



# Full wwPDB X-ray Structure Validation Report

Mar 5, 2026 – 09:36 PM UTC

PDB ID : 8CDQ / pdb\_00008cdq  
Title : Plasmodium falciparum Myosin A full-length, post-rigor state complexed to the inhibitor KNX-002 and Mg.ATP-gamma-S  
Authors : Moussaoui, D.; Robblee, J.P.; Robert-Paganin, J.; Auguin, D.; Fisher, F.; Fagnant, P.M.; MacFarlane, J.E.; Schaletzky, J.; Wehri, E.; Mueller-Dieckmann, C.; Baum, J.; Trybus, K.M.; Houdusse, A.  
Deposited on : 2023-01-31  
Resolution : 2.21 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

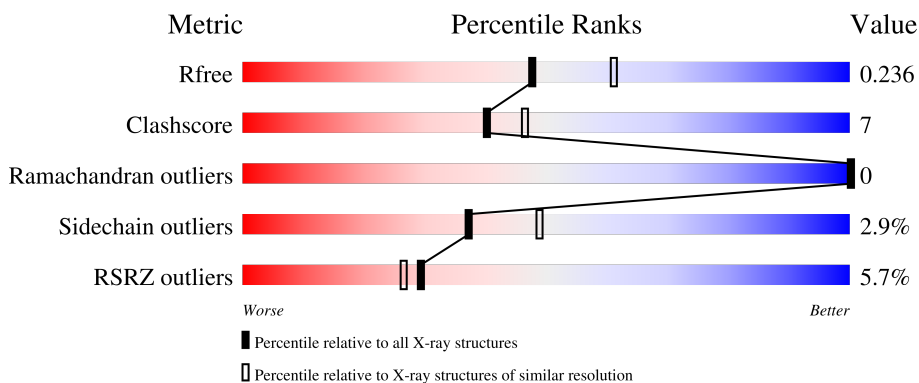
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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  $\geq 3$ , 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	B	204	
3	C	134	

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	GOL	A	905	-	X	-	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 8998 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
			Total	C	N	O	P	S			
1	A	814	6481	4123	1101	1223	1	33	0	2	0

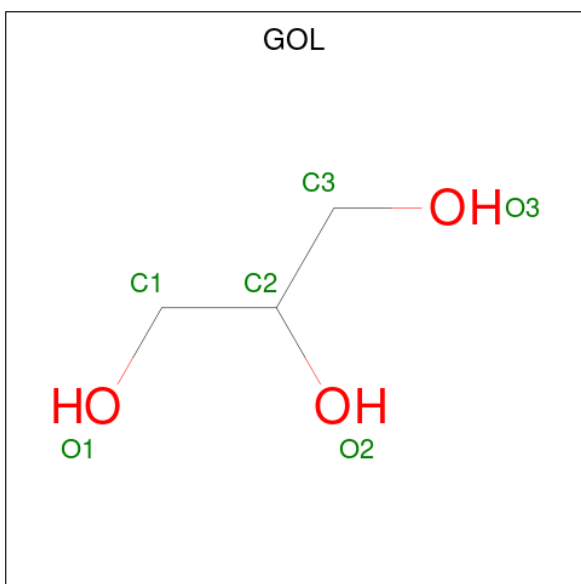
- Molecule 2 is a protein called Myosin A tail domain interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	1051	661	167	218	5	0	0	0

- Molecule 3 is a protein called Myosin essential light chain ELC.

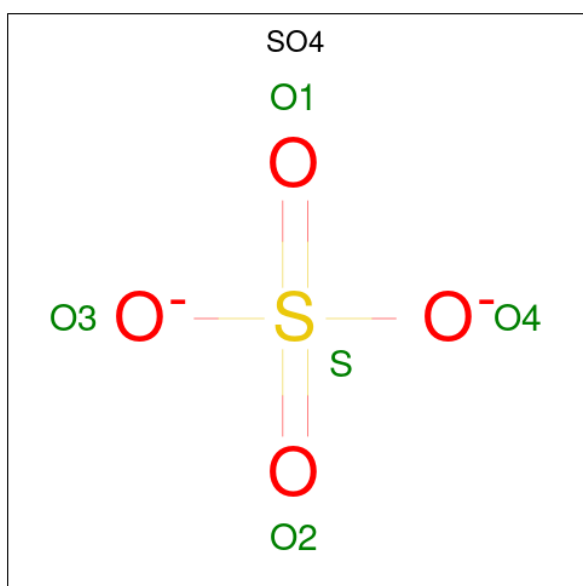
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	128	1051	673	170	202	6	0	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



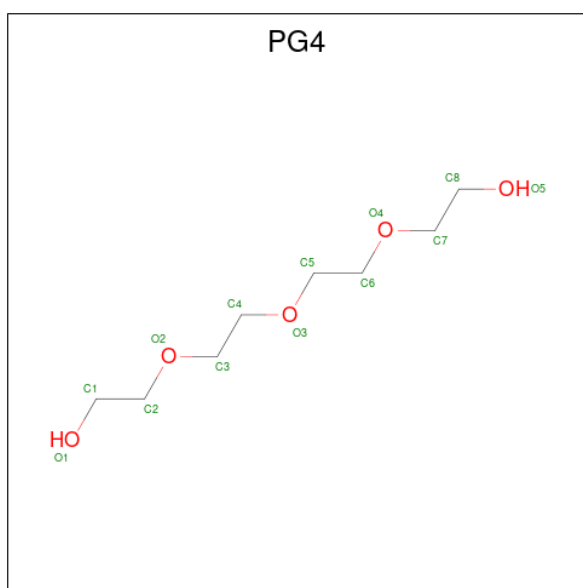
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

