



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:56 pm GMT

PDB ID : 5MCP
Title : Structure of IMP dehydrogenase from *Ashbya gossypii* bound to ATP
Authors : Winter, G.; Fernandez-Justel, D.; de Pereda, J.M.; Revuelta, J.L.; Buey, R.M.
Deposited on : 2016-11-10
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

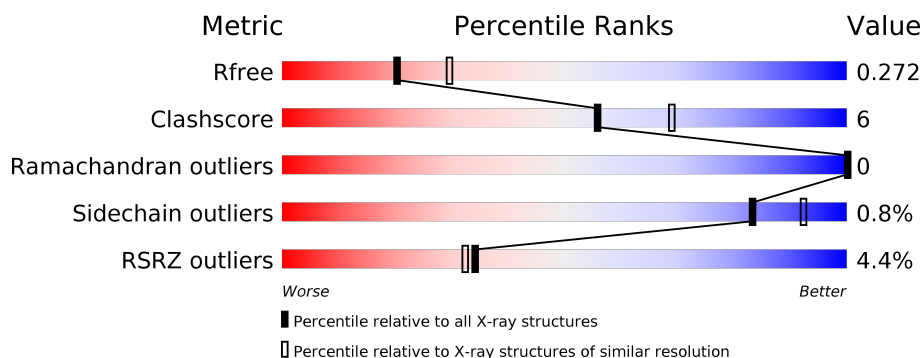
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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. 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	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 77%, green 16%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 77% 7% 16% </div> </div>
1	B	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 76%, green 15%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 76% 8% 15% </div> </div>
1	C	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 79%, green 15%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 79% 6% 15% </div> </div>
1	D	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 76%, green 15%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 9% 15% </div> </div>
1	E	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 66%, green 26%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 66% 8% 26% </div> </div>
1	F	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 59%, green 35%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 59% 6% 35% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	523	<div><div></div><div>7%</div><div>64%</div><div>9%</div><div>27%</div></div>
1	H	523	<div><div></div><div>8%</div><div>57%</div><div>5%</div><div>39%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45606 atoms, of which 21090 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	H	N	O	S	0	0	0
			6568	2057	3293	563	632	23			
1	B	444	Total	C	H	N	O	S	0	0	0
			6442	2039	3187	564	631	21			
1	C	446	Total	C	H	N	O	S	0	1	0
			6556	2068	3260	567	637	24			
1	D	443	Total	C	H	N	O	S	0	1	0
			6541	2060	3267	566	625	23			
1	E	387	Total	C	H	N	O	S	0	0	0
			5039	1659	2384	464	517	15			
1	F	342	Total	C	H	N	O	S	0	1	0
			4054	1379	1832	407	423	13			
1	G	382	Total	C	H	N	O	S	0	0	0
			4580	1561	2066	455	484	14			
1	H	321	Total	C	H	N	O	S	0	0	0
			3526	1225	1529	374	387	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q756Z6
B	0	HIS	-	expression tag	UNP Q756Z6
C	0	HIS	-	expression tag	UNP Q756Z6
D	0	HIS	-	expression tag	UNP Q756Z6
E	0	HIS	-	expression tag	UNP Q756Z6
F	0	HIS	-	expression tag	UNP Q756Z6
G	0	HIS	-	expression tag	UNP Q756Z6
H	0	HIS	-	expression tag	UNP Q756Z6

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	E	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	E	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	F	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	G	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	G	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	G	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	H	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	H	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	H	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O	0	0
			277	277		

