



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 02:50 AM EDT

PDB ID : 1G8M / pdb_00001g8m
Title : CRYSTAL STRUCTURE OF AVIAN ATIC, A BIFUNCTIONAL TRANSFORMYLASE AND CYCLOHYDROLASE ENZYME IN PURINE BIOSYNTHESIS AT 1.75 ANG. RESOLUTION
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Deposited on : 2000-11-17
Resolution : 1.75 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

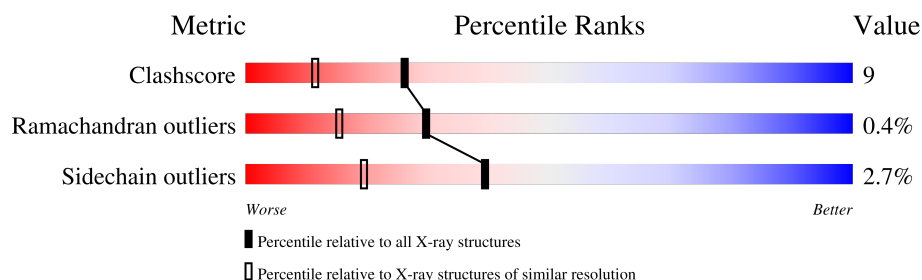
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	593	 79% 17% ...
1	B	593	 82% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9795 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 AICAR TRANSFORMYLASE-IMP CYCLOHYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	Se	0	5	0
			4516	2846	799	852	9	10			
1	B	590	Total	C	N	O	S	Se	0	2	0
			4509	2840	799	851	9	10			

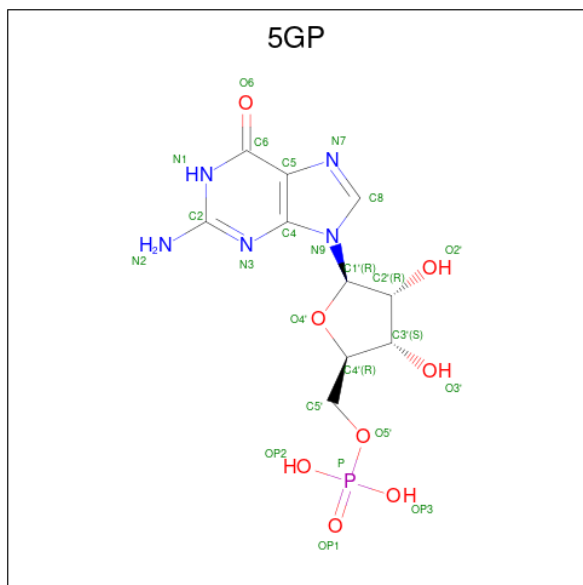
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MSE	MET	cloning artifact	UNP P31335
A	89	MSE	MET	cloning artifact	UNP P31335
A	159	MSE	MET	cloning artifact	UNP P31335
A	211	MSE	MET	cloning artifact	UNP P31335
A	289	MSE	MET	cloning artifact	UNP P31335
A	313	MSE	MET	cloning artifact	UNP P31335
A	368	MSE	MET	cloning artifact	UNP P31335
A	388	MSE	MET	cloning artifact	UNP P31335
A	477	MSE	MET	cloning artifact	UNP P31335
A	512	MSE	MET	cloning artifact	UNP P31335
B	61	MSE	MET	cloning artifact	UNP P31335
B	89	MSE	MET	cloning artifact	UNP P31335
B	159	MSE	MET	cloning artifact	UNP P31335
B	211	MSE	MET	cloning artifact	UNP P31335
B	289	MSE	MET	cloning artifact	UNP P31335
B	313	MSE	MET	cloning artifact	UNP P31335
B	368	MSE	MET	cloning artifact	UNP P31335
B	388	MSE	MET	cloning artifact	UNP P31335
B	477	MSE	MET	cloning artifact	UNP P31335
B	512	MSE	MET	cloning artifact	UNP P31335

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is water.