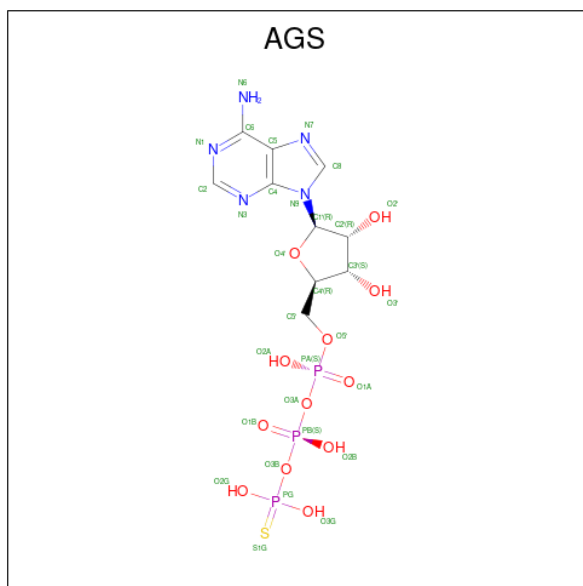
- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID:

AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).

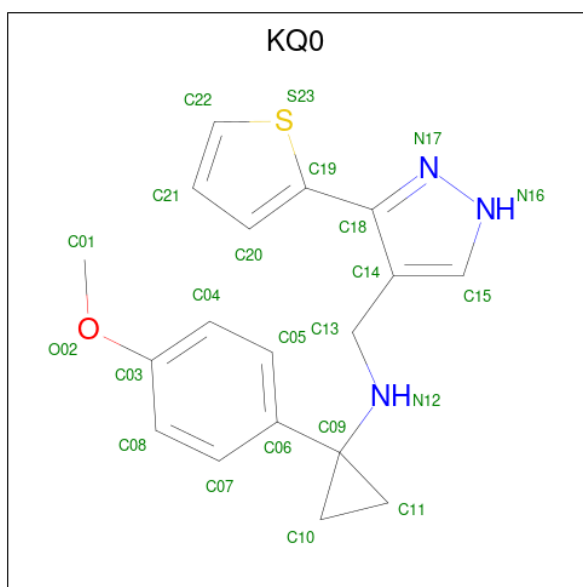


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
8	A	1	31	10	5	12	3	1	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 10 is 1-(4-methoxyphenyl)- {N}-[(3-thiophen-2-yl-1 {H}-pyrazol-4-yl)methyl]cyclopropan-1-amine (CCD ID: KQ0) (formula: C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	A	1	23	18	3	1	1	0	0

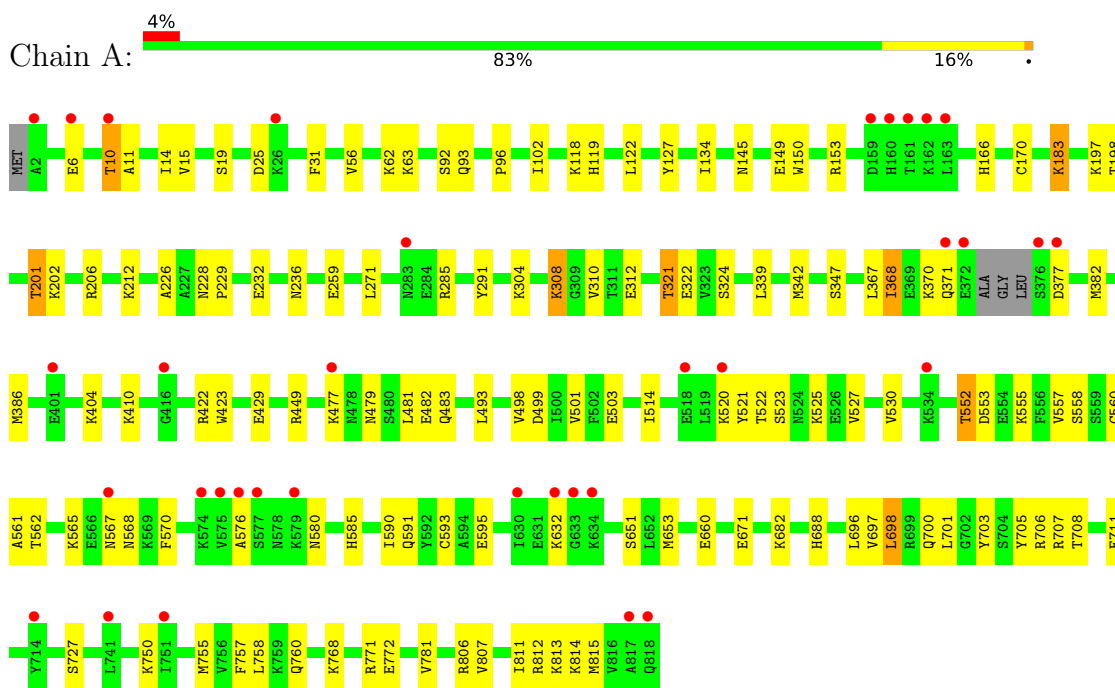
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	261	Total	O	0	0
			261	261		
11	B	17	Total	O	0	0
			17	17		
11	C	27	Total	O	0	0
			27	27		

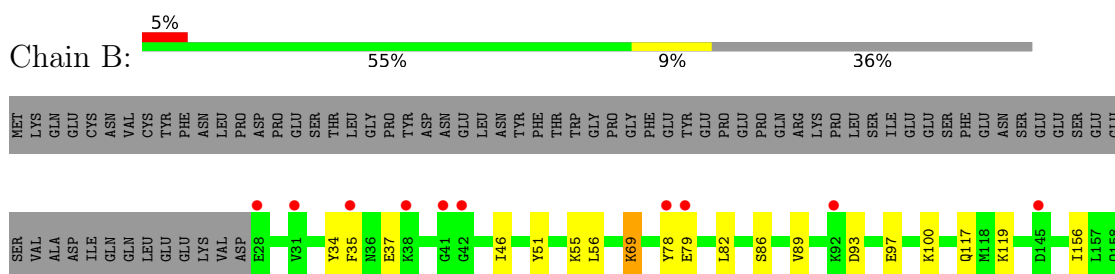
### 3 Residue-property plots

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.