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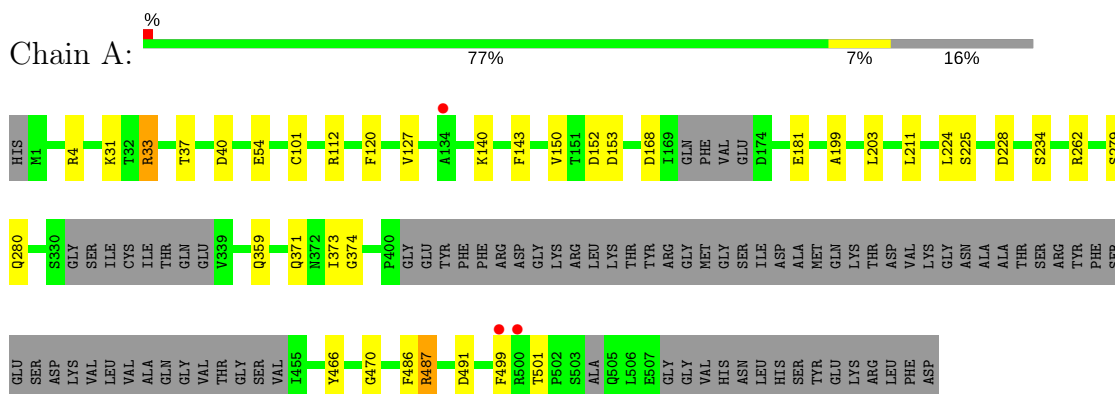
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	283	Total 283	O 283	0	0
4	C	301	Total 301	O 301	0	0
4	D	285	Total 285	O 285	0	0
4	E	51	Total 51	O 51	0	0
4	F	38	Total 38	O 38	0	0
4	G	24	Total 24	O 24	0	0
4	H	17	Total 17	O 17	0	0

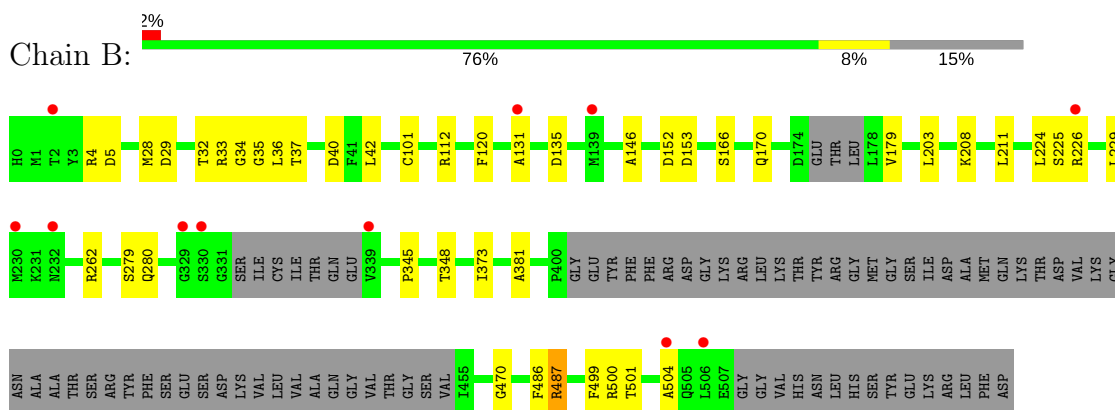
3 Residue-property plots [i](#)

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.

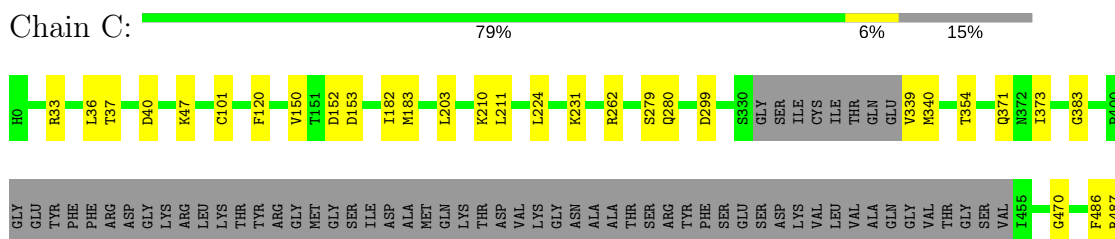
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

