



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:42 AM UTC

PDB ID : 2X9H / pdb_00002x9h
Title : CRYSTAL STRUCTURE OF MYOSIN-2 MOTOR DOMAIN IN COMPLEX
WITH ADP- METAVANADATE AND PENTACHLOROCARBAZOLE
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Deposited on : 2010-03-19
Resolution : 2.70 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

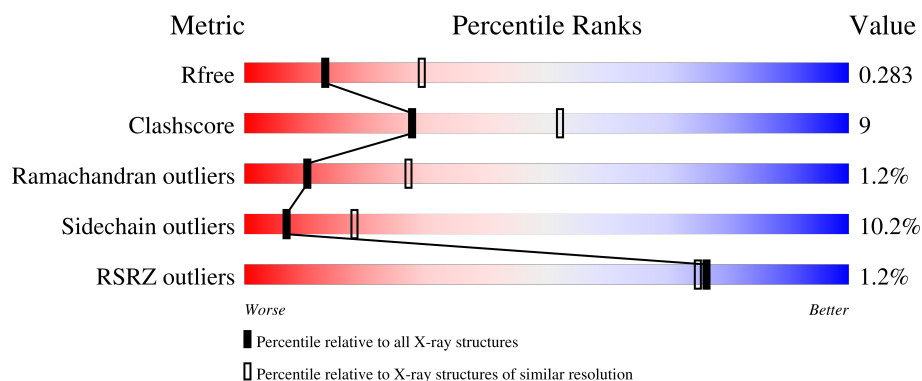
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	695	

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
4	KI9	A	4001	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5781 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.

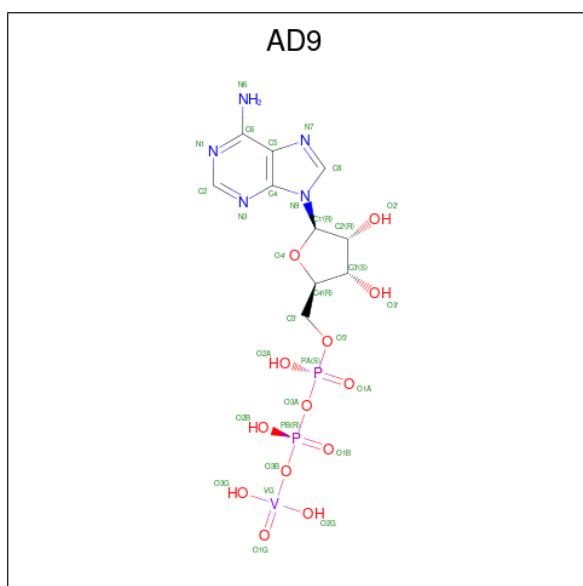
- Molecule 1 is a protein called MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	691	5532	3516	949	1051	16	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	ASN	conflict	UNP P08799
A	131	ILE	ARG	conflict	UNP P08799
A	435	ILE	LYS	conflict	UNP P08799

- Molecule 2 is ADP METAVANADATE (CCD ID: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).

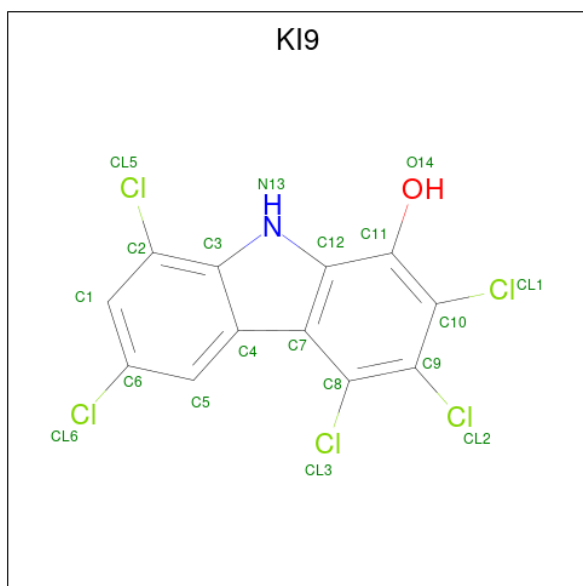


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	V		
2	A	1	31	10	5	13	2	1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 2,3,4,6,8-PENTACHLORO-9H-CARBAZOL-1-OL (CCD ID: KI9) (formula: C₁₂H₄Cl₅NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			19	12	5	1	1		

