Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:58 am BST

PDB ID	:	1DGS
Title	:	CRYSTAL STRUCTURE OF NAD+-DEPENDENT DNA LIGASE FROM T. FILIFORMIS
Authors	:	Lee, J.Y.; Chang, C.; Song, H.K.; Kwon, S.T.; Suh, S.W.
Deposited on	:	1999-11-25
Resolution	:	2.90 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:

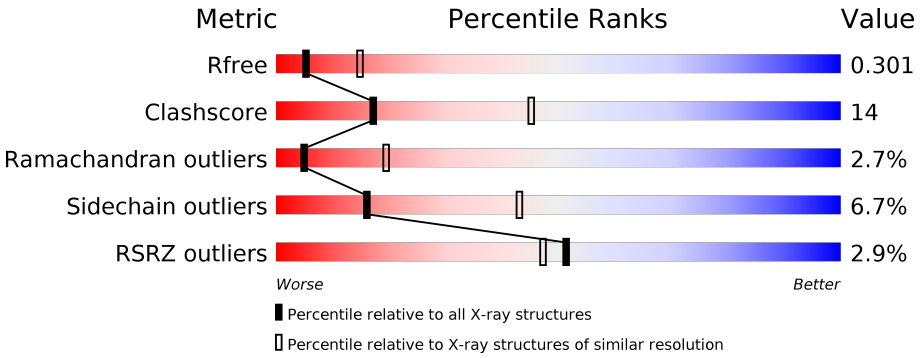
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	667	2% 58% 26% • 13%
1	B	667	3% 59% 24% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9674 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.

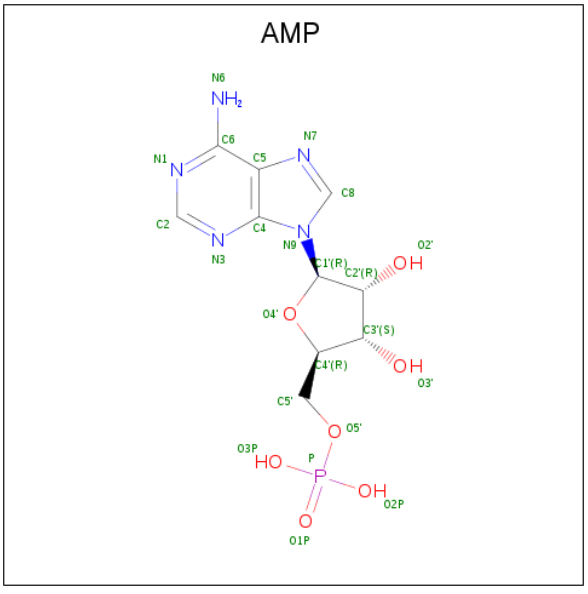
- Molecule 1 is a protein called DNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4693	2965	845	871	12			
1	B	581	Total	C	N	O	S	0	0	0
			4693	2965	845	871	12			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 4 is water.

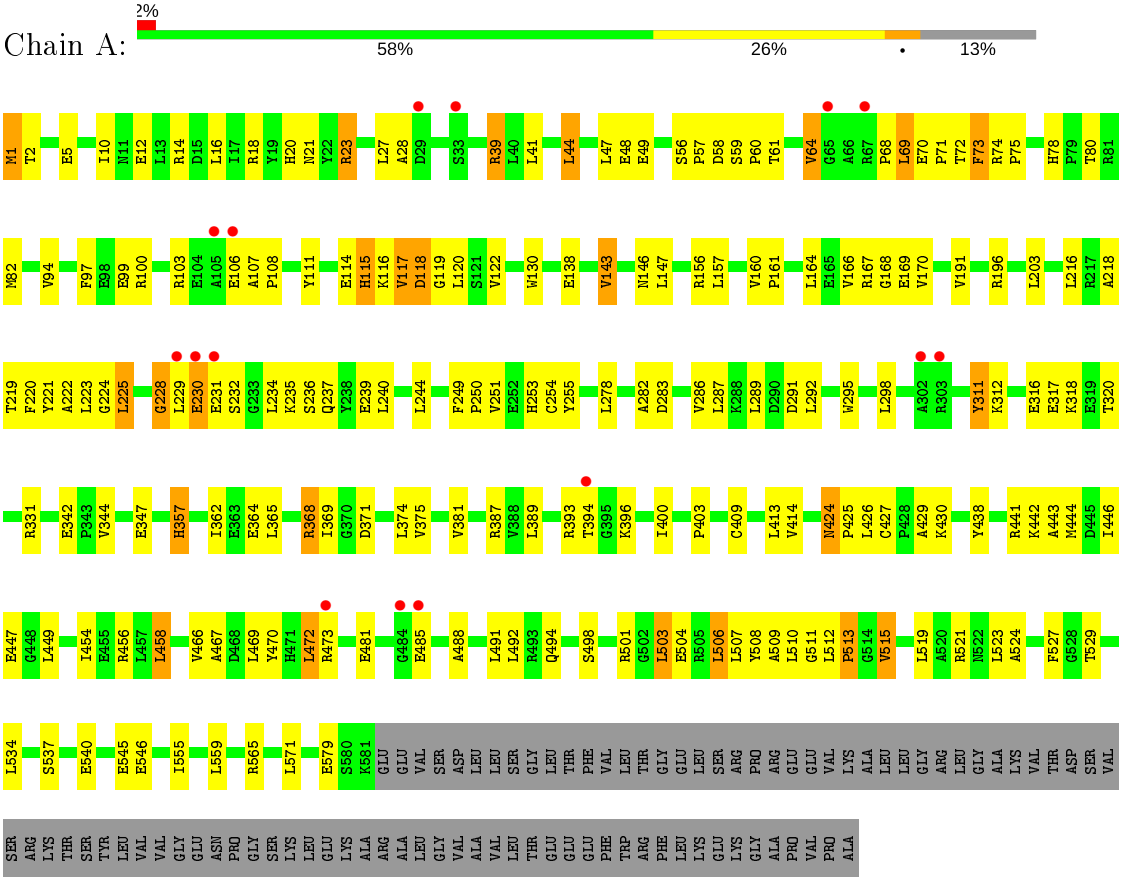
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	119	Total	O	0	0
			119	119		

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.

