



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:50 PM UTC

PDB ID : 1DGS / pdb_00001dgs
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 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

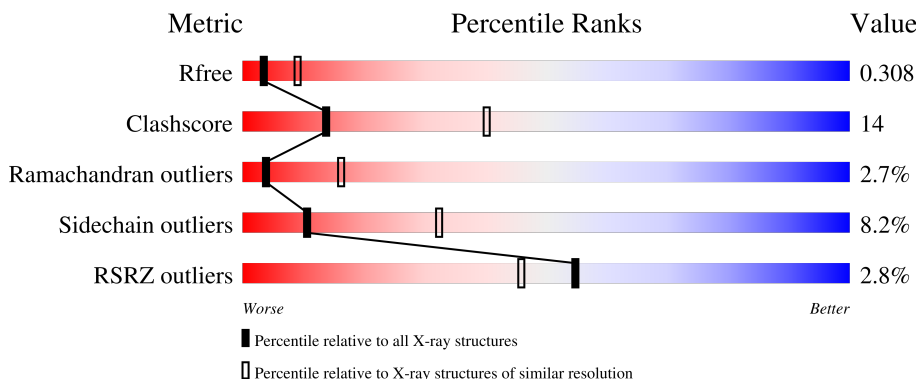
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 $\leq 5\%$. 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	
1	B	667	

2 Entry composition [i](#)

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.

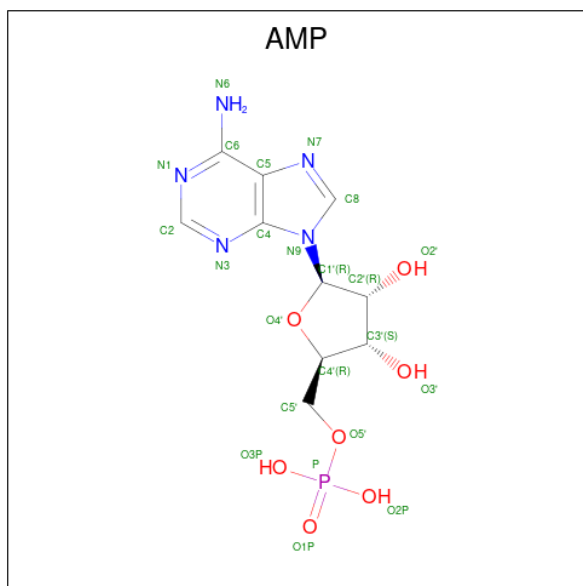
- Molecule 1 is a protein called DNA LIGASE.

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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		