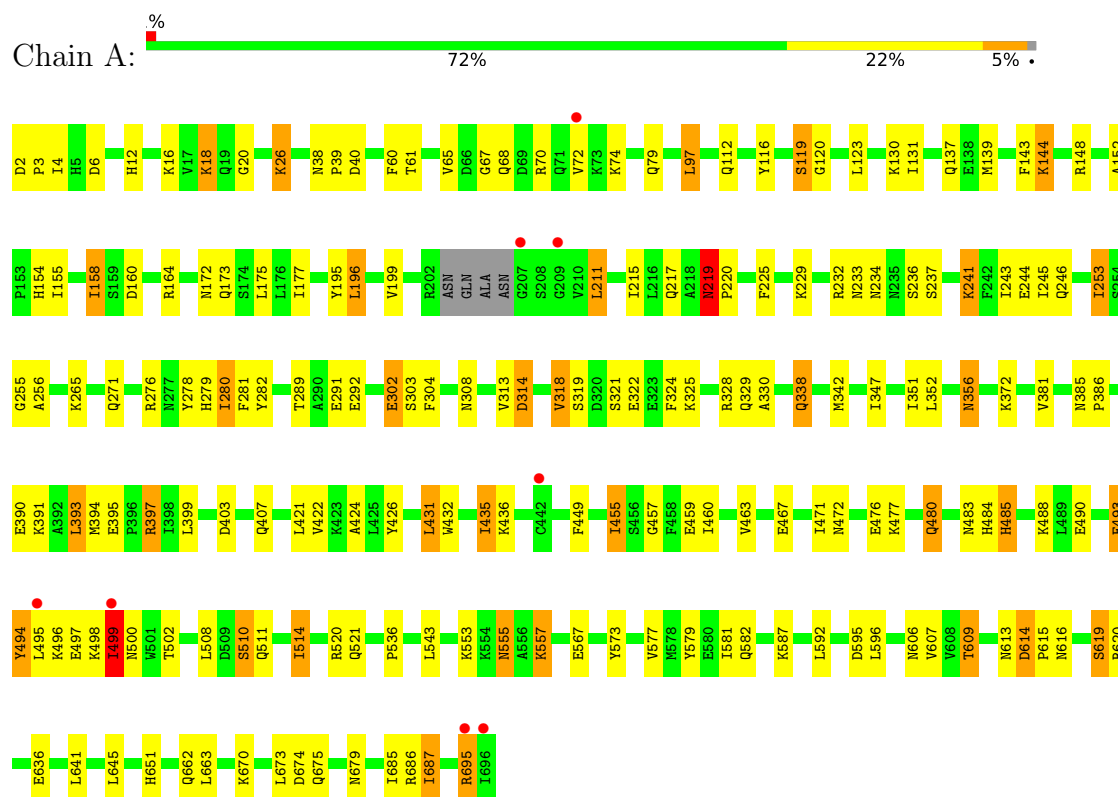
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total	O	0	0
			198	198		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYOSIN-2 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.16Å 146.63Å 153.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 2.70 19.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.77-2.70) 98.2 (19.77-2.70)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.53 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.289 0.200 , 0.283	Depositor DCC
R_{free} test set	1377 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5781	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: AD9, KI9, 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	1.12	8/5639 (0.1%)	1.20	18/7608 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	ILE	CA-CB	7.17	1.63	1.54
1	A	695	ARG	CA-C	6.35	1.59	1.52
1	A	499	ILE	CA-CB	5.94	1.62	1.54
1	A	313	VAL	CA-CB	5.60	1.60	1.54
1	A	65	VAL	CA-CB	5.54	1.61	1.54
1	A	219	ASN	CA-C	5.24	1.59	1.52
1	A	318	VAL	CA-CB	5.13	1.61	1.54
1	A	463	VAL	CA-CB	5.02	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	LEU	N-CA-C	6.91	119.38	110.39
1	A	152	ALA	CA-C-N	-6.75	113.01	119.76
1	A	152	ALA	C-N-CA	-6.75	113.01	119.76
1	A	674	ASP	N-CA-C	-6.23	104.41	111.07
1	A	485	HIS	N-CA-C	6.22	118.14	111.36
1	A	543	LEU	N-CA-C	6.12	117.61	111.07
1	A	40	ASP	CA-C-N	-6.04	113.75	120.45
1	A	40	ASP	C-N-CA	-6.04	113.75	120.45
1	A	614	ASP	CA-C-N	6.00	125.71	119.05
1	A	614	ASP	C-N-CA	6.00	125.71	119.05
1	A	38	ASN	CA-C-N	5.92	125.79	119.28
1	A	38	ASN	C-N-CA	5.92	125.79	119.28
1	A	536	PRO	N-CA-C	5.62	122.00	114.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ILE	N-CA-C	-5.25	104.49	111.05
1	A	432	TRP	N-CA-C	5.19	116.63	111.07
1	A	253	ILE	N-CA-C	5.10	115.57	108.84
1	A	510	SER	CA-C-N	5.01	126.96	120.44
1	A	510	SER	C-N-CA	5.01	126.96	120.44

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	5532	0	5494	100	0
2	A	31	0	14	2	0
3	A	1	0	0	0	0
4	A	19	0	3	7	0
5	A	198	0	0	12	0
All	All	5781	0	5511	100	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 9.