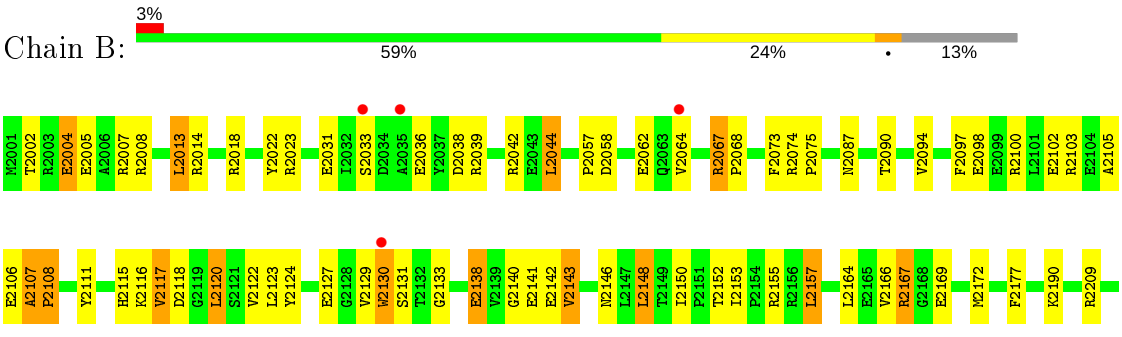
- Molecule 1: DNA LIGASE

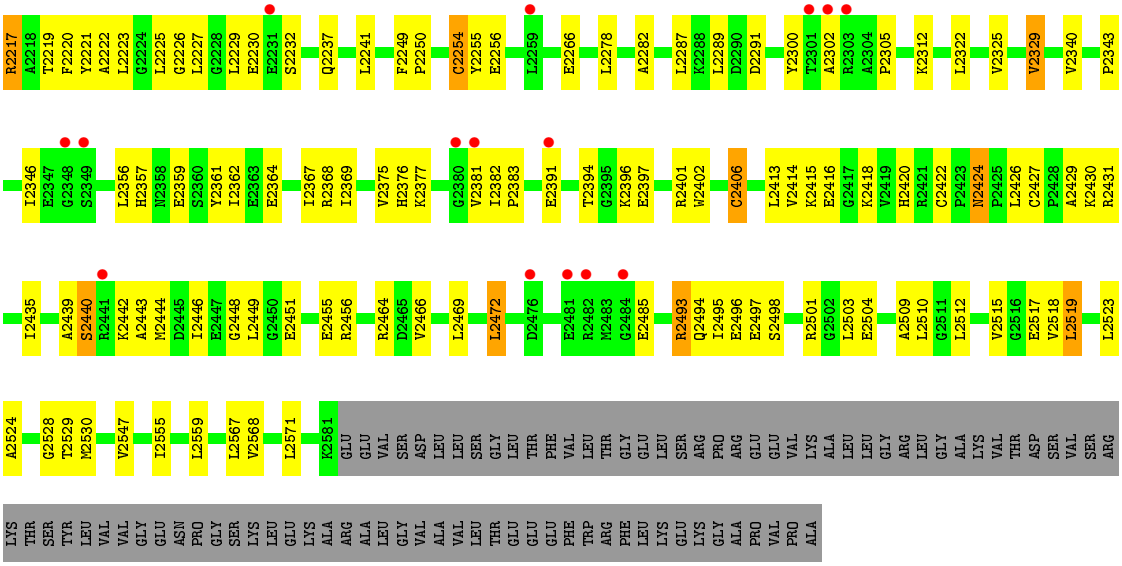
Chain A:



- Molecule 1: DNA LIGASE

Chain B:




R2217 A2218 T2219 F2220 Y2221 A2222 L2223 G2224 L2225 G2226 L2227 G2228 L2229 E2230 E2231 S2232 Q2237 L2241 F2249 P2250 C2254 Y2255 E2256 L2259 E2266 L2278 A2282 L2287 K2288 L2289 D2290 D2291 Y2300 T2301 A2302 R2303 A2304 P2305 K2312 L2322 V2325 V2329 V2340 P2343
I2346 E2347 G2348 S2349 L2356 H2357 N2358 E2359 S2360 Y2361 I2362 E2363 E2364 I2367 R2368 I2369 V2375 H2376 K2377 G2380 V2381 I2382 P2383 E2391 T2394 G2395 K2396 E2397 R2401 W2402 C2406 L2413 V2414 K2415 E2416 G2417 K2418 V2419 H2420 R2421 C2422 P2423 N2424 P2425 L2426 C2427 P2428 A2429 K2430 R2431
I2435 A2439 S2440 R2441 K2442 A2443 M2444 D2445 I2446 E2447 G2448 L2449 G2450 E2451 E2455 R2456 R2464 D2465 V2466 L2469 L2472 D2476 E2481 R2482 M2483 G2484 E2485 R2493 Q2494 I2495 E2496 E2497 S2498 R2501 G2502 L2503 E2504 A2509 L2510 G2511 L2512 V2515 G2516 E2517 V2518 L2519 L2523
A2524 G2528 T2529 M2530 V2547 I2555 L2559 L2567 V2568 L2571 K2581 GLU GLU VAL SER ASP LEU LEU SER GLY LEU THR PHE VAL LEU THR GLY GLU LEU SER ARG PRO ARG GLU GLU VAL LYS ALA LEU LEU GLY ARG LEU GLY ALA LYS VAL THR ASP SER VAL SER ARG
LYS THR SER TYR LEU VAL VAL GLY GLU ASN PRO GLY SER LYS LEU GLU LYS ALA ARG ALA LEU GLY VAL ALA VAL LEU THR GLU GLU GLU PHE TRP ARG PHE LEU LYS GLU LYS GLY ALA PRO VAL PRO ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.21Å 117.33Å 97.48Å 90.00° 115.09° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 24.75 – 2.88	Depositor EDS
% Data completeness (in resolution range)	89.5 (20.00-2.90) 94.4 (24.75-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.89Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.228 , 0.298 0.234 , 0.301	Depositor DCC
R_{free} test set	3869 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9674	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AMP, ZN

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	0.38	0/4782	0.65	2/6451 (0.0%)
1	B	0.37	0/4782	0.65	0/6451
All	All	0.37	0/9564	0.65	2/12902 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	GLY	N-CA-C	-5.08	100.39	113.10
1	A	64	VAL	N-CA-C	5.00	124.51	111.00

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	4693	0	4732	134	0
1	B	4693	0	4727	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	12	0	0
3	B	22	0	12	1	0
4	A	123	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	119	0	0	0	0
All	All	9674	0	9483	263	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 14.