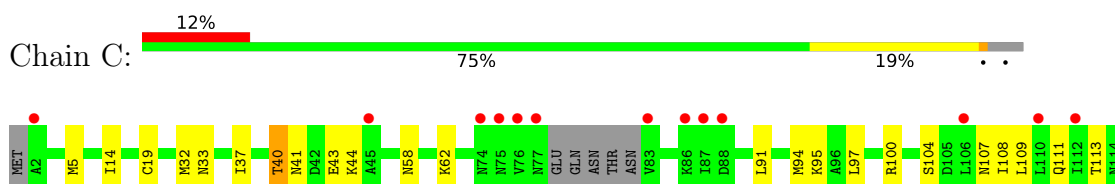
- Molecule 1: Myosin-A

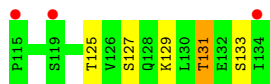


- Molecule 2: Myosin A tail domain interacting protein



- Molecule 3: Myosin essential light chain ELC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.42Å 170.92Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.08 – 2.21 95.08 – 2.21	Depositor EDS
% Data completeness (in resolution range)	64.0 (95.08-2.21) 64.0 (95.08-2.21)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.20.1	Depositor
R, $R_{free}$	0.188 , 0.235 0.189 , 0.236	Depositor DCC
$R_{free}$ test set	2835 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, PG4, MG, AGS, KQ0, SO4, GOL, SEP

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	0.40	0/6583	0.56	0/8874
2	B	0.33	0/1068	0.51	0/1440
3	C	0.38	0/1070	0.50	0/1441
All	All	0.39	0/8721	0.54	0/11755

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6481	0	6580	88	0
2	B	1051	0	1005	14	0
3	C	1051	0	1037	19	0
4	A	24	0	32	2	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	A	8	0	12	0	0
7	A	13	0	18	3	0
8	A	31	0	12	2	0
9	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	23	0	0	0	0
11	A	261	0	0	6	0
11	B	17	0	0	0	0
11	C	27	0	0	1	0
All	All	8998	0	8696	114	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 7.

