



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:47 am BST

PDB ID : 4FUT
Title : Crystal structure of ATP bound MatB from Rhodopseudomonas palustris
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Deposited on : 2012-06-28
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

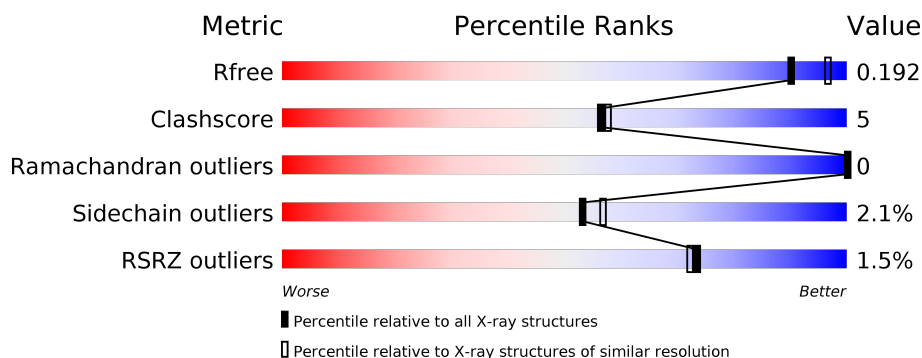
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	503	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; left: 0; top: -10px; width: 5px; height: 5px; background-color: red;"></div> <div style="position: absolute; left: 95%; top: -10px; width: 5px; height: 5px; background-color: yellow;"></div> <div style="position: absolute; left: 50%; top: -10px; width: 5px; height: 5px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 91% 8% </div> </div>

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
1	MLY	A	62	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4604 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.

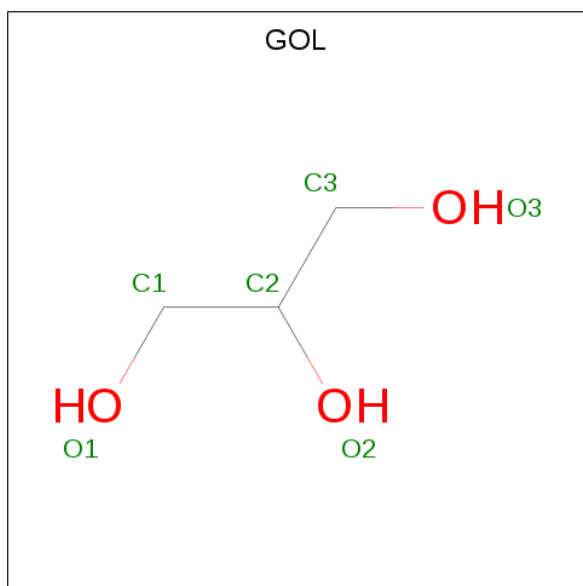
- Molecule 1 is a protein called Malonyl CoA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	1	9	0
			3927	2513	663	737	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	ALA	LYS	ENGINEERED MUTATION	UNP Q6ND88

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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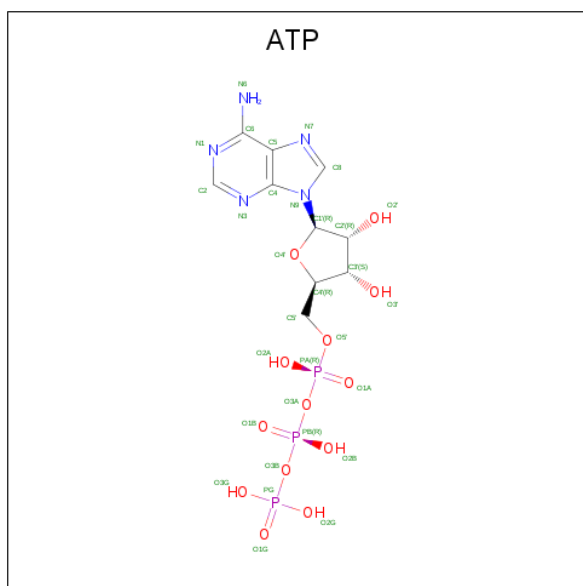
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