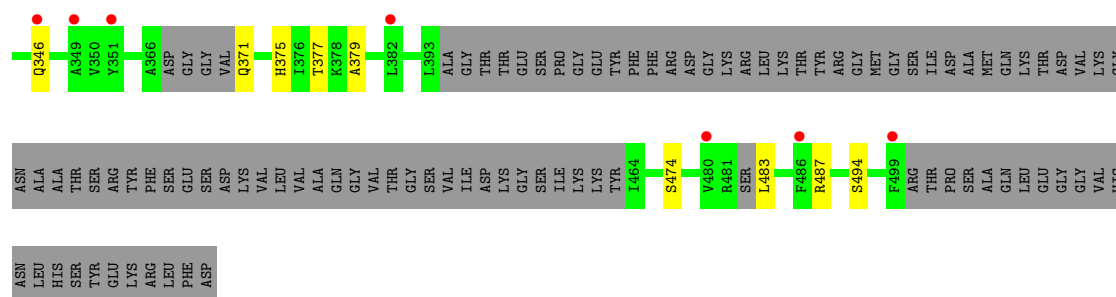


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

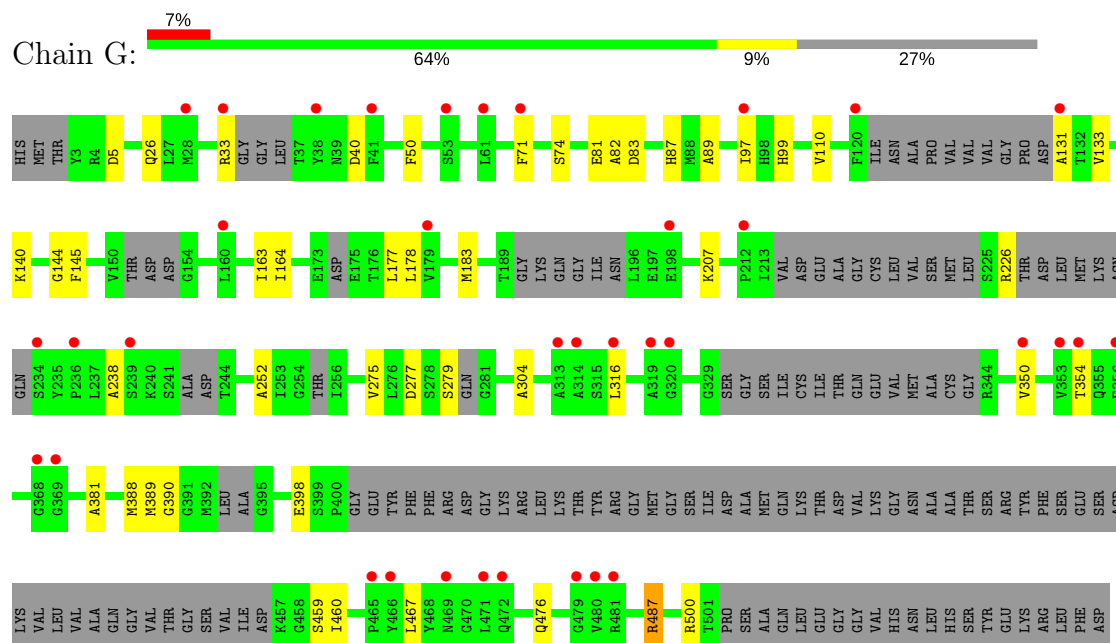


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

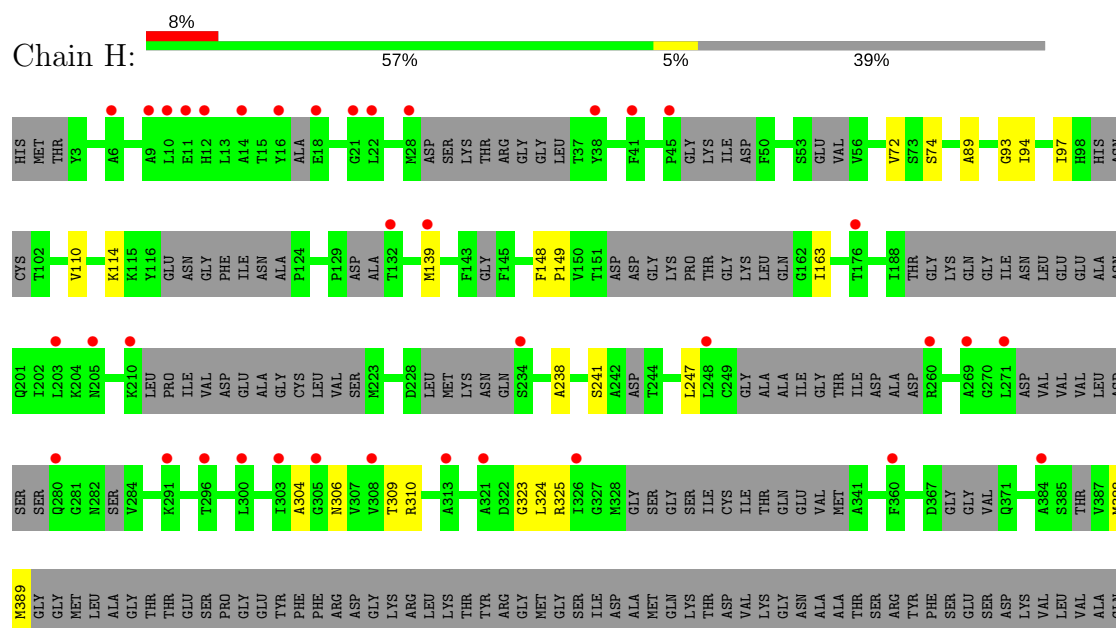




• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase



GLY	VAL	THR	GLY	SER	VAL	ILE	ASP	LYS	GLY	SER	ILE	LYS	LYS	Y463	L467	F485	R487	F499	ARG	THR	PRO	SER	ALA	GLN	LEU	GLU	GLY	GLY	VAL	HIS	ASN	LEU	HIS	SER	TYR	GLU	LYS	ARG	LEU	PHE	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.89Å 152.09Å 152.25Å 90.00° 93.03° 90.00°	Depositor
Resolution (Å)	152.04 – 2.40 152.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.04-2.40) 92.3 (152.04-2.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.249 , 0.271 0.250 , 0.272	Depositor DCC
R_{free} test set	11359 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	45606	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, 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	0.36	2/3318 (0.1%)	0.48	0/4484
1	B	0.32	0/3300	0.49	0/4469