All (263) 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:115:HIS:ND1	1:A:254:CYS:SG	2.39	0.94
1:A:316:GLU:HG2	1:A:347:GLU:HG3	1.52	0.91
1:A:534:LEU:HD22	1:A:565:ARG:HE	1.40	0.86
1:B:2039:ARG:HG3	1:B:2042:ARG:HH21	1.40	0.85
1:B:2004:GLU:HG3	1:B:2007:ARG:HH21	1.44	0.82
1:B:2107:ALA:HB3	1:B:2108:PRO:HD3	1.62	0.81
1:B:2359:GLU:HG3	1:B:2418:LYS:O	1.82	0.80
1:A:10:ILE:HG23	1:A:14:ARG:NH1	1.95	0.80
1:A:449:LEU:HD12	1:A:454:ILE:HG12	1.62	0.79
1:A:20:HIS:HA	1:A:23:ARG:HB2	1.67	0.77
1:B:2115:HIS:CG	1:B:2254:CYS:SG	2.78	0.77
1:A:424:ASN:HD22	1:A:426:LEU:H	1.36	0.74
1:B:2120:LEU:H	1:B:2120:LEU:HD12	1.52	0.74
1:B:2381:VAL:HG13	1:B:2382:ILE:H	1.51	0.74
1:A:234:LEU:HD13	1:A:240:LEU:HD12	1.71	0.72
1:B:2067:ARG:HG2	1:B:2068:PRO:HD2	1.72	0.72
1:B:2039:ARG:HG3	1:B:2042:ARG:NH2	2.06	0.71
1:A:228:GLY:HA2	1:A:232:SER:O	1.92	0.70
1:B:2120:LEU:HA	1:B:2169:GLU:HG2	1.74	0.70
1:B:2117:VAL:HG12	1:B:2118:ASP:H	1.56	0.69
1:A:424:ASN:ND2	1:A:426:LEU:H	1.91	0.69
1:B:2023:ARG:HH11	1:B:2031:GLU:HG3	1.57	0.68
1:B:2115:HIS:ND1	1:B:2254:CYS:SG	2.66	0.68
1:A:166:VAL:HG21	1:A:249:PHE:CE1	2.28	0.68
1:A:115:HIS:HD1	1:A:254:CYS:HG	1.42	0.67
1:B:2167:ARG:HG2	1:B:2167:ARG:HH21	1.58	0.67
1:A:442:LYS:HB3	1:A:508:TYR:HE2	1.60	0.66
1:B:2427:CYS:HB3	1:B:2430:LYS:HG2	1.79	0.65
1:A:115:HIS:HB2	1:A:254:CYS:SG	2.38	0.63
1:B:2406:CYS:HB2	1:B:2413:LEU:HD21	1.79	0.63
1:B:2100:ARG:O	1:B:2103:ARG:HG2	1.98	0.63
1:B:2368:ARG:HB3	1:B:2397:GLU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:HA	1:A:250:PRO:O	1.98	0.63
1:A:537:SER:OG	1:A:540:GLU:HG3	1.99	0.63
1:B:2530:MET:HG2	1:B:2568:VAL:HG21	1.82	0.62
1:A:236:SER:HB3	1:A:239:GLU:HG2	1.80	0.62
1:A:223:LEU:HG	1:A:240:LEU:HD11	1.81	0.61
1:B:2217:ARG:HH21	1:B:2217:ARG:HG2	1.66	0.61
1:A:365:LEU:HD12	1:A:387:ARG:HA	1.84	0.60
1:B:2498:SER:O	1:B:2501:ARG:HG2	2.01	0.60
1:A:424:ASN:HD22	1:A:426:LEU:N	1.98	0.60
1:B:2115:HIS:CE1	1:B:2254:CYS:SG	2.94	0.60
1:B:2157:LEU:HD21	1:B:2249:PHE:CE2	2.37	0.60
1:A:78:HIS:ND1	1:A:122:VAL:HG11	2.16	0.60
1:B:2431:ARG:O	1:B:2435:ILE:HG12	2.02	0.60
1:A:16:LEU:HD11	1:A:156:ARG:HH22	1.66	0.60
1:B:2014:ARG:HD3	1:B:2018:ARG:HH21	1.67	0.59
1:A:442:LYS:HB3	1:A:508:TYR:CE2	2.38	0.59
1:B:2008:ARG:HG3	1:B:2127:GLU:HG3	1.83	0.59
1:A:143:VAL:HG22	1:A:146:ASN:HB2	1.84	0.58
1:A:21:ASN:CG	1:A:69:LEU:HB2	2.24	0.58
1:B:2130:TRP:CZ3	1:B:2148:LEU:HD13	2.39	0.58
1:A:14:ARG:O	1:A:18:ARG:HG3	2.04	0.57
1:B:2217:ARG:NH2	1:B:2217:ARG:HG2	2.18	0.57
1:A:230:GLU:O	1:A:231:GLU:HG3	2.04	0.57
1:A:529:THR:HG22	1:A:579:GLU:HG2	1.87	0.56
1:A:515:VAL:HG13	1:A:515:VAL:O	2.05	0.56
1:B:2038:ASP:O	1:B:2042:ARG:HG3	2.06	0.56
1:B:2143:VAL:HG22	1:B:2146:ASN:HB2	1.87	0.56
1:A:234:LEU:CD1	1:A:240:LEU:HD12	2.35	0.56
1:B:2190:LYS:HE3	1:B:2361:TYR:CD1	2.41	0.55
1:B:2117:VAL:HB	1:B:2169:GLU:OE2	2.06	0.55
1:B:2116:LYS:O	1:B:2282:ALA:HA	2.06	0.55
1:A:320:THR:OG1	1:A:342:GLU:HB3	2.07	0.55
1:B:2157:LEU:HD21	1:B:2249:PHE:HE2	1.69	0.55
1:A:519:LEU:O	1:A:523:LEU:HB2	2.07	0.55
1:A:16:LEU:HD11	1:A:156:ARG:NH2	2.22	0.55
1:B:2217:ARG:HH21	1:B:2217:ARG:CG	2.19	0.55
1:A:534:LEU:HD22	1:A:565:ARG:NE	2.18	0.55
1:B:2123:LEU:HG	1:B:2130:TRP:CZ2	2.42	0.55
1:B:2442:LYS:HD3	1:B:2517:GLU:OE1	2.07	0.54
1:A:147:LEU:HD23	1:A:203:LEU:HD11	1.89	0.54
1:A:57:PRO:HG2	1:A:74:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2172:MET:HG2	1:B:2177:PHE:HB2	1.90	0.54
1:B:2241:LEU:HD23	1:B:2255:TYR:CD1	2.43	0.54
1:A:444:MET:CE	1:A:506:LEU:HD23	2.38	0.54
1:B:2152:THR:O	1:B:2250:PRO:HD3	2.08	0.53
1:A:119:GLY:N	1:A:196:ARG:HD2	2.23	0.53
1:B:2448:GLY:H	1:B:2494:GLN:NE2	2.07	0.53
1:A:498:SER:O	1:A:501:ARG:HG2	2.08	0.52
1:A:427:CYS:HB3	1:A:430:LYS:HD3	1.92	0.52
1:A:10:ILE:HG23	1:A:14:ARG:HH11	1.75	0.52
1:A:119:GLY:H	1:A:196:ARG:HD2	1.74	0.52
1:B:2287:LEU:H	1:B:2287:LEU:HD23	1.75	0.52
1:B:2300:TYR:CD2	1:B:2305:PRO:HB3	2.44	0.52
1:A:120:LEU:HA	1:A:169:GLU:HG2	1.92	0.52
1:B:2058:ASP:OD2	1:B:2142:GLU:HG3	2.09	0.52
1:A:251:VAL:HG23	1:A:253:HIS:CE1	2.44	0.52