All (100) 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:424:ALA:HB2	4:A:4001:KI9:CL5	1.91	1.07
1:A:614:ASP:OD1	1:A:616:ASN:HB2	1.54	1.05
1:A:325:LYS:O	1:A:329:GLN:HG3	1.81	0.81
1:A:477:LYS:HD2	1:A:514:ILE:HD12	1.68	0.74
1:A:18:LYS:H	1:A:112:GLN:HE22	1.31	0.74
1:A:620:ARG:HD3	4:A:4001:KI9:CL3	2.25	0.74
1:A:246:GLN:HE21	1:A:255:GLY:HA3	1.54	0.73
1:A:338:GLN:NE2	1:A:338:GLN:H	1.86	0.73
1:A:241:LYS:HE2	1:A:243:ILE:HD11	1.71	0.71
1:A:455:ILE:HG13	5:A:2055:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD12	1:A:686:ARG:HG3	1.73	0.71
1:A:459:GLU:H	1:A:472:ASN:HD21	1.38	0.70
1:A:480:GLN:HE21	1:A:483:ASN:HD22	1.41	0.67
1:A:480:GLN:HE21	1:A:480:GLN:HA	1.59	0.67
1:A:555:ASN:HD22	1:A:557:LYS:H	1.42	0.66
1:A:490:GLU:HA	1:A:490:GLU:OE1	1.96	0.65
1:A:480:GLN:NE2	1:A:483:ASN:HD22	1.93	0.65
1:A:219:ASN:HD22	1:A:220:PRO:HD3	1.61	0.64
1:A:338:GLN:H	1:A:338:GLN:HE21	1.46	0.62
1:A:493:GLU:O	1:A:496:LYS:N	2.33	0.61
1:A:18:LYS:H	1:A:112:GLN:NE2	1.98	0.59
1:A:265:LYS:HD3	4:A:4001:KI9:O14	2.03	0.59
1:A:457:GLY:H	2:A:1001:AD9:H2G1	1.50	0.59
1:A:510:SER:O	1:A:514:ILE:HG12	2.03	0.58
1:A:289:THR:OG1	1:A:292:GLU:OE1	2.21	0.58
1:A:393:LEU:HD13	1:A:596:LEU:HD21	1.86	0.58
1:A:234:ASN:H	1:A:662:GLN:HE22	1.51	0.57
1:A:567:GLU:HA	1:A:579:TYR:O	2.05	0.57
1:A:172:ASN:ND2	1:A:449:PHE:H	2.03	0.57
1:A:244:GLU:O	1:A:256:ALA:HA	2.03	0.57
1:A:493:GLU:O	1:A:495:LEU:N	2.37	0.57
1:A:397:ARG:HD3	1:A:595:ASP:OD2	2.05	0.56
1:A:511:GLN:NE2	5:A:2133:HOH:O	2.38	0.56
1:A:511:GLN:CD	5:A:2133:HOH:O	2.48	0.56
1:A:233:ASN:HB3	1:A:236:SER:HB2	1.87	0.55
1:A:493:GLU:O	1:A:494:TYR:C	2.49	0.55
1:A:615:PRO:O	1:A:619:SER:HB2	2.06	0.55
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.88	0.54
1:A:510:SER:HA	5:A:2135:HOH:O	2.07	0.54
1:A:319:SER:HB3	1:A:322:GLU:HB2	1.89	0.54
1:A:347:ILE:HD11	1:A:607:VAL:HG12	1.90	0.54
1:A:620:ARG:HG3	4:A:4001:KI9:CL6	2.45	0.54
1:A:421:LEU:HB2	1:A:596:LEU:HD13	1.91	0.53
1:A:246:GLN:NE2	1:A:255:GLY:HA3	2.22	0.53
1:A:476:GLU:OE1	1:A:510:SER:HB2	2.10	0.52
1:A:246:GLN:HE21	1:A:255:GLY:CA	2.21	0.52
1:A:3:PRO:HA	5:A:2001:HOH:O	2.11	0.51
1:A:229:LYS:HB3	1:A:276:ARG:HB2	1.92	0.50
1:A:276:ARG:HG2	1:A:282:TYR:CZ	2.46	0.50
1:A:225:PHE:O	1:A:426:TYR:OH	2.28	0.50
1:A:609:THR:O	1:A:613:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HE3	5:A:2003:HOH:O	2.11	0.49