1	C	0.36	0/3345	0.51	0/4526
1	D	0.30	0/3322	0.48	0/4493
1	E	0.38	0/2678	0.51	0/3629
1	F	0.27	0/2241	0.44	0/3038
1	G	0.36	0/2544	0.50	0/3459
1	H	0.32	0/2004	0.46	0/2716
All	All	0.34	2/22752 (0.0%)	0.49	0/30814

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ARG	CZ-NH2	7.18	1.42	1.33
1	A	33	ARG	CZ-NH1	6.72	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	305	GLY	Peptide

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	3275	3293	3286	38	0
1	B	3255	3187	3194	39	0
1	C	3296	3260	3260	25	0
1	D	3274	3267	3262	40	0
1	E	2655	2384	2365	42	0
1	F	2222	1832	1816	21	0
1	G	2514	2066	2057	38	0
1	H	1997	1529	1508	15	0
2	A	93	34	36	6	0
2	B	155	56	60	4	0
2	C	93	34	36	3	0
2	D	93	34	36	4	0
2	E	93	34	36	1	0
2	F	31	12	12	1	0
2	G	93	34	36	4	0
2	H	93	34	36	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	277	0	0	11	0
4	B	283	0	0	7	0
4	C	301	0	0	9	2
4	D	285	0	0	8	2
4	E	51	0	0	5	0
4	F	38	0	0	4	0
4	G	24	0	0	3	0
4	H	17	0	0	0	0
All	All	24516	21090	21036	244	2

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 6.