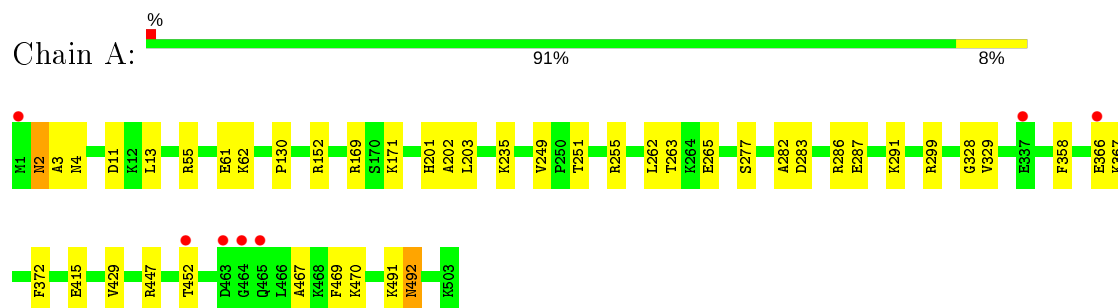
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	609	Total	O	0	0
			609	609		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Malonyl CoA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	173.14 Å 173.14 Å 47.74 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.99 – 2.00 24.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (24.99-2.00) 95.9 (24.99-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.72 (at 1.99 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.158 , 0.196 0.154 , 0.192	Depositor DCC
R_{free} test set	2828 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4604	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, MG, MLY, ATP

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	0.34	0/3720	0.51	0/5080

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

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	3927	0	3975	40	0
2	A	36	0	48	5	0
3	A	1	0	0	0	0
4	A	31	0	12	0	0
5	A	609	0	0	4	0
All	All	4604	0	4035	40	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 5.