1:A:265:LYS:CD	4:A:4001:KI9:O14	2.59	0.49
1:A:116:TYR:CD2	1:A:154:HIS:HA	2.48	0.49
1:A:324:PHE:CE2	1:A:328:ARG:HD2	2.49	0.48
1:A:173:GLN:OE1	1:A:651:HIS:HE1	1.98	0.47
1:A:641:LEU:O	1:A:645:LEU:HG	2.14	0.47
1:A:271:GLN:NE2	5:A:2074:HOH:O	2.48	0.46
1:A:139:MET:O	1:A:143:PHE:HD1	1.98	0.46
1:A:347:ILE:HD11	1:A:607:VAL:CG1	2.45	0.46
1:A:39:PRO:HD2	5:A:2015:HOH:O	2.14	0.46
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.81	0.46
1:A:573:TYR:HB2	5:A:2191:HOH:O	2.15	0.46
1:A:457:GLY:N	2:A:1001:AD9:O2G	2.37	0.45
1:A:467:GLU:O	1:A:471:ILE:HG12	2.17	0.44
1:A:302:GLU:O	1:A:308:ASN:ND2	2.42	0.44
1:A:581:ILE:O	1:A:582:GLN:C	2.60	0.44
1:A:424:ALA:CB	4:A:4001:KI9:CL5	2.83	0.44
1:A:164:ARG:HD3	1:A:164:ARG:HA	1.79	0.44
1:A:211:LEU:CD2	1:A:215:ILE:HD11	2.48	0.44
1:A:460:ILE:HG12	1:A:577:VAL:HG22	2.00	0.43
1:A:116:TYR:HB3	1:A:123:LEU:HD11	2.00	0.43
1:A:431:LEU:O	1:A:435:ILE:HG23	2.18	0.43
1:A:119:SER:OG	1:A:685:ILE:HD11	2.18	0.43
1:A:196:LEU:HD23	1:A:245:ILE:HG13	2.01	0.43
1:A:687:ILE:HD13	1:A:687:ILE:O	2.18	0.43
1:A:79:GLN:NE2	5:A:2025:HOH:O	2.36	0.43
1:A:484:HIS:HB2	5:A:2128:HOH:O	2.18	0.42
1:A:225:PHE:CE2	1:A:280:ILE:HG12	2.55	0.42
1:A:395:GLU:HA	1:A:407:GLN:O	2.19	0.42
1:A:281:PHE:CD1	1:A:352:LEU:HD21	2.54	0.42
1:A:160:ASP:OD2	1:A:195:TYR:OH	2.37	0.42
1:A:26:LYS:HE3	1:A:26:LYS:HB2	1.80	0.42
1:A:497:GLU:O	1:A:499:ILE:N	2.53	0.42
1:A:120:GLY:O	1:A:148:ARG:NH1	2.47	0.42
1:A:399:LEU:HA	1:A:403:ASP:O	2.20	0.42
1:A:338:GLN:NE2	1:A:338:GLN:N	2.61	0.41
1:A:217:GLN:HG3	1:A:330:ALA:HA	2.02	0.41
1:A:467:GLU:OE2	1:A:587:LYS:HE2	2.20	0.41
1:A:2:ASP:HA	1:A:3:PRO:HD3	1.89	0.41
1:A:385:ASN:HA	1:A:386:PRO:HD2	1.94	0.41
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD1	1:A:314:ASP:N	2.53	0.41
1:A:61:THR:HA	1:A:70:ARG:O	2.20	0.41
1:A:20:GLY:HA2	5:A:2008:HOH:O	2.20	0.41
1:A:278:TYR:O	1:A:279:HIS:C	2.63	0.41
1:A:431:LEU:HD13	1:A:431:LEU:HA	1.98	0.41
1:A:592:LEU:HB2	4:A:4001:KI9:CL5	2.58	0.41
1:A:675:GLN:O	1:A:679:ASN:HB2	2.21	0.41
1:A:390:GLU:HG2	1:A:394:MET:CE	2.52	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	687/695 (99%)	644 (94%)	35 (5%)	8 (1%)	10	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	493	GLU
1	A	494	TYR
1	A	498	LYS
1	A	67	GLY
1	A	144	LYS
1	A	500	ASN
1	A	499	ILE