All (114) 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:449:ARG:NH2	11:A:1001:HOH:O	2.06	0.87
1:A:62:LYS:HD2	1:A:63:LYS:H	1.40	0.86
1:A:271:LEU:H	4:A:903:GOL:H31	1.39	0.84
1:A:483:GLN:HE22	7:A:907:PG4:H41	1.48	0.77
1:A:708:THR:OG1	1:A:711:GLU:HG3	1.92	0.70
3:C:127:SER:O	3:C:131:THR:OG1	2.09	0.70
1:A:149:GLU:OE2	1:A:153:ARG:NH2	2.24	0.69
1:A:700:GLN:HG2	1:A:760:GLN:HE22	1.60	0.67
3:C:40:THR:N	3:C:43:GLU:OE1	2.28	0.67
1:A:499:ASP:O	1:A:503:GLU:HG3	1.96	0.65
1:A:700:GLN:HG2	1:A:760:GLN:NE2	2.11	0.65
1:A:339:LEU:HD23	1:A:342:MET:HE2	1.79	0.64
1:A:145:ASN:HA	1:A:150:TRP:CD1	2.32	0.64
1:A:814:LYS:HE2	2:B:156:ILE:HA	1.80	0.63
1:A:552:THR:HG23	1:A:555:LYS:H	1.64	0.63
1:A:781:VAL:HG22	3:C:94:MET:HE2	1.82	0.62
2:B:79:GLU:H	2:B:79:GLU:CD	2.08	0.61
1:A:62:LYS:HD2	1:A:63:LYS:HD2	1.83	0.60
1:A:812:ARG:HA	1:A:815:MET:HG3	1.83	0.60
1:A:386:MET:HE1	1:A:404:LYS:HD2	1.84	0.60
1:A:558:SER:O	1:A:562:THR:HG23	2.01	0.59
1:A:368:ILE:HD13	1:A:382:MET:HG2	1.84	0.58
1:A:585:HIS:CD2	1:A:590:ILE:HD12	2.38	0.58
2:B:97:GLU:OE1	2:B:100:LYS:HE3	2.03	0.58
2:B:35:PHE:CE2	2:B:78:TYR:HA	2.39	0.57
1:A:321:THR:HB	11:A:1076:HOH:O	2.04	0.57
1:A:96:PRO:HG2	1:A:119[B]:HIS:CG	2.39	0.57
1:A:62:LYS:HD2	1:A:63:LYS:N	2.17	0.56
1:A:226:ALA:O	1:A:229:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:VAL:HG22	3:C:94:MET:CE	2.36	0.56
1:A:561:ALA:O	1:A:565:LYS:HD3	2.06	0.55
3:C:125:THR:O	3:C:129:LYS:HG2	2.07	0.55
3:C:5:MET:HA	3:C:5:MET:HE2	1.90	0.54
1:A:671:GLU:HG3	1:A:682:LYS:NZ	2.23	0.54
1:A:514:ILE:O	11:A:1002:HOH:O	2.19	0.53
1:A:498:VAL:HG12	1:A:521:TYR:CE1	2.43	0.53
1:A:410:LYS:HB2	1:A:423:TRP:CE2	2.44	0.53
1:A:197:LYS:O	1:A:201:THR:HG23	2.09	0.52
1:A:706:ARG:HB3	1:A:755:MET:HE2	1.92	0.52
3:C:14:ILE:HB	3:C:19:CYS:HA	1.92	0.52
1:A:321:THR:HG22	1:A:322:GLU:HG2	1.93	0.51
1:A:6:GLU:O	1:A:10:THR:HG22	2.11	0.51
1:A:62:LYS:CD	1:A:63:LYS:H	2.18	0.51
1:A:93:GLN:HB3	3:C:100:ARG:HH11	1.76	0.51
1:A:202:LYS:O	1:A:206:ARG:HG3	2.11	0.50
1:A:25:ASP:HB3	1:A:31:PHE:CE1	2.46	0.50
1:A:771:ARG:HG3	3:C:97:LEU:HD22	1.92	0.50
1:A:806:ARG:NH1	2:B:93:ASP:OD2	2.43	0.50
1:A:10:THR:O	1:A:14:ILE:HG13	2.11	0.49
1:A:367:LEU:HD12	1:A:429:GLU:HG3	1.94	0.49
2:B:86:SER:O	2:B:89:VAL:HG22	2.13	0.49
1:A:553:ASP:O	1:A:557:VAL:HG23	2.13	0.49
3:C:91:LEU:O	3:C:95:LYS:HG3	2.12	0.49
1:A:14:ILE:HG21	1:A:688:HIS:HB2	1.93	0.49
1:A:212:LYS:HB2	1:A:259:GLU:HB3	1.94	0.49
3:C:33:ASN:ND2	11:C:301:HOH:O	2.39	0.49
1:A:183:LYS:HG3	11:A:1249:HOH:O	2.13	0.48
3:C:40:THR:O	3:C:44:LYS:HB2	2.13	0.48
3:C:109:LEU:O	3:C:113:THR:OG1	2.24	0.48
1:A:530:VAL:HB	1:A:567:ASN:HD21	1.78	0.47
1:A:482:GLU:CD	7:A:907:PG4:H42	2.40	0.47
1:A:493:LEU:HD21	1:A:653:MET:HE1	1.96	0.47
1:A:271:LEU:N	4:A:903:GOL:H31	2.17	0.47
1:A:697:VAL:O	1:A:701:LEU:HD13	2.14	0.47
1:A:118:LYS:HE2	1:A:122:LEU:HD11	1.96	0.46
2:B:51:TYR:CE2	2:B:55:LYS:HD2	2.50	0.46
1:A:183:LYS:HD2	1:A:660:GLU:HG2	1.98	0.46
1:A:483:GLN:NE2	7:A:907:PG4:H41	2.25	0.46
1:A:768:LYS:O	1:A:772:GLU:HG3	2.15	0.45
1:A:698:LEU:HD23	1:A:698:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:VAL:O	1:A:811:ILE:HG13	2.16	0.45
1:A:501:VAL:HG11	1:A:698:LEU:HD13	1.99	0.45
2:B:78:TYR:CE2	2:B:82:LEU:HD11	2.51	0.45
1:A:521:TYR:HE2	1:A:523:SER:HB2	1.81	0.45
1:A:479:ASN:HB2	1:A:591:GLN:O	2.17	0.44
1:A:304:LYS:HB3	1:A:304:LYS:HE2	1.84	0.44
2:B:46:ILE:HD12	2:B:69:LYS:HG3	1.99	0.44
1:A:197:LYS:HG3	8:A:909:AGS:O2B	2.17	0.44
1:A:760:GLN:HG3	11:A:1151:HOH:O	2.17	0.44
1:A:806:ARG:HD3	2:B:93:ASP:OD1	2.18	0.43
1:A:134:ILE:CD1	1:A:170:CYS:HB2	2.48	0.43
1:A:371:GLN:HB3	1:A:377:ASP:OD1	2.18	0.43
1:A:576:ALA:O	1:A:580:ASN:HB2	2.19	0.43
8:A:909:AGS:O5'	8:A:909:AGS:H8	2.19	0.43
1:A:410:LYS:HB2	1:A:423:TRP:CD2	2.54	0.43
2:B:35:PHE:CD2	2:B:78:TYR:HD1	2.37	0.43
1:A:705:TYR:HB3	1:A:758:LEU:HB2	2.01	0.43
2:B:117:GLN:HA	3:C:19:CYS:O	2.19	0.42
1:A:232:GLU:O	1:A:236:ASN:HB2	2.19	0.42
1:A:703:TYR:HB3	1:A:757:PHE:HB3	2.00	0.42
3:C:41:ASN:OD1	3:C:41:ASN:N	2.52	0.42
3:C:104:SER:O	3:C:108:ILE:HG13	2.19	0.42
1:A:11:ALA:O	1:A:15:VAL:HG23	2.20	0.42
1:A:308:LYS:HB3	1:A:312:GLU:OE1	2.19	0.42
3:C:58:ASN:O	3:C:62:LYS:HG3	2.19	0.42
2:B:34:TYR:CD2	2:B:56:LEU:HD11	2.55	0.41
1:A:527:VAL:O	1:A:530:VAL:HG12	2.20	0.41
1:A:14:ILE:HD13	1:A:688:HIS:CB	2.50	0.41
1:A:632:LYS:HA	1:A:632:LYS:HD3	1.77	0.41
1:A:102:ILE:HB	1:A:696:LEU:HD21	2.01	0.41
1:A:422:ARG:HG2	1:A:422:ARG:HH11	1.86	0.41
1:A:560:CYS:HB3	1:A:570:PHE:CE2	2.56	0.41
1:A:127:TYR:CD2	1:A:166:HIS:HA	2.56	0.41
1:A:593:CYS:SG	1:A:595:GLU:HB2	2.61	0.41
2:B:119:LYS:HE2	2:B:119:LYS:HB3	1.94	0.41
1:A:285:ARG:HB3	1:A:291:TYR:CZ	2.56	0.40
1:A:520:LYS:HA	1:A:520:LYS:HD3	1.89	0.40
1:A:552:THR:HG23	1:A:555:LYS:HB2	2.02	0.40
3:C:32:MET:HB2	3:C:37:ILE:HB	2.03	0.40
1:A:228:ASN:HB2	1:A:229:PRO:HD3	2.03	0.40
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:HB3	1:A:711:GLU:HB2	2.02	0.40
1:A:555:LYS:NZ	11:A:1022:HOH:O	2.51	0.40
3:C:107:ASN:O	3:C:111:GLN:HG3	2.21	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	811/818 (99%)	786 (97%)	25 (3%)	0	100	100
2	B	129/204 (63%)	123 (95%)	6 (5%)	0	100	100
3	C	124/134 (92%)	117 (94%)	7 (6%)	0	100	100
All	All	1064/1156 (92%)	1026 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	725/725 (100%)	702 (97%)	23 (3%)	34	45
2	B	117/186 (63%)	115 (98%)	2 (2%)	53	68
3	C	120/126 (95%)	117 (98%)	3 (2%)	42	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	962/1037 (93%)	934 (97%)	28 (3%)	37 49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	56	VAL
1	A	92	SER
1	A	183	LYS
1	A	198	THR
1	A	201	THR
1	A	308	LYS
1	A	310	VAL
1	A	321	THR
1	A	324	SER
1	A	347	SER
1	A	368	ILE
1	A	370	LYS
1	A	477	LYS
1	A	522	THR
1	A	525	LYS
1	A	552	THR
1	A	568	ASN
1	A	651	SER
1	A	698	LEU
1	A	727	SER
1	A	750	LYS
1	A	813	LYS
2	B	37	GLU
2	B	69	LYS
3	C	40	THR
3	C	131	THR
3	C	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	496	ASN
1	A	584	GLN
1	A	622	GLN