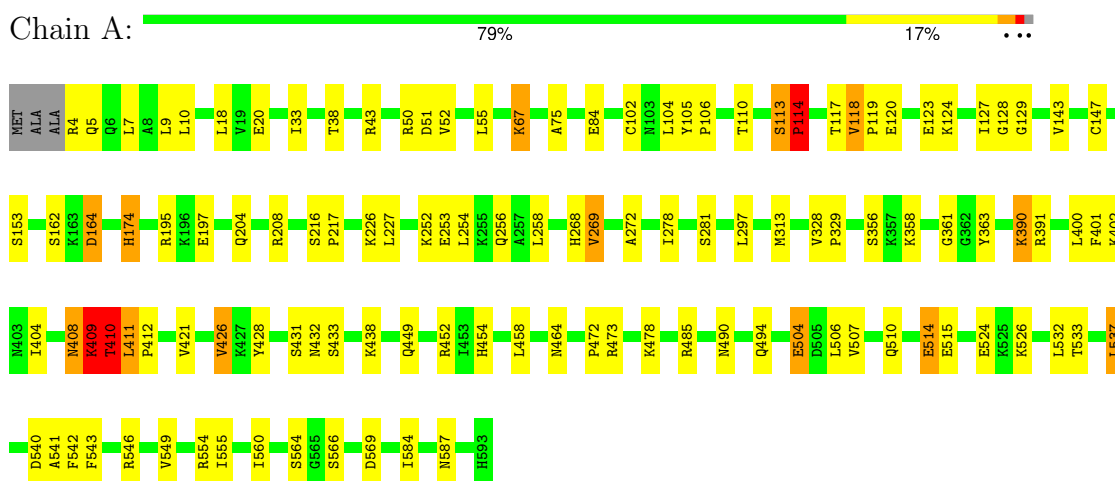
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	383	Total O 383 383	0	0
4	B	361	Total O 361 361	0	0

3 Residue-property plots

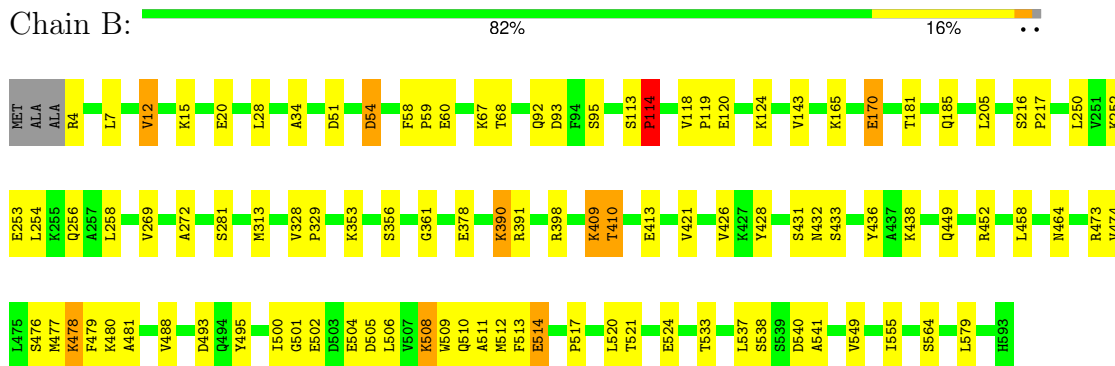
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: AICAR TRANSFORMYLASE-IMP CYCLOHYDROLASE



• Molecule 1: AICAR TRANSFORMYLASE-IMP CYCLOHYDROLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.10 Å 106.00 Å 103.50 Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.75	Depositor
% Data completeness (in resolution range)	89.1 (50.00-1.75)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.200 , 0.216	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9795	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP, K