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	606/609 (100%)	544 (90%)	62 (10%)	7 18

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	ASP
1	A	12	HIS
1	A	18	LYS
1	A	26	LYS
1	A	72	VAL
1	A	97	LEU
1	A	119	SER
1	A	130	LYS
1	A	131	ILE
1	A	137	GLN
1	A	144	LYS
1	A	155	ILE
1	A	158	ILE
1	A	175	LEU
1	A	177	ILE
1	A	196	LEU
1	A	199	VAL
1	A	211	LEU
1	A	219	ASN
1	A	232	ARG
1	A	237	SER
1	A	241	LYS
1	A	253	ILE
1	A	291	GLU
1	A	302	GLU
1	A	303	SER
1	A	314	ASP
1	A	318	VAL
1	A	321	SER

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	342	MET
1	A	356	ASN
1	A	372	LYS
1	A	381	VAL
1	A	391	LYS
1	A	393	LEU
1	A	397	ARG
1	A	431	LEU
1	A	435	ILE
1	A	436	LYS
1	A	455	ILE
1	A	480	GLN
1	A	485	HIS
1	A	488	LYS
1	A	499	ILE
1	A	502	THR
1	A	508	LEU
1	A	514	ILE
1	A	520	ARG
1	A	521	GLN
1	A	553	LYS
1	A	555	ASN
1	A	557	LYS
1	A	606	ASN
1	A	609	THR
1	A	619	SER
1	A	636	GLU
1	A	670	LYS
1	A	673	LEU
1	A	687	ILE
1	A	695	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	12	HIS
1	A	38	ASN
1	A	78	ASN
1	A	112	GLN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	172	ASN
1	A	188	ASN
1	A	217	GLN
1	A	219	ASN
1	A	246	GLN
1	A	271	GLN
1	A	297	HIS
1	A	309	GLN
1	A	329	GLN
1	A	338	GLN
1	A	356	ASN
1	A	443	GLN
1	A	472	ASN
1	A	480	GLN
1	A	485	HIS
1	A	532	GLN
1	A	555	ASN
1	A	594	GLN
1	A	651	HIS
1	A	660	ASN
1	A	662	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	AD9	A	1001	3	29,33,33	1.38	1 (3%)	42,52,52	1.91	10 (23%)
4	KI9	A	4001	-	21,21,21	2.09	8 (38%)	28,33,33	1.98	11 (39%)

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	AD9	A	1001	3	-	0/16/38/38	0/3/3/3
4	KI9	A	4001	-	-	-	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	AD9	O3B-VG	5.61	2.05	1.80
4	A	4001	KI9	C4-C7	-3.98	1.37	1.46
4	A	4001	KI9	C10-CL1	3.26	1.79	1.72
4	A	4001	KI9	C9-CL2	3.19	1.79	1.72
4	A	4001	KI9	C4-C3	-3.17	1.37	1.41
4	A	4001	KI9	C8-CL3	3.06	1.79	1.72
4	A	4001	KI9	C3-C2	-2.78	1.36	1.40
4	A	4001	KI9	C7-C12	-2.42	1.37	1.41
4	A	4001	KI9	C6-CL6	2.12	1.79	1.74

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	AD9	N3-C2-N1	-5.87	119.70	128.58
2	A	1001	AD9	C5-C4-N3	-5.41	119.27	126.72
4	A	4001	KI9	C5-C6-CL6	4.13	124.35	119.17
2	A	1001	AD9	C2-N3-C4	4.03	121.68	111.83
4	A	4001	KI9	C11-C10-CL1	-3.60	113.72	118.09
4	A	4001	KI9	C9-C10-CL1	3.29	126.08	120.00
4	A	4001	KI9	C1-C6-CL6	-3.28	115.06	119.17
2	A	1001	AD9	N3-C4-N9	3.15	132.53	127.17
2	A	1001	AD9	C4-C5-N7	-3.14	106.99	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4001	KI9	C3-C2-CL5	-2.81	116.09	119.28
4	A	4001	KI9	C1-C2-CL5	2.70	122.87	118.45
4	A	4001	KI9	C2-C3-N13	2.69	132.12	128.94
2	A	1001	AD9	O2B-PB-O1B	2.65	124.79	112.44
2	A	1001	AD9	N9-C8-N7	-2.63	110.20	113.94
2	A	1001	AD9	C5-N7-C8	2.63	107.59	103.45
2	A	1001	AD9	C2-N1-C6	2.56	122.94	118.73
4	A	4001	KI9	C12-C7-C8	2.51	121.56	117.27
4	A	4001	KI9	C7-C12-N13	-2.41	106.34	108.89
2	A	1001	AD9	C5-C4-N9	2.19	108.19	105.81
4	A	4001	KI9	C9-C8-CL3	2.10	123.89	120.00
4	A	4001	KI9	C5-C4-C3	2.03	121.92	119.67

There are no chirality outliers.