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Mol	Chain	Res	Type
1	A	760	GLN
3	C	74	ASN
3	C	75	ASN
3	C	77	ASN
3	C	114	ASN
3	C	128	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](#)

1 non-standard protein/DNA/RNA residue is 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	A	19	1	8,9,10	1.60	1 (12%)	7,12,14	1.79	1 (14%)

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	A	19	1	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	SEP	P-O1P	3.50	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	SEP	OG-CB-CA	3.96	112.00	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	SEP	C-CA-CB-OG
1	A	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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
5	SO4	A	904	-	4,4,4	0.30	0	6,6,6	0.39	0
6	EDO	A	908	-	3,3,3	0.38	0	2,2,2	0.70	0
4	GOL	A	902	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
5	SO4	C	201	-	4,4,4	0.39	0	6,6,6	0.33	0
6	EDO	A	906	-	3,3,3	0.51	0	2,2,2	0.40	0
8	AGS	A	909	9	32,33,33	0.69	2 (6%)	45,52,52	0.65	1 (2%)
10	KQ0	A	911	-	25,26,26	1.66	4 (16%)	30,37,37	4.18	8 (26%)
4	GOL	A	905	-	5,5,5	2.20	2 (40%)	5,5,5	0.69	0
4	GOL	A	903	-	5,5,5	0.91	0	5,5,5	1.19	1 (20%)
4	GOL	A	901	-	5,5,5	1.76	1 (20%)	5,5,5	0.62	0
7	PG4	A	907	-	12,12,12	0.59	0	11,11,11	0.54	0