All (40) 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:492:ASN:HD22	1:A:492:ASN:H	1.21	0.86
1:A:171:MLY:HH12	1:A:367:MLY:HE3	1.58	0.85
1:A:62:MLY:HH12	1:A:203:LEU:O	1.86	0.75
1:A:491:MLY:HH11	5:A:1016:HOH:O	1.85	0.74
1:A:62:MLY:HH22	1:A:62:MLY:CG	2.18	0.72
1:A:492:ASN:ND2	1:A:492:ASN:H	1.87	0.71
1:A:62:MLY:HH13	1:A:201:HIS:ND1	2.13	0.63
1:A:329:VAL:O	2:A:604:GOL:H2	2.01	0.61
1:A:2:ASN:HD21	1:A:152:ARG:H	1.48	0.59
1:A:61:GLU:HG3	1:A:130:PRO:HG3	1.84	0.58
1:A:251[A]:THR:HG22	1:A:255:ARG:NE	2.20	0.56
1:A:2:ASN:ND2	1:A:4:ASN:H	2.05	0.55
1:A:62:MLY:CB	1:A:62:MLY:HH22	2.37	0.53
1:A:467:ALA:HB3	1:A:470:MLY:HD2	1.89	0.53
1:A:251[A]:THR:HG22	1:A:255:ARG:HE	1.74	0.52
1:A:2:ASN:ND2	1:A:152:ARG:H	2.08	0.51
1:A:62:MLY:HH13	1:A:201:HIS:O	2.11	0.51
1:A:328:GLY:H	2:A:604:GOL:H31	1.76	0.51
1:A:262:LEU:O	1:A:291:MLY:HE3	2.10	0.50
1:A:263:THR:OG1	1:A:265[B]:GLU:HG2	2.11	0.50
1:A:62:MLY:HH11	1:A:202:ALA:HA	1.93	0.50
1:A:171:MLY:CH1	1:A:367:MLY:HE3	2.37	0.49
1:A:62:MLY:HG3	1:A:62:MLY:HH22	1.95	0.48
1:A:2:ASN:HD22	1:A:3:ALA:N	2.12	0.48
1:A:235:MLY:HH23	5:A:1105:HOH:O	2.14	0.47
1:A:492:ASN:ND2	1:A:492:ASN:N	2.58	0.46
1:A:249:VAL:HG12	1:A:277:SER:HB2	1.98	0.46
1:A:283:ASP:O	1:A:287:GLU:HG3	2.16	0.46
1:A:171:MLY:HH12	1:A:171:MLY:HD2	1.78	0.44
1:A:11[B]:ASP:OD1	5:A:1078:HOH:O	2.20	0.44
1:A:469:PHE:CE2	1:A:470:MLY:HG2	2.54	0.43
1:A:366:GLU:CD	1:A:367:MLY:H	2.22	0.42
1:A:169:ARG:HB3	5:A:1265:HOH:O	2.20	0.42
1:A:282:ALA:HB2	2:A:603:GOL:H31	2.01	0.42
1:A:429:VAL:O	1:A:491:MLY:HH22	2.20	0.42
1:A:286:ARG:HH22	2:A:603:GOL:H12	1.86	0.41
1:A:62:MLY:CH1	1:A:201:HIS:ND1	2.83	0.41
1:A:62:MLY:CH1	1:A:201:HIS:O	2.69	0.40
1:A:415:GLU:OE2	1:A:491:MLY:NZ	2.54	0.40
1:A:372:PHE:CG	2:A:602:GOL:H11	2.57	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	483/503 (96%)	478 (99%)	5 (1%)	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	383/374 (102%)	375 (98%)	8 (2%)	53	57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	13	LEU
1	A	55	ARG
1	A	299	ARG
1	A	358	PHE
1	A	447	ARG
1	A	452	THR
1	A	492	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	408	ASN
1	A	457	GLN
1	A	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 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	MLY	A	264	1	9,10,11	0.60	0	6,11,13	0.56	0
1	MLY	A	367	1	9,10,11	0.52	0	6,11,13	0.93	0
1	MLY	A	120	1	9,10,11	0.51	0	6,11,13	0.77	0
1	MLY	A	473	1	9,10,11	0.50	0	6,11,13	0.82	0
1	MLY	A	412	1	9,10,11	0.53	0	6,11,13	0.81	0
1	MLY	A	470	1	9,10,11	0.52	0	6,11,13	0.72	0
1	MLY	A	110	1	9,10,11	0.48	0	6,11,13	1.09	0
1	MLY	A	468	1	9,10,11	0.54	0	6,11,13	0.94	0
1	MLY	A	353	1	9,10,11	0.62	0	6,11,13	0.82	0
1	MLY	A	449	1	9,10,11	0.59	0	6,11,13	0.78	0
1	MLY	A	359	1	9,10,11	0.63	0	6,11,13	0.70	0
1	MLY	A	385	1	9,10,11	0.46	0	6,11,13	0.83	0
1	MLY	A	28	1	9,10,11	0.48	0	6,11,13	0.87	0
1	MLY	A	62	1	9,10,11	0.66	0	6,11,13	1.59	1 (16%)
1	MLY	A	291	1	9,10,11	0.60	0	6,11,13	0.67	0
1	MLY	A	491	1	9,10,11	0.44	0	6,11,13	0.99	0
1	MLY	A	171	1	9,10,11	0.46	0	6,11,13	0.84	0
1	MLY	A	230	1	9,10,11	0.56	0	6,11,13	0.81	0
1	MLY	A	102	1	9,10,11	0.61	0	6,11,13	0.73	0
1	MLY	A	369	1	9,10,11	0.49	0	6,11,13	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	503	1	7,11,11	0.48	0	7,13,13	0.78	0
1	MLY	A	340	1	9,10,11	0.46	0	6,11,13	0.97	0
1	MLY	A	12	1	9,10,11	0.53	0	6,11,13	0.84	0
1	MLY	A	474	1	9,10,11	0.59	0	6,11,13	0.84	0
1	MLY	A	235	1	9,10,11	0.47	0	6,11,13	0.75	0
1	MLY	A	499	1	9,10,11	0.50	0	6,11,13	0.78	0
1	MLY	A	399	1	9,10,11	0.47	0	6,11,13	0.90	0
1	MLY	A	18	1	9,10,11	0.55	0	6,11,13	0.78	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
1	MLY	A	264	1	-	0/8/9/11	-
1	MLY	A	367	1	-	3/8/9/11	-
1	MLY	A	120	1	-	1/8/9/11	-
1	MLY	A	473	1	-	1/8/9/11	-
1	MLY	A	412	1	-	0/8/9/11	-
1	MLY	A	470	1	-	1/8/9/11	-
1	MLY	A	110	1	-	0/8/9/11	-
1	MLY	A	468	1	-	0/8/9/11	-
1	MLY	A	353	1	-	1/8/9/11	-
1	MLY	A	449	1	-	0/8/9/11	-
1	MLY	A	359	1	-	2/8/9/11	-
1	MLY	A	385	1	-	0/8/9/11	-
1	MLY	A	28	1	-	0/8/9/11	-
1	MLY	A	62	1	-	4/8/9/11	-
1	MLY	A	291	1	-	1/8/9/11	-
1	MLY	A	491	1	-	2/8/9/11	-
1	MLY	A	171	1	-	1/8/9/11	-
1	MLY	A	230	1	-	3/8/9/11	-
1	MLY	A	102	1	-	1/8/9/11	-
1	MLY	A	369	1	-	0/8/9/11	-
1	MLY	A	503	1	-	2/7/11/11	-
1	MLY	A	340	1	-	1/8/9/11	-
1	MLY	A	12	1	-	2/8/9/11	-
1	MLY	A	474	1	-	3/8/9/11	-
1	MLY	A	235	1	-	1/8/9/11	-
1	MLY	A	499	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	399	1	-	3/8/9/11	-
1	MLY	A	18	1	-	3/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	MLY	CH2-NZ-CH1	-2.75	102.62	109.73