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	0.41	0/4615	1.01	20/6243 (0.3%)
1	B	0.40	0/4593	0.90	10/6213 (0.2%)
All	All	0.40	0/9208	0.96	30/12456 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	LEU	CA-C-N	16.77	137.03	119.76
1	A	411	LEU	C-N-CA	16.77	137.03	119.76
1	A	113	SER	CA-C-N	15.34	139.01	119.84
1	A	113	SER	C-N-CA	15.34	139.01	119.84
1	A	104	LEU	N-CA-C	10.20	125.61	110.52
1	B	272	ALA	N-CA-C	-8.22	102.14	112.90
1	A	272	ALA	N-CA-C	-8.21	102.15	112.90
1	A	514	GLU	N-CA-C	-6.33	104.25	112.23
1	B	514	GLU	N-CA-C	-6.20	104.42	112.23
1	B	433	SER	N-CA-C	6.16	118.49	108.76
1	A	143	VAL	N-CA-C	6.11	118.16	108.87
1	A	278	ILE	N-CA-C	-6.00	103.47	108.63
1	B	281	SER	N-CA-C	-5.85	102.98	110.53
1	A	105	TYR	N-CA-C	-5.83	102.89	109.60
1	A	390	LYS	N-CA-C	-5.75	101.11	110.20
1	B	143	VAL	N-CA-C	5.72	117.57	108.87
1	B	390	LYS	N-CA-C	-5.62	101.32	110.20
1	A	408	ASN	N-CA-C	5.59	117.81	108.02
1	A	153	SER	N-CA-C	5.54	117.32	111.28
1	A	564	SER	N-CA-C	-5.47	101.87	110.36
1	A	113	SER	N-CA-C	5.41	117.49	110.40
1	A	281	SER	N-CA-C	-5.41	103.55	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ALA	N-CA-C	5.40	118.73	110.20
1	B	7	LEU	N-CA-C	5.32	118.38	110.14
1	A	587	ASN	N-CA-C	-5.22	104.52	111.87
1	B	12	VAL	N-CA-C	5.19	116.19	108.46
1	B	564	SER	N-CA-C	-5.15	102.37	110.36
1	A	118	VAL	CB-CA-C	-5.15	108.81	113.70
1	A	297	LEU	N-CA-C	5.11	117.72	110.10
1	A	75	ALA	N-CA-C	-5.10	105.80	111.36