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
6	EDO	A	908	-	-	0/1/1/1	-
4	GOL	A	902	-	-	1/4/4/4	-
6	EDO	A	906	-	-	1/1/1/1	-
10	KQ0	A	911	-	-	8/15/22/22	0/4/4/4
8	AGS	A	909	9	-	2/21/38/38	0/3/3/3
4	GOL	A	905	-	-	4/4/4/4	-
4	GOL	A	903	-	-	1/4/4/4	-
4	GOL	A	901	-	-	2/4/4/4	-
7	PG4	A	907	-	-	5/10/10/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	911	KQ0	C18-C19	4.49	1.52	1.46
10	A	911	KQ0	C11-C09	3.49	1.55	1.51
4	A	901	GOL	C3-C2	3.24	1.64	1.51
4	A	905	GOL	C1-C2	3.23	1.64	1.51
4	A	905	GOL	C3-C2	3.09	1.63	1.51
10	A	911	KQ0	C15-C14	2.76	1.42	1.38
10	A	911	KQ0	C10-C09	2.76	1.54	1.51
8	A	909	AGS	PG-S1G	2.23	1.95	1.90
8	A	909	AGS	PB-O3B	-2.04	1.57	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	911	KQ0	C10-C09-C06	16.93	140.26	118.78
10	A	911	KQ0	C10-C09-N12	-8.95	108.81	117.30
10	A	911	KQ0	C11-C09-C06	-7.86	108.80	118.78
10	A	911	KQ0	C11-C09-N12	-6.24	111.38	117.30
10	A	911	KQ0	C22-S23-C19	3.74	99.04	92.33
10	A	911	KQ0	C01-O02-C03	-3.18	110.68	117.50
10	A	911	KQ0	C21-C22-S23	-2.86	106.02	113.02
10	A	911	KQ0	C18-N17-N16	2.45	107.29	104.73
4	A	903	GOL	C3-C2-C1	-2.17	103.82	111.80
4	A	902	GOL	C3-C2-C1	-2.11	104.05	111.80
8	A	909	AGS	O3G-PG-O3B	2.07	111.54	104.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	905	GOL	O1-C1-C2-C3
4	A	905	GOL	C1-C2-C3-O3
10	A	911	KQ0	C14-C13-N12-C09
10	A	911	KQ0	C05-C06-C09-N12
10	A	911	KQ0	C07-C06-C09-N12
7	A	907	PG4	O3-C5-C6-O4
4	A	901	GOL	C1-C2-C3-O3
4	A	905	GOL	O1-C1-C2-O2
4	A	905	GOL	O2-C2-C3-O3
7	A	907	PG4	O4-C7-C8-O5
6	A	906	EDO	O1-C1-C2-O2
4	A	902	GOL	O2-C2-C3-O3
7	A	907	PG4	O2-C3-C4-O3
10	A	911	KQ0	N17-C18-C19-C20
10	A	911	KQ0	N17-C18-C19-S23
4	A	903	GOL	O2-C2-C3-O3
7	A	907	PG4	C4-C3-O2-C2
4	A	901	GOL	O2-C2-C3-O3
8	A	909	AGS	PG-O3B-PB-O1B
8	A	909	AGS	PG-O3B-PB-O2B
7	A	907	PG4	C8-C7-O4-C6
10	A	911	KQ0	C14-C18-C19-S23
10	A	911	KQ0	C05-C06-C09-C10
10	A	911	KQ0	C07-C06-C09-C10

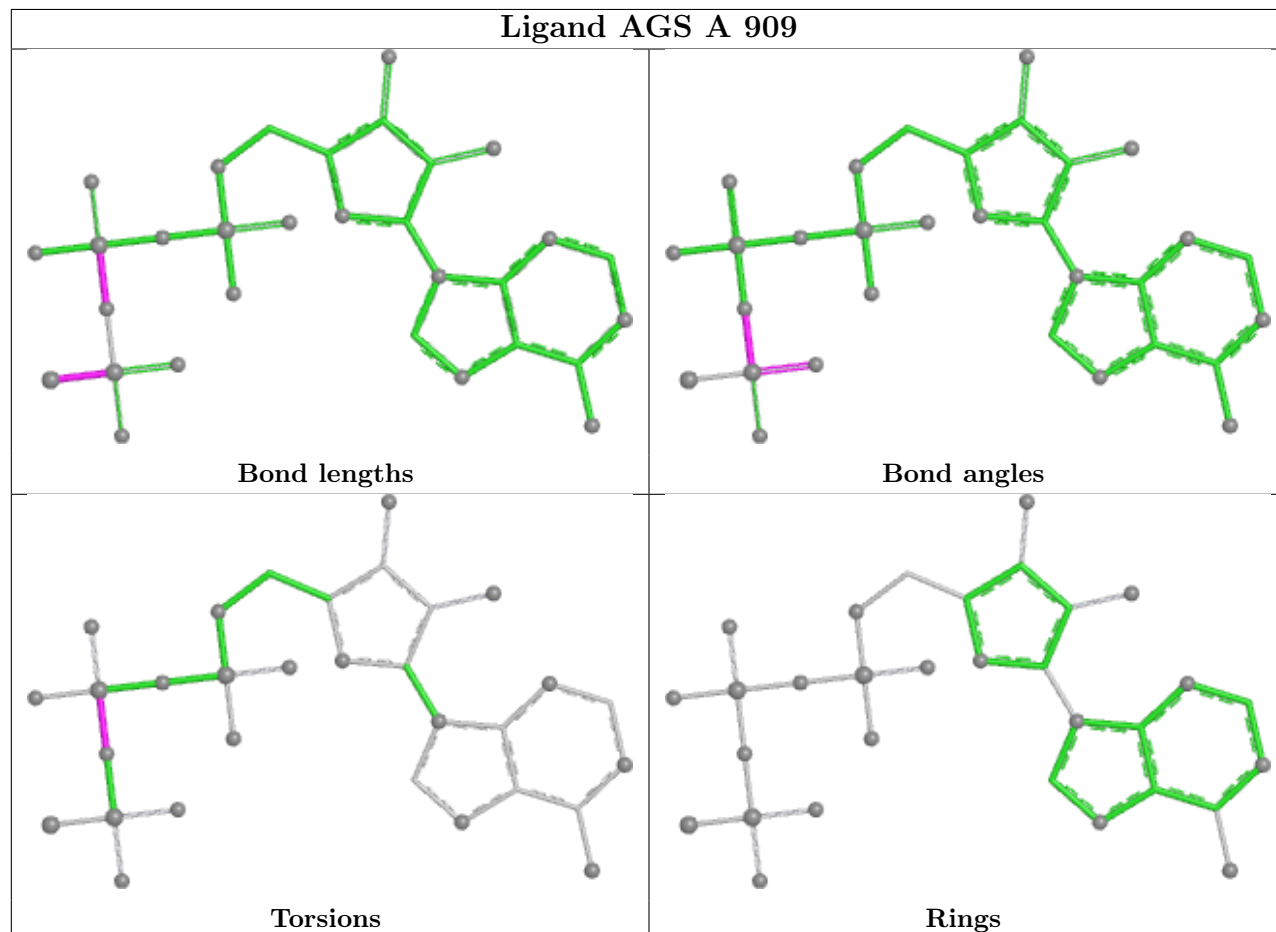
There are no ring outliers.