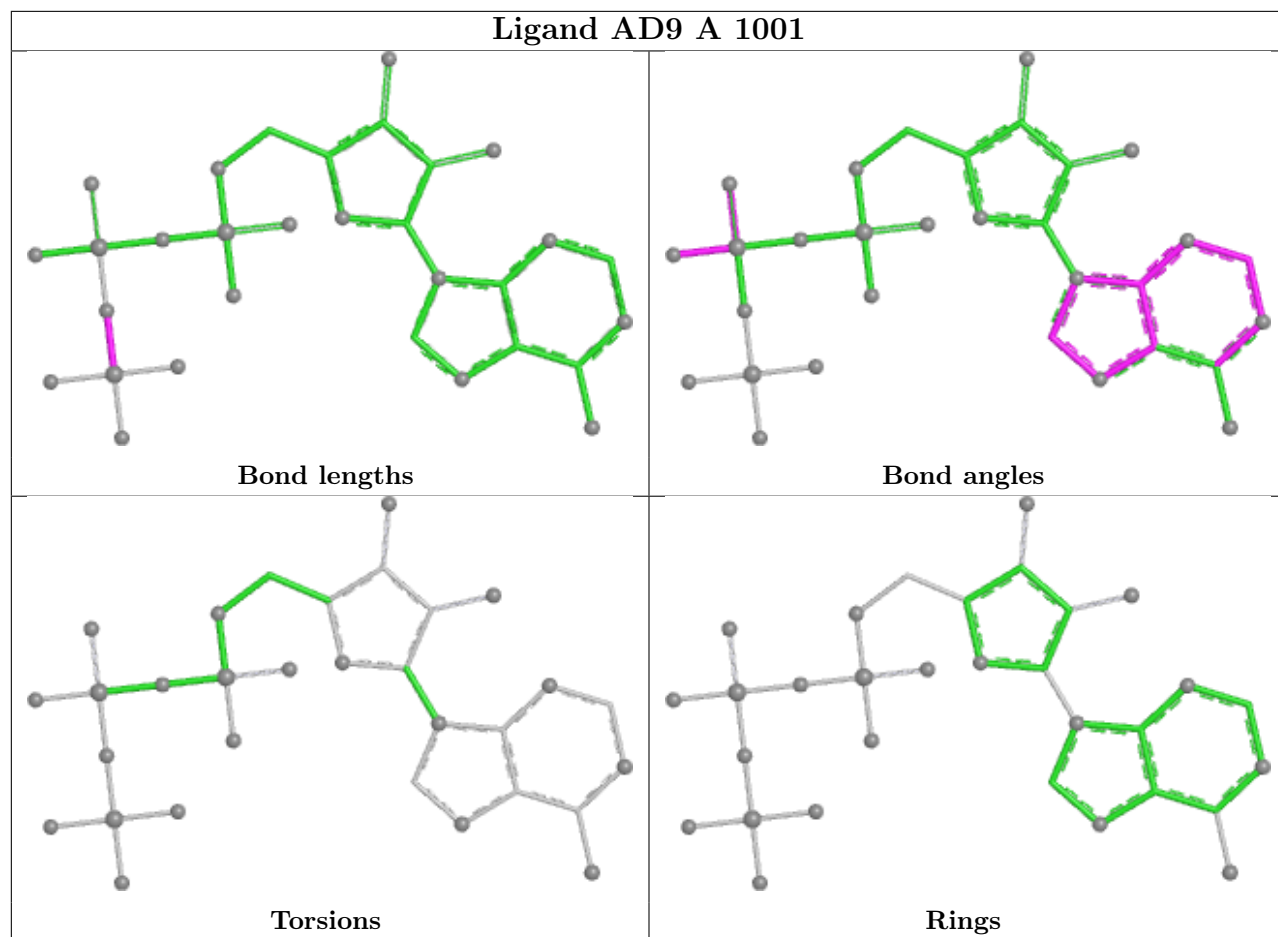
There are no torsion outliers.