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	4516	0	4566	93	0
1	B	4509	0	4552	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	12	3	0
4	A	383	0	0	15	0
4	B	361	0	0	6	0
All	All	9795	0	9130	171	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 (171) 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:404:ILE:HD12	1:A:409:LYS:HG2	1.35	1.05
1:A:478:LYS:HG3	1:A:515:GLU:OE2	1.75	0.85
4:A:2099:HOH:O	1:B:390:LYS:HD2	1.77	0.85
1:A:404:ILE:CD1	1:A:409:LYS:HG2	2.08	0.83
1:B:170:GLU:H	1:B:170:GLU:CD	1.88	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:OE1	1:A:507:VAL:HB	1.80	0.81
1:A:438:LYS:HE2	1:A:532:LEU:HD11	1.63	0.80
1:B:479:PHE:O	1:B:512:MSE:O	2.01	0.79
1:B:313:MSE:HG2	4:B:1137:HOH:O	1.83	0.78
1:B:438:LYS:HE3	1:B:533:THR:O	1.85	0.77
1:A:409:LYS:O	1:A:411:LEU:N	2.19	0.75
1:B:500:ILE:HD12	4:B:1306:HOH:O	1.86	0.75
1:A:110[B]:THR:HG21	1:A:124:LYS:HG2	1.70	0.74
1:A:526:LYS:HG3	4:A:2367:HOH:O	1.87	0.74
1:A:546:ARG:O	1:A:549:VAL:HG22	1.87	0.73
1:A:504:GLU:OE1	1:A:504:GLU:HA	1.91	0.71
1:A:454:HIS:HE1	1:B:313:MSE:CE	2.05	0.69
1:A:208:ARG:HG2	4:A:2233:HOH:O	1.93	0.69
1:A:454:HIS:HE1	1:B:313:MSE:HE3	1.58	0.69
1:A:18:LEU:HD21	1:A:38:THR:HG23	1.77	0.66
1:A:485:ARG:NH1	4:A:2238:HOH:O	2.28	0.66
1:A:174:HIS:CD2	1:A:174:HIS:C	2.74	0.65
1:A:164:ASP:N	1:A:164:ASP:OD1	2.28	0.65
1:B:409:LYS:O	1:B:409:LYS:HD2	1.97	0.65
1:B:258:LEU:HB2	4:B:1158:HOH:O	1.96	0.65
1:B:432:ASN:OD1	1:B:449:GLN:HB2	1.97	0.64
1:A:390:LYS:HD3	1:A:391:ARG:O	1.98	0.64
1:A:252:LYS:O	1:A:256:GLN:HG3	1.98	0.64
1:A:438:LYS:HE2	1:A:532:LEU:CD1	2.27	0.63
1:A:43:ARG:HH22	1:A:51:ASP:CG	2.07	0.63
1:A:118:VAL:HB	1:A:119:PRO:HD3	1.81	0.63
1:A:113:SER:HB2	1:A:114:PRO:HD2	1.80	0.62
1:B:480:LYS:CB	1:B:514:GLU:HG2	2.28	0.62
1:A:50:ARG:NH1	1:A:55:LEU:HD12	2.16	0.61
1:B:67:LYS:HG3	1:B:68:THR:HG23	1.82	0.61
1:B:480:LYS:HB3	1:B:514:GLU:HG2	1.81	0.61
1:A:409:LYS:NZ	1:A:410:THR:HA	2.16	0.60
1:A:110[B]:THR:HG21	1:A:124:LYS:CG	2.31	0.60
1:A:195:ARG:HG2	1:A:204:GLN:HB2	1.82	0.60
1:B:477:MSE:HE2	1:B:517:PRO:HG3	1.83	0.60
1:A:537:LEU:HD23	1:A:560:ILE:HG23	1.85	0.59
1:A:402:LYS:HA	1:A:402:LYS:HE2	1.85	0.59
1:A:409:LYS:HZ2	1:A:411:LEU:H	1.50	0.59
1:A:410:THR:C	1:A:412:PRO:HD3	2.28	0.59
1:A:473:ARG:NH2	1:A:524:GLU:OE2	2.36	0.58
1:A:84:GLU:OE1	1:A:84:GLU:N	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:O	1:B:256:GLN:HG3	2.04	0.58
1:B:409:LYS:O	1:B:410:THR:C	2.46	0.58
1:A:52[B]:VAL:HG11	4:A:2263:HOH:O	2.04	0.58
1:A:258:LEU:HB2	4:A:2303:HOH:O	2.04	0.57
1:A:432:ASN:OD1	1:A:449:GLN:HB2	2.04	0.57
1:A:555:ILE:O	1:A:555:ILE:HG13	2.03	0.57
1:B:473:ARG:NH1	1:B:520:LEU:HD23	2.20	0.57
1:B:398:ARG:NH2	1:B:413:GLU:OE2	2.32	0.56