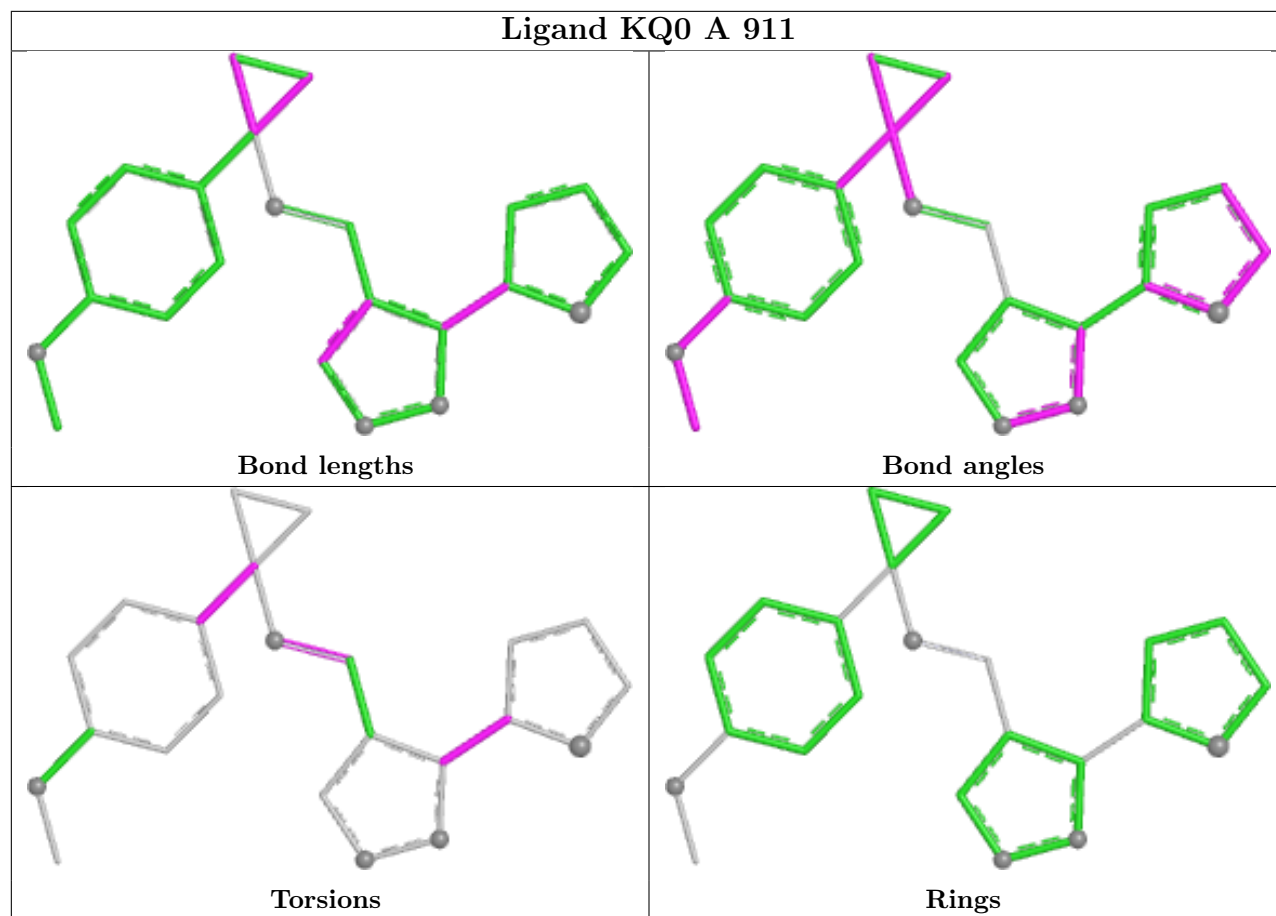
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	909	AGS	2	0
4	A	903	GOL	2	0
7	A	907	PG4	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	813/818 (99%)	0.06	35 (4%) 40 37	17, 43, 73, 108	2 (0%)
2	B	131/204 (64%)	0.63	10 (7%) 20 17	40, 65, 87, 106	0
3	C	128/134 (95%)	0.67	16 (12%) 8 6	39, 58, 87, 102	0
All	All	1072/1156 (92%)	0.21	61 (5%) 29 26	17, 47, 80, 108	2 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	83	VAL	6.2
1	A	160	HIS	6.2
1	A	2	ALA	5.3
1	A	575	VAL	4.5
3	C	2	ALA	4.2
1	A	376	SER	4.1
1	A	632	LYS	4.0
1	A	372	GLU	4.0
1	A	159	ASP	3.9
1	A	634	LYS	3.9
1	A	818	GLN	3.6
1	A	633	GLY	3.6
1	A	714	TYR	3.4
1	A	161	THR	3.3
1	A	477	LYS	3.1
1	A	630	ILE	3.1
3	C	134	ILE	3.0
1	A	518	GLU	3.0
1	A	817	ALA	2.9
1	A	283	ASN	2.9
1	A	377	ASP	2.9
2	B	92	LYS	2.8
2	B	38	LYS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	162	LYS	2.7
3	C	77	ASN	2.7
1	A	10	THR	2.6
1	A	741	LEU	2.6
1	A	576	ALA	2.5
3	C	88	ASP	2.5
1	A	577	SER	2.4
2	B	78	TYR	2.4
1	A	534	LYS	2.4
3	C	86	LYS	2.3
3	C	119	SER	2.3
2	B	41	GLY	2.3
2	B	42	GLY	2.3
1	A	574	LYS	2.3
3	C	115	PRO	2.3
3	C	87	ILE	2.3
1	A	751	ILE	2.2
1	A	163	LEU	2.2
2	B	31	VAL	2.2
3	C	76	VAL	2.2
1	A	416	GLY	2.2
3	C	112	ILE	2.2
2	B	145	ASP	2.1
1	A	26	LYS	2.1
3	C	110	LEU	2.1
1	A	579	LYS	2.1
1	A	6	GLU	2.1
1	A	401	GLU	2.1
1	A	520	LYS	2.1
2	B	28	GLU	2.1
2	B	79	GLU	2.1
2	B	35	PHE	2.1
3	C	45	ALA	2.0
1	A	371	GLN	2.0
3	C	75	ASN	2.0
3	C	106	LEU	2.0
1	A	567	ASN	2.0
3	C	74	ASN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	19	10/11	0.97	0.08	44,57,61,62	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