1:B:2130:TRP:HZ3	1:B:2148:LEU:HD13	1.74	0.52
1:B:2222:ALA:O	1:B:2223:LEU:HD23	2.10	0.52
1:B:2226:GLY:O	1:B:2232:SER:HB3	2.10	0.52
1:A:161:PRO:HG3	1:A:231:GLU:HB2	1.93	0.51
1:B:2493:ARG:O	1:B:2497:GLU:HG3	2.10	0.51
1:A:82:MET:CE	1:A:122:VAL:HB	2.41	0.51
1:B:2346:ILE:HD11	1:B:2375:VAL:HG13	1.93	0.51
1:A:12:GLU:O	1:A:16:LEU:HD13	2.10	0.51
1:B:2014:ARG:HG2	1:B:2044:LEU:HD11	1.93	0.51
1:A:485:GLU:HA	1:A:488:ALA:HB3	1.92	0.51
1:A:16:LEU:CD1	1:A:156:ARG:HH22	2.24	0.50
1:A:317:GLU:C	1:A:318:LYS:HD2	2.31	0.50
1:A:235:LYS:O	1:A:292:LEU:HB2	2.10	0.50
1:B:2087:ASN:HD22	1:B:2312:LYS:HG3	1.76	0.50
1:B:2122:VAL:O	1:B:2133:GLY:HA2	2.11	0.50
1:B:2014:ARG:O	1:B:2018:ARG:HG3	2.11	0.50
1:B:2515:VAL:HG23	1:B:2519:LEU:HB3	1.92	0.50
1:A:438:TYR:CD1	1:A:509:ALA:HB1	2.46	0.50
1:B:2225:LEU:HA	1:B:2229:LEU:HD11	1.93	0.50
1:A:512:LEU:HB2	1:A:515:VAL:CG1	2.42	0.50
1:A:555:ILE:O	1:A:559:LEU:HG	2.12	0.50
1:B:2377:LYS:HA	1:B:2383:PRO:HA	1.94	0.50
1:B:2422:CYS:SG	1:B:2424:ASN:HB3	2.52	0.50
1:B:2123:LEU:HG	1:B:2130:TRP:HZ2	1.75	0.49
1:A:504:GLU:HG2	1:A:521:ARG:HG3	1.94	0.49
1:A:80:THR:HG23	1:A:225:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:CG	1:A:347:GLU:HG3	2.36	0.49
1:B:2152:THR:HB	1:B:2250:PRO:HB3	1.95	0.49
1:A:170:VAL:HG22	1:A:218:ALA:HB2	1.94	0.49
1:A:143:VAL:O	1:A:143:VAL:HG22	2.13	0.49
1:A:545:GLU:O	1:A:546:GLU:HB2	2.12	0.49
1:B:2002:THR:HG22	1:B:2005:GLU:HG3	1.94	0.49
1:A:168:GLY:HA3	1:A:220:PHE:HA	1.95	0.49
1:A:71:PRO:HG2	1:A:73:PHE:CE2	2.48	0.49
1:B:2512:LEU:O	1:B:2515:VAL:HG12	2.13	0.48
1:B:2515:VAL:O	1:B:2515:VAL:HG13	2.13	0.48
1:A:115:HIS:CE1	1:A:278:LEU:HD11	2.49	0.48
1:B:2444:MET:HG2	1:B:2509:ALA:CB	2.42	0.48
1:A:44:LEU:HD11	1:A:60:PRO:HD2	1.96	0.48
1:B:2166:VAL:HG21	1:B:2249:PHE:CZ	2.49	0.48
1:B:2097:PHE:HA	1:B:2100:ARG:NH2	2.29	0.47
1:A:470:TYR:O	1:A:473:ARG:HG3	2.15	0.47
1:A:244:LEU:O	1:A:249:PHE:HB2	2.14	0.47
1:B:2033:SER:OG	1:B:2036:GLU:HG3	2.14	0.47
1:B:2115:HIS:CE1	1:B:2278:LEU:HD11	2.49	0.47
1:A:116:LYS:NZ	1:A:312:LYS:HD3	2.30	0.47
1:B:2503:LEU:HB3	1:B:2524:ALA:HB1	1.97	0.47
1:A:512:LEU:HB3	1:A:513:PRO:HD2	1.95	0.47
1:B:2226:GLY:HA2	1:B:2230:GLU:HB2	1.96	0.47
1:B:2150:ILE:HB	1:B:2153:ILE:HD12	1.95	0.47
1:B:2120:LEU:HD21	3:B:2700:AMP:O2'	2.14	0.47
1:B:2167:ARG:NH2	1:B:2167:ARG:HG2	2.23	0.47
1:A:82:MET:HE3	1:A:167:ARG:HG3	1.96	0.47
1:A:116:LYS:O	1:A:282:ALA:HA	2.15	0.47
1:B:2166:VAL:HG12	1:B:2220:PHE:HD1	1.80	0.47
1:B:2394:THR:HG23	1:B:2396:LYS:H	1.79	0.47
1:B:2519:LEU:HD11	1:B:2547:VAL:HG22	1.97	0.47
1:A:449:LEU:HD22	1:A:491:LEU:HD11	1.97	0.46
1:A:94:VAL:HG21	1:A:311:TYR:CD1	2.50	0.46
1:A:14:ARG:NH2	1:A:59:SER:HB2	2.30	0.46
1:B:2023:ARG:NH1	1:B:2031:GLU:HG3	2.29	0.46
1:B:2220:PHE:CD2	1:B:2220:PHE:N	2.83	0.46
1:B:2014:ARG:HD3	1:B:2018:ARG:NH2	2.30	0.46
1:B:2148:LEU:HD11	1:B:2155:ARG:HG2	1.97	0.46
1:B:2402:TRP:CG	1:B:2420:HIS:ND1	2.84	0.46
1:A:295:TRP:O	1:A:298:LEU:O	2.34	0.46
1:A:44:LEU:HD13	1:A:61:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2255:TYR:O	1:B:2256:GLU:HB3	2.16	0.46
1:A:438:TYR:CE1	1:A:466:VAL:HG11	2.51	0.46
1:A:56:SER:C	1:A:58:ASP:H	2.19	0.46
1:B:2143:VAL:HG22	1:B:2143:VAL:O	2.16	0.46
1:A:504:GLU:HG3	1:A:524:ALA:HB3	1.98	0.46
1:A:94:VAL:HG21	1:A:311:TYR:CE1	2.51	0.45
1:B:2013:LEU:HB3	1:B:2044:LEU:HG	1.98	0.45
1:A:117:VAL:HG12	1:A:118:ASP:H	1.81	0.45
1:A:519:LEU:O	1:A:519:LEU:HD13	2.16	0.45
1:B:2111:TYR:HD2	1:B:2289:LEU:HA	1.81	0.45
1:B:2555:ILE:O	1:B:2559:LEU:HG	2.16	0.45
1:A:107:ALA:HB3	1:A:108:PRO:HD3	1.98	0.45
1:A:116:LYS:CG	1:A:286:VAL:HG23	2.47	0.45
1:A:456:ARG:HG3	1:A:481:GLU:HG2	1.99	0.45
1:B:2226:GLY:N	1:B:2230:GLU:HB2	2.32	0.45
1:A:80:THR:HG23	1:A:225:LEU:CD2	2.46	0.45
1:A:114:GLU:HB3	1:A:255:TYR:HB3	1.99	0.45
1:A:369:ILE:O	1:A:371:ASP:N	2.50	0.45
1:A:394:THR:HG23	1:A:396:LYS:H	1.80	0.45
1:A:446:ILE:HG21	1:A:449:LEU:HD23	1.99	0.45
1:A:467:ALA:HB2	1:A:571:LEU:HG	1.98	0.44
1:B:2362:ILE:HG23	1:B:2367:ILE:HB	1.98	0.44
1:A:221:TYR:CD2	1:A:222:ALA:N	2.86	0.44