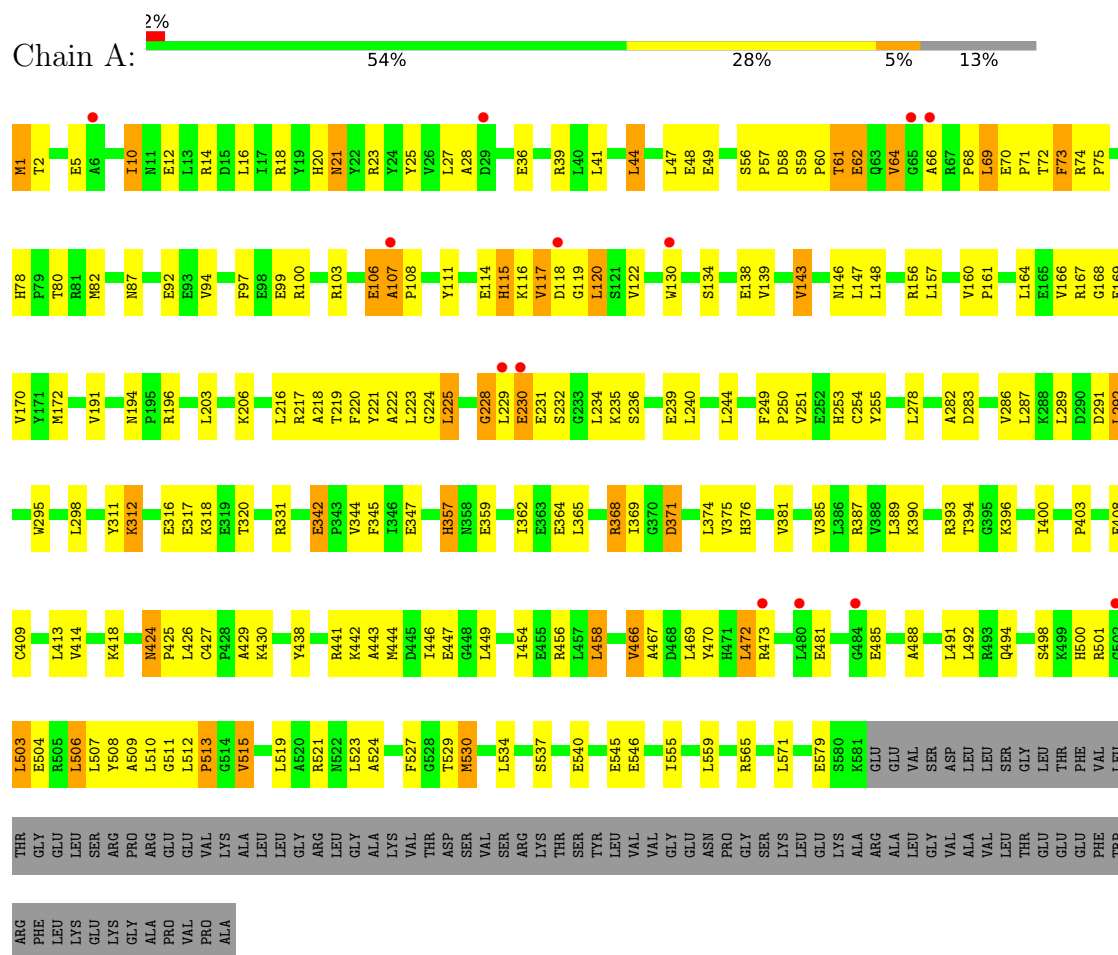
- Molecule 4 is water.

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

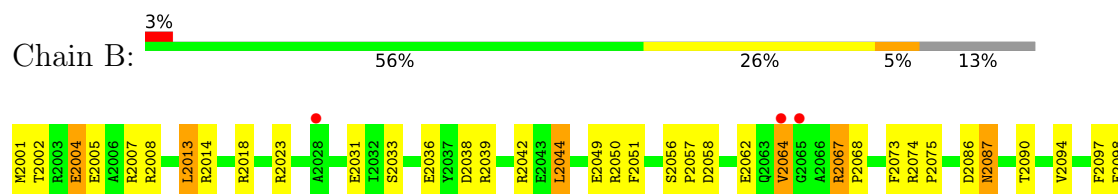
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA LIGASE



• Molecule 1: DNA LIGASE





4 Data and refinement statistics

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 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.5 (20.00-2.90) 95.5 (20.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.89Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.228 , 0.298 0.242 , 0.308	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)	0.30 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	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.*

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AMP

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	0.48	2/4782 (0.0%)	1.01	24/6451 (0.4%)
1	B	0.46	1/4782 (0.0%)	1.02	27/6451 (0.4%)
All	All	0.47	3/9564 (0.0%)	1.01	51/12902 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	MET	SD-CE	-5.67	1.65	1.79
1	B	2444	MET	SD-CE	-5.58	1.65	1.79
1	A	172	MET	SD-CE	-5.50	1.65	1.79