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	367	MLY	O-C-CA-CB
1	A	120	MLY	O-C-CA-CB
1	A	503	MLY	C-CA-CB-CG
1	A	12	MLY	C-CA-CB-CG
1	A	62	MLY	CD-CE-NZ-CH1
1	A	399	MLY	CD-CE-NZ-CH1
1	A	399	MLY	CD-CE-NZ-CH2
1	A	291	MLY	CG-CD-CE-NZ
1	A	62	MLY	CD-CE-NZ-CH2
1	A	171	MLY	CD-CE-NZ-CH1
1	A	474	MLY	CD-CE-NZ-CH2
1	A	474	MLY	CG-CD-CE-NZ
1	A	230	MLY	CG-CD-CE-NZ
1	A	18	MLY	CD-CE-NZ-CH2
1	A	230	MLY	CA-CB-CG-CD
1	A	359	MLY	CA-CB-CG-CD
1	A	491	MLY	CG-CD-CE-NZ
1	A	340	MLY	CD-CE-NZ-CH2
1	A	62	MLY	CA-CB-CG-CD
1	A	18	MLY	CA-CB-CG-CD
1	A	367	MLY	CA-CB-CG-CD
1	A	503	MLY	CA-CB-CG-CD
1	A	359	MLY	CD-CE-NZ-CH1
1	A	62	MLY	CE-CD-CG-CB
1	A	474	MLY	CD-CE-NZ-CH1
1	A	367	MLY	CD-CE-NZ-CH2
1	A	102	MLY	CD-CE-NZ-CH2
1	A	12	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	470	MLY	CA-CB-CG-CD
1	A	491	MLY	CE-CD-CG-CB
1	A	230	MLY	CE-CD-CG-CB
1	A	353	MLY	CD-CE-NZ-CH1
1	A	235	MLY	CD-CE-NZ-CH1
1	A	399	MLY	CA-CB-CG-CD
1	A	18	MLY	CD-CE-NZ-CH1
1	A	473	MLY	CA-CB-CG-CD