1:B:2120:LEU:CD1	1:B:2120:LEU:H	2.25	0.44
1:B:2073:PHE:HD2	1:B:2141:GLU:HG2	1.82	0.44
1:A:157:LEU:HD23	1:A:160:VAL:HG11	1.99	0.44
1:A:27:LEU:O	1:A:28:ALA:HB3	2.18	0.44
1:A:2:THR:HG23	1:A:5:GLU:H	1.83	0.44
1:B:2115:HIS:CD2	1:B:2254:CYS:SG	3.10	0.44
1:B:2300:TYR:CE2	1:B:2305:PRO:HB3	2.53	0.44
1:B:2424:ASN:ND2	1:B:2426:LEU:H	2.15	0.44
1:B:2469:LEU:O	1:B:2472:LEU:HB2	2.18	0.44
1:A:44:LEU:O	1:A:48:GLU:HB2	2.18	0.44
1:B:2057:PRO:HG2	1:B:2074:ARG:NE	2.33	0.44
1:B:2529:THR:HG22	1:B:2530:MET:N	2.32	0.44
1:B:2446:ILE:HD13	1:B:2495:ILE:HG12	2.00	0.44
1:A:289:LEU:HD23	1:A:291:ASP:H	1.83	0.44
1:B:2004:GLU:O	1:B:2008:ARG:HB2	2.18	0.44
1:B:2097:PHE:HD1	1:B:2100:ARG:NH2	2.15	0.44
1:A:161:PRO:HB3	1:A:231:GLU:HB2	2.00	0.43
1:A:115:HIS:CG	1:A:254:CYS:SG	3.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ARG:CG	1:A:481:GLU:HG2	2.46	0.43
1:B:2075:PRO:HA	1:B:2140:GLY:O	2.18	0.43
1:B:2129:VAL:HG12	1:B:2130:TRP:N	2.33	0.43
1:A:424:ASN:HA	1:A:425:PRO:HD3	1.84	0.43
1:A:503:LEU:HD22	1:A:507:LEU:HG	2.00	0.43
1:A:94:VAL:O	1:A:97:PHE:HB3	2.18	0.43
1:A:228:GLY:O	1:A:230:GLU:N	2.52	0.43
1:A:68:PRO:O	1:A:70:GLU:HG3	2.18	0.43
1:A:442:LYS:CB	1:A:508:TYR:HE2	2.30	0.43
1:B:2002:THR:HG23	1:B:2005:GLU:H	1.84	0.43
1:A:100:ARG:O	1:A:103:ARG:HG2	2.18	0.43
1:A:523:LEU:O	1:A:527:PHE:HD1	2.02	0.43
1:B:2226:GLY:H	1:B:2230:GLU:HB2	1.83	0.43
1:A:164:LEU:HA	1:A:225:LEU:O	2.18	0.43
1:B:2381:VAL:HG13	1:B:2382:ILE:N	2.28	0.43
1:A:292:LEU:O	1:A:295:TRP:HB2	2.19	0.42
1:A:444:MET:HA	1:A:501:ARG:HG3	2.01	0.42
1:A:446:ILE:CG2	1:A:449:LEU:HD23	2.49	0.42
1:A:512:LEU:HB2	1:A:515:VAL:HG11	2.00	0.42
1:B:2002:THR:HG22	1:B:2005:GLU:CG	2.49	0.42
1:B:2098:GLU:O	1:B:2102:GLU:HG3	2.18	0.42
1:B:2451:GLU:O	1:B:2455:GLU:HG2	2.19	0.42
1:A:221:TYR:HD2	1:A:222:ALA:N	2.18	0.42
1:B:2057:PRO:HA	1:B:2062:GLU:HG3	2.01	0.42
1:B:2223:LEU:HB2	1:B:2227:LEU:HD13	2.01	0.42
1:A:368:ARG:HD3	1:A:393:ARG:NH1	2.33	0.42
1:A:447:GLU:HB2	1:A:494:GLN:HE22	1.84	0.42
1:A:454:ILE:O	1:A:458:LEU:HD23	2.18	0.42
1:B:2456:ARG:HD2	1:B:2456:ARG:HA	1.85	0.42
1:A:565:ARG:HA	1:A:565:ARG:HD3	1.87	0.42
1:A:427:CYS:SG	1:A:429:ALA:HB3	2.60	0.42
1:A:191:VAL:HG21	1:A:357:HIS:CE1	2.55	0.42
1:A:1:MET:SD	1:A:47:LEU:HD21	2.60	0.42
1:B:2329:VAL:HG22	1:B:2429:ALA:CB	2.50	0.42
1:B:2503:LEU:HB3	1:B:2524:ALA:CB	2.50	0.42
1:A:116:LYS:HE2	1:A:116:LYS:HB3	1.82	0.41
1:A:14:ARG:NH1	1:A:44:LEU:HD21	2.36	0.41
1:A:469:LEU:O	1:A:472:LEU:HB2	2.21	0.41
1:A:362:ILE:HD13	1:A:400:ILE:HG21	2.03	0.41
1:B:2090:THR:O	1:B:2094:VAL:HG23	2.20	0.41
1:B:2498:SER:HA	1:B:2501:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PRO:CB	1:A:231:GLU:HB2	2.51	0.41
1:A:515:VAL:HA	1:A:519:LEU:HD12	2.03	0.41
1:B:2124:TYR:HD2	1:B:2131:SER:HB2	1.85	0.41
1:B:2322:LEU:HD12	1:B:2340:VAL:O	2.20	0.41
1:B:2466:VAL:HG23	1:B:2571:LEU:HD21	2.02	0.41
1:B:2401:ARG:HB3	1:B:2401:ARG:HH21	1.85	0.41
1:A:39:ARG:HA	1:A:39:ARG:HE	1.85	0.40
1:B:2164:LEU:HD12	1:B:2225:LEU:O	2.21	0.40
1:A:103:ARG:HD3	1:A:103:ARG:HA	1.89	0.40
1:B:2322:LEU:O	1:B:2369:ILE:O	2.39	0.40
1:B:2518:VAL:HG13	1:B:2519:LEU:N	2.37	0.40
1:B:2466:VAL:HG22	1:B:2567:LEU:HD11	2.03	0.40
1:A:130:TRP:HH2	1:A:147:LEU:HB2	1.87	0.40
1:A:369:ILE:C	1:A:371:ASP:H	2.25	0.40
1:B:2123:LEU:HD22	1:B:2220:PHE:CZ	2.56	0.40
1:B:2356:LEU:HD22	1:B:2367:ILE:HD12	2.02	0.40
1:B:2414:VAL:HG22	1:B:2415:LYS:N	2.36	0.40
1:B:2431:ARG:HG2	1:B:2464:ARG:O	2.20	0.40
1:B:2439:ALA:HB2	1:B:2449:LEU:HD23	2.03	0.40
1:A:111:TYR:HD2	1:A:289:LEU:HA	1.86	0.40
1:A:506:LEU:O	1:A:510:LEU:HD13	2.21	0.40
1:A:74:ARG:HA	1:A:75:PRO:HD3	1.93	0.40
1:B:2219:THR:O	1:B:2219:THR:HG23	2.22	0.40
1:B:2241:LEU:HD23	1:B:2255:TYR:CG	2.57	0.40
1:A:403:PRO:O	1:A:413:LEU:HD12	2.21	0.40
1:B:2097:PHE:HD1	1:B:2100:ARG:HH21	1.70	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	579/667 (87%)	508 (88%)	56 (10%)	15 (3%)	5 20
1	B	579/667 (87%)	504 (87%)	59 (10%)	16 (3%)	5 19
All	All	1158/1334 (87%)	1012 (87%)	115 (10%)	31 (3%)	5 19