The worst 5 of 244 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:E:71:PHE:CD1	1:E:389:MET:HE3	1.74	1.22
1:G:133:VAL:HG23	1:G:177:LEU:O	1.38	1.22
1:E:64:LYS:HB2	1:E:301:GLN:NE2	1.54	1.20
1:E:71:PHE:CD1	1:E:389:MET:CE	2.26	1.18
1:E:71:PHE:HD1	1:E:389:MET:CE	1.57	1.14

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:705:HOH:O	4:D:802:HOH:O[2_554]	2.09	0.11
4:C:975:HOH:O	4:D:873:HOH:O[2_554]	2.14	0.06

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	430/523 (82%)	421 (98%)	9 (2%)	0	100	100
1	B	436/523 (83%)	430 (99%)	6 (1%)	0	100	100
1	C	441/523 (84%)	432 (98%)	9 (2%)	0	100	100
1	D	436/523 (83%)	426 (98%)	10 (2%)	0	100	100
1	E	356/523 (68%)	343 (96%)	13 (4%)	0	100	100
1	F	306/523 (58%)	295 (96%)	11 (4%)	0	100	100
1	G	354/523 (68%)	346 (98%)	8 (2%)	0	100	100
1	H	279/523 (53%)	272 (98%)	7 (2%)	0	100	100
All	All	3038/4184 (73%)	2965 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	350/430 (81%)	347 (99%)	3 (1%)	81	91
1	B	337/430 (78%)	334 (99%)	3 (1%)	81	91
1	C	345/430 (80%)	342 (99%)	3 (1%)	81	91
1	D	343/430 (80%)	339 (99%)	4 (1%)	74	87
1	E	234/430 (54%)	234 (100%)	0	100	100
1	F	165/430 (38%)	164 (99%)	1 (1%)	87	95
1	G	191/430 (44%)	190 (100%)	1 (0%)	90	96
1	H	128/430 (30%)	127 (99%)	1 (1%)	83	92
All	All	2093/3440 (61%)	2077 (99%)	16 (1%)	83	92

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	486	PHE
1	C	487	ARG
1	D	487	ARG
1	C	280	GLN
1	F	487	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	GLN
1	E	286	GLN
1	E	301	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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	ATP	A	601	3	27,33,33	2.76	5 (18%)	27,52,52	2.47	10 (37%)
2	ATP	A	602	3	27,33,33	2.87	4 (14%)	27,52,52	2.42	9 (33%)
2	ATP	A	603	-	27,33,33	2.76	5 (18%)	27,52,52	2.44	8 (29%)
2	ATP	B	601	3	27,33,33	2.80	5 (18%)	27,52,52	2.44	8 (29%)
2	ATP	B	602	3	27,33,33	2.78	5 (18%)	27,52,52	2.45	9 (33%)
2	ATP	B	603	-	27,33,33	2.70	5 (18%)	27,52,52	2.44	9 (33%)
2	ATP	B	605	3	27,33,33	2.81	5 (18%)	27,52,52	2.45	6 (22%)
2	ATP	B	606	3	27,33,33	2.86	5 (18%)	27,52,52	2.42	8 (29%)
2	ATP	C	601	3	27,33,33	2.85	5 (18%)	27,52,52	2.43	8 (29%)
2	ATP	C	602	3	27,33,33	2.81	4 (14%)	27,52,52	2.45	8 (29%)
2	ATP	C	603	-	27,33,33	2.75	5 (18%)	27,52,52	2.38	7 (25%)
2	ATP	D	601	3	27,33,33	2.65	5 (18%)	27,52,52	2.45	9 (33%)
2	ATP	D	602	3	27,33,33	2.72	5 (18%)	27,52,52	2.35	8 (29%)
2	ATP	D	603	-	27,33,33	2.74	5 (18%)	27,52,52	2.48	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	E	601	3	27,33,33	2.92	5 (18%)	27,52,52	2.26	8 (29%)
2	ATP	E	602	3	27,33,33	2.81	5 (18%)	27,52,52	2.45	8 (29%)
2	ATP	E	603	-	27,33,33	2.84	6 (22%)	27,52,52	2.37	6 (22%)
2	ATP	F	601	-	27,33,33	2.78	5 (18%)	27,52,52	2.41	9 (33%)
2	ATP	G	601	3	27,33,33	2.89	5 (18%)	27,52,52	2.48	9 (33%)
2	ATP	G	602	3	27,33,33	2.83	5 (18%)	27,52,52	2.39	6 (22%)
2	ATP	G	603	-	27,33,33	2.88	5 (18%)	27,52,52	2.30	8 (29%)
2	ATP	H	601	3	27,33,33	2.77	5 (18%)	27,52,52	2.48	9 (33%)
2	ATP	H	602	3	27,33,33	2.77	5 (18%)	27,52,52	2.43	9 (33%)
2	ATP	H	603	-	27,33,33	2.81	5 (18%)	27,52,52	2.40	8 (29%)