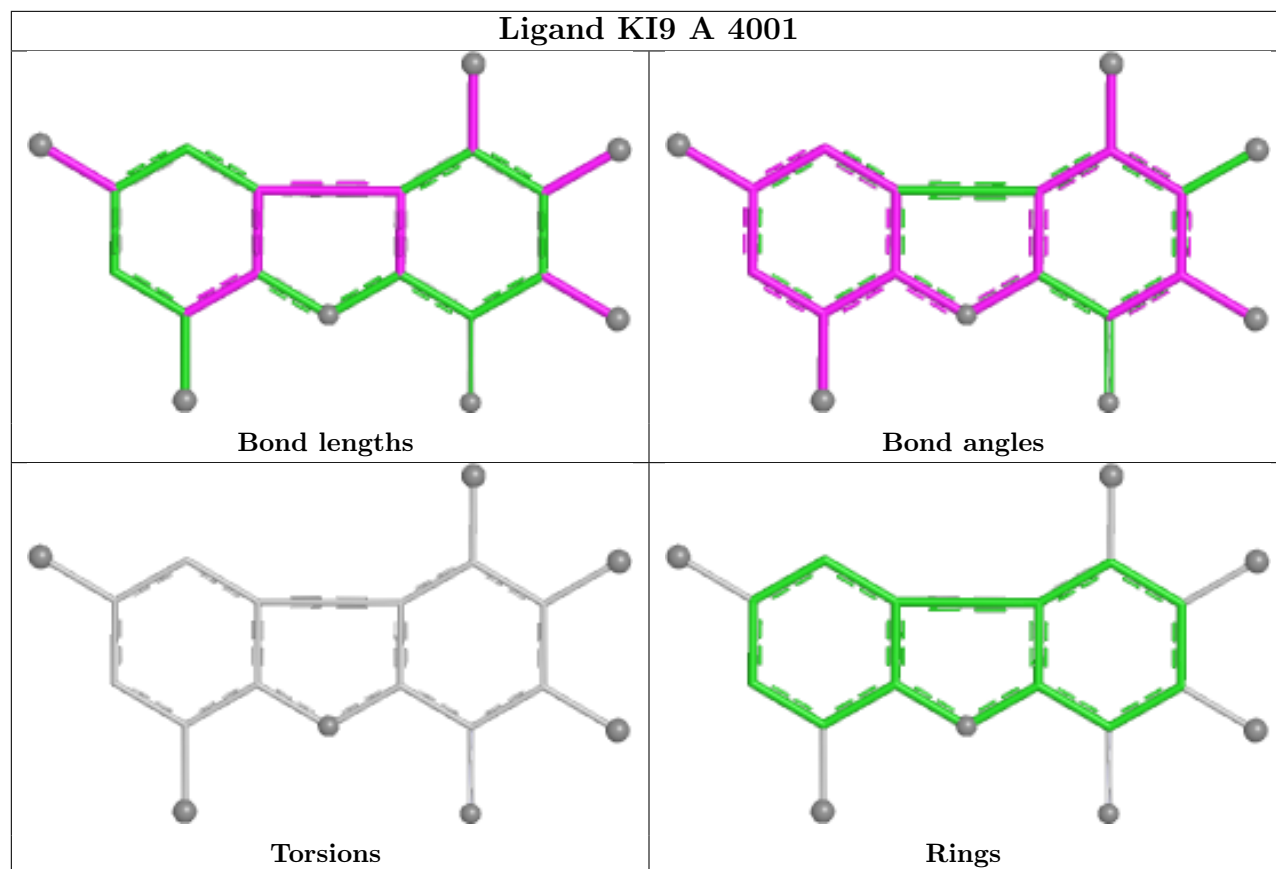
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	AD9	2	0
4	A	4001	KI9	7	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	691/695 (99%)	-0.24	8 (1%) 76 75	2, 20, 42, 56	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ILE	3.9
1	A	695	ARG	3.6
1	A	442	CYS	3.1
1	A	696	ILE	3.1
1	A	209	GLY	2.8
1	A	495	LEU	2.6
1	A	72	VAL	2.6
1	A	207	GLY	2.3

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](#)

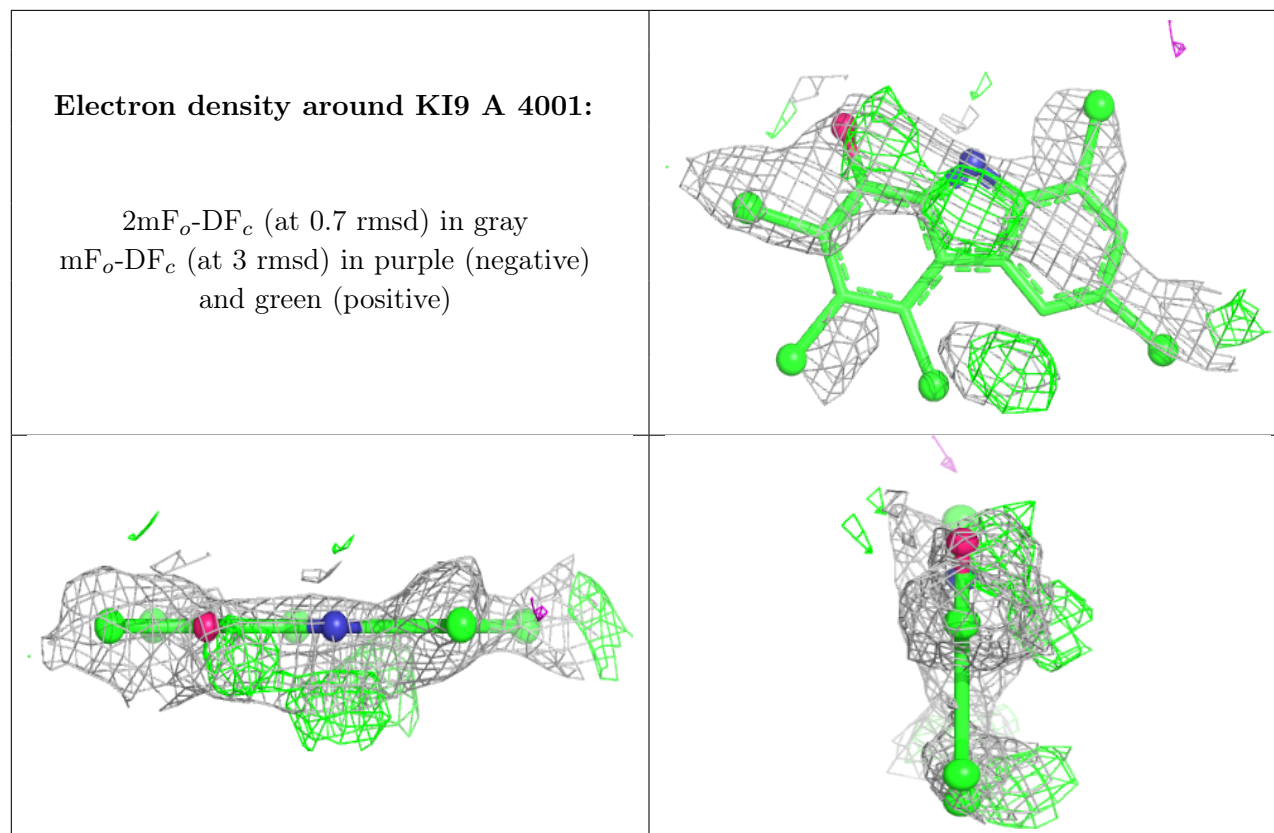
There are no oligosaccharides in this entry.