1:A:124:LYS:N	1:A:124:LYS:HD2	2.19	0.56
1:B:521:THR:OG1	1:B:524:GLU:HG3	2.06	0.56
1:A:408:ASN:C	1:A:408:ASN:OD1	2.47	0.56
1:A:106:PRO:O	1:A:110[B]:THR:HG23	2.06	0.55
1:B:12:VAL:HG23	1:B:15:LYS:HG2	1.89	0.55
1:A:123:GLU:C	1:A:124:LYS:HD2	2.32	0.55
1:A:554:ARG:NH1	4:A:2152:HOH:O	2.39	0.55
1:A:124:LYS:HD3	4:A:2281:HOH:O	2.06	0.55
1:B:410:THR:O	1:B:410:THR:HG23	2.06	0.55
1:B:549:VAL:HG12	1:B:579:LEU:HD12	1.87	0.54
1:A:464:ASN:OD1	1:A:555:ILE:HD13	2.07	0.54
1:A:504:GLU:OE1	1:A:504:GLU:CA	2.54	0.54
1:A:458[B]:LEU:HD12	4:A:2172:HOH:O	2.07	0.53
1:B:356:SER:O	1:B:361:GLY:HA2	2.08	0.53
1:B:495:TYR:HA	1:B:500:ILE:HD11	1.90	0.53
1:B:34:ALA:O	1:B:51:ASP:HA	2.09	0.53
1:A:452:ARG:NH2	1:A:541:ALA:HB3	2.23	0.53
1:A:67:LYS:HB2	4:A:2263:HOH:O	2.09	0.53
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.39	0.53
1:B:216[B]:SER:OG	1:B:217:PRO:HA	2.08	0.53
1:B:555:ILE:O	1:B:555:ILE:HG13	2.10	0.52
1:B:431:SER:HB3	1:B:432:ASN:HA	1.90	0.52
1:B:508:LYS:O	1:B:511:ALA:HB3	2.10	0.52
1:A:128:GLY:HA3	3:A:2001:5GP:C6	2.38	0.52
1:A:409:LYS:O	1:A:409:LYS:HD2	2.09	0.52
1:B:170:GLU:OE1	1:B:170:GLU:N	2.42	0.52
1:A:431:SER:HB3	1:A:432:ASN:HA	1.92	0.51
1:B:464:ASN:OD1	1:B:555:ILE:HD13	2.09	0.51
1:B:124:LYS:HE2	4:B:1103:HOH:O	2.10	0.51
1:B:410:THR:CG2	4:B:1163:HOH:O	2.59	0.51
1:A:478:LYS:HG3	1:A:515:GLU:CD	2.34	0.51
1:A:411:LEU:N	1:A:412:PRO:HD3	2.25	0.51
1:B:479:PHE:O	1:B:480:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LEU:C	1:B:537:LEU:HD23	2.36	0.50
1:A:409:LYS:O	1:A:410:THR:C	2.54	0.50
1:A:542:PHE:CD1	1:A:566:SER:HB2	2.47	0.50
1:B:118:VAL:HB	1:B:119:PRO:HD3	1.94	0.50
1:B:390:LYS:HE2	1:B:391:ARG:O	2.12	0.50
1:B:452:ARG:NH2	1:B:541:ALA:HB3	2.27	0.50
1:B:476:SER:O	1:B:478:LYS:HE3	2.11	0.49
1:B:502:GLU:HA	1:B:502:GLU:OE1	2.11	0.49
1:A:404:ILE:HD12	1:A:409:LYS:CG	2.25	0.49
1:A:7:LEU:HD13	1:A:33:ILE:HD13	1.93	0.49
1:A:431:SER:CB	1:A:432:ASN:HA	2.42	0.49
1:B:500:ILE:O	1:B:505:ASP:HB3	2.13	0.49
1:A:404:ILE:HG21	1:A:409:LYS:HA	1.95	0.49
1:A:356:SER:O	1:A:361:GLY:HA2	2.13	0.48
1:B:506:LEU:O	1:B:510:GLN:HG3	2.14	0.48
1:B:458:LEU:C	1:B:458:LEU:HD23	2.38	0.48
1:B:473:ARG:HD2	1:B:495:TYR:OH	2.13	0.48
4:A:2221:HOH:O	1:B:493:ASP:HB3	2.14	0.48
1:B:474:VAL:O	1:B:477:MSE:HG3	2.14	0.48
1:A:52[B]:VAL:CG1	4:A:2263:HOH:O	2.61	0.48
1:B:4:ARG:CZ	1:B:95:SER:OG	2.62	0.48
1:A:408:ASN:O	1:A:410:THR:N	2.47	0.48
1:A:537:LEU:HD21	1:A:543:PHE:HZ	1.78	0.48
1:A:490:ASN:O	1:A:494:GLN:HG3	2.14	0.47
1:A:506:LEU:O	1:A:510:GLN:HG3	2.14	0.47
1:A:566:SER:HB3	1:A:569:ASP:OD1	2.14	0.47
1:A:409:LYS:HZ1	1:A:410:THR:HA	1.79	0.47
1:A:129:GLY:HA3	3:A:2001:5GP:O2'	2.15	0.47
1:B:253:GLU:OE2	1:B:428:TYR:OH	2.31	0.47
