A	270	PHE	2.7
1	B	353	PHE	2.7
3	F	39	LEU	2.7
1	A	2	ALA	2.6
2	D	88	GLY	2.6
1	A	543	GLU	2.5
2	H	88	GLY	2.5
1	A	667	ILE	2.5
2	H	173	ASP	2.5
1	B	21	VAL	2.5
1	B	11	ALA	2.5
1	B	609	LEU	2.5
1	B	293	PHE	2.4
1	B	39[A]	ASP	2.4
1	B	356	VAL	2.4
1	A	741	LEU	2.4
1	B	23	ALA	2.4
1	A	38	THR	2.4
3	F	83	VAL	2.4
3	F	79	GLN	2.4
1	B	440	TYR	2.4
1	B	138	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	348	ASP	2.3
1	B	589	PRO	2.3
1	B	272	LEU	2.2
1	A	15	VAL	2.2
1	B	804	LEU	2.2
3	F	41	ASN	2.2
1	A	352	ILE	2.2
1	B	34	TYR	2.2
1	A	323	VAL	2.2
1	B	723	ALA	2.2
1	B	235	GLY	2.2
1	B	626	GLU	2.2
1	B	751	ILE	2.2
1	B	339	LEU	2.2
2	H	98	ASN	2.2
1	B	246	SER	2.1
1	A	409	ILE	2.1
1	A	363	GLY	2.1
1	B	539	LEU	2.1
1	B	610	VAL	2.1
1	B	18	VAL	2.1
1	B	451	LEU	2.1
3	F	56	TRP	2.1
1	B	645	PHE	2.1
2	D	87	GLY	2.0
1	B	410	LYS	2.0
1	B	603	ASP	2.0
3	F	3	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	19	10/11	0.93	0.11	3,3,3,3	0
1	SEP	B	19	10/11	0.95	0.07	13,16,18,18	0

6.3 Carbohydrates [i](#)

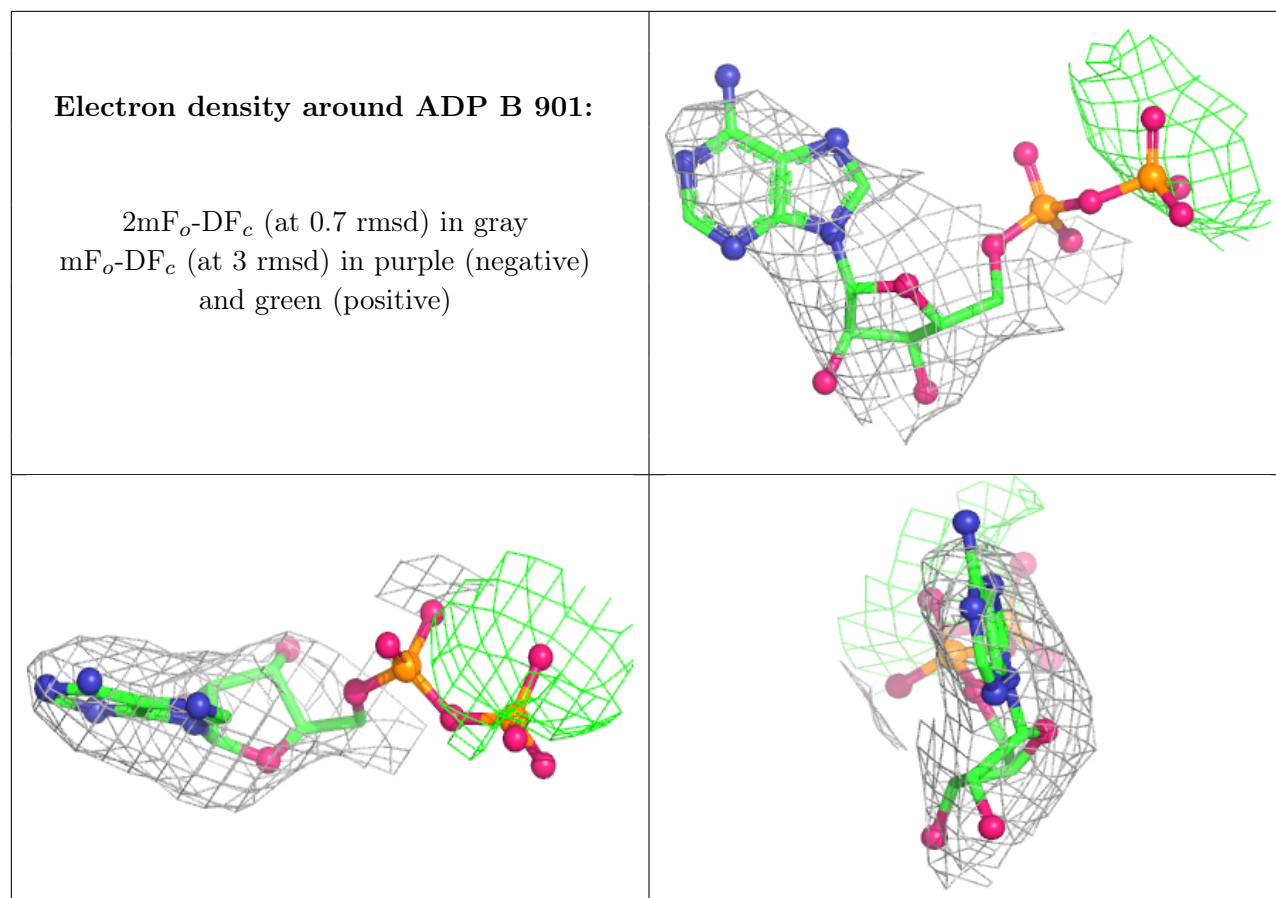
There are no oligosaccharides in this entry.

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
5	ADP	B	901	27/27	0.91	0.13	31,37,42,44	0
6	VO4	B	902	5/5	0.91	0.10	42,43,44,46	0
7	MG	B	903	1/1	0.93	0.17	27,27,27,27	0
5	ADP	A	901	27/27	0.95	0.10	3,6,10,12	0
7	MG	A	903	1/1	0.98	0.18	27,27,27,27	0
6	VO4	A	902	5/5	0.98	0.06	7,8,9,9	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.