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2150	ILE	N-CA-C	-8.97	99.27	108.15
1	A	87	ASN	N-CA-C	7.94	121.67	108.73
1	B	2134	SER	N-CA-C	7.84	120.31	109.18
1	B	2120	LEU	N-CA-C	7.44	120.47	110.35
1	A	64	VAL	N-CA-C	7.29	124.51	109.34
1	A	120	LEU	N-CA-C	7.27	120.87	109.96
1	B	2550	LEU	N-CA-C	7.23	118.81	111.07
1	A	466	VAL	N-CA-C	7.09	117.86	110.62
1	B	2342	GLU	CA-C-N	7.04	128.64	119.84
1	B	2342	GLU	C-N-CA	7.04	128.64	119.84
1	A	371	ASP	N-CA-C	6.81	120.11	110.23
1	A	500	HIS	N-CA-C	6.77	121.37	113.18
1	B	2118	ASP	N-CA-C	6.53	119.10	108.26
1	A	342	GLU	N-CA-C	-6.44	101.53	109.65
1	B	2371	ASP	N-CA-C	6.24	118.60	110.43
1	A	408	GLU	N-CA-C	6.14	120.09	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2086	ASP	N-CA-C	-6.06	101.98	110.35
1	B	2447	GLU	N-CA-C	6.01	119.44	111.75
1	A	194	ASN	CA-C-N	5.92	125.60	119.56
1	A	194	ASN	C-N-CA	5.92	125.60	119.56
1	A	134	SER	N-CA-C	5.86	118.78	109.81
1	A	312	LYS	N-CA-C	5.79	119.26	109.76
1	A	194	ASN	N-CA-C	5.74	113.30	108.13
1	B	2569	ARG	N-CA-C	-5.61	104.56	111.40
1	B	2112	THR	N-CA-C	-5.59	99.41	108.52
1	A	345	PHE	N-CA-C	5.57	117.77	108.02
1	A	21	ASN	N-CA-C	-5.54	105.39	111.82
1	B	2115	HIS	N-CA-C	-5.52	102.34	110.52
1	B	2139	VAL	N-CA-C	-5.52	100.23	108.46
1	B	2150	ILE	CA-C-N	5.46	125.81	119.47
1	B	2150	ILE	C-N-CA	5.46	125.81	119.47
1	A	107	ALA	N-CA-C	5.45	121.85	109.81
1	A	390	LYS	N-CA-C	5.43	120.27	111.37
1	A	224	GLY	N-CA-C	-5.40	100.39	113.18
1	B	2252	GLU	N-CA-C	5.39	119.86	113.28
1	B	2316	GLU	N-CA-C	5.39	118.04	109.96
1	B	2400	ILE	N-CA-C	5.36	116.17	108.93
1	A	61	THR	N-CA-C	5.33	117.84	111.71
1	A	106	GLU	N-CA-C	5.30	122.08	110.80
1	B	2127	GLU	N-CA-C	-5.23	105.55	112.24
1	B	2051	PHE	CA-C-N	5.21	125.52	119.47
1	B	2051	PHE	C-N-CA	5.21	125.52	119.47
1	B	2056	SER	CA-C-N	5.19	124.86	119.56
1	B	2056	SER	C-N-CA	5.19	124.86	119.56
1	A	25	TYR	N-CA-C	5.18	119.09	112.87
1	B	2087	ASN	N-CA-C	5.17	117.27	109.41
1	B	2064	VAL	N-CA-C	5.10	119.94	109.34
1	A	139	VAL	N-CA-C	-5.09	100.79	108.12
1	A	62	GLU	N-CA-C	5.07	119.22	113.19
1	A	66	ALA	N-CA-C	-5.04	106.98	112.72
1	B	2466	VAL	N-CA-C	5.03	117.34	111.05