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	106	GLU
1	A	216	LEU
1	B	2064	VAL
1	B	2106	GLU
1	B	2138	GLU
1	B	2343	PRO
1	A	69	LEU
1	A	228	GLY
1	A	229	LEU
1	B	2105	ALA
1	B	2443	ALA
1	A	357	HIS
1	A	381	VAL
1	A	409	CYS
1	B	2357	HIS
1	B	2440	SER
1	B	2485	GLU
1	A	73	PHE
1	A	515	VAL
1	B	2107	ALA
1	B	2108	PRO
1	A	443	ALA
1	B	2302	ALA
1	A	143	VAL
1	B	2325	VAL
1	A	513	PRO
1	A	511	GLY
1	B	2528	GLY
1	B	2117	VAL
1	B	2143	VAL

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	495/566 (88%)	462 (93%)	33 (7%)	16	43
1	B	495/566 (88%)	462 (93%)	33 (7%)	16	43
All	All	990/1132 (88%)	924 (93%)	66 (7%)	16	43

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	ARG
1	A	39	ARG
1	A	41	LEU
1	A	44	LEU
1	A	49	GLU
1	A	72	THR
1	A	99	GLU
1	A	115	HIS
1	A	117	VAL
1	A	118	ASP
1	A	138	GLU
1	A	225	LEU
1	A	230	GLU
1	A	237	GLN
1	A	283	ASP
1	A	287	LEU
1	A	311	TYR
1	A	331	ARG
1	A	344	VAL
1	A	364	GLU
1	A	368	ARG
1	A	374	LEU
1	A	375	VAL
1	A	389	LEU
1	A	414	VAL
1	A	424	ASN