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	ATP	A	601	3	-	0/18/38/38	0/3/3/3
2	ATP	A	602	3	-	0/18/38/38	0/3/3/3
2	ATP	A	603	-	-	0/18/38/38	0/3/3/3
2	ATP	B	601	3	-	0/18/38/38	0/3/3/3
2	ATP	B	602	3	-	0/18/38/38	0/3/3/3
2	ATP	B	603	-	-	0/18/38/38	0/3/3/3
2	ATP	B	605	3	-	0/18/38/38	0/3/3/3
2	ATP	B	606	3	-	0/18/38/38	0/3/3/3
2	ATP	C	601	3	-	0/18/38/38	0/3/3/3
2	ATP	C	602	3	-	0/18/38/38	0/3/3/3
2	ATP	C	603	-	-	0/18/38/38	0/3/3/3
2	ATP	D	601	3	-	0/18/38/38	0/3/3/3
2	ATP	D	602	3	-	0/18/38/38	0/3/3/3
2	ATP	D	603	-	-	0/18/38/38	0/3/3/3
2	ATP	E	601	3	-	0/18/38/38	0/3/3/3
2	ATP	E	602	3	-	0/18/38/38	0/3/3/3
2	ATP	E	603	-	-	0/18/38/38	0/3/3/3
2	ATP	F	601	-	-	0/18/38/38	0/3/3/3
2	ATP	G	601	3	-	0/18/38/38	0/3/3/3
2	ATP	G	602	3	-	0/18/38/38	0/3/3/3
2	ATP	G	603	-	-	0/18/38/38	0/3/3/3
2	ATP	H	601	3	-	0/18/38/38	0/3/3/3
2	ATP	H	602	3	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	H	603	-	-	0/18/38/38	0/3/3/3

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	ATP	O5'-C5'	-2.75	1.34	1.44
2	G	601	ATP	O5'-C5'	-2.74	1.34	1.44
2	A	602	ATP	O5'-C5'	-2.69	1.34	1.44
2	B	602	ATP	O5'-C5'	-2.66	1.34	1.44
2	E	602	ATP	O5'-C5'	-2.65	1.34	1.44

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	603	ATP	PA-O3A-PB	-7.11	108.74	132.63
2	B	606	ATP	PA-O3A-PB	-6.99	109.12	132.63
2	H	601	ATP	PA-O3A-PB	-6.94	109.31	132.63
2	G	601	ATP	PA-O3A-PB	-6.91	109.41	132.63
2	A	601	ATP	PA-O3A-PB	-6.89	109.47	132.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ATP	2	0
2	A	602	ATP	2	0
2	A	603	ATP	2	0
2	B	602	ATP	1	0
2	B	603	ATP	1	0
2	B	605	ATP	2	0
2	C	601	ATP	2	0
2	C	602	ATP	1	0
2	C	603	ATP	1	0
2	D	602	ATP	3	0
2	D	603	ATP	1	0
2	E	601	ATP	1	0
2	F	601	ATP	1	0
2	G	602	ATP	1	0
2	G	603	ATP	3	0