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	138	0
1	B	4693	0	4727	136	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
4	B	119	0	0	0	0
All	All	9674	0	9483	274	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 (274) 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:HD12	1:B:2120:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2167:ARG:HG2	1:B:2167:ARG:HH21	1.58	0.67
1:A:115:HIS:HD1	1:A:254:CYS:HG	1.43	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
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:21:ASN:CG	1:A:69:LEU:HB2	2.24	0.62
1:A:223:LEU:HG	1:A:240:LEU:HD11	1.81	0.61
1:B:2217:ARG:HG2	1:B:2217:ARG:HH21	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:B:2530:MET:HE3	1:B:2568:VAL:HG21	1.83	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: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:HG2	1:B:2217:ARG:NH2	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:B:2038:ASP:O	1:B:2042:ARG:HG3	2.06	0.56
1:A:515:VAL:O	1:A:515:VAL:HG13	2.05	0.56
1:B:2143:VAL:HG22	1:B:2146:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2001:MET:HE3	1:B:2050:ARG:HH21	1.69	0.55
1:B:2157:LEU:HD21	1:B:2249:PHE:HE2	1.69	0.55
1:A:317:GLU:C	1:A:318:LYS:HD2	2.31	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
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:2001:MET:HE3	1:B:2050:ARG:NH2	2.23	0.53
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:HD23	1:B:2287:LEU:H	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:A:82:MET:HE3	1:A:122:VAL:HB	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:56:SER:C	1:A:58:ASP:H	2.19	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:80:THR:HG23	1:A:225:LEU:HD23	1.93	0.49
1:A:504:GLU:HG2	1:A:521:ARG:HG3	1.94	0.49
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:B:2402:TRP:CG	1:B:2420:HIS:HD1	2.30	0.49
1:A:143:VAL:HG22	1:A:143:VAL:O	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:71:PRO:HG2	1:A:73:PHE:CE2	2.48	0.49
1:A:168:GLY:HA3	1:A:220:PHE:HA	1.95	0.49
1:B:2512:LEU:O	1:B:2515:VAL:HG12	2.13	0.48
1:B:2515:VAL:HG13	1:B:2515:VAL:O	2.13	0.48
1:A:115:HIS:CE1	1:A:278:LEU:HD11	2.49	0.48
1:A:530:MET:HE3	1:A:534:LEU:HG	1.94	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:A:82:MET:HE3	1:A:167:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2150:ILE:HB	1:B:2153:ILE:HD12	1.95	0.47
1:B:2226:GLY:HA2	1:B:2230:GLU:HB2	1.96	0.47
1:B:2120:LEU:HD21	3:B:2700:AMP:O2'	2.14	0.47
1:B:2167:ARG:HG2	1:B:2167:ARG:NH2	2.23	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:94:VAL:HG21	1:A:311:TYR:CD1	2.50	0.46
1:A:449:LEU:HD22	1:A:491:LEU:HD11	1.97	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:N	1:B:2220:PHE:CD2	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:44:LEU:HD13	1:A:61:THR:HG23	1.98	0.46
1:A:295:TRP:O	1:A:298:LEU:O	2.34	0.46
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: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:A:369:ILE:C	1:A:371:ASP:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2073:PHE:HD2	1:B:2141:GLU:HG2	1.82	0.44
1:B:2120:LEU:H	1:B:2120:LEU:CD1	2.25	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:B:2102:GLU:C	1:B:2104:GLU:H	2.24	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:115:HIS:CG	1:A:254:CYS:SG	3.11	0.43
1:A:161:PRO:HB3	1:A:231:GLU:HB2	2.00	0.43
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:94:VAL:O	1:A:97:PHE:HB3	2.18	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:68:PRO:O	1:A:70:GLU:HG3	2.18	0.43
1:A:228:GLY:O	1:A:230:GLU:N	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:444:MET:HE2	1:A:506:LEU:HD23	2.00	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:2172:MET:HE3	1:B:2172:MET:HB2	1.72	0.42
1:B:2456:ARG:HA	1:B:2456:ARG:HD2	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:1:MET:SD	1:A:47:LEU:HD21	2.60	0.42
1:A:191:VAL:HG21	1:A:357:HIS:CE1	2.55	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:14:ARG:NH1	1:A:44:LEU:HD21	2.36	0.41
1:A:116:LYS:HE2	1:A:116:LYS:HB3	1.82	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:2424:ASN:C	1:B:2424:ASN:HD22	2.28	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
1:A:161:PRO:CB	1:A:231:GLU:HB2	2.51	0.41
1:A:424:ASN:HD22	1:A:424:ASN:C	2.28	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:HH21	1:B:2401:ARG:HB3	1.85	0.41
1:A:39:ARG:HE	1:A:39:ARG:HA	1.85	0.40
1:B:2164:LEU:HD12	1:B:2225:LEU:O	2.21	0.40
1:A:103:ARG:HA	1:A:103:ARG:HD3	1.89	0.40
1:B:2262:GLU:H	1:B:2262:GLU:CD	2.29	0.40
1:B:2322:LEU:O	1:B:2369:ILE:O	2.39	0.40
1:B:2466:VAL:HG22	1:B:2567:LEU:HD11	2.03	0.40
1:B:2518:VAL:HG13	1:B:2519:LEU:N	2.37	0.40
1:A:130:TRP:HH2	1:A:147:LEU:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:ARG:HA	1:A:75:PRO:HD3	1.93	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: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%)	4	17
1	B	579/667 (87%)	504 (87%)	59 (10%)	16 (3%)	4	15
All	All	1158/1334 (87%)	1012 (87%)	115 (10%)	31 (3%)	4	16