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Mol	Chain	Res	Type
1	A	441	ARG
1	A	458	LEU
1	A	472	LEU
1	A	492	LEU
1	A	503	LEU
1	A	506	LEU
1	B	2004	GLU
1	B	2013	LEU
1	B	2022	TYR
1	B	2044	LEU
1	B	2067	ARG
1	B	2120	LEU
1	B	2130	TRP
1	B	2138	GLU
1	B	2148	LEU
1	B	2157	LEU
1	B	2167	ARG
1	B	2209	ARG
1	B	2217	ARG
1	B	2221	TYR
1	B	2237	GLN
1	B	2254	CYS
1	B	2266	GLU
1	B	2291	ASP
1	B	2329	VAL
1	B	2364	GLU
1	B	2376	HIS
1	B	2391	GLU
1	B	2406	CYS
1	B	2416	GLU
1	B	2424	ASN
1	B	2440	SER
1	B	2472	LEU
1	B	2493	ARG
1	B	2496	GLU
1	B	2504	GLU
1	B	2510	LEU
1	B	2519	LEU
1	B	2523	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	197	ASN
1	A	276	HIS
1	A	424	ASN
1	B	2087	ASN
1	B	2145	GLN
1	B	2146	ASN
1	B	2197	ASN
1	B	2205	GLN
1	B	2237	GLN
1	B	2424	ASN
1	B	2494	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AMP	B	2700	1	18,24,25	1.03	2 (11%)	18,35,38	1.70	2 (11%)
3	AMP	A	700	1	18,24,25	0.95	2 (11%)	18,35,38	1.78	4 (22%)

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	AMP	B	2700	1	-	2/3/25/26	0/3/3/3
3	AMP	A	700	1	-	1/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2700	AMP	O4'-C1'	2.86	1.45	1.41
3	B	2700	AMP	C5-N7	-2.30	1.31	1.39
3	A	700	AMP	C5-N7	-2.28	1.31	1.39
3	A	700	AMP	O4'-C1'	2.06	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2700	AMP	N3-C2-N1	-6.01	119.28	128.68
3	A	700	AMP	N3-C2-N1	-5.92	119.42	128.68
3	A	700	AMP	C4-C5-N7	-2.28	107.02	109.40
3	B	2700	AMP	C4-C5-N7	-2.25	107.05	109.40
3	A	700	AMP	C3'-C2'-C1'	2.20	104.29	100.98
3	A	700	AMP	C2'-C3'-C4'	2.13	106.78	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2700	AMP	O4'-C4'-C5'-O5'
3	A	700	AMP	O4'-C4'-C5'-O5'
3	B	2700	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

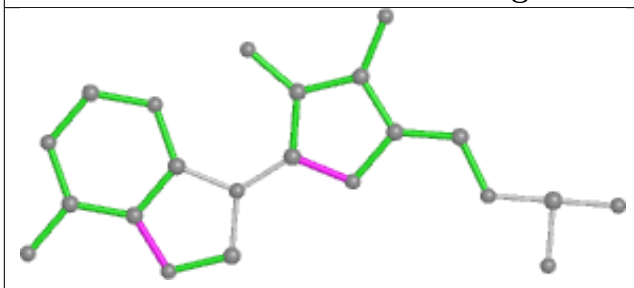
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2700	AMP	1	0

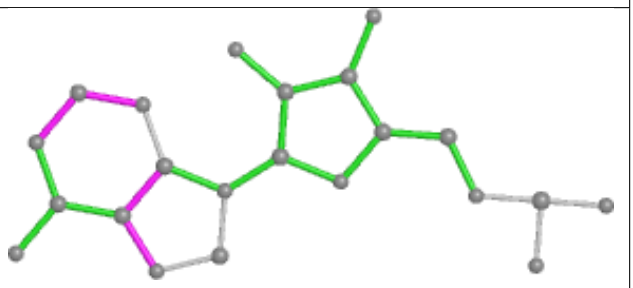
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