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	440/523 (84%)	-0.10	3 (0%) 87 86	19, 36, 92, 167	0
1	B	444/523 (84%)	-0.09	11 (2%) 57 55	22, 37, 100, 144	0
1	C	446/523 (85%)	-0.11	0 100 100	20, 36, 95, 159	0
1	D	443/523 (84%)	-0.07	7 (1%) 72 69	20, 35, 91, 124	0
1	E	387/523 (73%)	0.23	18 (4%) 31 29	23, 99, 141, 182	0
1	F	342/523 (65%)	0.42	26 (7%) 14 12	71, 110, 146, 183	0
1	G	382/523 (73%)	0.52	36 (9%) 8 7	30, 106, 152, 182	0
1	H	321/523 (61%)	0.62	40 (12%) 4 3	80, 114, 153, 183	0
All	All	3205/4184 (76%)	0.15	141 (4%) 34 32	19, 77, 137, 183	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	320	GLY	5.6
1	G	38	TYR	5.4
1	H	9	ALA	4.8
1	H	326	ILE	4.8
1	F	38	TYR	4.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	MG	C	605	1/1	0.54	0.17	113,113,113,113	0
3	MG	B	604	1/1	0.60	0.13	79,79,79,79	0
3	MG	C	604	1/1	0.69	0.37	89,89,89,89	0
2	ATP	G	603	31/31	0.74	0.26	100,106,122,125	43
3	MG	E	605	1/1	0.76	0.17	93,93,93,93	0
2	ATP	B	606	31/31	0.77	0.19	97,103,121,123	0
2	ATP	H	603	31/31	0.80	0.19	101,111,126,129	43
2	ATP	E	603	31/31	0.80	0.20	133,141,164,166	0
2	ATP	F	601	31/31	0.84	0.13	118,133,146,153	0
2	ATP	E	602	31/31	0.84	0.17	100,102,121,124	0
2	ATP	G	602	31/31	0.86	0.15	98,105,122,123	0
2	ATP	H	602	31/31	0.86	0.14	92,97,112,117	0
3	MG	G	604	1/1	0.87	0.28	64,64,64,64	0
2	ATP	E	601	31/31	0.87	0.13	83,90,105,109	0
2	ATP	H	601	31/31	0.88	0.13	89,97,114,119	0
2	ATP	C	601	31/31	0.89	0.16	64,69,81,82	0
2	ATP	C	602	31/31	0.89	0.16	46,54,70,93	0
2	ATP	B	603	31/31	0.90	0.13	54,62,72,72	0
2	ATP	A	603	31/31	0.91	0.13	47,57,71,71	0
2	ATP	B	605	31/31	0.91	0.12	92,100,118,127	0
2	ATP	D	603	31/31	0.91	0.14	53,59,73,74	0
2	ATP	G	601	31/31	0.91	0.12	81,89,103,108	0
3	MG	F	602	1/1	0.92	0.24	95,95,95,95	0
2	ATP	C	603	31/31	0.92	0.14	50,59,70,73	0
2	ATP	D	602	31/31	0.93	0.13	45,49,63,68	0
2	ATP	A	601	31/31	0.93	0.16	50,58,67,70	0
2	ATP	B	601	31/31	0.94	0.14	63,67,80,84	0
2	ATP	B	602	31/31	0.94	0.12	49,59,67,68	0
2	ATP	A	602	31/31	0.94	0.15	49,55,64,68	0
3	MG	D	604	1/1	0.95	0.18	87,87,87,87	0
3	MG	E	604	1/1	0.95	0.34	86,86,86,86	0
2	ATP	D	601	31/31	0.95	0.13	49,51,61,75	0

6.5 Other polymers

There are no such residues in this entry.