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	367	MLY	3	0
1	A	470	MLY	2	0
1	A	62	MLY	9	0
1	A	291	MLY	1	0
1	A	491	MLY	3	0
1	A	171	MLY	3	0
1	A	235	MLY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	GOL	A	603	-	5,5,5	0.34	0	5,5,5	0.17	0
2	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.21	0
2	GOL	A	601	-	5,5,5	0.36	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	606	-	5,5,5	0.37	0	5,5,5	0.25	0
2	GOL	A	605	-	5,5,5	0.38	0	5,5,5	0.30	0
4	ATP	A	608	3	26,33,33	0.92	1 (3%)	31,52,52	1.24	2 (6%)
2	GOL	A	604	-	5,5,5	0.48	0	5,5,5	0.17	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
2	GOL	A	603	-	-	4/4/4/4	-
2	GOL	A	602	-	-	4/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	A	606	-	-	2/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-
4	ATP	A	608	3	-	4/18/38/38	0/3/3/3
2	GOL	A	604	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	ATP	C5-C4	2.50	1.47	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	ATP	N3-C2-N1	-2.92	124.12	128.68
4	A	608	ATP	C4-C5-N7	-2.74	106.54	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-C3
2	A	606	GOL	O1-C1-C2-C3

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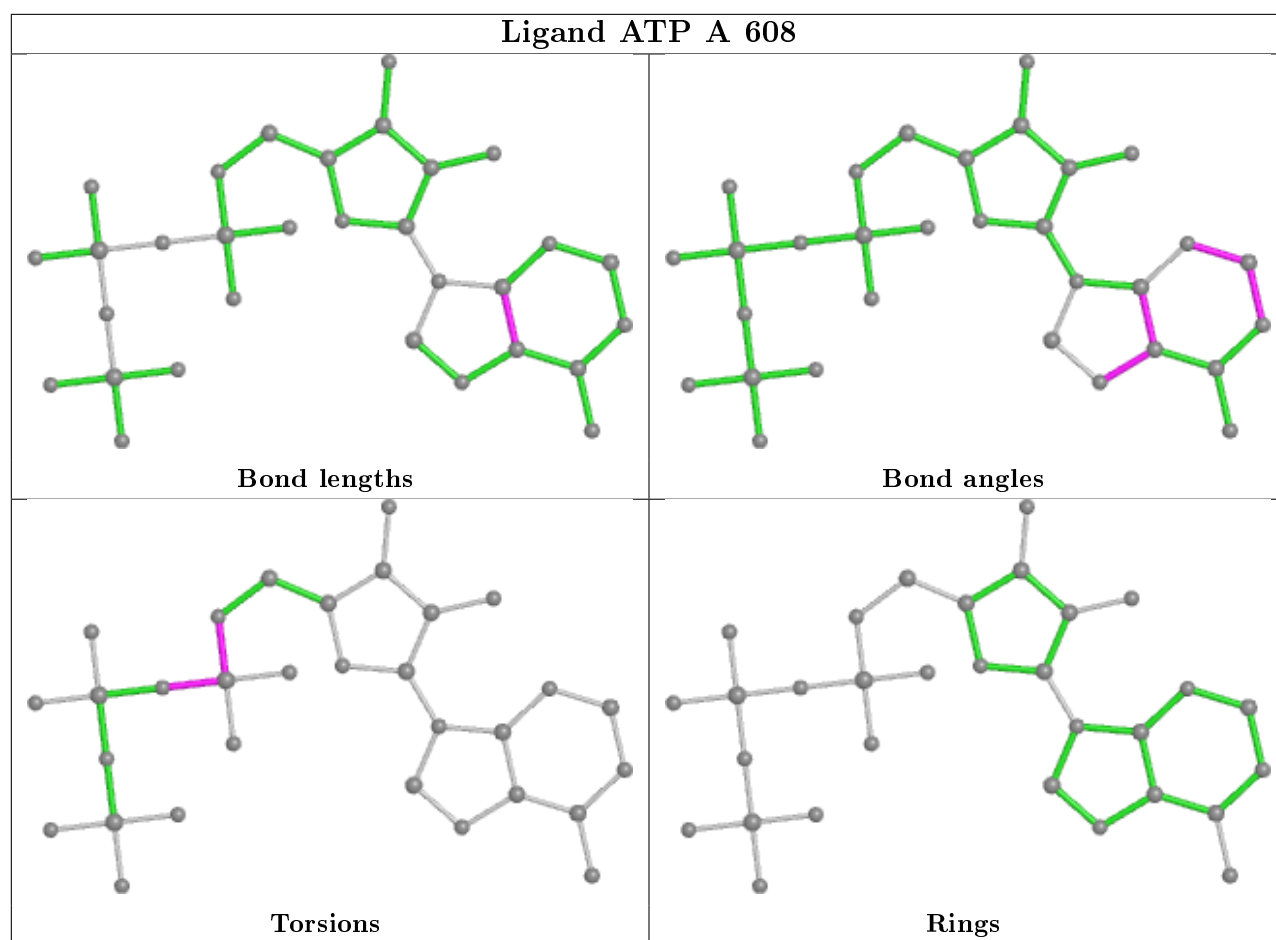
Mol	Chain	Res	Type	Atoms
2	A	605	GOL	O1-C1-C2-C3
4	A	608	ATP	PB-O3A-PA-O5'
4	A	608	ATP	C5'-O5'-PA-O1A
4	A	608	ATP	C5'-O5'-PA-O2A
2	A	604	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	A	602	GOL	C1-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
2	A	606	GOL	O1-C1-C2-O2
2	A	605	GOL	O1-C1-C2-O2
2	A	604	GOL	O1-C1-C2-O2
2	A	602	GOL	O2-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3
4	A	608	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	GOL	2	0