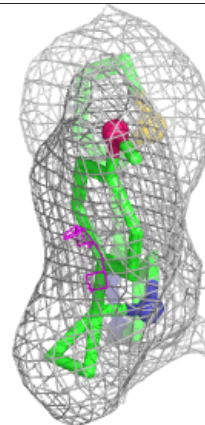
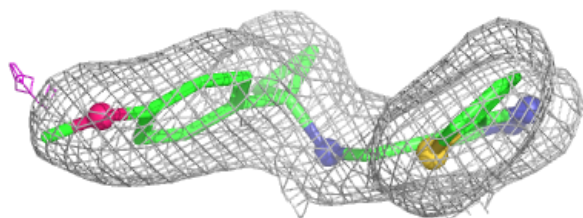
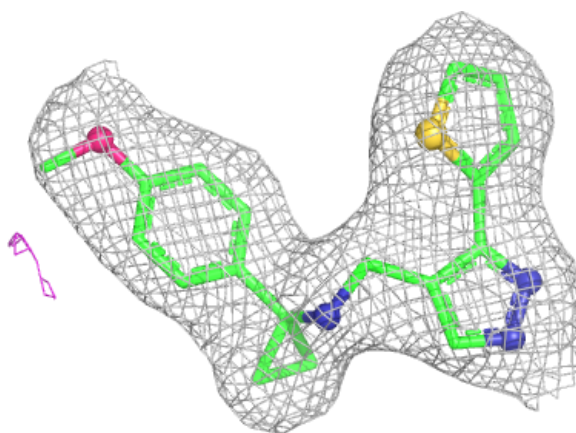
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	A	908	4/4	0.82	0.15	43,45,46,51	0
5	SO4	A	904	5/5	0.84	0.10	68,75,80,84	0
4	GOL	A	905	6/6	0.86	0.17	31,42,50,54	0
4	GOL	A	901	6/6	0.87	0.15	47,48,52,52	0
5	SO4	C	201	5/5	0.88	0.11	64,65,73,91	0
7	PG4	A	907	13/13	0.90	0.13	39,47,61,63	0
4	GOL	A	902	6/6	0.91	0.10	47,51,52,57	0
6	EDO	A	906	4/4	0.91	0.15	41,46,49,54	0
4	GOL	A	903	6/6	0.93	0.11	44,47,50,57	0
9	MG	A	910	1/1	0.97	0.05	41,41,41,41	0
10	KQ0	A	911	23/23	0.97	0.06	29,34,37,40	0
8	AGS	A	909	31/31	0.99	0.05	27,31,34,41	0

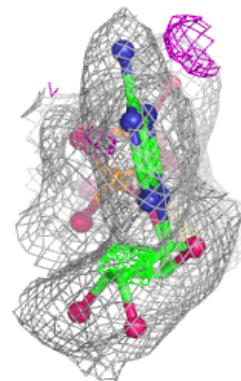
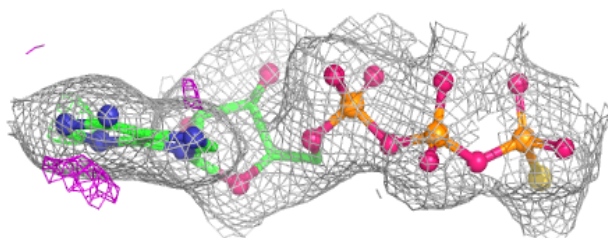
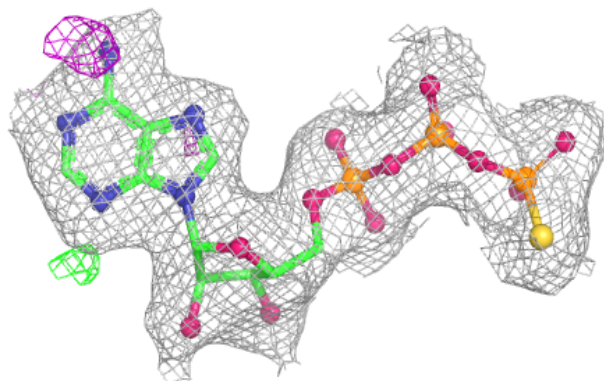
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around KQ0 A 911:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around AGS A 909:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.