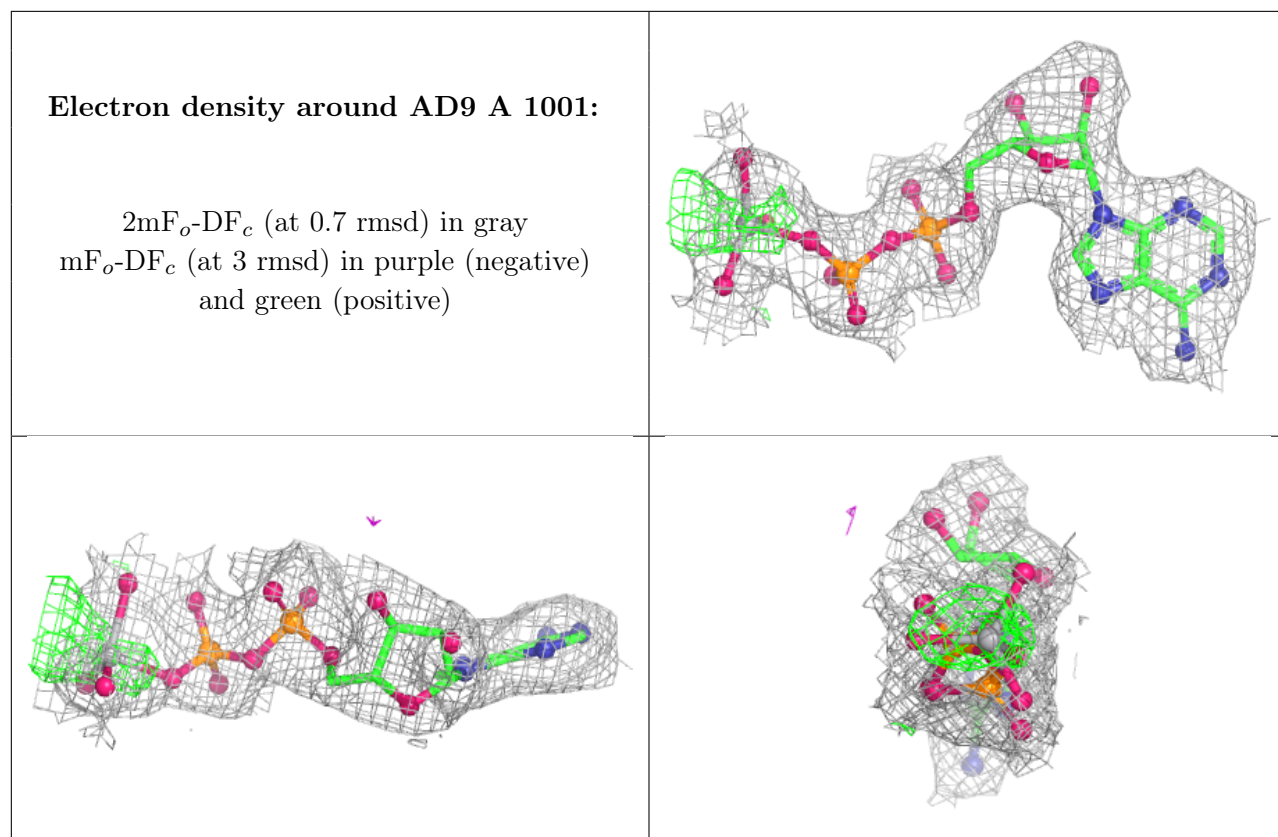
6.4 Ligands [i](#)

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
4	KI9	A	4001	19/19	0.70	0.36	57,60,61,62	19
3	MG	A	3001	1/1	0.97	0.08	20,20,20,20	0
2	AD9	A	1001	31/31	0.99	0.05	4,11,15,16	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.