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	455 (92%)	40 (8%)	11	33
1	B	495/566 (88%)	454 (92%)	41 (8%)	10	32
All	All	990/1132 (88%)	909 (92%)	81 (8%)	10	32

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	10	ILE
1	A	36	GLU
1	A	41	LEU
1	A	44	LEU
1	A	49	GLU
1	A	62	GLU
1	A	72	THR
1	A	92	GLU
1	A	99	GLU
1	A	115	HIS
1	A	117	VAL
1	A	138	GLU
1	A	148	LEU
1	A	206	LYS
1	A	217	ARG
1	A	225	LEU
1	A	230	GLU
1	A	283	ASP
1	A	287	LEU
1	A	292	LEU
1	A	331	ARG
1	A	344	VAL
1	A	359	GLU
1	A	364	GLU
1	A	368	ARG
1	A	374	LEU
1	A	375	VAL
1	A	376	HIS
1	A	385	VAL
1	A	389	LEU
1	A	414	VAL
1	A	418	LYS
1	A	424	ASN
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	2044	LEU

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Mol	Chain	Res	Type
1	B	2049	GLU
1	B	2067	ARG
1	B	2117	VAL
1	B	2120	LEU
1	B	2138	GLU
1	B	2145	GLN
1	B	2148	LEU
1	B	2157	LEU
1	B	2209	ARG
1	B	2216	LEU
1	B	2217	ARG
1	B	2229	LEU
1	B	2230	GLU
1	B	2237	GLN
1	B	2251	VAL
1	B	2254	CYS
1	B	2266	GLU
1	B	2275	ARG
1	B	2291	ASP
1	B	2325	VAL
1	B	2329	VAL
1	B	2343	PRO
1	B	2364	GLU
1	B	2376	HIS
1	B	2386	LEU
1	B	2391	GLU
1	B	2406	CYS
1	B	2416	GLU
1	B	2440	SER
1	B	2458	LEU
1	B	2472	LEU
1	B	2493	ARG
1	B	2495	ILE
1	B	2496	GLU
1	B	2504	GLU
1	B	2510	LEU
1	B	2519	LEU
1	B	2523	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	197	ASN
1	A	237	GLN
1	A	276	HIS
1	A	376	HIS
1	A	424	ASN
1	A	522	ASN
1	B	2078	HIS
1	B	2087	ASN
1	B	2115	HIS
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
1	B	2500	HIS

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 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	A	700	1	21,24,25	1.32	2 (9%)	30,35,38	2.32	8 (26%)
3	AMP	B	2700	1	21,24,25	1.32	2 (9%)	30,35,38	2.30	7 (23%)