1:B:113:SER:HB3	1:B:114:PRO:HD2	1.97	0.46
1:B:431:SER:CB	1:B:432:ASN:HA	2.45	0.46
1:B:480:LYS:HA	1:B:514:GLU:OE2	2.15	0.46
1:B:170:GLU:CD	1:B:170:GLU:N	2.65	0.46
1:A:426:VAL:CG1	1:A:540:ASP:HB3	2.45	0.45
1:B:432:ASN:OD1	1:B:432:ASN:C	2.58	0.45
1:A:50:ARG:CZ	1:A:55:LEU:HD12	2.46	0.45
1:B:20:GLU:HA	1:B:20:GLU:OE1	2.15	0.45
1:A:426:VAL:HG13	1:A:540:ASP:HB3	1.98	0.45
1:B:479:PHE:CZ	1:B:488:VAL:HG13	2.50	0.45
1:A:409:LYS:O	1:A:409:LYS:CD	2.65	0.45
1:B:120:GLU:O	1:B:124:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:GLU:HG3	1:B:391:ARG:HB3	1.98	0.45
1:A:216:SER:OG	1:A:217:PRO:HA	2.17	0.44
1:A:401:PHE:HA	1:A:584:ILE:HG21	2.00	0.44
1:B:436:TYR:CE2	1:B:555:ILE:HG21	2.53	0.44
1:A:20:GLU:HA	1:A:20:GLU:OE1	2.17	0.44
1:A:197:GLU:HG2	4:A:2338:HOH:O	2.18	0.43
1:A:358:LYS:HB2	1:A:363:TYR:HB2	1.99	0.43
1:B:51:ASP:O	1:B:54:ASP:HB2	2.18	0.43
1:B:501:GLY:O	1:B:506:LEU:HB2	2.19	0.43
1:A:400:LEU:HB2	4:A:2129:HOH:O	2.18	0.43
1:B:254:LEU:HD21	1:B:421:VAL:HA	2.00	0.43
1:A:254:LEU:HD21	1:A:421:VAL:HA	2.00	0.42
1:B:4:ARG:HD3	1:B:95:SER:OG	2.19	0.42
1:A:226:LYS:HG2	1:A:227:LEU:N	2.33	0.42
1:A:268:HIS:C	1:A:269:VAL:HG23	2.44	0.42
1:A:478:LYS:CE	1:A:515:GLU:OE2	2.67	0.42
1:B:477:MSE:CE	1:B:517:PRO:HG3	2.46	0.42
1:B:537:LEU:HD23	1:B:538:SER:N	2.34	0.42
1:B:92:GLN:O	1:B:93:ASP:HB3	2.19	0.42
1:A:253:GLU:OE2	1:A:428:TYR:OH	2.33	0.42
1:B:181:THR:O	1:B:185:GLN:HG3	2.19	0.42
1:A:533:THR:HG22	4:A:2330:HOH:O	2.19	0.42
1:B:28:LEU:O	1:B:165:LYS:NZ	2.40	0.42
1:A:127:ILE:HB	3:A:2001:5GP:HN21	1.85	0.42
1:B:479:PHE:CE1	1:B:488:VAL:HG13	2.55	0.42
1:A:9:LEU:HA	1:A:33:ILE:HG13	2.01	0.41
1:A:328:VAL:HB	1:A:329:PRO:HD3	2.02	0.41
1:A:409:LYS:HB3	1:A:409:LYS:HE3	1.59	0.41
1:B:58:PHE:CG	1:B:59:PRO:HD2	2.55	0.41
1:B:353:LYS:HG2	4:B:1356:HOH:O	2.20	0.41
1:B:520:LEU:HA	1:B:524:GLU:OE1	2.20	0.41
1:A:124:LYS:N	1:A:124:LYS:CD	2.83	0.41
1:A:102:CYS:O	1:A:147:CYS:HA	2.21	0.41
1:B:504:GLU:H	1:B:504:GLU:HG2	1.53	0.41
1:B:480:LYS:HB3	1:B:514:GLU:CG	2.49	0.40
1:B:431:SER:HA	1:B:432:ASN:C	2.47	0.40
1:A:113:SER:HA	1:A:114:PRO:HD3	1.78	0.40
1:B:328:VAL:HB	1:B:329:PRO:HD3	2.02	0.40
1:B:509:TRP:CE2	1:B:513:PHE:HZ	2.40	0.40
1:A:10:LEU:HD23	1:A:18:LEU:HD11	2.04	0.40
1:A:117:THR:OG1	1:A:120:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:C	1:B:250:LEU:HD23	2.47	0.40
1:B:513:PHE:CD1	1:B:513:PHE:N	2.89	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	593/593 (100%)	574 (97%)	16 (3%)	3 (0%)	24	11
1	B	590/593 (100%)	571 (97%)	17 (3%)	2 (0%)	36	21
All	All	1183/1186 (100%)	1145 (97%)	33 (3%)	5 (0%)	30	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	LYS
1	A	410	THR
1	B	114	PRO
1	A	114	PRO
1	B	410	THR