2	A	602	GOL	1	0
2	A	604	GOL	2	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	475/503 (94%)	-0.46	7 (1%) 73 72	17, 27, 55, 91	3 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	ASP	3.0
1	A	452	THR	2.8
1	A	337	GLU	2.8
1	A	464	GLY	2.7
1	A	1	MET	2.6
1	A	465	GLN	2.3
1	A	366	GLU	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	MLY	A	503	12/12	0.89	0.33	53,77,111,111	0
1	MLY	A	449	11/12	0.90	0.30	61,75,86,87	3
1	MLY	A	399	11/12	0.90	0.24	42,70,112,113	1
1	MLY	A	367	11/12	0.92	0.28	43,57,100,101	2
1	MLY	A	359	11/12	0.92	0.12	27,42,53,55	0
1	MLY	A	264	11/12	0.93	0.12	23,29,31,32	0
1	MLY	A	470	11/12	0.93	0.11	41,50,67,69	0
1	MLY	A	291	11/12	0.94	0.14	30,37,87,93	0
1	MLY	A	491	11/12	0.94	0.12	29,34,46,69	0
1	MLY	A	171	11/12	0.94	0.12	25,45,82,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	A	468	11/12	0.94	0.23	45,63,81,82	2
1	MLY	A	385	11/12	0.94	0.10	25,31,67,67	0
1	MLY	A	369	11/12	0.95	0.25	32,49,77,78	1
1	MLY	A	120	11/12	0.95	0.19	39,46,75,76	0
1	MLY	A	12	11/12	0.95	0.22	31,47,90,90	4
1	MLY	A	474	11/12	0.95	0.11	31,45,58,66	0
1	MLY	A	473	11/12	0.95	0.10	36,48,60,60	0
1	MLY	A	28	11/12	0.96	0.12	23,36,52,54	0
1	MLY	A	340	11/12	0.96	0.19	34,53,82,89	0
1	MLY	A	62	11/12	0.96	0.13	23,31,55,69	0
1	MLY	A	230	11/12	0.96	0.12	34,47,85,89	0
1	MLY	A	235	11/12	0.96	0.13	23,36,68,77	0
1	MLY	A	499	11/12	0.96	0.21	33,47,74,75	0
1	MLY	A	110	11/12	0.96	0.10	28,39,62,67	0
1	MLY	A	18	11/12	0.96	0.13	22,30,62,70	0
1	MLY	A	412	11/12	0.97	0.10	27,31,36,38	0
1	MLY	A	353	11/12	0.97	0.08	21,26,59,64	0
1	MLY	A	102	11/12	0.98	0.10	19,26,54,68	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