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	A	700	1	-	0/7/25/26	0/3/3/3
3	AMP	B	2700	1	-	1/7/25/26	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	C5-N7	-4.21	1.31	1.39
3	A	700	AMP	C5-N7	-4.18	1.31	1.39
3	A	700	AMP	C4-N9	-2.37	1.32	1.37
3	B	2700	AMP	C4-N9	-2.28	1.32	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	AMP	N3-C2-N1	-6.14	119.28	128.58
3	A	700	AMP	N3-C2-N1	-6.05	119.42	128.58
3	B	2700	AMP	C5-C4-N3	-5.76	118.79	126.72
3	A	700	AMP	C5-C4-N3	-5.66	118.92	126.72
3	B	2700	AMP	C2-N3-C4	4.45	122.71	111.83
3	A	700	AMP	C2-N3-C4	4.42	122.62	111.83
3	B	2700	AMP	N3-C4-N9	4.07	134.08	127.17
3	A	700	AMP	N3-C4-N9	3.91	133.81	127.17
3	B	2700	AMP	C5-N7-C8	3.29	108.62	103.45
3	A	700	AMP	C5-N7-C8	3.25	108.56	103.45
3	A	700	AMP	N9-C8-N7	-3.20	109.39	113.94
3	A	700	AMP	C4-C5-N7	-3.12	107.02	110.58
3	B	2700	AMP	C4-C5-N7	-3.09	107.05	110.58
3	B	2700	AMP	N9-C8-N7	-3.07	109.58	113.94
3	A	700	AMP	C2'-C3'-C4'	2.16	106.78	102.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

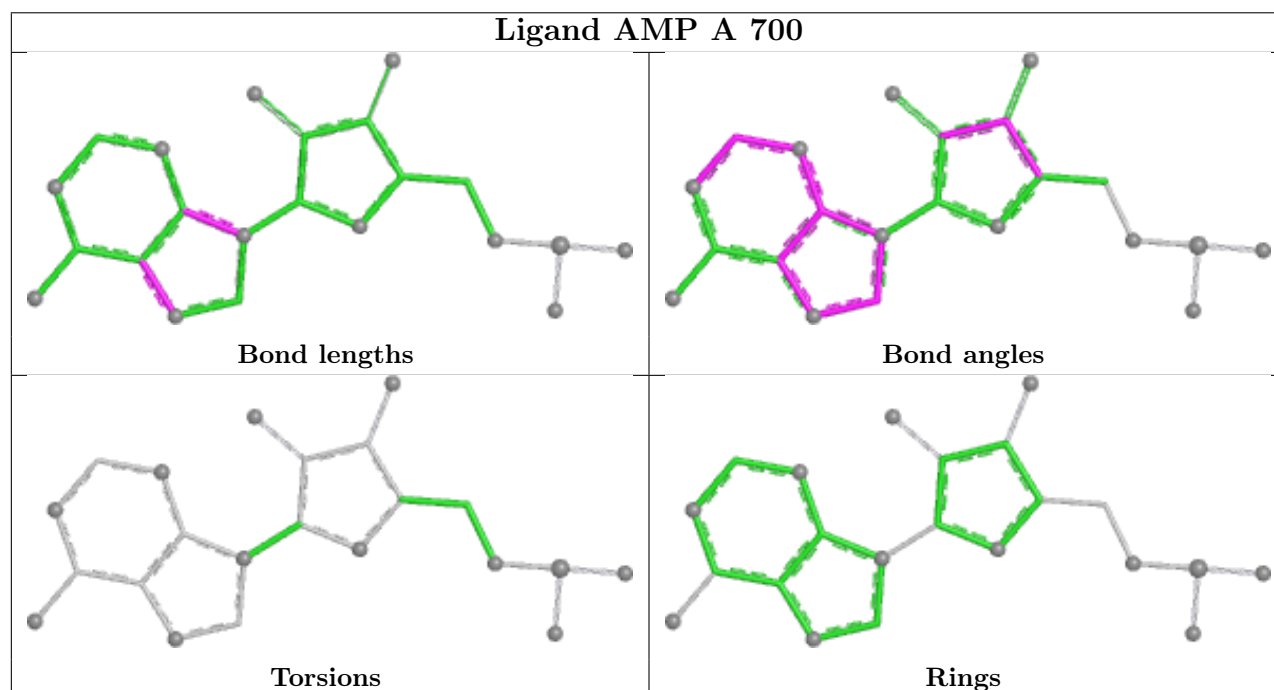
Mol	Chain	Res	Type	Atoms
3	B	2700	AMP	O4'-C4'-C5'-O5'