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	488/475 (103%)	471 (96%)	17 (4%)	32	12
1	B	485/475 (102%)	476 (98%)	9 (2%)	50	31
All	All	973/950 (102%)	947 (97%)	26 (3%)	39	19

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	GLN
1	A	67	LYS
1	A	114	PRO
1	A	162	SER
1	A	164	ASP
1	A	174	HIS
1	A	269	VAL
1	A	313	MSE
1	A	409	LYS
1	A	410	THR
1	A	426	VAL
1	A	433	SER
1	A	472	PRO
1	A	504	GLU
1	A	514	GLU
1	A	537	LEU
1	B	54	ASP
1	B	60	GLU
1	B	114	PRO
1	B	170	GLU
1	B	205	LEU
1	B	269	VAL
1	B	409	LYS
1	B	478	LYS
1	B	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	174	HIS
1	A	377	ASN
1	A	386	GLN

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Mol	Chain	Res	Type
1	A	494	GLN
1	A	510	GLN
1	A	558	GLN
1	B	90	ASN
1	B	246	ASN
1	B	367	GLN
1	B	377	ASN
1	B	386	GLN
1	B	408	ASN

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, 2 are monoatomic - leaving 1 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	$\# Z > 2$
3	5GP	A	2001	-	26,26,26	1.81	6 (23%)	39,40,40	2.07	7 (17%)

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
3	5GP	A	2001	-	-	2/10/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	5GP	C4-N3	5.19	1.46	1.34
3	A	2001	5GP	C2-N1	3.93	1.47	1.37
3	A	2001	5GP	C5-C6	3.40	1.57	1.44
3	A	2001	5GP	P-OP1	3.33	1.60	1.50
3	A	2001	5GP	C5-C4	2.09	1.44	1.38
3	A	2001	5GP	C8-N7	2.05	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	5GP	C2-N3-C4	6.35	123.23	112.30
3	A	2001	5GP	C5-C4-N3	-5.78	119.19	128.39
3	A	2001	5GP	N9-C8-N7	4.47	121.69	113.40
3	A	2001	5GP	C8-N7-C5	-4.13	96.90	104.26
3	A	2001	5GP	C8-N9-C4	-3.44	99.57	106.03
3	A	2001	5GP	N9-C4-N3	3.22	132.40	125.95
3	A	2001	5GP	N1-C2-N3	-2.26	119.19	123.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	5GP	O4'-C4'-C5'-O5'
3	A	2001	5GP	C3'-C4'-C5'-O5'

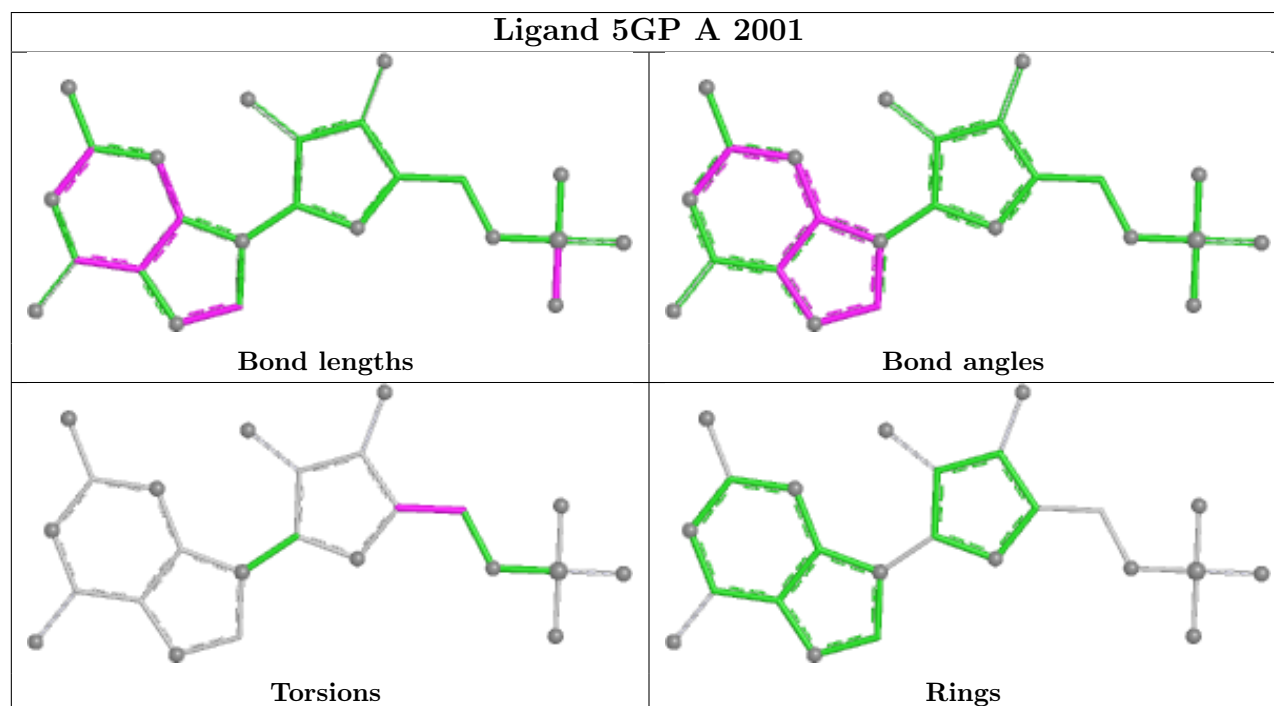
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	5GP	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.