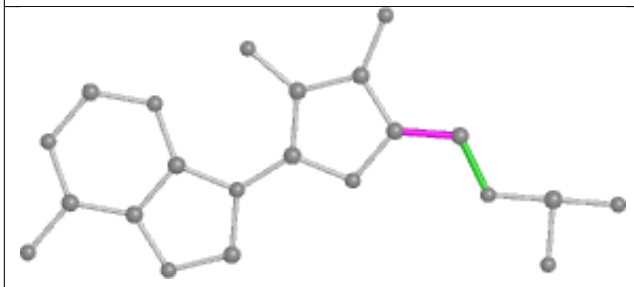
Ligand AMP B 2700



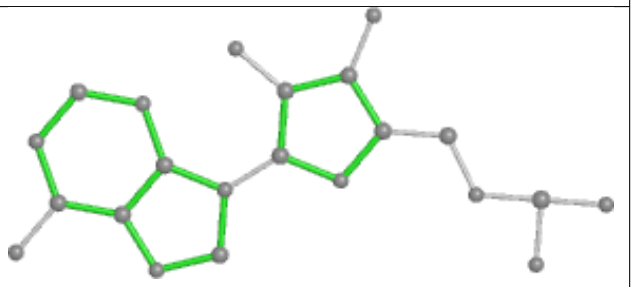
Bond lengths



Bond angles

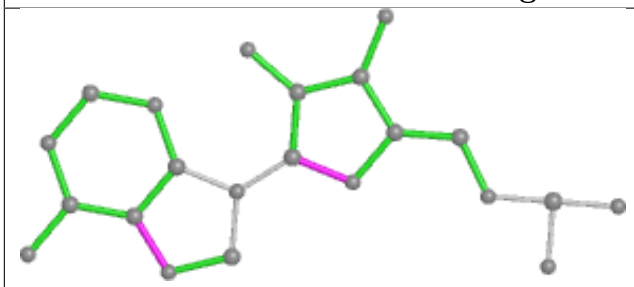


Torsions

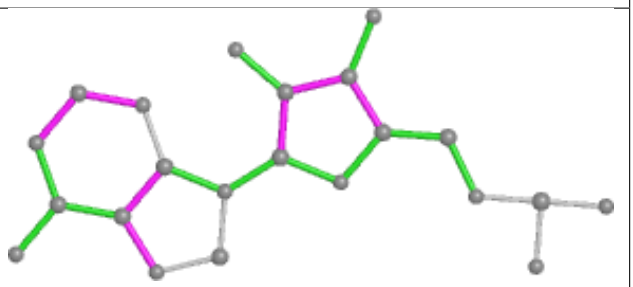


Rings

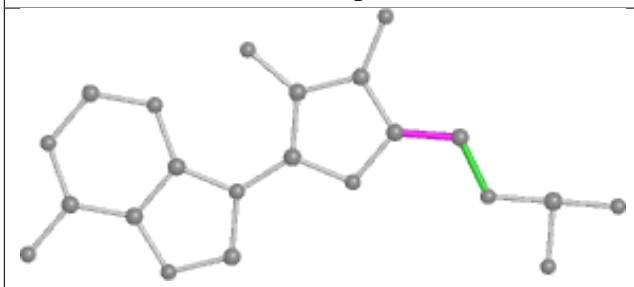
Ligand AMP A 700



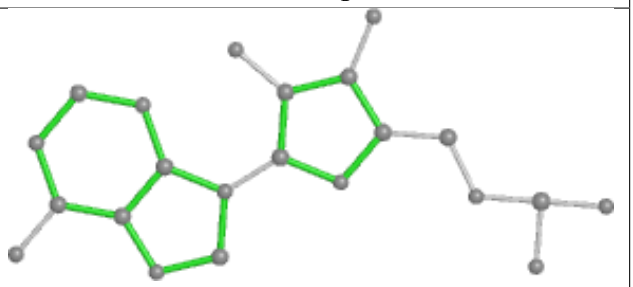
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	581/667 (87%)	-0.18	15 (2%) 56 52	11, 43, 87, 101	0
1	B	581/667 (87%)	-0.07	19 (3%) 46 41	11, 47, 89, 101	0
All	All	1162/1334 (87%)	-0.13	34 (2%) 51 47	11, 45, 89, 101	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2348	GLY	5.1
1	B	2303	ARG	4.8
1	A	230	GLU	4.0
1	B	2035	ALA	3.9
1	A	106	GLU	3.8
1	A	302	ALA	3.7
1	A	65	GLY	3.6
1	B	2482	ARG	3.5
1	A	484	GLY	3.5
1	B	2302	ALA	3.4
1	A	229	LEU	3.1
1	A	394	THR	3.0
1	B	2484	GLY	2.9
1	B	2301	THR	2.9
1	A	303	ARG	2.8
1	A	33	SER	2.8
1	A	473	ARG	2.8
1	A	485	GLU	2.8
1	A	29	ASP	2.7
1	B	2033	SER	2.7
1	B	2231	GLU	2.7
1	B	2481	GLU	2.6
1	B	2441	ARG	2.5
1	B	2064	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	2381	VAL	2.5
1	A	105	ALA	2.3
1	B	2391	GLU	2.3
1	B	2349	SER	2.3
1	B	2259	LEU	2.1
1	A	67	ARG	2.1
1	B	2380	GLY	2.1
1	A	231	GLU	2.1
1	B	2476	ASP	2.1
1	B	2130	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

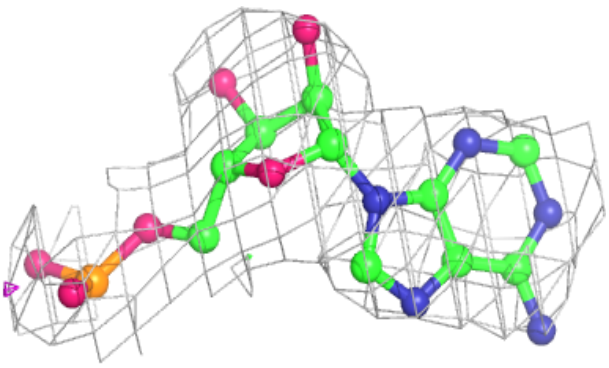
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

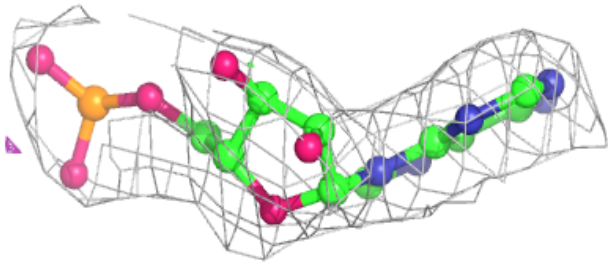
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AMP	B	2700	22/23	0.91	0.18	75,84,92,94	0
3	AMP	A	700	22/23	0.95	0.12	36,43,52,62	0
2	ZN	B	2701	1/1	0.97	0.14	33,33,33,33	0
2	ZN	A	701	1/1	0.99	0.10	20,20,20,20	0

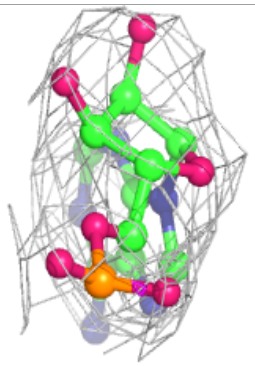
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP B 2700:

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

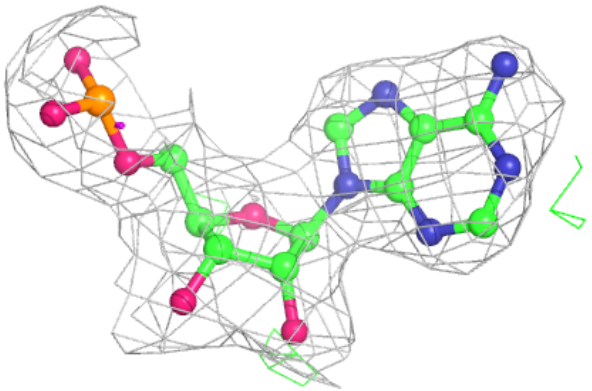


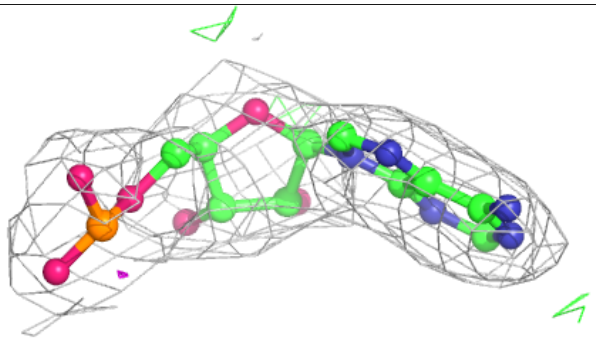


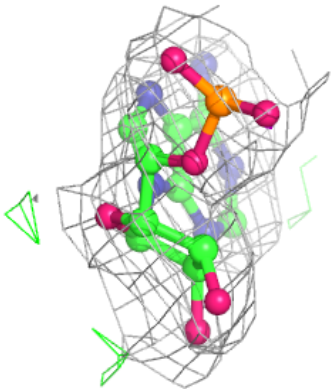


Electron density around AMP A 700:

$2mF_o$-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.