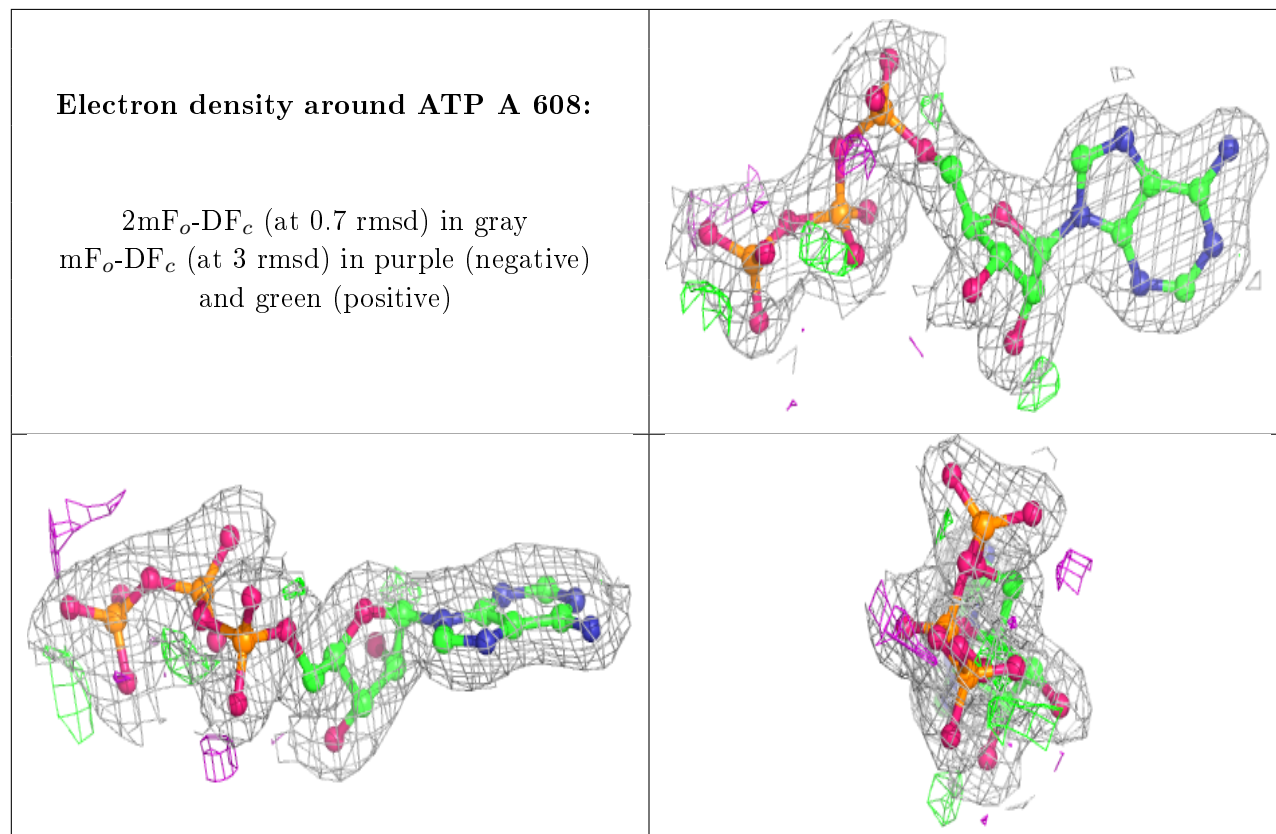
6.4 Ligands

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(\AA^2)	Q<0.9
2	GOL	A	602	6/6	0.65	0.23	74,79,83,84	0
2	GOL	A	604	6/6	0.66	0.33	39,58,66,70	0
2	GOL	A	603	6/6	0.67	0.33	59,65,72,72	0
2	GOL	A	606	6/6	0.84	0.22	52,67,74,74	0
2	GOL	A	605	6/6	0.86	0.31	56,64,67,68	0
2	GOL	A	601	6/6	0.92	0.14	53,59,66,76	0
3	MG	A	607	1/1	0.96	0.09	31,31,31,31	0
4	ATP	A	608	31/31	0.98	0.09	20,25,36,45	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 ⓘ

There are no such residues in this entry.