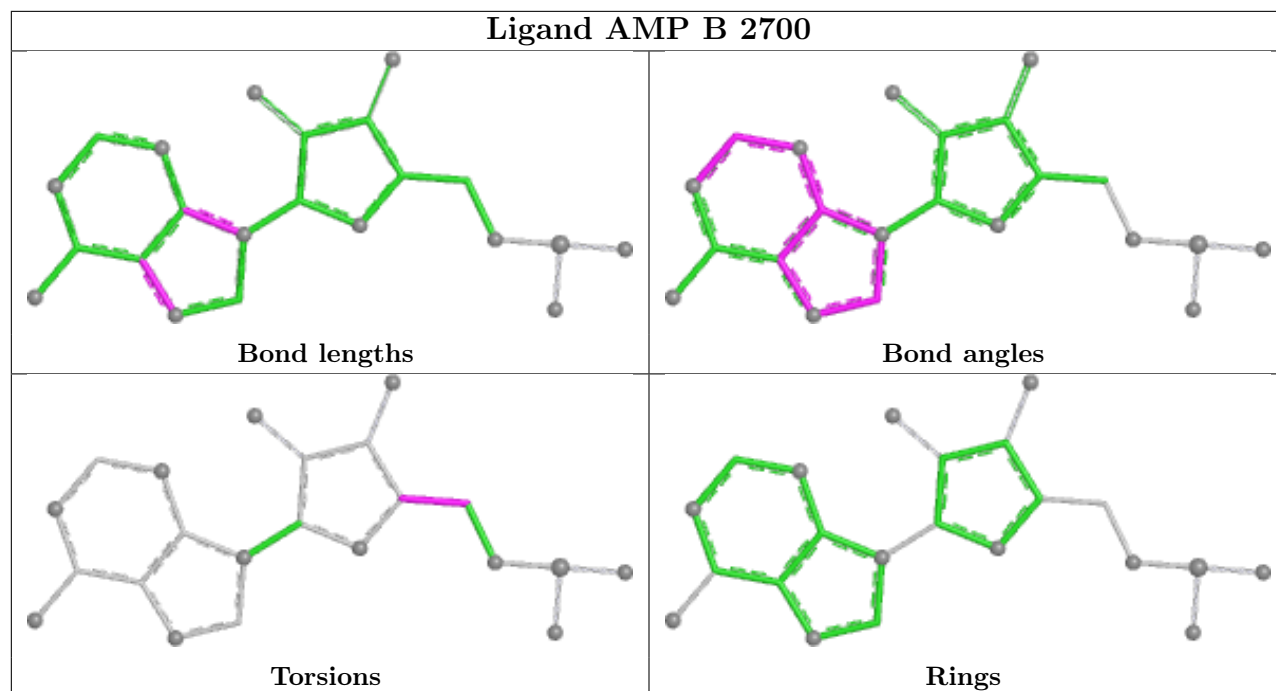
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	581/667 (87%)	-0.03	13 (2%) 62 53	10, 43, 87, 101	0
1	B	581/667 (87%)	0.04	19 (3%) 49 40	11, 47, 89, 101	0
All	All	1162/1334 (87%)	0.00	32 (2%) 55 46	10, 45, 89, 101	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	TRP	4.6
1	B	2130	TRP	4.3
1	B	2064	VAL	4.3
1	A	229	LEU	4.3
1	A	480	LEU	3.2
1	B	2137	GLY	3.2
1	B	2484	GLY	3.2
1	A	65	GLY	3.2
1	B	2380	GLY	3.1
1	A	107	ALA	3.0
1	B	2107	ALA	2.9
1	B	2135	GLY	2.8
1	B	2381	VAL	2.8
1	A	230	GLU	2.8
1	B	2379	GLY	2.8
1	B	2477	LEU	2.6
1	A	29	ASP	2.5
1	A	473	ARG	2.5
1	B	2232	SER	2.4
1	B	2474	LYS	2.4
1	A	6	ALA	2.3
1	A	484	GLY	2.3
1	B	2370	GLY	2.3
1	B	2136	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2065	GLY	2.3
1	A	502	GLY	2.1
1	A	66	ALA	2.1
1	B	2301	THR	2.1
1	B	2028	ALA	2.1
1	A	118	ASP	2.0
1	B	2481	GLU	2.0
1	B	2108	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

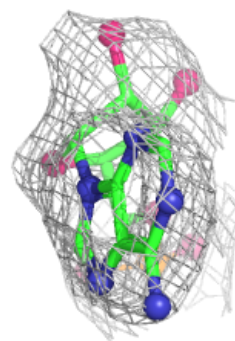
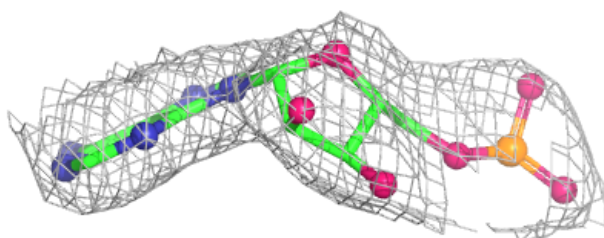
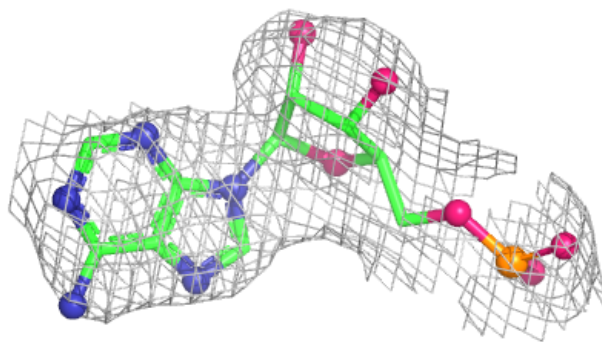
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	B	2700	22/23	0.90	0.11	75,84,92,94	0
3	AMP	A	700	22/23	0.94	0.07	36,43,52,62	0
2	ZN	A	701	1/1	0.99	0.04	20,20,20,20	0
2	ZN	B	2701	1/1	1.00	0.07	33,33,33,33	0

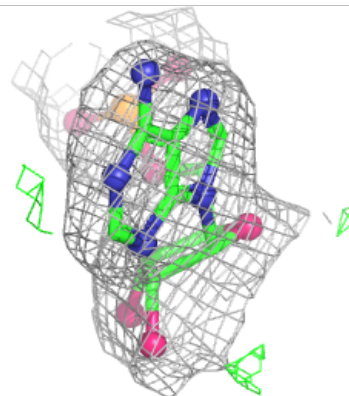
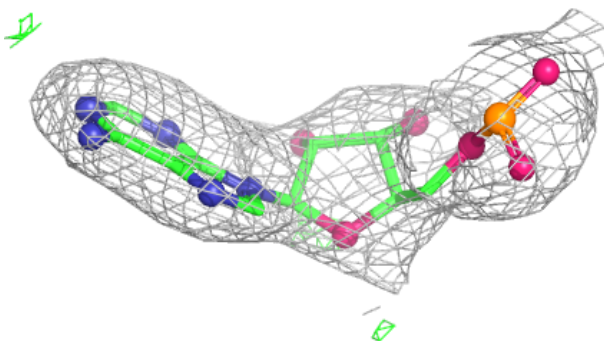
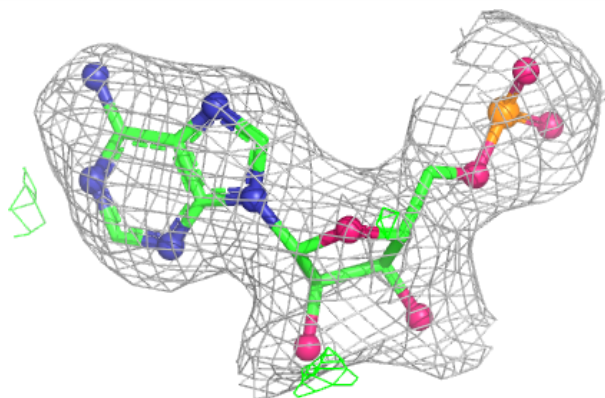
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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